



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:01 PM GMT

PDB ID : 1VQM
Title : The structure of the transition state analogue "DAN" bound to the large 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

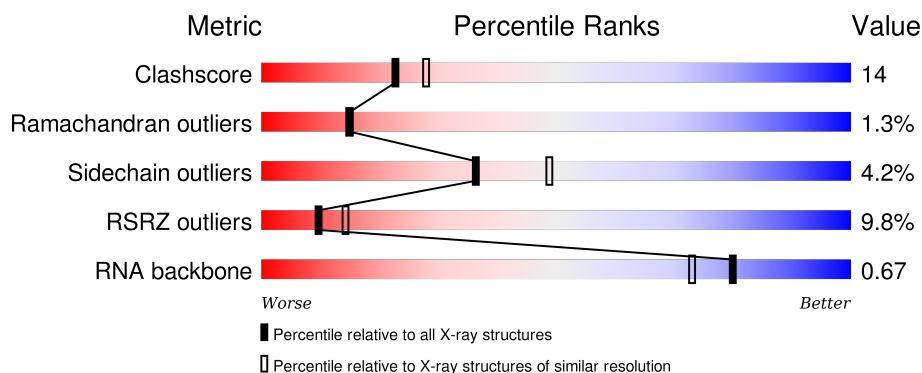
1 Overall quality at a glance

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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)
RNA backbone	2183	1011 (2.84-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>64% 25% 5% 6%</div> </div>
2	9	122	<div> <div>5%</div> <div>61% 29% 10%</div> </div>
3	4	7	<div> <div>29% 14% 57%</div> </div>
4	A	240	<div> <div>9%</div> <div>59% 36%</div> </div>
5	B	338	<div> <div>5%</div> <div>56% 41%</div> </div>

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	MG	0	8001	-	-	-	X
34	MG	0	8008	-	-	-	X
34	MG	0	8012	-	-	-	X
34	MG	0	8013	-	-	-	X
34	MG	0	8014	-	-	-	X
34	MG	0	8020	-	-	-	X
34	MG	0	8021	-	-	-	X
34	MG	0	8022	-	-	-	X
34	MG	0	8027	-	-	-	X
34	MG	0	8038	-	-	-	X
34	MG	0	8054	-	-	-	X
34	MG	0	8057	-	-	-	X
34	MG	0	8060	-	-	-	X
34	MG	0	8065	-	-	-	X
34	MG	0	8080	-	-	-	X
34	MG	0	8097	-	-	-	X
35	K	0	9001	-	-	-	X
36	NA	0	9115	-	-	-	X
36	NA	0	9120	-	-	-	X
36	NA	0	9125	-	-	-	X
36	NA	0	9127	-	-	-	X
36	NA	0	9131	-	-	-	X
36	NA	0	9135	-	-	-	X
36	NA	0	9150	-	-	-	X
36	NA	0	9156	-	-	-	X
36	NA	0	9159	-	-	-	X
36	NA	0	9161	-	-	-	X
36	NA	0	9162	-	-	-	X
36	NA	0	9165	-	-	-	X
36	NA	0	9167	-	-	-	X
36	NA	0	9168	-	-	-	X
36	NA	0	9171	-	-	-	X
36	NA	0	9172	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	NA	0	9173	-	-	-	X
36	NA	0	9174	-	-	-	X
36	NA	0	9178	-	-	-	X
36	NA	0	9185	-	-	-	X
36	NA	R	9186	-	-	-	X
37	CL	0	9316	-	-	-	X
37	CL	B	9319	-	-	-	X
38	SR	0	9406	-	-	-	X
38	SR	0	9407	-	-	-	X
38	SR	0	9482	-	-	-	X
38	SR	B	9521	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 99045 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 5 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*(PPU)P*(PO2)P*(DA)P*C*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	3	Total	C	N	O	P	0	0	0
			74	40	13	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	S	0	0	0
			1118	670	222	226				

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

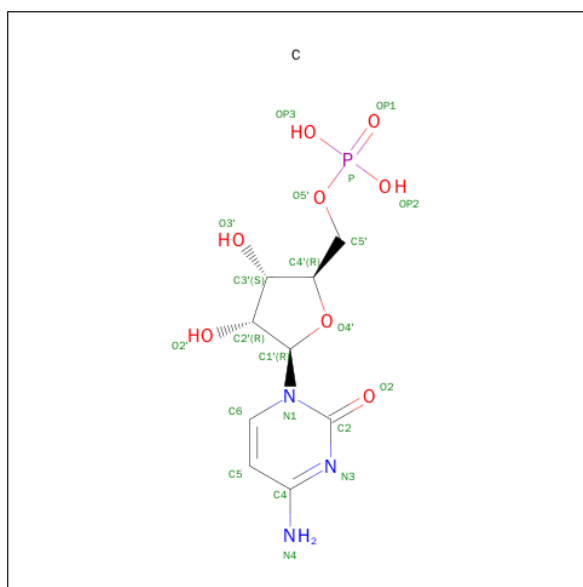
- Molecule 31 is a protein called 50S ribosomal protein L44E.

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

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

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

- Molecule 33 is HYPOPHOSPHITE (three-letter code: C, PO2, DA) (formula: $C_9H_{14}N_3O_8P$, O_2P , $C_{10}H_{14}N_5O_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	4	4	Total	C	N	O	P	0	0
			61	28	11	19	3		

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	87	Total	Mg	0	0
			87	87		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	Y	1	Total 1	Mg 1	0	0
34	K	1	Total 1	Mg 1	0	0
34	B	1	Total 1	Mg 1	0	0
34	A	1	Total 1	Mg 1	0	0
34	T	1	Total 1	Mg 1	0	0
34	2	1	Total 1	Mg 1	0	0
34	9	1	Total 1	Mg 1	0	0

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	2	Total 2	K 2	0	0

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	62	Total 62	Na 62	0	0
36	J	1	Total 1	Na 1	0	0
36	Q	1	Total 1	Na 1	0	0
36	H	1	Total 1	Na 1	0	0
36	C	1	Total 1	Na 1	0	0
36	3	1	Total 1	Na 1	0	0
36	R	3	Total 3	Na 3	0	0
36	9	3	Total 3	Na 3	0	0
36	S	1	Total 1	Na 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	M	1	Total	Na	0	0
			1	1		

- Molecule 37 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	10	Total	Cl	0	0
			10	10		
37	J	3	Total	Cl	0	0
			3	3		
37	B	1	Total	Cl	0	0
			1	1		
37	A	1	Total	Cl	0	0
			1	1		
37	N	1	Total	Cl	0	0
			1	1		
37	O	1	Total	Cl	0	0
			1	1		
37	R	1	Total	Cl	0	0
			1	1		
37	Y	1	Total	Cl	0	0
			1	1		
37	L	1	Total	Cl	0	0
			1	1		
37	3	1	Total	Cl	0	0
			1	1		
37	M	1	Total	Cl	0	0
			1	1		

- Molecule 38 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	98	Total	Sr	0	0
			98	98		
38	1	2	Total	Sr	0	0
			2	2		
38	H	1	Total	Sr	0	0
			1	1		
38	B	2	Total	Sr	0	0
			2	2		
38	3	1	Total	Sr	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	3	Total 3	Sr 3	0	0
38	R	1	Total 1	Sr 1	0	0
38	9	3	Total 3	Sr 3	0	0
38	L	1	Total 1	Sr 1	0	0
38	S	1	Total 1	Sr 1	0	0
38	F	1	Total 1	Sr 1	0	0

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

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5739	Total 5739	O 5739	0	0
40	9	132	Total 132	O 132	0	0
40	4	8	Total 8	O 8	0	0
40	A	123	Total 123	O 123	0	0
40	B	139	Total 139	O 139	0	0
40	C	177	Total 177	O 177	0	0

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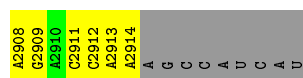
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	D	50	Total 50	O 50	0	0
40	E	43	Total 43	O 43	0	0
40	F	28	Total 28	O 28	0	0
40	G	16	Total 16	O 16	0	0
40	H	71	Total 71	O 71	0	0
40	J	53	Total 53	O 53	0	0
40	K	57	Total 57	O 57	0	0
40	L	82	Total 82	O 82	0	0
40	M	125	Total 125	O 125	0	0
40	N	59	Total 59	O 59	0	0
40	O	35	Total 35	O 35	0	0
40	P	59	Total 59	O 59	0	0
40	Q	48	Total 48	O 48	0	0
40	R	86	Total 86	O 86	0	0
40	S	31	Total 31	O 31	0	0
40	T	36	Total 36	O 36	0	0
40	U	26	Total 26	O 26	0	0
40	V	11	Total 11	O 11	0	0
40	W	68	Total 68	O 68	0	0
40	X	23	Total 23	O 23	0	0
40	Y	93	Total 93	O 93	0	0

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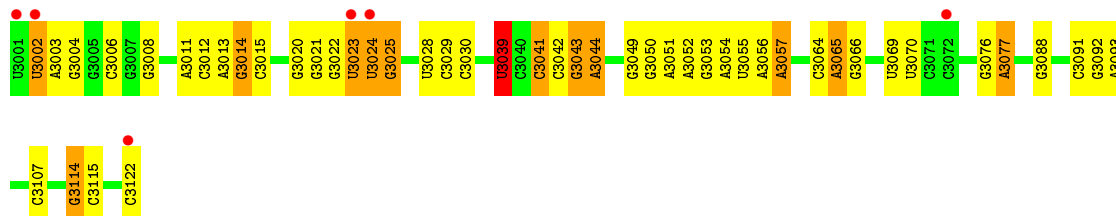
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	Z	28	Total 28	O 28	0	0
40	1	51	Total 51	O 51	0	0
40	2	41	Total 41	O 41	0	0
40	3	67	Total 67	O 67	0	0
40	I	9	Total 9	O 9	0	0





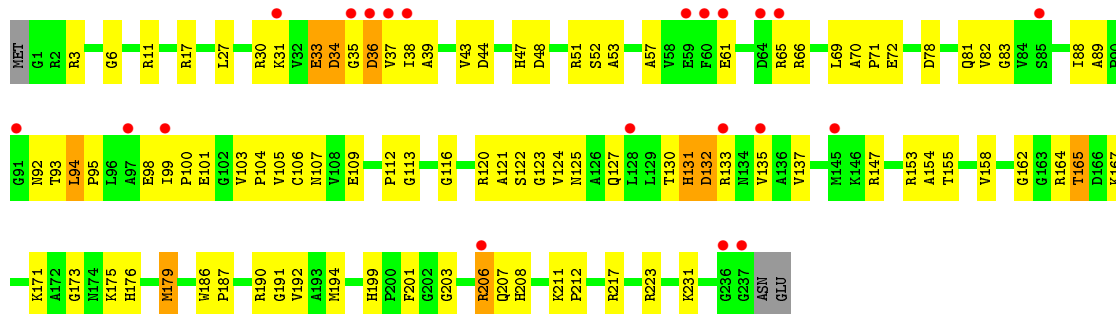
- Molecule 2: 5S ribosomal RNA



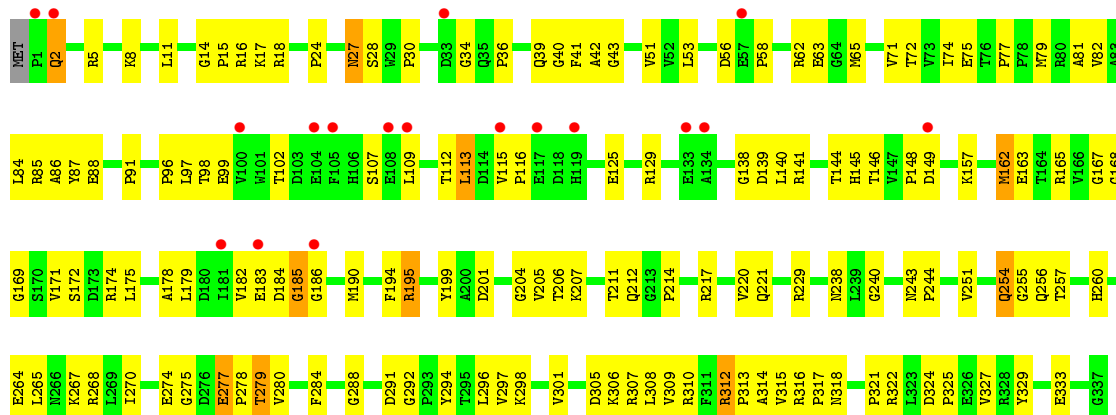
- Molecule 3: 5'-R(*CP*CP*(PPU)P*(PO2)P*(DA)P*C*C)-3'



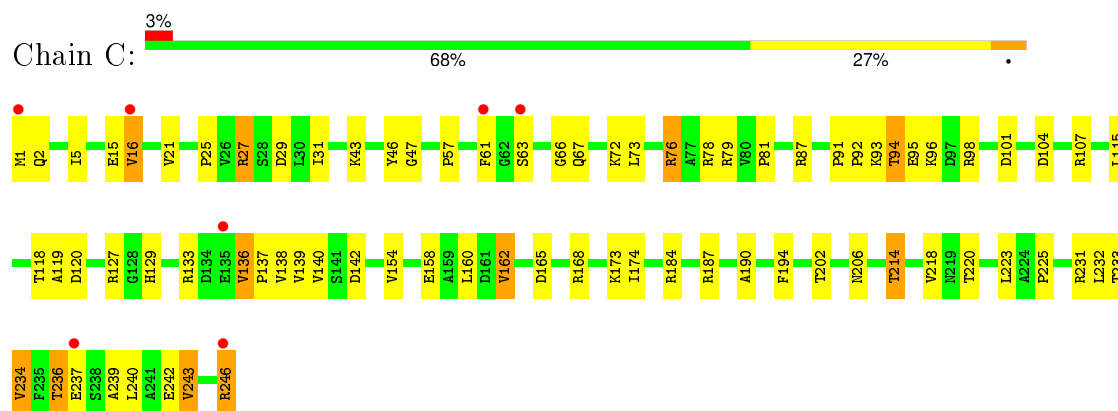
- Molecule 4: 50S ribosomal protein L2P



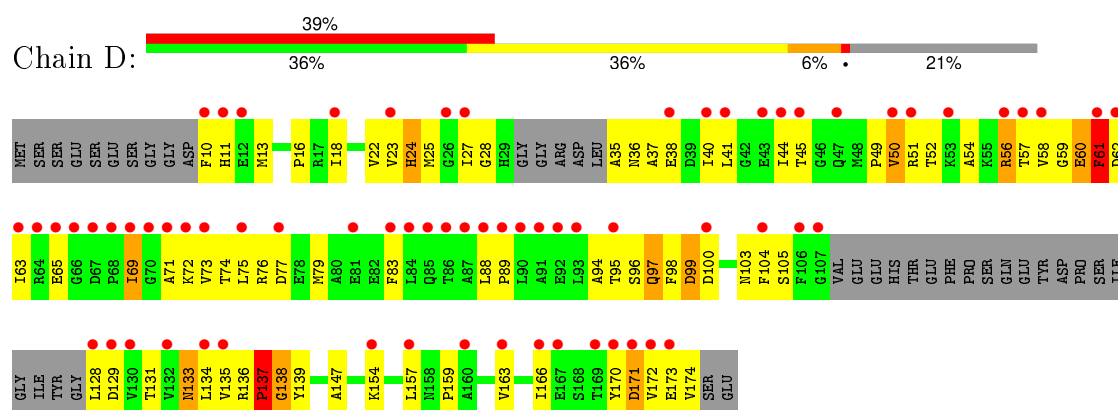
- Molecule 5: 50S ribosomal protein L3P



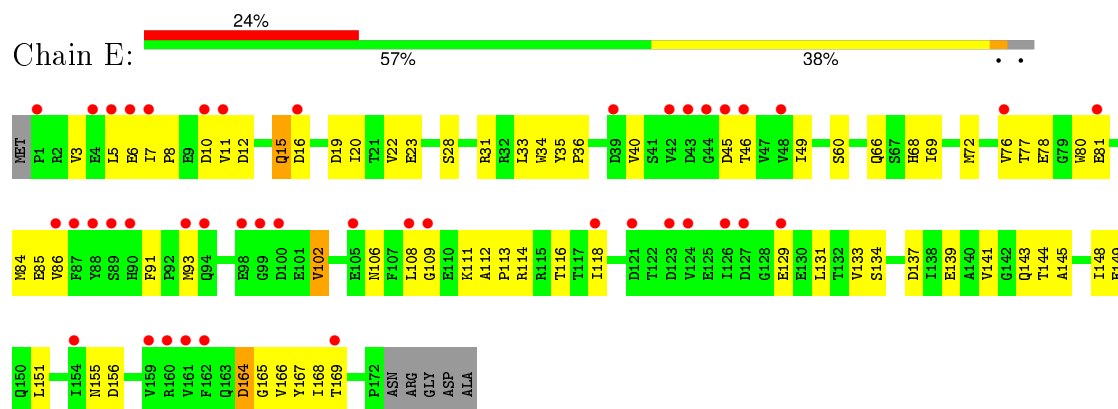
- Molecule 6: 50S ribosomal protein L4E



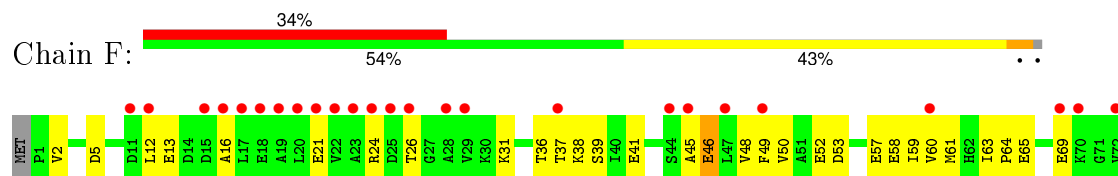
- Molecule 7: 50S ribosomal protein L5P

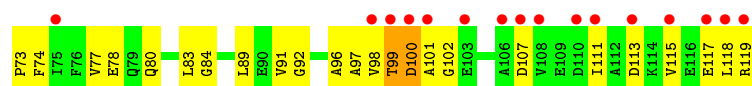


- Molecule 8: 50S ribosomal protein L6P

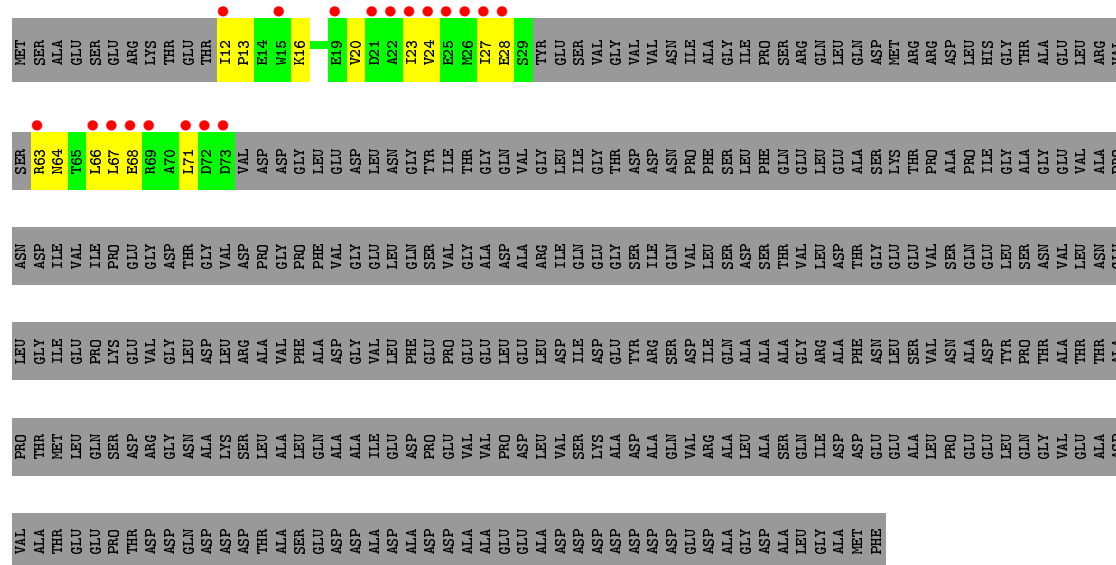


- Molecule 9: 50S ribosomal protein L7AE

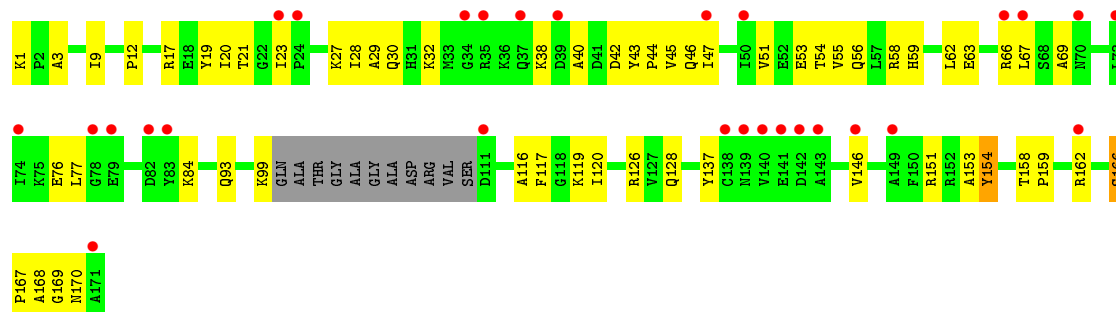




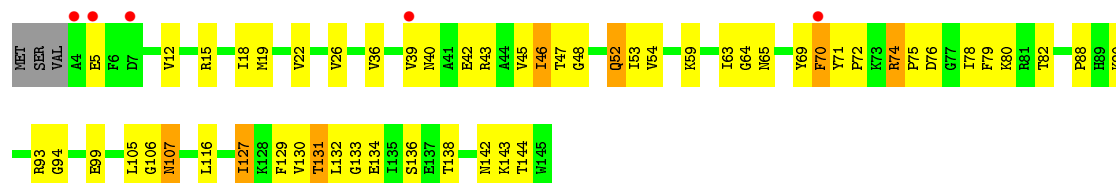
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



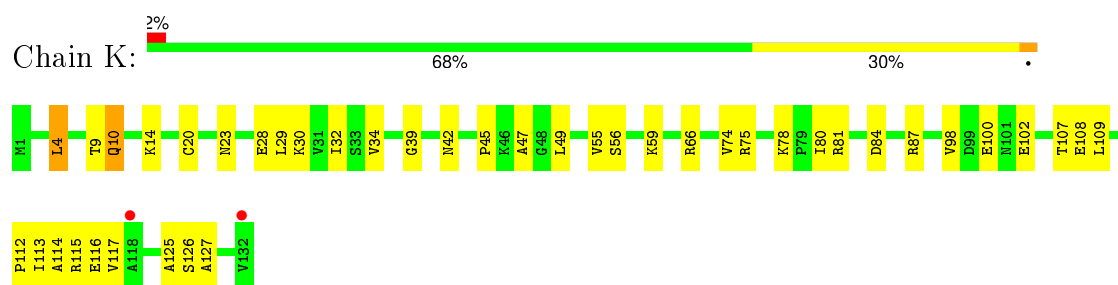
• Molecule 11: 50S RIBOSOMAL PROTEIN L10E



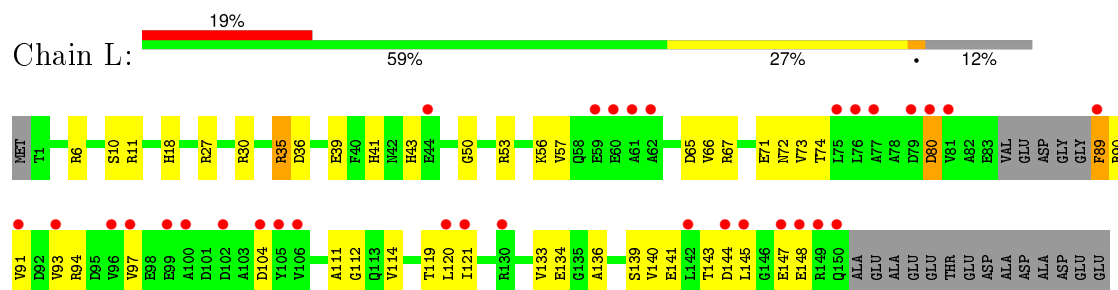
• Molecule 12: 50S ribosomal protein L13P



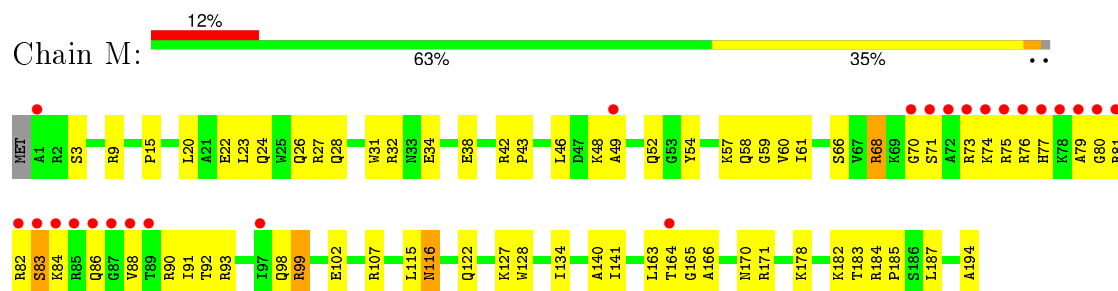
• Molecule 13: 50S ribosomal protein L14P



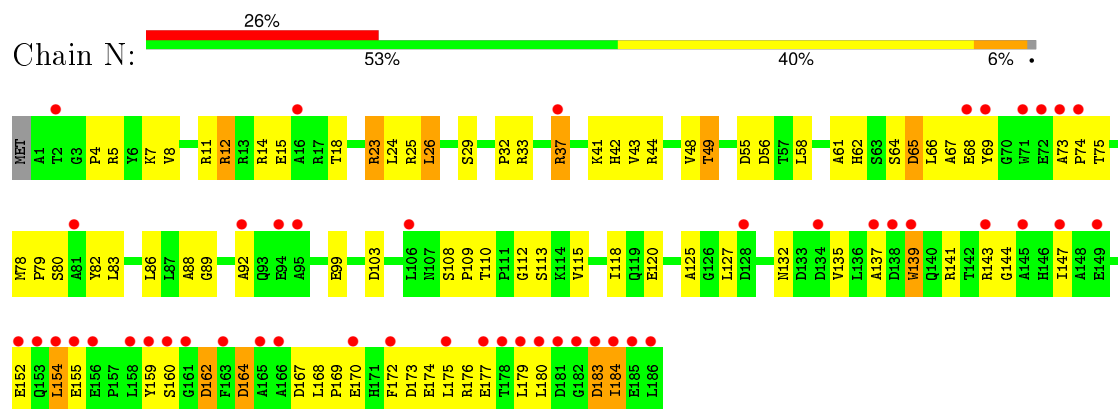
- Molecule 14: 50S ribosomal protein L15P



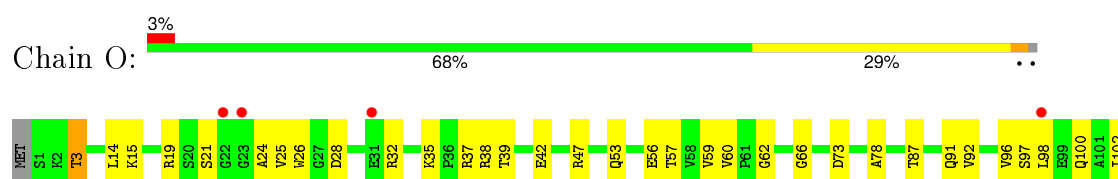
- Molecule 15: 50S Ribosomal Protein L15E



- Molecule 16: 50S ribosomal protein L18P



- Molecule 17: 50S ribosomal protein L18e

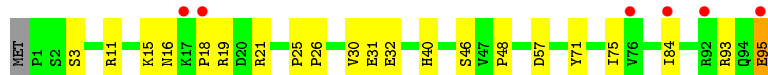
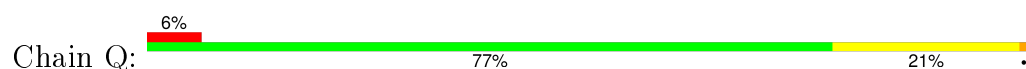




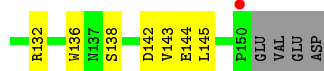
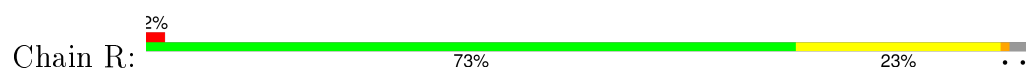
- Molecule 18: 50S ribosomal protein L19E



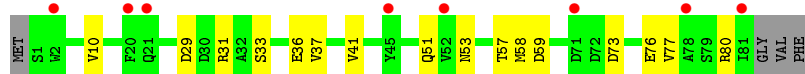
- Molecule 19: 50S ribosomal protein L21e



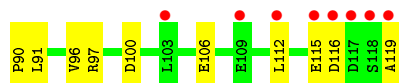
- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P

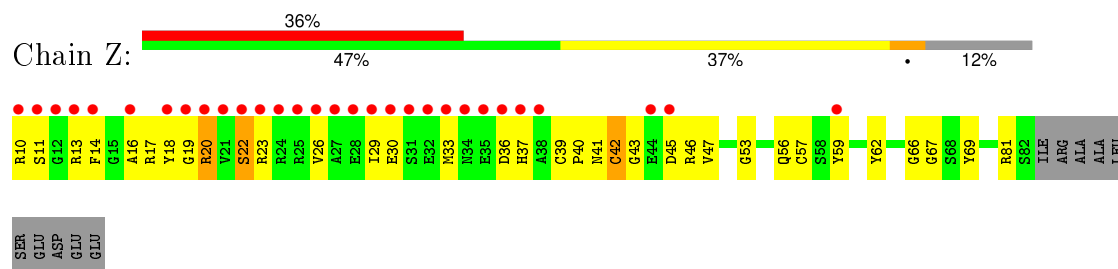


- Molecule 22: 50S ribosomal protein L24P

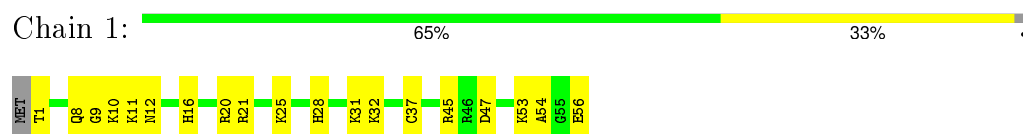


- Molecule 23: 50S ribosomal protein L24E

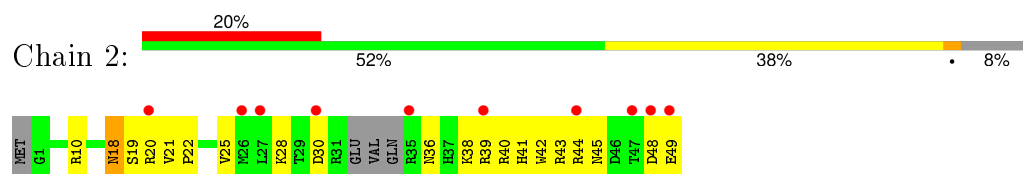
● Molecule 28: 50S ribosomal protein L37Ae



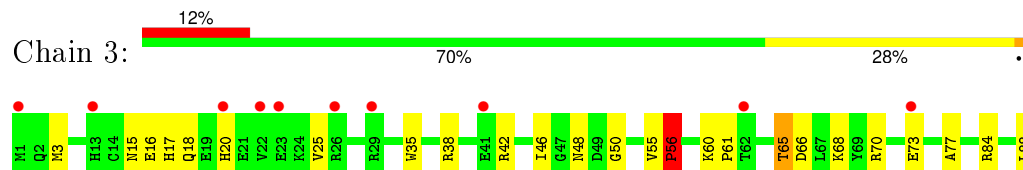
● Molecule 29: 50S ribosomal protein L37e



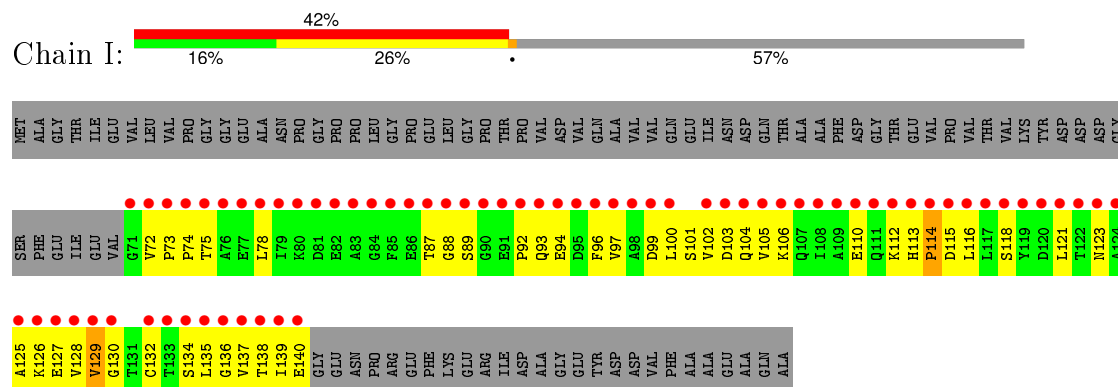
● Molecule 30: 50S ribosomal protein L39e



● Molecule 31: 50S ribosomal protein L44E



● Molecule 32: 50S RIBOSOMAL PROTEIN L11P



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.44Å 298.56Å 574.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.30) 89.8 (49.61-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.247 0.208 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 789252 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99045	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, PPU, CL, SR, NA, K, PO2, 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	0.38	0/65959	0.70	24/102870 (0.0%)
2	9	0.32	0/2905	0.70	1/4528 (0.0%)
3	4	0.48	0/40	0.61	0/60
4	A	0.33	0/1786	0.65	0/2408
5	B	0.32	0/2690	0.64	0/3652
6	C	0.37	0/1884	0.65	0/2551
7	D	0.29	0/1111	0.53	0/1498
8	E	0.31	0/1382	0.56	0/1880
9	F	0.30	0/901	0.53	0/1224
10	G	0.27	0/241	0.46	0/324
11	H	0.33	0/1287	0.64	0/1725
12	J	0.34	0/1136	0.60	0/1530
13	K	0.35	0/1001	0.66	0/1347
14	L	0.32	0/1130	0.63	0/1509
15	M	0.35	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.60	0/1999
17	O	0.32	0/874	0.58	1/1181 (0.1%)
18	P	0.34	0/1147	0.55	0/1528
19	Q	0.35	0/749	0.68	0/1005
20	R	0.35	0/1172	0.66	1/1578 (0.1%)
21	S	0.32	0/648	0.58	0/875
22	T	0.30	0/958	0.62	0/1289
23	U	0.34	0/417	0.56	0/562
24	V	0.26	0/502	0.50	0/675
25	W	0.33	0/1219	0.59	0/1655
26	X	0.32	0/664	0.59	0/895
27	Y	0.35	0/1146	0.65	0/1536
28	Z	0.33	0/589	0.59	0/787
29	1	0.44	0/438	0.66	0/578
30	2	0.34	0/401	0.58	0/529
31	3	0.35	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	0/98732	0.67	27/147637 (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	0	44
2	9	0	1
All	All	0	45

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1819	G	C5'-C4'-C3'	7.74	128.38	116.00
1	0	871	G	C5'-C4'-O4'	-7.70	99.86	109.10
1	0	1942	A	C5'-C4'-C3'	7.40	127.83	116.00
2	9	3039	U	N1-C1'-C2'	6.97	123.06	114.00
1	0	1979	G	C2'-C3'-O3'	6.95	124.81	113.70
1	0	1592	G	N9-C1'-C2'	6.57	122.55	114.00
1	0	777	U	O4'-C1'-N1	6.41	113.33	108.20
1	0	1819	G	C4'-C3'-C2'	-6.14	96.46	102.60
1	0	1819	G	C1'-O4'-C4'	-6.12	105.01	109.90
1	0	1504	A	C1'-O4'-C4'	-6.09	105.03	109.90
1	0	389	G	C5'-C4'-C3'	-5.79	106.74	116.00
1	0	883	U	N1-C1'-C2'	5.75	121.47	114.00
1	0	2467	A	C1'-O4'-C4'	-5.66	105.37	109.90
1	0	2291	A	N9-C1'-C2'	5.62	121.31	114.00
1	0	206	G	C5'-C4'-C3'	-5.50	107.19	116.00
1	0	2726	U	N1-C1'-C2'	5.31	120.90	114.00
1	0	1261	A	N9-C1'-C2'	5.26	120.84	114.00
1	0	2313	C	C5'-C4'-O4'	5.21	115.36	109.10
1	0	1504	A	N9-C1'-C2'	5.17	120.73	114.00
17	O	66	GLY	N-CA-C	5.17	126.03	113.10
1	0	1615	A	C5'-C4'-C3'	5.12	124.18	116.00
1	0	841	A	C1'-O4'-C4'	-5.11	105.81	109.90
1	0	921	G	N9-C1'-C2'	5.09	120.62	114.00
1	0	1120	U	C5'-C4'-C3'	-5.09	107.85	116.00
1	0	69	A	C5'-C4'-O4'	-5.06	103.03	109.10
1	0	1452	G	C5'-C4'-C3'	-5.03	107.96	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	R	128	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1132	A	Sidechain
1	0	1327	G	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1361	C	Sidechain
1	0	1458	A	Sidechain
1	0	1777	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	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1979	G	Sidechain
1	0	2036	C	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2599	A	Sidechain
1	0	2607	U	Sidechain
1	0	2632	G	Sidechain
1	0	2842	G	Sidechain
1	0	396	U	Sidechain
1	0	460	A	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	518	G	Sidechain
1	0	554	G	Sidechain
1	0	619	U	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

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	714	0
2	9	2600	0	1326	52	0
3	4	74	0	49	1	0
4	A	1753	0	1766	108	0
5	B	2625	0	2532	133	0
6	C	1859	0	1816	89	0
7	D	1094	0	1085	77	0
8	E	1357	0	1266	55	0
9	F	890	0	843	47	0
10	G	240	0	231	14	0
11	H	1266	0	1268	57	0
12	J	1120	0	1098	78	0
13	K	992	0	1031	46	0
14	L	1118	0	1076	50	0
15	M	1560	0	1568	72	0
16	N	1445	0	1401	86	0
17	O	865	0	873	37	0
18	P	1136	0	1123	38	0
19	Q	735	0	729	17	0
20	R	1149	0	1122	36	0
21	S	641	0	605	16	0
22	T	950	0	924	49	0
23	U	410	0	364	21	0
24	V	499	0	511	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	W	1196	0	1137	91	0
26	X	654	0	653	38	0
27	Y	1130	0	1133	61	0
28	Z	578	0	539	39	0
29	1	431	0	426	26	0
30	2	396	0	413	28	0
31	3	755	0	728	28	0
32	I	519	0	500	50	0
33	4	61	0	34	2	0
34	0	87	0	0	0	0
34	2	1	0	0	0	0
34	9	1	0	0	0	0
34	A	1	0	0	0	0
34	B	1	0	0	0	0
34	K	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	2	0	0	0	0
36	0	62	0	0	0	0
36	3	1	0	0	0	0
36	9	3	0	0	0	0
36	C	1	0	0	0	0
36	H	1	0	0	0	0
36	J	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	3	0	0	0	0
36	S	1	0	0	0	0
37	0	10	0	0	0	0
37	3	1	0	0	0	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0
37	J	3	0	0	1	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	N	1	0	0	1	0
37	O	1	0	0	0	0
37	R	1	0	0	0	0
37	Y	1	0	0	0	0
38	0	98	0	0	0	0
38	1	2	0	0	0	0
38	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	9	3	0	0	0	0
38	A	3	0	0	0	0
38	B	2	0	0	0	0
38	F	1	0	0	0	0
38	H	1	0	0	0	0
38	L	1	0	0	0	0
38	R	1	0	0	0	0
38	S	1	0	0	0	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5739	0	0	94	0
40	1	51	0	0	1	0
40	2	41	0	0	1	0
40	3	67	0	0	3	0
40	4	8	0	0	0	0
40	9	132	0	0	8	0
40	A	123	0	0	14	0
40	B	139	0	0	19	0
40	C	177	0	0	16	0
40	D	50	0	0	5	0
40	E	43	0	0	2	0
40	F	28	0	0	2	0
40	G	16	0	0	2	0
40	H	71	0	0	8	0
40	I	9	0	0	1	0
40	J	53	0	0	3	0
40	K	57	0	0	4	0
40	L	82	0	0	11	0
40	M	125	0	0	7	0
40	N	59	0	0	7	0
40	O	35	0	0	3	0
40	P	59	0	0	0	0
40	Q	48	0	0	5	0
40	R	86	0	0	2	0
40	S	31	0	0	1	0
40	T	36	0	0	1	0
40	U	26	0	0	1	0
40	V	11	0	0	1	0
40	W	68	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	X	23	0	0	3	0
40	Y	93	0	0	9	0
40	Z	28	0	0	3	0
All	All	99045	0	59983	2061	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 (2061) 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	1.23	1.17
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.31	1.10
2:9:3076:G:H3'	2:9:3077:A:H5''	1.35	1.08
6:C:236:THR:HG22	6:C:239:ALA:H	1.14	1.06
1:0:133:U:H2'	1:0:134:U:H5''	1.37	1.02
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.42	0.99
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.78	0.99
7:D:25:MET:HE2	7:D:41:LEU:HG	1.45	0.98
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.07	0.98
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.29	0.98
1:0:156:C:H5''	15:M:171:ARG:HD3	1.44	0.97
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.29	0.97
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.46	0.97
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.45	0.97
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.47	0.96
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.80	0.96
30:2:18:ASN:HD21	30:2:40:ARG:H	1.05	0.96
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.48	0.96
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.13	0.95
9:F:91:VAL:HG12	9:F:92:GLY:H	1.27	0.95
1:0:2812:A:H2	1:0:2814:A:H62	1.11	0.95
29:1:25:LYS:HD2	30:2:49:GLU:H	1.29	0.94
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.46	0.94
13:K:10:GLN:H	13:K:10:GLN:NE2	1.64	0.93
1:0:542:A:H5'	1:0:542:A:H8	1.34	0.93
1:0:1242:A:H5'	12:J:82:THR:HG23	1.50	0.93
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.48	0.92
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.53	0.91
1:0:1160:G:H5'	1:0:1161:A:H5'	1.51	0.91
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.36	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:10:GLN:N	13:K:10:GLN:HE21	1.69	0.90
30:2:41:HIS:H	30:2:45:ASN:HD22	1.13	0.90
1:0:2717:C:H2'	1:0:2718:C:H5''	1.53	0.90
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.52	0.89
1:0:1372:A:H3'	40:0:7657:HOH:O	1.71	0.89
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.53	0.89
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.55	0.89
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.53	0.89
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.56	0.88
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.54	0.88
6:C:1:MET:HG2	6:C:2:GLN:H	1.39	0.88
6:C:5:ILE:HD11	6:C:16:VAL:HG22	1.56	0.88
1:0:1466:C:H42	1:0:1476:A:H61	1.18	0.87
2:9:3056:A:H2'	2:9:3057:A:H5''	1.55	0.87
13:K:10:GLN:H	13:K:10:GLN:HE21	0.87	0.87
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.57	0.86
1:0:2506:A:HO2'	1:0:2507:G:H8	0.87	0.86
1:0:541:C:H2'	1:0:542:A:H5''	1.57	0.86
1:0:1835:U:H5	1:0:1840:A:N7	1.74	0.86
13:K:39:GLY:HA2	40:K:4183:HOH:O	1.74	0.86
7:D:58:VAL:HB	7:D:62:ASP:HB3	1.57	0.86
5:B:238:ASN:HD22	5:B:240:GLY:H	1.20	0.86
1:0:2840:A:OP1	5:B:211:THR:HG23	1.77	0.84
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.77	0.84
1:0:2717:C:C2'	1:0:2718:C:H5''	2.06	0.84
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.59	0.84
6:C:236:THR:HG22	6:C:239:ALA:N	1.91	0.84
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.12	0.84
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.59	0.84
1:0:1593:C:OP1	18:P:117:SER:HB3	1.78	0.84
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.59	0.84
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.43	0.84
1:0:289:G:H22	1:0:363:A:H2	1.25	0.83
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.60	0.83
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.91	0.83
25:W:13:MET:HE1	25:W:18:GLN:HA	1.60	0.83
4:A:206:ARG:HD3	4:A:206:ARG:H	1.41	0.83
1:0:2073:G:H5''	40:0:4402:HOH:O	1.77	0.82
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.44	0.82
25:W:122:ARG:NH2	25:W:154:ARG:HG2	1.94	0.82
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:871:G:C8	1:0:871:G:H5'	2.15	0.82
4:A:81:GLN:HB2	4:A:92:ASN:ND2	1.94	0.82
6:C:115:LEU:HD21	6:C:243:VAL:HG13	1.62	0.82
25:W:88:THR:HB	40:W:6679:HOH:O	1.80	0.82
4:A:191:GLY:HA2	4:A:194:MET:CE	2.09	0.82
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.62	0.81
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.80	0.81
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.45	0.81
7:D:172:VAL:HG12	7:D:173:GLU:H	1.43	0.81
24:V:1:THR:HG23	24:V:2:VAL:H	1.46	0.81
16:N:144:GLY:O	16:N:147:ILE:HG22	1.79	0.81
6:C:104:ASP:HA	6:C:107:ARG:NH1	1.96	0.81
4:A:69:LEU:HD23	4:A:107:ASN:HB2	1.62	0.81
1:0:1116:U:O2'	1:0:1118:A:H2	1.64	0.81
1:0:2851:G:C2'	1:0:2852:A:H5'	2.11	0.81
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.63	0.81
1:0:1603:A:H5'	1:0:1605:G:O4'	1.82	0.80
4:A:192:VAL:HG22	40:A:9620:HOH:O	1.79	0.80
1:0:133:U:C2'	1:0:134:U:H5''	2.11	0.80
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.63	0.80
1:0:560:C:H42	1:0:597:A:H61	1.27	0.80
1:0:1474:C:H6	1:0:1474:C:H5'	1.47	0.80
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.62	0.80
1:0:1159:G:H21	1:0:1189:A:H8	1.30	0.80
22:T:9:LYS:HE3	22:T:13:ARG:CZ	2.12	0.80
17:O:32:ARG:HD3	17:O:32:ARG:O	1.82	0.80
18:P:115:SER:H	18:P:118:GLN:HE21	1.30	0.80
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.63	0.80
1:0:541:C:C2'	1:0:542:A:H5''	2.12	0.79
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.63	0.79
16:N:113:SER:HB2	40:N:9354:HOH:O	1.82	0.79
4:A:192:VAL:HB	40:A:9583:HOH:O	1.81	0.79
40:O:5382:HOH:O	12:J:47:THR:HB	1.80	0.79
15:M:79:ALA:HB3	15:M:81:ARG:HH12	1.45	0.79
1:0:2506:A:O2'	1:0:2507:G:H8	1.64	0.79
15:M:28:GLN:O	15:M:32:ARG:HG3	1.83	0.79
7:D:154:LYS:HD2	7:D:154:LYS:H	1.47	0.79
20:R:99:ALA:HB1	20:R:109:MET:CE	2.13	0.79
1:0:2054:A:N3	20:R:128:ARG:NH2	2.31	0.79
29:1:25:LYS:HD2	30:2:49:GLU:N	1.98	0.79
1:0:1838:U:H1'	1:0:2644:C:H5'	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1041:U:H5'	40:L:9490:HOH:O	1.82	0.79
1:0:1701:A:H4'	1:0:1702:U:H5''	1.65	0.79
1:0:1118:A:H62	1:0:1244:U:H3	1.30	0.79
27:Y:154:ARG:HH12	27:Y:155:ARG:HG3	1.48	0.79
32:I:78:LEU:HD12	32:I:112:LYS:HZ2	1.49	0.78
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.64	0.78
22:T:63:ILE:HD11	22:T:75:GLU:HB2	1.66	0.78
16:N:11:ARG:HG3	16:N:14:ARG:HH12	1.49	0.78
15:M:79:ALA:HB3	15:M:81:ARG:NH1	1.99	0.77
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.65	0.77
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.10	0.77
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.66	0.77
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.46	0.77
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.85	0.77
14:L:91:VAL:HG13	14:L:120:LEU:HD23	1.67	0.77
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.67	0.77
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.66	0.77
1:0:870:G:H2'	1:0:871:G:H5''	1.67	0.77
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.32	0.77
1:0:1667:A:H8	1:0:1667:A:H5'	1.50	0.77
6:C:246:ARG:HH11	6:C:246:ARG:HB3	1.49	0.76
1:0:1116:U:HO2'	1:0:1118:A:H2	0.80	0.76
1:0:1751:G:H2'	1:0:1752:G:H5''	1.67	0.76
1:0:1973:A:H5'	1:0:1973:A:H8	1.50	0.76
1:0:1119:G:H2'	12:J:52:GLN:NE2	2.01	0.76
2:9:3039:U:H1'	2:9:3044:A:H61	1.50	0.76
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.66	0.76
8:E:15:GLN:HG2	8:E:19:ASP:O	1.84	0.76
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.68	0.76
1:0:2851:G:H2'	1:0:2852:A:H5'	1.68	0.76
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.15	0.76
1:0:1165:G:H4'	1:0:1174:A:O2'	1.86	0.76
1:0:1119:G:N2	1:0:1246:A:C2	2.53	0.76
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.66	0.76
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.02	0.75
11:H:27:LYS:H	11:H:59:HIS:HD2	1.30	0.75
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.68	0.75
1:0:544:G:H2'	1:0:545:G:H5''	1.68	0.75
14:L:143:THR:HG22	14:L:144:ASP:H	1.49	0.75
1:0:559:U:H5'	1:0:559:U:H6	1.51	0.75
1:0:288:A:H61	1:0:364:C:H42	1.32	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:78:LEU:HD12	32:I:112:LYS:NZ	2.02	0.75
1:O:871:G:C8	1:O:871:G:C5'	2.70	0.74
18:P:115:SER:OG	18:P:118:GLN:HG3	1.87	0.74
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.68	0.74
1:O:281:U:H2'	1:O:282:C:O4'	1.86	0.74
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.68	0.74
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.69	0.74
21:S:57:THR:HG22	21:S:59:ASP:H	1.52	0.74
16:N:132:ASN:O	16:N:135:VAL:HG12	1.87	0.74
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.53	0.74
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.70	0.74
1:O:506:G:H22	1:O:509:A:H5''	1.52	0.74
40:O:7902:HOH:O	5:B:211:THR:HG21	1.87	0.73
1:O:470:U:O2'	29:1:16:HIS:HD2	1.71	0.73
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.71	0.73
9:F:58:GLU:HG3	9:F:61:MET:HE1	1.70	0.73
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.70	0.73
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.18	0.73
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.69	0.73
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.19	0.73
1:O:871:G:H8	1:O:871:G:C5'	2.00	0.73
5:B:51:VAL:HG23	5:B:329:TYR:O	1.89	0.73
1:O:2468:A:H61	31:3:48:ASN:HD21	1.37	0.73
1:O:1175:G:H1'	1:O:1193:A:H2'	1.69	0.73
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.71	0.73
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.86	0.73
1:O:380:A:OP2	15:M:9:ARG:HD2	1.89	0.73
1:O:1878:G:H1'	40:O:6632:HOH:O	1.89	0.73
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.70	0.73
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.19	0.73
1:O:1160:G:C5'	1:O:1161:A:H5'	2.19	0.73
1:O:2491:G:H1'	40:O:7349:HOH:O	1.87	0.73
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.12	0.72
6:C:246:ARG:NH1	6:C:246:ARG:HB3	2.04	0.72
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.72	0.72
17:O:32:ARG:NE	17:O:35:LYS:HD2	2.03	0.72
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.90	0.72
1:O:1206:U:H5'	1:O:1206:U:H6	1.53	0.72
16:N:37:ARG:HG3	37:N:9307:CL:CL	2.26	0.72
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.70	0.72
26:X:71:ARG:HD3	40:X:2171:HOH:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:141:ARG:HD2	5:B:163:GLU:OE2	1.90	0.72
1:0:2765:C:H4'	40:0:6049:HOH:O	1.90	0.72
40:0:6049:HOH:O	5:B:298:LYS:HG2	1.88	0.72
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.20	0.72
1:0:2748:G:H2'	40:0:7984:HOH:O	1.90	0.72
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.25	0.71
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.72	0.71
9:F:96:ALA:HA	40:F:3111:HOH:O	1.91	0.71
1:0:960:G:H4'	40:0:7878:HOH:O	1.89	0.71
6:C:236:THR:H	6:C:239:ALA:HB3	1.55	0.71
1:0:481:U:H5''	40:0:6176:HOH:O	1.89	0.71
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.73	0.71
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.73	0.71
1:0:2716:G:H5''	5:B:206:THR:HG21	1.72	0.71
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.09	0.71
1:0:2291:A:C8	1:0:2309:C:H5'	2.26	0.71
21:S:51:GLN:HE21	21:S:53:ASN:ND2	1.85	0.71
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.73	0.71
14:L:143:THR:HG22	14:L:144:ASP:N	2.05	0.71
2:9:3014:G:H8	2:9:3014:G:H5'	1.56	0.71
21:S:51:GLN:NE2	21:S:53:ASN:HD21	1.86	0.71
1:0:506:G:H22	1:0:509:A:C5'	2.04	0.71
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.21	0.71
27:Y:141:THR:HG23	40:Y:9388:HOH:O	1.90	0.71
1:0:93:C:H5''	24:V:1:THR:HB	1.73	0.70
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.02	0.70
26:X:25:ARG:HD3	26:X:64:ALA:O	1.90	0.70
1:0:1118:A:H3'	1:0:1118:A:H8	1.56	0.70
23:U:14:GLU:O	23:U:17:THR:HB	1.92	0.70
5:B:179:LEU:O	5:B:183:GLU:HG2	1.92	0.70
24:V:12:THR:HG22	24:V:15:GLU:CG	2.20	0.70
9:F:58:GLU:HA	9:F:61:MET:HE2	1.73	0.70
25:W:88:THR:HG22	25:W:89:ASP:N	2.06	0.70
1:0:1700:C:H5''	1:0:1701:A:OP2	1.90	0.70
10:G:12:ILE:N	10:G:13:PRO:HD3	2.06	0.70
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.91	0.70
6:C:236:THR:CG2	6:C:239:ALA:H	1.98	0.70
6:C:1:MET:HG2	6:C:2:GLN:N	2.06	0.70
17:O:32:ARG:HH21	17:O:35:LYS:NZ	1.88	0.70
5:B:16:ARG:NH1	40:B:9609:HOH:O	2.25	0.70
15:M:164:THR:HG22	15:M:166:ALA:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:80:GLY:O	15:M:81:ARG:HD2	1.91	0.70
11:H:59:HIS:HA	11:H:62:LEU:HD23	1.72	0.70
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.54	0.70
1:0:2481:G:H5''	40:0:5097:HOH:O	1.91	0.70
1:0:1206:U:H2'	1:0:1207:A:O4'	1.92	0.70
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.57	0.70
1:0:1474:C:C6	1:0:1474:C:H5'	2.27	0.70
16:N:11:ARG:HA	16:N:14:ARG:NH1	2.07	0.70
1:0:969:G:H1	1:0:999:C:H42	1.40	0.69
1:0:1182:C:H1'	1:0:1192:A:H8	1.56	0.69
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.75	0.69
6:C:2:GLN:HB3	40:C:9192:HOH:O	1.92	0.69
1:0:2073:G:OP2	1:0:2490:A:H5'	1.92	0.69
25:W:80:ASP:O	25:W:84:VAL:HG23	1.90	0.69
1:0:1118:A:H3'	1:0:1118:A:C8	2.27	0.69
2:9:3039:U:H1'	2:9:3044:A:N6	2.06	0.69
9:F:37:THR:O	9:F:41:GLU:HG3	1.93	0.69
27:Y:144:ARG:HG3	27:Y:144:ARG:HH11	1.58	0.69
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.92	0.69
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.74	0.69
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.73	0.69
1:0:1187:U:HO2'	1:0:1189:A:H2	1.41	0.69
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.89	0.69
1:0:545:G:H8	1:0:545:G:H5'	1.57	0.69
1:0:1184:C:H4'	32:I:126:LYS:HB3	1.75	0.69
1:0:1184:C:H1'	40:0:7912:HOH:O	1.93	0.69
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.41	0.69
20:R:39:THR:HB	20:R:42:GLU:HG3	1.74	0.69
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.75	0.69
5:B:275:GLY:O	5:B:291:ASP:HA	1.92	0.69
1:0:541:C:H2'	1:0:542:A:C5'	2.23	0.69
16:N:164:ASP:CG	16:N:167:ASP:HA	2.13	0.69
1:0:1166:A:H1'	1:0:1192:A:C2	2.28	0.69
5:B:140:LEU:HA	40:B:9575:HOH:O	1.92	0.69
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.73	0.69
1:0:542:A:H5'	1:0:542:A:C8	2.23	0.68
12:J:19:MET:CE	12:J:132:LEU:HD11	2.23	0.68
9:F:77:VAL:HG21	9:F:83:LEU:HD13	1.76	0.68
25:W:4:LEU:HD11	25:W:45:VAL:HG12	1.76	0.68
25:W:137:GLN:NE2	25:W:141:HIS:HE1	1.91	0.68
1:0:2534:C:H1'	40:0:4086:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.76	0.68
24:V:39:ALA:N	24:V:40:PRO:HD2	2.07	0.68
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.73	0.68
1:O:381:G:H5''	40:M:9376:HOH:O	1.93	0.68
22:T:115:GLU:HG3	22:T:116:ASP:N	2.08	0.68
1:O:1730:G:H5'	1:O:1731:C:C5	2.29	0.68
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.90	0.68
7:D:170:TYR:O	7:D:171:ASP:HB3	1.94	0.68
1:O:2005:G:H3'	1:O:2005:G:OP2	1.94	0.68
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.76	0.68
25:W:48:VAL:HG12	25:W:48:VAL:O	1.93	0.68
2:9:3051:A:H5'	16:N:160:SER:HB3	1.76	0.68
4:A:199:HIS:HD2	4:A:201:PHE:H	1.39	0.67
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.77	0.67
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.76	0.67
1:O:2480:G:H3'	40:O:4754:HOH:O	1.94	0.67
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.76	0.67
1:O:1299:G:O6	14:L:6:ARG:HD3	1.95	0.67
1:O:1244:U:OP1	12:J:18:ILE:HD13	1.94	0.67
1:O:1528:A:H2'	1:O:1529:G:O4'	1.95	0.67
31:3:35:TRP:HB2	40:3:9488:HOH:O	1.93	0.67
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.76	0.67
15:M:24:GLN:O	15:M:28:GLN:HG3	1.94	0.67
25:W:88:THR:HG22	25:W:89:ASP:H	1.58	0.67
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.76	0.67
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.24	0.67
1:O:280:C:H2'	1:O:281:U:O4'	1.95	0.67
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.13	0.67
4:A:48:ASP:HB3	40:A:9595:HOH:O	1.94	0.67
1:O:1116:U:H3	1:O:1246:A:H62	1.41	0.66
1:O:2780:C:H1'	8:E:143:GLN:HE21	1.60	0.66
1:O:1377:C:H6	1:O:1377:C:H5'	1.59	0.66
1:O:1666:C:H2'	1:O:1667:A:H5'	1.76	0.66
11:H:27:LYS:N	11:H:59:HIS:HD2	1.93	0.66
4:A:51:ARG:HB2	40:A:9595:HOH:O	1.94	0.66
1:O:1681:G:H5''	1:O:1682:A:H5'	1.77	0.66
1:O:2003:U:H4'	1:O:2004:U:H5	1.61	0.66
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.26	0.66
28:Z:17:ARG:HD3	40:Z:9218:HOH:O	1.95	0.66
1:O:338:C:H4'	6:C:174:ILE:CD1	2.26	0.66
16:N:62:HIS:HB3	16:N:65:ASP:OD1	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.26	0.66
7:D:172:VAL:HG12	7:D:173:GLU:N	2.10	0.66
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.11	0.66
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.11	0.66
1:O:1209:C:H2'	1:O:1210:G:H8	1.59	0.66
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.28	0.66
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.25	0.66
1:O:709:G:O2'	17:O:25:VAL:HG12	1.94	0.66
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.77	0.66
15:M:77:HIS:HD2	15:M:79:ALA:O	1.79	0.66
40:O:4937:HOH:O	15:M:83:SER:HB3	1.96	0.66
11:H:166:SER:CB	11:H:167:PRO:CD	2.74	0.65
1:O:871:G:H8	1:O:871:G:H5'	1.60	0.65
25:W:52:VAL:HG22	25:W:53:ALA:H	1.61	0.65
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.26	0.65
14:L:35:ARG:HB2	14:L:35:ARG:NH1	2.11	0.65
1:O:134:U:H6	1:O:134:U:C5'	2.09	0.65
6:C:107:ARG:NE	40:C:9263:HOH:O	2.29	0.65
30:2:18:ASN:ND2	30:2:40:ARG:H	1.86	0.65
40:O:9737:HOH:O	15:M:82:ARG:HD2	1.95	0.65
5:B:109:LEU:HG	5:B:113:LEU:HD11	1.78	0.65
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.60	0.65
27:Y:144:ARG:CZ	40:Y:9409:HOH:O	2.44	0.65
18:P:115:SER:H	18:P:118:GLN:NE2	1.93	0.65
20:R:44:VAL:O	20:R:48:GLU:HG3	1.95	0.65
1:O:553:G:P	27:Y:204:ARG:HH22	2.19	0.65
13:K:49:LEU:HD12	13:K:80:ILE:HG21	1.79	0.65
1:O:2676:C:H4'	12:J:70:PHE:CE1	2.32	0.65
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.20	0.65
1:O:1119:G:H22	1:O:1246:A:H2	1.38	0.65
1:O:1166:A:H61	1:O:1180:U:H3	1.44	0.65
1:O:2676:C:H4'	12:J:70:PHE:CD1	2.32	0.65
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.62	0.65
28:Z:37:HIS:O	28:Z:45:ASP:HA	1.97	0.65
1:O:282:C:O2'	1:O:283:U:H5'	1.96	0.65
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.97	0.65
1:O:1201:C:H5''	40:O:6742:HOH:O	1.97	0.65
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.97	0.65
1:O:544:G:C2'	1:O:545:G:H5''	2.26	0.65
21:S:57:THR:HG22	21:S:59:ASP:N	2.11	0.65
1:O:1426:C:H2'	40:O:3204:HOH:O	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:99:ARG:NH2	15:M:170:ASN:HD22	1.89	0.64
14:L:73:VAL:HG23	14:L:74:THR:H	1.62	0.64
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.23	0.64
16:N:80:SER:HB2	40:N:9333:HOH:O	1.95	0.64
1:O:263:U:O4'	9:F:59:ILE:HD13	1.98	0.64
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.12	0.64
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.80	0.64
18:P:91:LYS:O	18:P:95:GLU:HG3	1.97	0.64
1:O:2749:U:H5'	40:O:8438:HOH:O	1.96	0.64
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.78	0.64
23:U:52:THR:HG22	23:U:54:THR:N	2.13	0.64
2:9:3029:C:O3'	7:D:138:GLY:HA2	1.97	0.64
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.32	0.64
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.13	0.64
12:J:75:PRO:HD3	12:J:136:SER:OG	1.97	0.64
17:O:32:ARG:HH21	17:O:35:LYS:HZ2	1.43	0.64
24:V:56:ILE:O	24:V:60:GLN:HG3	1.97	0.64
1:O:1201:C:H2'	1:O:1202:A:H5'	1.79	0.64
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.62	0.64
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.32	0.64
1:O:1771:U:H5'	28:Z:20:ARG:HH21	1.63	0.64
7:D:159:PRO:O	7:D:163:VAL:HG23	1.97	0.64
2:9:3056:A:C2'	2:9:3057:A:H5''	2.27	0.64
1:O:2908:A:H2'	1:O:2909:G:O4'	1.98	0.64
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.27	0.64
1:O:134:U:H5'	1:O:134:U:H6	1.63	0.64
4:A:107:ASN:OD1	4:A:120:ARG:HD2	1.97	0.64
1:O:1119:G:H2'	12:J:52:GLN:HE22	1.61	0.64
2:9:3029:C:H2'	2:9:3030:C:H5'	1.80	0.64
1:O:1943:C:H4'	4:A:211:LYS:O	1.98	0.64
5:B:53:LEU:HD11	5:B:327:VAL:HG22	1.78	0.63
1:O:1183:C:N4	1:O:1184:C:H41	1.96	0.63
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.81	0.63
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.28	0.63
31:3:65:THR:HG22	31:3:88:LEU:HD22	1.78	0.63
1:O:1641:A:H2'	1:O:1642:A:H5'	1.79	0.63
5:B:53:LEU:HD21	5:B:270:ILE:HD12	1.80	0.63
17:O:57:THR:HB	17:O:111:VAL:HG23	1.78	0.63
19:Q:25:PRO:HB2	40:Q:4350:HOH:O	1.98	0.63
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.80	0.63
1:O:2426:G:H1'	40:O:6603:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:165:GLU:HB3	40:Y:9393:HOH:O	1.98	0.63
1:O:2541:U:H5'	40:O:3025:HOH:O	1.96	0.63
7:D:105:SER:HB2	7:D:131:THR:HG23	1.81	0.63
6:C:242:GLU:HG3	40:C:9189:HOH:O	1.99	0.63
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.28	0.63
1:O:834:G:H4'	1:O:835:U:OP2	1.99	0.63
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.26	0.63
25:W:84:VAL:HG12	40:W:6679:HOH:O	1.98	0.63
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.32	0.63
1:O:282:C:H1'	1:O:368:C:N4	2.13	0.63
4:A:113:GLY:HA2	4:A:153:ARG:NH2	2.14	0.63
9:F:91:VAL:HG12	9:F:92:GLY:N	2.05	0.63
8:E:34:TRP:O	12:J:127:ILE:HD11	1.99	0.63
2:9:3013:A:O2'	2:9:3014:G:H5''	1.98	0.63
7:D:57:THR:HG23	7:D:63:ILE:HA	1.80	0.63
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.34	0.63
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.80	0.63
7:D:136:ARG:HH12	7:D:157:LEU:HA	1.63	0.63
1:O:1328:A:OP1	27:Y:169:ARG:HD2	1.98	0.63
1:O:2578:G:H5'	1:O:2578:G:H8	1.63	0.63
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.81	0.63
32:I:99:ASP:OD1	32:I:138:THR:HB	1.98	0.63
5:B:305:ASP:O	5:B:306:LYS:HB2	1.99	0.63
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.79	0.63
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.27	0.62
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.81	0.62
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.80	0.62
9:F:21:GLU:O	9:F:24:ARG:HG3	1.99	0.62
12:J:19:MET:HE1	12:J:132:LEU:HD11	1.81	0.62
17:O:21:SER:OG	17:O:106:PRO:HB2	2.00	0.62
22:T:85:GLU:HG2	22:T:86:GLU:N	2.14	0.62
1:O:2346:C:O2'	7:D:52:THR:HG21	1.98	0.62
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.82	0.62
1:O:902:G:N7	14:L:18:HIS:HD2	1.98	0.62
1:O:2896:A:N3	1:O:2896:A:H2'	2.13	0.62
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.62	0.62
1:O:1160:G:H5'	1:O:1161:A:C5'	2.28	0.62
8:E:81:GLU:HG2	8:E:134:SER:CB	2.29	0.62
14:L:133:VAL:HA	40:L:9469:HOH:O	1.99	0.62
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.35	0.62
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:254:GLN:HG2	5:B:255:GLY:N	2.12	0.62
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.82	0.62
9:F:13:GLU:OE2	9:F:78:GLU:HG2	1.99	0.62
5:B:238:ASN:ND2	5:B:240:GLY:H	1.96	0.62
22:T:115:GLU:HG3	22:T:116:ASP:H	1.63	0.62
1:0:877:G:H5'	1:0:878:G:OP1	1.98	0.62
17:O:87:THR:O	17:O:91:GLN:HG3	1.99	0.62
1:0:2064:U:H5'	1:0:2652:U:H4'	1.81	0.62
29:1:10:LYS:HG3	40:1:9489:HOH:O	1.99	0.62
32:I:110:GLU:HA	32:I:113:HIS:CE1	2.35	0.62
11:H:63:GLU:HA	40:H:9544:HOH:O	1.98	0.62
1:0:1555:G:H4'	1:0:1630:A:H2	1.65	0.62
13:K:55:VAL:HG12	13:K:56:SER:N	2.15	0.62
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.15	0.62
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.15	0.62
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.14	0.62
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.29	0.62
1:0:1666:C:O2'	1:0:1667:A:H5''	1.99	0.62
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.03	0.62
4:A:131:HIS:O	4:A:132:ASP:HB2	1.98	0.62
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.64	0.62
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.82	0.62
1:0:625:U:H5''	1:0:1044:C:N4	2.14	0.62
22:T:47:THR:HB	22:T:100:ASP:HB3	1.82	0.62
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.29	0.61
1:0:2541:U:H4'	1:0:2542:C:OP1	1.99	0.61
11:H:30:GLN:H	11:H:66:ARG:NH1	1.98	0.61
4:A:179:MET:HG2	4:A:186:TRP:CB	2.30	0.61
22:T:38:ARG:NH1	40:T:6217:HOH:O	2.33	0.61
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.31	0.61
10:G:20:VAL:O	10:G:24:VAL:HG23	2.00	0.61
4:A:33:GLU:O	4:A:34:ASP:HB2	1.99	0.61
1:0:2505:G:O2'	1:0:2506:A:H5'	2.00	0.61
1:0:558:C:C2'	1:0:559:U:H5''	2.30	0.61
16:N:176:ARG:HG3	16:N:180:LEU:HD13	1.82	0.61
1:0:111:C:O2'	29:1:20:ARG:HG2	2.01	0.61
7:D:25:MET:CE	7:D:41:LEU:HG	2.26	0.61
29:1:25:LYS:CD	30:2:49:GLU:H	2.09	0.61
5:B:175:LEU:O	5:B:175:LEU:HD23	2.01	0.61
1:0:1116:U:O2'	1:0:1118:A:C2	2.45	0.61
12:J:74:ARG:O	12:J:78:ILE:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:39:VAL:HG13	12:J:106:GLY:O	2.01	0.61
1:0:244:C:OP2	9:F:38:LYS:HE3	2.00	0.61
15:M:76:ARG:HG3	15:M:88:VAL:HG21	1.83	0.61
15:M:107:ARG:NH1	15:M:107:ARG:HG3	2.10	0.61
4:A:82:VAL:HG13	4:A:93:THR:HB	1.80	0.61
4:A:33:GLU:CD	4:A:33:GLU:H	2.03	0.61
4:A:35:GLY:O	4:A:36:ASP:HB3	1.99	0.61
5:B:307:ARG:NH1	5:B:307:ARG:HG3	2.16	0.61
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.65	0.61
1:0:681:G:N3	1:0:681:G:H5'	2.16	0.61
1:0:2661:U:H3	1:0:2812:A:H62	1.48	0.61
15:M:164:THR:HG22	15:M:166:ALA:N	2.14	0.61
25:W:13:MET:CE	25:W:17:ILE:HG22	2.31	0.61
1:0:1701:A:H4'	1:0:1702:U:C5'	2.30	0.61
1:0:2032:U:H2'	1:0:2033:G:H5''	1.83	0.61
1:0:2032:U:H2'	1:0:2033:G:C5'	2.31	0.61
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.15	0.61
1:0:2533:C:H5'	1:0:2533:C:H6	1.65	0.61
25:W:38:THR:HG22	25:W:39:ASP:N	2.15	0.61
1:0:2524:G:H21	1:0:2526:C:N4	1.99	0.61
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.66	0.61
8:E:68:HIS:O	8:E:72:MET:HG3	2.00	0.61
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.34	0.61
21:S:77:VAL:O	21:S:80:ARG:HG2	2.00	0.61
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.82	0.61
2:9:3020:G:O2'	2:9:3021:G:H5'	2.00	0.61
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.31	0.60
1:0:447:A:P	22:T:1:SER:HB2	2.40	0.60
14:L:80:ASP:HB2	14:L:90:ARG:O	2.01	0.60
1:0:2748:G:H1'	40:0:8415:HOH:O	2.01	0.60
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.16	0.60
1:0:1406:A:H4'	1:0:1407:A:H5''	1.83	0.60
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.01	0.60
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.00	0.60
14:L:67:ARG:O	14:L:71:GLU:HG3	2.01	0.60
8:E:108:LEU:HD11	8:E:164:ASP:HB2	1.82	0.60
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.83	0.60
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.82	0.60
7:D:94:ALA:HA	7:D:174:VAL:HA	1.84	0.60
1:0:558:C:H2'	1:0:559:U:C5'	2.31	0.60
14:L:35:ARG:HB2	14:L:35:ARG:HH11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.49	0.60
40:O:6281:HOH:O	22:T:106:GLU:HG3	2.00	0.60
9:F:60:VAL:HG12	9:F:60:VAL:O	2.02	0.60
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.35	0.60
1:O:1168:C:H5''	32:I:87:THR:CG2	2.32	0.60
25:W:130:HIS:O	25:W:136:GLY:HA3	2.02	0.60
2:9:3008:G:O6	16:N:11:ARG:NH1	2.34	0.60
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.84	0.60
1:O:2420:G:O2'	1:O:2421:G:H5'	2.02	0.60
1:O:137:U:H2'	1:O:139:C:C5	2.37	0.60
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.82	0.60
15:M:99:ARG:HH21	15:M:170:ASN:ND2	1.93	0.60
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.83	0.60
7:D:50:VAL:O	7:D:71:ALA:HA	2.02	0.60
1:O:1687:C:O2	29:I:9:GLY:HA2	2.02	0.60
27:Y:115:ARG:HH11	27:Y:115:ARG:HB3	1.66	0.60
6:C:107:ARG:HH11	6:C:107:ARG:HB3	1.66	0.60
16:N:115:VAL:HG22	40:N:9354:HOH:O	2.00	0.60
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.66	0.60
1:O:1183:C:H2'	40:O:6752:HOH:O	2.01	0.60
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.31	0.60
13:K:107:THR:HG22	13:K:108:GLU:HG3	1.84	0.60
4:A:165:THR:HG22	40:A:9608:HOH:O	2.02	0.60
15:M:68:ARG:HD3	15:M:68:ARG:O	2.02	0.60
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.67	0.60
2:9:3014:G:C8	2:9:3014:G:H5'	2.36	0.60
2:9:3076:G:H3'	2:9:3077:A:C5'	2.24	0.59
32:I:102:VAL:O	32:I:106:LYS:HG3	2.02	0.59
1:O:316:A:N3	1:O:336:G:O2'	2.33	0.59
4:A:121:ALA:O	4:A:124:VAL:HG22	2.02	0.59
1:O:271:C:H41	1:O:378:A:H2	1.46	0.59
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.00	0.59
1:O:289:G:N2	1:O:363:A:H2	1.97	0.59
1:O:1838:U:O2'	1:O:2644:C:H5'	2.03	0.59
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.32	0.59
1:O:1168:C:H5''	32:I:87:THR:HG23	1.83	0.59
1:O:1159:G:H1	1:O:1208:C:H42	1.51	0.59
12:J:45:VAL:HG23	12:J:130:VAL:O	2.01	0.59
22:T:19:ARG:HD3	22:T:67:LEU:O	2.03	0.59
17:O:39:THR:O	17:O:115:ARG:NH2	2.36	0.59
32:I:92:PRO:C	32:I:94:GLU:H	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.84	0.59
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.38	0.59
40:0:3151:HOH:O	18:P:81:LYS:HG2	2.01	0.59
25:W:122:ARG:HG2	25:W:152:ALA:O	2.02	0.59
24:V:1:THR:HG23	24:V:2:VAL:N	2.17	0.59
1:0:797:A:H4'	28:Z:10:ARG:N	2.18	0.59
10:G:24:VAL:O	10:G:28:GLU:HB2	2.02	0.59
4:A:105:VAL:HG12	4:A:106:CYS:N	2.18	0.59
1:0:328:U:O4'	6:C:202:THR:HG22	2.03	0.59
6:C:236:THR:HG21	40:C:9181:HOH:O	2.03	0.59
1:0:2812:A:C2	1:0:2814:A:N6	2.66	0.59
22:T:71:VAL:HG12	22:T:72:ILE:N	2.18	0.59
16:N:154:LEU:O	16:N:155:GLU:HB3	2.02	0.59
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.84	0.59
1:0:121:U:OP2	30:2:10:ARG:NH2	2.33	0.59
12:J:75:PRO:HB3	12:J:132:LEU:HB3	1.85	0.59
8:E:85:GLU:HG3	8:E:169:THR:OG1	2.03	0.59
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.68	0.59
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.36	0.58
1:0:797:A:C4'	28:Z:10:ARG:N	2.66	0.58
25:W:119:HIS:HD2	25:W:120:PRO:O	1.86	0.58
1:0:775:G:OP1	29:1:16:HIS:HE1	1.85	0.58
1:0:1626:A:H2'	1:0:1627:G:O4'	2.03	0.58
1:0:2878:U:H2'	1:0:2879:A:O4'	2.03	0.58
1:0:1119:G:H8	12:J:52:GLN:HE22	1.52	0.58
4:A:199:HIS:CD2	4:A:201:PHE:H	2.19	0.58
4:A:206:ARG:N	4:A:206:ARG:HD3	2.14	0.58
1:0:1878:G:O2'	1:0:1879:U:OP2	2.20	0.58
5:B:125:GLU:O	5:B:129:ARG:HG3	2.03	0.58
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.68	0.58
1:0:256:C:H2'	1:0:257:G:O4'	2.03	0.58
25:W:149:LEU:HG	25:W:153:MET:CE	2.33	0.58
1:0:272:A:H5'	1:0:273:G:OP2	2.04	0.58
5:B:72:THR:HB	40:B:9598:HOH:O	2.02	0.58
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.17	0.58
1:0:558:C:O2'	1:0:559:U:H5''	2.04	0.58
1:0:1745:G:H22	1:0:2033:G:H5'	1.68	0.58
22:T:78:THR:HB	22:T:87:VAL:O	2.04	0.58
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.85	0.58
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.28	0.58
32:I:113:HIS:N	32:I:114:PRO:HD2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.86	0.58
4:A:125:ASN:CB	4:A:158:VAL:HG12	2.34	0.58
1:0:2526:C:O2'	1:0:2527:U:H5'	2.03	0.58
40:0:9972:HOH:O	29:1:1:THR:HA	2.02	0.58
11:H:154:TYR:HB2	40:H:9557:HOH:O	2.04	0.58
1:0:1973:A:H5'	1:0:1973:A:C8	2.37	0.58
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.72	0.58
1:0:396:U:O2'	1:0:418:C:H4'	2.04	0.58
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.86	0.58
18:P:16:VAL:HG12	18:P:17:GLY:N	2.18	0.58
1:0:871:G:H8	1:0:871:G:H5''	1.68	0.57
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.86	0.57
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.85	0.57
15:M:182:LYS:O	15:M:194:ALA:HB2	2.04	0.57
1:0:1333:U:H2'	1:0:1334:C:C6	2.40	0.57
1:0:1736:A:H1'	40:0:8095:HOH:O	2.03	0.57
1:0:2502:C:H2'	1:0:2503:A:H5'	1.86	0.57
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.03	0.57
8:E:102:VAL:HG11	8:E:148:ILE:HG12	1.86	0.57
1:0:516:A:H5'	40:0:6176:HOH:O	2.05	0.57
18:P:40:VAL:O	18:P:44:VAL:HG23	2.04	0.57
1:0:1080:C:H4'	1:0:1081:A:OP1	2.03	0.57
15:M:71:SER:HB2	15:M:92:THR:HG22	1.85	0.57
15:M:57:LYS:HE2	15:M:140:ALA:O	2.04	0.57
8:E:8:PRO:HB2	8:E:11:VAL:HG23	1.86	0.57
1:0:138:U:H5''	1:0:139:C:OP2	2.04	0.57
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.70	0.57
1:0:447:A:OP1	22:T:2:LYS:HG2	2.05	0.57
13:K:114:ALA:HB3	13:K:117:VAL:HG23	1.85	0.57
1:0:2769:C:O2'	1:0:2770:G:H5'	2.05	0.57
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.87	0.57
1:0:2502:C:C2'	1:0:2503:A:H5'	2.35	0.57
1:0:2769:C:C2'	1:0:2770:G:H5'	2.35	0.57
32:I:125:ALA:O	32:I:129:VAL:HG23	2.04	0.57
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.39	0.57
6:C:139:VAL:HG13	40:C:9253:HOH:O	2.05	0.57
25:W:125:HIS:CD2	25:W:127:GLY:H	2.23	0.57
16:N:23:ARG:HD3	40:N:9344:HOH:O	2.03	0.57
15:M:74:LYS:HG2	15:M:75:ARG:N	2.20	0.57
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.34	0.57
1:0:1119:G:H8	12:J:52:GLN:NE2	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:297:VAL:HB	40:B:9598:HOH:O	2.03	0.57
32:I:134:SER:O	32:I:135:LEU:HD23	2.04	0.57
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.87	0.57
1:0:485:A:N3	1:0:487:G:H5''	2.20	0.57
1:0:474:C:O3'	6:C:73:LEU:HD21	2.04	0.57
1:0:69:A:H5'	1:0:69:A:C8	2.39	0.57
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.34	0.57
15:M:68:ARG:NH2	15:M:73:ARG:HD3	2.18	0.57
40:0:7990:HOH:O	15:M:91:ILE:HG23	2.04	0.57
1:0:450:C:OP1	6:C:184:ARG:NH2	2.37	0.57
1:0:1205:U:H2'	1:0:1206:U:C5'	2.35	0.56
1:0:475:G:OP1	6:C:73:LEU:HD22	2.05	0.56
6:C:93:LYS:O	6:C:98:ARG:NH2	2.38	0.56
6:C:25:PRO:HG2	40:C:9125:HOH:O	2.05	0.56
15:M:107:ARG:CG	15:M:107:ARG:HH11	2.14	0.56
1:0:1786:C:OP1	18:P:74:GLN:HG2	2.05	0.56
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.71	0.56
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.86	0.56
1:0:2524:G:H21	1:0:2526:C:H41	1.54	0.56
1:0:2883:A:H2'	1:0:2884:G:O4'	2.06	0.56
5:B:62:ARG:HA	5:B:65:MET:CE	2.36	0.56
16:N:169:PRO:O	16:N:172:PHE:HB3	2.05	0.56
22:T:26:THR:HA	22:T:39:ASN:HB3	1.87	0.56
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.77	0.56
2:9:3024:U:H3'	2:9:3025:G:H5'	1.87	0.56
1:0:1185:U:H4'	32:I:123:ASN:HB3	1.87	0.56
18:P:16:VAL:HG13	18:P:20:ARG:NH1	2.20	0.56
6:C:194:PHE:CD2	6:C:234:VAL:HG11	2.39	0.56
29:1:25:LYS:HE2	40:2:7213:HOH:O	2.04	0.56
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.87	0.56
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.03	0.56
15:M:15:PRO:HA	15:M:20:LEU:HD23	1.87	0.56
1:0:291:C:H2'	1:0:292:G:O4'	2.05	0.56
1:0:2586:U:H3	1:0:2592:G:H22	1.54	0.56
9:F:84:GLY:O	9:F:89:LEU:HB2	2.05	0.56
1:0:1189:A:H3'	40:0:8201:HOH:O	2.06	0.56
1:0:2421:G:H1'	40:0:4283:HOH:O	2.05	0.56
1:0:2670:G:O2'	1:0:2671:U:H5'	2.05	0.56
5:B:85:ARG:NH1	40:B:9628:HOH:O	2.37	0.56
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.87	0.56
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:710:G:H5'	17:O:25:VAL:CG1	2.35	0.56
1:0:2419:U:H5''	1:0:2420:G:H5'	1.87	0.56
24:V:5:VAL:HG23	40:V:2271:HOH:O	2.06	0.56
11:H:166:SER:CB	11:H:167:PRO:HD3	2.36	0.56
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.88	0.56
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.88	0.56
1:0:316:A:H5'	22:T:54:ASP:OD2	2.05	0.56
12:J:90:LYS:HB2	37:J:9302:CL:CL	2.43	0.56
1:0:1979:G:O2'	1:0:1980:U:OP1	2.21	0.56
1:0:151:A:H2'	1:0:152:A:O4'	2.06	0.56
1:0:2718:C:H6	1:0:2718:C:H5'	1.70	0.56
7:D:59:GLY:O	7:D:61:PHE:N	2.39	0.56
1:0:1118:A:H8	1:0:1119:G:H5''	1.71	0.56
23:U:17:THR:CG2	23:U:18:GLY:N	2.68	0.56
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.87	0.56
1:0:2866:U:H4'	1:0:2867:G:H5'	1.86	0.56
1:0:1819:G:H2'	1:0:1820:G:H4'	1.87	0.56
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.88	0.55
7:D:136:ARG:NH1	7:D:157:LEU:HA	2.21	0.55
7:D:138:GLY:N	40:D:7597:HOH:O	2.37	0.55
18:P:9:LEU:O	18:P:13:VAL:HG12	2.05	0.55
8:E:7:ILE:HG22	8:E:45:ASP:O	2.07	0.55
1:0:1979:G:H2'	40:0:3887:HOH:O	2.05	0.55
6:C:162:VAL:HG22	6:C:232:LEU:HD21	1.86	0.55
16:N:110:THR:HB	16:N:113:SER:OG	2.06	0.55
1:0:1753:C:O2	5:B:229:ARG:NH2	2.39	0.55
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.88	0.55
4:A:94:LEU:HD12	4:A:98:GLU:HB2	1.88	0.55
1:0:2769:C:H2'	1:0:2770:G:O4'	2.06	0.55
1:0:2320:U:H4'	1:0:2321:A:O4'	2.06	0.55
30:2:20:ARG:HD2	30:2:39:ARG:NH2	2.21	0.55
1:0:2807:U:P	5:B:27:ASN:HD21	2.29	0.55
25:W:26:ILE:O	25:W:26:ILE:HG13	2.06	0.55
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.88	0.55
1:0:1189:A:O2'	1:0:1208:C:H2'	2.06	0.55
10:G:12:ILE:N	10:G:13:PRO:CD	2.70	0.55
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.88	0.55
1:0:2904:U:H4'	26:X:8:ARG:NH1	2.22	0.55
5:B:238:ASN:HD22	5:B:240:GLY:N	1.99	0.55
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.87	0.55
1:0:558:C:H2'	1:0:559:U:H5'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:105:VAL:HG11	32:I:129:VAL:HG22	1.89	0.55
26:X:43:VAL:HG12	26:X:44:ASP:N	2.22	0.55
1:0:1634:G:H3'	40:0:4470:HOH:O	2.07	0.55
11:H:69:ALA:HB2	11:H:153:ALA:HB2	1.89	0.55
1:0:241:A:C2	1:0:378:A:H4'	2.42	0.55
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.72	0.55
24:V:64:GLY:O	24:V:65:ASP:HB2	2.05	0.55
31:3:55:VAL:HB	31:3:56:PRO:HD2	1.89	0.55
24:V:29:ASN:O	24:V:33:VAL:HG23	2.07	0.55
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.89	0.55
17:O:59:VAL:HG23	17:O:111:VAL:HG22	1.88	0.55
1:0:441:A:H1'	1:0:442:A:N7	2.21	0.55
12:J:39:VAL:HG11	12:J:107:ASN:CG	2.27	0.55
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.22	0.55
40:0:7355:HOH:O	15:M:178:LYS:HB2	2.05	0.55
16:N:162:ASP:HA	40:N:9328:HOH:O	2.06	0.55
1:0:2563:U:H2'	1:0:2565:C:O5'	2.07	0.55
1:0:236:A:H8	1:0:236:A:OP1	1.90	0.55
1:0:2645:U:OP2	1:0:2645:U:C6	2.60	0.55
12:J:19:MET:HE1	12:J:132:LEU:CD2	2.33	0.55
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.20	0.55
1:0:380:A:H2'	40:0:7695:HOH:O	2.06	0.55
1:0:90:A:H2'	1:0:91:G:O4'	2.07	0.55
1:0:1187:U:O2'	1:0:1189:A:H2	1.89	0.54
8:E:3:VAL:CG2	8:E:49:ILE:HB	2.37	0.54
10:G:12:ILE:HD12	40:G:692:HOH:O	2.06	0.54
1:0:848:C:H5'	40:0:7735:HOH:O	2.08	0.54
1:0:1595:G:O2'	1:0:1596:U:H5'	2.08	0.54
11:H:17:ARG:HD3	11:H:23:ILE:HD12	1.88	0.54
10:G:64:ASN:N	10:G:64:ASN:HD22	2.04	0.54
11:H:27:LYS:H	11:H:59:HIS:CD2	2.18	0.54
4:A:36:ASP:C	4:A:38:ILE:H	2.10	0.54
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.10	0.54
11:H:76:GLU:O	11:H:77:LEU:HD23	2.07	0.54
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.90	0.54
11:H:170:ASN:HD22	11:H:170:ASN:N	2.03	0.54
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.08	0.54
40:9:1361:HOH:O	16:N:41:LYS:HE3	2.08	0.54
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.06	0.54
40:9:4707:HOH:O	16:N:147:ILE:HD12	2.05	0.54
2:9:3051:A:H5'	16:N:160:SER:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:79:LEU:HG	22:T:89:ARG:HB2	1.88	0.54
7:D:135:VAL:HG22	7:D:136:ARG:N	2.23	0.54
1:O:2453:G:H5''	40:L:9439:HOH:O	2.07	0.54
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.35	0.54
30:2:36:ASN:HB3	30:2:39:ARG:HG3	1.89	0.54
16:N:183:ASP:O	16:N:184:ILE:O	2.25	0.54
22:T:40:VAL:HG22	22:T:41:ARG:N	2.23	0.54
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.55	0.54
17:O:25:VAL:HG23	17:O:26:TRP:N	2.22	0.54
12:J:131:THR:HG22	12:J:134:GLU:H	1.71	0.54
9:F:46:GLU:OE1	9:F:100:ASP:HA	2.07	0.54
1:O:20:G:H21	20:R:117:HIS:HD2	1.56	0.54
1:O:1189:A:H1'	1:O:1209:C:O4'	2.07	0.54
14:L:136:ALA:HB3	40:L:9469:HOH:O	2.07	0.54
4:A:33:GLU:CD	4:A:33:GLU:N	2.61	0.54
1:O:2032:U:C2'	1:O:2033:G:H5''	2.37	0.54
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.73	0.54
1:O:185:G:H4'	1:O:186:A:H4'	1.89	0.54
1:O:2851:G:O2'	1:O:2852:A:H5'	2.07	0.54
28:Z:29:ILE:O	28:Z:33:MET:HB2	2.08	0.54
16:N:42:HIS:CE1	16:N:75:THR:HG1	2.26	0.54
17:O:98:LEU:O	17:O:102:ILE:HG13	2.08	0.54
1:O:2827:A:H2'	1:O:2828:G:O4'	2.08	0.54
19:Q:26:PRO:O	19:Q:30:VAL:HG23	2.06	0.54
1:O:1477:C:H5'	1:O:1868:G:H5'	1.90	0.54
1:O:1730:G:H5'	1:O:1731:C:C6	2.43	0.53
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.90	0.53
40:O:4794:HOH:O	30:2:38:LYS:HE3	2.08	0.53
1:O:949:U:H4'	19:Q:95:GLU:HA	1.89	0.53
28:Z:10:ARG:HA	40:Z:9215:HOH:O	2.07	0.53
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.37	0.53
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.37	0.53
1:O:621:C:H5'	27:Y:132:ASP:OD2	2.07	0.53
1:O:1384:C:H5'	26:X:30:MET:HG2	1.88	0.53
1:O:1164:U:OP1	32:I:74:PRO:HA	2.08	0.53
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.90	0.53
32:I:138:THR:HG22	32:I:139:ILE:N	2.23	0.53
32:I:129:VAL:O	32:I:129:VAL:HG12	2.08	0.53
40:O:9697:HOH:O	5:B:214:PRO:HD2	2.08	0.53
1:O:1724:U:H5''	40:O:4314:HOH:O	2.08	0.53
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1835:U:C5	1:0:1840:A:N7	2.66	0.53
12:J:47:THR:HG22	12:J:48:GLY:N	2.24	0.53
4:A:34:ASP:OD1	4:A:35:GLY:N	2.38	0.53
1:0:466:A:OP1	30:2:38:LYS:HE2	2.08	0.53
1:0:182:G:H5'	40:M:9399:HOH:O	2.08	0.53
1:0:1189:A:H1'	1:0:1209:C:C1'	2.37	0.53
25:W:4:LEU:O	25:W:32:CYS:HA	2.08	0.53
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.90	0.53
1:0:12:U:H2'	1:0:13:G:H5'	1.91	0.53
1:0:500:G:H21	20:R:98:ASN:HD21	1.57	0.53
6:C:107:ARG:HH11	6:C:107:ARG:CB	2.21	0.53
24:V:55:ARG:O	24:V:59:ILE:HG12	2.08	0.53
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.21	0.53
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.38	0.53
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.09	0.53
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.09	0.53
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.39	0.53
1:0:1209:C:H2'	1:0:1210:G:C8	2.43	0.53
1:0:1766:U:O2	1:0:1778:A:H5'	2.09	0.53
16:N:32:PRO:HD2	16:N:99:GLU:O	2.09	0.53
1:0:288:A:H2'	1:0:289:G:C8	2.43	0.53
16:N:74:PRO:HG2	16:N:159:TYR:CE1	2.44	0.53
9:F:58:GLU:HA	9:F:61:MET:CE	2.37	0.53
16:N:11:ARG:O	16:N:15:GLU:HG3	2.08	0.53
25:W:139:GLY:O	25:W:141:HIS:HD2	1.91	0.53
1:0:1730:G:C5'	1:0:1731:C:C6	2.92	0.53
22:T:49:GLU:CB	22:T:59:GLU:HG2	2.38	0.53
9:F:46:GLU:O	9:F:73:PRO:HD2	2.08	0.53
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.08	0.53
7:D:104:PHE:CE2	7:D:166:ILE:HD13	2.44	0.53
7:D:99:ASP:HB2	7:D:103:ASN:O	2.08	0.53
7:D:24:HIS:HB2	7:D:72:LYS:HB3	1.91	0.53
1:0:2815:G:OP2	12:J:99:GLU:HG2	2.09	0.53
25:W:11:VAL:O	25:W:12:ASN:HB2	2.09	0.53
2:9:3076:G:C3'	2:9:3077:A:H5''	2.24	0.52
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.39	0.52
1:0:1406:A:H4'	1:0:1407:A:C5'	2.39	0.52
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.56	0.52
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.38	0.52
1:0:757:C:OP1	14:L:27:ARG:HD2	2.09	0.52
1:0:1741:U:H3'	40:0:3367:HOH:O	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2795:C:O2'	1:0:2796:U:H5'	2.09	0.52
18:P:105:LEU:CD2	18:P:137:LEU:HD21	2.39	0.52
1:0:603:A:H5''	1:0:604:G:OP1	2.08	0.52
40:0:5513:HOH:O	11:H:58:ARG:HG3	2.08	0.52
1:0:447:A:OP1	22:T:1:SER:HB2	2.10	0.52
1:0:2591:C:H2'	1:0:2592:G:O4'	2.08	0.52
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.91	0.52
33:4:179:DA:O4'	33:4:180:C:H2'	2.09	0.52
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.45	0.52
1:0:95:A:H5''	1:0:97:G:O4'	2.09	0.52
1:0:2265:U:H2'	1:0:2266:A:C8	2.44	0.52
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.39	0.52
27:Y:212:ARG:HD2	40:Y:9400:HOH:O	2.08	0.52
6:C:236:THR:HG22	6:C:239:ALA:CB	2.39	0.52
13:K:115:ARG:HG3	13:K:116:GLU:N	2.25	0.52
17:O:59:VAL:HG23	17:O:111:VAL:CG2	2.39	0.52
1:0:475:G:C5'	6:C:73:LEU:HD23	2.39	0.52
1:0:1119:G:N2	1:0:1246:A:N1	2.57	0.52
21:S:57:THR:CG2	21:S:58:MET:N	2.73	0.52
16:N:152:GLU:C	16:N:154:LEU:H	2.13	0.52
12:J:15:ARG:CZ	12:J:43:ARG:NH1	2.72	0.52
1:0:2894:C:O2'	1:0:2895:C:H5'	2.09	0.52
18:P:103:THR:O	18:P:107:GLU:HG3	2.09	0.52
1:0:793:A:H5''	18:P:83:LYS:HG2	1.91	0.52
1:0:248:A:H5'	1:0:249:G:OP2	2.10	0.52
1:0:920:C:H5''	1:0:921:G:O5'	2.10	0.52
1:0:1252:A:H2'	1:0:1253:C:O4'	2.10	0.52
5:B:171:VAL:HG23	5:B:172:SER:N	2.25	0.52
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.74	0.52
6:C:246:ARG:NE	40:C:9230:HOH:O	2.42	0.52
1:0:1972:U:H2'	1:0:1973:A:H5'	1.92	0.52
17:O:14:LEU:HG	17:O:102:ILE:HD11	1.91	0.52
19:Q:11:ARG:HD3	40:Q:5620:HOH:O	2.10	0.52
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.10	0.52
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.74	0.52
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.39	0.52
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.92	0.52
1:0:870:G:C2'	1:0:871:G:H5''	2.37	0.52
4:A:192:VAL:HG11	4:A:207:GLN:HB3	1.90	0.52
1:0:1751:G:C2'	1:0:1752:G:H5''	2.39	0.52
25:W:64:THR:O	25:W:68:THR:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1926:G:H2'	1:0:1927:A:C8	2.44	0.52
23:U:5:GLU:HG2	23:U:10:GLY:O	2.10	0.52
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.90	0.52
1:0:2587:OMU:H6	1:0:2587:OMU:O5'	2.09	0.52
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.10	0.52
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.92	0.52
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.92	0.52
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.43	0.52
6:C:233:THR:HG22	6:C:234:VAL:N	2.24	0.52
11:H:40:ALA:HB1	11:H:137:TYR:CE2	2.45	0.52
40:0:5938:HOH:O	4:A:164:ARG:CZ	2.57	0.52
1:0:156:C:H5''	15:M:171:ARG:CD	2.28	0.52
6:C:246:ARG:CB	6:C:246:ARG:HH11	2.20	0.52
1:0:2781:U:H1'	8:E:139:GLU:OE2	2.10	0.52
7:D:36:ASN:HA	40:D:7500:HOH:O	2.10	0.52
6:C:140:VAL:HB	40:C:9256:HOH:O	2.09	0.51
1:0:1981:A:H1'	1:0:1983:C:N4	2.25	0.51
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.50	0.51
11:H:166:SER:HB2	11:H:167:PRO:CD	2.41	0.51
20:R:96:VAL:HG13	20:R:106:GLY:HA3	1.92	0.51
1:0:545:G:C8	1:0:545:G:H5'	2.41	0.51
16:N:37:ARG:NH2	40:N:9316:HOH:O	2.29	0.51
27:Y:112:GLU:OE1	27:Y:112:GLU:HA	2.11	0.51
6:C:57:PRO:HG2	6:C:73:LEU:HD13	1.92	0.51
12:J:99:GLU:HA	40:J:7377:HOH:O	2.11	0.51
1:0:164:G:H4'	14:L:30:ARG:HD3	1.93	0.51
13:K:75:ARG:HD3	13:K:112:PRO:O	2.10	0.51
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.24	0.51
29:1:56:GLU:HG2	29:1:56:GLU:OXT	2.10	0.51
6:C:142:ASP:CG	6:C:237:GLU:HB3	2.30	0.51
25:W:88:THR:CG2	25:W:89:ASP:H	2.23	0.51
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.46	0.51
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.08	0.51
15:M:86:GLN:O	15:M:88:VAL:HG23	2.11	0.51
5:B:199:TYR:CE2	5:B:268:ARG:HB2	2.45	0.51
18:P:135:ALA:HB1	18:P:139:ARG:NH1	2.26	0.51
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.92	0.51
1:0:969:G:H1	1:0:999:C:N4	2.08	0.51
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.75	0.51
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.09	0.51
31:3:16:GLU:HG3	31:3:18:GLN:HE21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:K:7438:HOH:O	23:U:20:MET:HE1	2.10	0.51
13:K:81:ARG:HD3	13:K:87:ARG:CZ	2.40	0.51
7:D:173:GLU:HG3	7:D:174:VAL:N	2.25	0.51
28:Z:33:MET:HG3	28:Z:69:TYR:O	2.11	0.51
1:0:119:A:H2'	1:0:120:A:H5''	1.92	0.51
18:P:16:VAL:HG13	18:P:20:ARG:CZ	2.40	0.51
25:W:29:VAL:O	25:W:30:ASN:HB2	2.11	0.51
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.93	0.51
40:9:6497:HOH:O	16:N:23:ARG:HD2	2.09	0.51
1:0:204:A:C2'	1:0:205:U:H5'	2.41	0.51
11:H:45:VAL:HA	11:H:167:PRO:O	2.10	0.51
8:E:15:GLN:NE2	8:E:40:VAL:O	2.43	0.51
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.92	0.51
1:0:2456:A:H2'	1:0:2457:U:C6	2.46	0.51
13:K:125:ALA:C	13:K:127:ALA:H	2.13	0.51
1:0:2649:A:H5'	1:0:2649:A:H8	1.76	0.51
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.40	0.51
1:0:1205:U:H2'	1:0:1206:U:H5'	1.93	0.51
30:2:20:ARG:HG3	30:2:21:VAL:N	2.26	0.51
5:B:81:ALA:O	5:B:186:GLY:HA3	2.11	0.51
12:J:12:VAL:HG21	12:J:116:LEU:HD11	1.92	0.51
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.92	0.51
13:K:30:LYS:O	13:K:55:VAL:HG13	2.10	0.51
12:J:93:ARG:NH1	12:J:93:ARG:HB3	2.19	0.51
25:W:88:THR:CG2	25:W:89:ASP:N	2.74	0.51
31:3:55:VAL:HG22	40:3:9444:HOH:O	2.10	0.51
1:0:432:G:O2'	1:0:433:C:H5'	2.11	0.51
5:B:42:ALA:HB1	5:B:308:LEU:HD11	1.92	0.51
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.23	0.51
1:0:776:A:OP1	29:1:28:HIS:HE1	1.94	0.51
1:0:625:U:H5'	40:0:3777:HOH:O	2.11	0.51
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.26	0.51
7:D:25:MET:HE1	7:D:37:ALA:O	2.11	0.50
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.11	0.50
2:9:3003:A:H2'	40:9:2430:HOH:O	2.11	0.50
25:W:149:LEU:HG	25:W:153:MET:HE2	1.93	0.50
5:B:62:ARG:HA	5:B:65:MET:HE2	1.93	0.50
1:0:1946:C:H2'	1:0:1971:G:C8	2.46	0.50
11:H:63:GLU:O	11:H:67:LEU:HB2	2.11	0.50
12:J:15:ARG:CZ	12:J:43:ARG:HH11	2.24	0.50
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:63:ILE:HG22	12:J:64:GLY:N	2.25	0.50
26:X:31:ILE:O	26:X:35:GLU:HG3	2.11	0.50
2:9:3004:G:H21	16:N:44:ARG:NH1	2.09	0.50
1:0:171:C:OP2	15:M:84:LYS:HG3	2.10	0.50
30:2:20:ARG:HD2	30:2:39:ARG:HH21	1.76	0.50
26:X:20:GLU:HG3	26:X:21:PRO:HD2	1.91	0.50
1:0:968:G:H1'	11:H:32:LYS:HD2	1.92	0.50
1:0:653:C:H2'	1:0:654:A:C8	2.45	0.50
40:0:5240:HOH:O	28:Z:13:ARG:HD3	2.12	0.50
4:A:39:ALA:O	4:A:61:GLU:HG3	2.11	0.50
1:0:734:U:H1'	1:0:737:A:N6	2.26	0.50
32:I:75:THR:OG1	32:I:112:LYS:HE2	2.11	0.50
5:B:41:PHE:CG	5:B:79:MET:HE2	2.47	0.50
25:W:108:ARG:HE	25:W:114:PRO:CG	2.24	0.50
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.12	0.50
1:0:2064:U:H5'	1:0:2652:U:O3'	2.11	0.50
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.94	0.50
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.93	0.50
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.93	0.50
4:A:109:GLU:HG2	4:A:116:GLY:N	2.25	0.50
4:A:81:GLN:HB2	4:A:92:ASN:HD21	1.75	0.50
4:A:105:VAL:HG12	4:A:106:CYS:H	1.77	0.50
9:F:57:GLU:O	9:F:61:MET:HG3	2.12	0.50
1:0:284:C:H4'	1:0:285:A:H8	1.76	0.50
1:0:1180:U:H2'	1:0:1181:A:C8	2.46	0.50
1:0:69:A:H5'	1:0:69:A:H8	1.77	0.50
17:O:78:ALA:C	17:O:98:LEU:HD13	2.32	0.50
1:0:1234:U:N3	5:B:244:PRO:HB3	2.27	0.50
8:E:149:GLU:OE1	8:E:167:TYR:HA	2.12	0.50
11:H:116:ALA:O	11:H:117:PHE:C	2.50	0.50
5:B:41:PHE:CD2	5:B:190:MET:HE3	2.47	0.50
8:E:11:VAL:HG12	8:E:12:ASP:N	2.27	0.50
5:B:96:PRO:HG3	40:B:9628:HOH:O	2.11	0.50
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.46	0.50
1:0:2472:C:O2'	1:0:2634:G:H4'	2.11	0.50
1:0:1118:A:C8	1:0:1118:A:C3'	2.90	0.50
4:A:192:VAL:HG12	4:A:207:GLN:CB	2.41	0.50
1:0:558:C:H2'	1:0:559:U:H5''	1.92	0.50
5:B:87:TYR:O	5:B:138:GLY:N	2.38	0.50
2:9:3028:U:H2'	2:9:3029:C:C6	2.46	0.50
1:0:2649:A:C8	1:0:2649:A:H5'	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:79:ARG:O	6:C:87:ARG:HG2	2.11	0.50
27:Y:154:ARG:HH11	27:Y:154:ARG:HB3	1.77	0.50
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.93	0.50
1:O:1730:G:H5'	1:O:1731:C:H5	1.76	0.50
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.93	0.50
25:W:105:THR:HA	25:W:109:GLU:OE1	2.11	0.50
5:B:145:HIS:HD2	5:B:146:THR:O	1.95	0.50
32:I:128:VAL:C	32:I:130:GLY:H	2.15	0.50
1:O:1342:C:C2'	1:O:1343:C:H5'	2.42	0.50
1:O:299:U:H5'	40:O:7794:HOH:O	2.11	0.50
2:9:3012:C:H5'	2:9:3070:U:O4'	2.12	0.50
28:Z:11:SER:O	28:Z:14:PHE:HB2	2.12	0.49
24:V:8:ILE:HA	24:V:11:MET:CE	2.42	0.49
14:L:145:LEU:O	14:L:145:LEU:HD23	2.12	0.49
30:2:22:PRO:HG2	30:2:25:VAL:HG21	1.93	0.49
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.41	0.49
25:W:125:HIS:HD2	25:W:127:GLY:H	1.59	0.49
1:O:1363:G:OP1	6:C:76:ARG:NH2	2.44	0.49
14:L:36:ASP:HB2	40:L:9433:HOH:O	2.12	0.49
7:D:154:LYS:H	7:D:154:LYS:CD	2.22	0.49
32:I:113:HIS:N	32:I:114:PRO:CD	2.75	0.49
2:9:3039:U:O2'	2:9:3042:C:C5	2.63	0.49
24:V:56:ILE:HG22	24:V:60:GLN:HE21	1.77	0.49
11:H:54:THR:O	11:H:55:VAL:HG13	2.13	0.49
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.77	0.49
40:O:8006:HOH:O	31:3:60:LYS:HG3	2.12	0.49
5:B:17:LYS:O	5:B:260:HIS:HD2	1.95	0.49
1:O:951:A:C2'	1:O:952:G:H5'	2.41	0.49
14:L:89:PHE:CD1	14:L:89:PHE:N	2.80	0.49
27:Y:96:GLU:O	27:Y:235:GLU:HA	2.12	0.49
1:O:1666:C:H2'	1:O:1667:A:C5'	2.41	0.49
1:O:1730:G:C5'	1:O:1731:C:H6	2.24	0.49
22:T:96:VAL:CG1	22:T:97:ARG:N	2.75	0.49
18:P:105:LEU:HD21	18:P:137:LEU:HD21	1.94	0.49
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.94	0.49
1:O:1189:A:H1'	1:O:1209:C:H1'	1.95	0.49
1:O:1972:U:H2'	1:O:1973:A:C5'	2.43	0.49
4:A:167:LYS:HB2	28:Z:29:ILE:HD13	1.94	0.49
17:O:96:VAL:CG1	17:O:100:GLN:HB2	2.41	0.49
12:J:39:VAL:CG1	12:J:40:ASN:N	2.75	0.49
26:X:41:PHE:O	26:X:43:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.26	0.49
4:A:104:PRO:HG3	4:A:127:GLN:OE1	2.12	0.49
1:0:1462:C:H2'	1:0:1463:A:C8	2.48	0.49
11:H:58:ARG:O	11:H:62:LEU:HD22	2.12	0.49
14:L:143:THR:CG2	14:L:144:ASP:N	2.75	0.49
14:L:148:GLU:HB2	40:L:9485:HOH:O	2.12	0.49
12:J:74:ARG:HH12	12:J:76:ASP:CB	2.25	0.49
8:E:22:VAL:O	8:E:28:SER:HA	2.12	0.49
11:H:28:ILE:HG23	40:H:9544:HOH:O	2.12	0.49
1:0:949:U:O2'	19:Q:40:HIS:HE1	1.95	0.49
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.45	0.49
1:0:2326:U:H4'	1:0:2412:G:C4'	2.42	0.49
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.95	0.49
14:L:104:ASP:HB2	40:L:9458:HOH:O	2.12	0.49
13:K:55:VAL:CG1	13:K:56:SER:N	2.75	0.49
30:2:48:ASP:O	30:2:49:GLU:HB2	2.13	0.49
30:2:41:HIS:HD2	30:2:44:ARG:H	1.60	0.49
32:I:113:HIS:HE1	32:I:121:LEU:HD22	1.75	0.49
14:L:145:LEU:O	14:L:148:GLU:HG3	2.11	0.49
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.12	0.49
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.94	0.49
12:J:15:ARG:NH1	12:J:43:ARG:NH1	2.61	0.49
5:B:139:ASP:HB3	40:B:9547:HOH:O	2.12	0.49
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.93	0.49
1:0:2852:A:H5''	40:0:5766:HOH:O	2.11	0.49
32:I:138:THR:HG22	32:I:139:ILE:H	1.77	0.49
24:V:39:ALA:N	24:V:40:PRO:CD	2.73	0.49
7:D:103:ASN:ND2	7:D:134:LEU:H	2.10	0.49
1:0:2815:G:N7	12:J:80:LYS:NZ	2.60	0.49
1:0:449:A:N7	6:C:43:LYS:HG2	2.27	0.49
1:0:1466:C:H42	1:0:1476:A:N6	1.98	0.49
12:J:52:GLN:HG3	12:J:53:ILE:N	2.27	0.49
27:Y:148:GLY:O	27:Y:154:ARG:HD3	2.12	0.49
1:0:558:C:C2'	1:0:559:U:C5'	2.91	0.49
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.33	0.49
20:R:122:GLN:HB3	20:R:138:SER:HB2	1.93	0.49
1:0:816:G:H5'	1:0:1598:A:H4'	1.94	0.49
20:R:29:LYS:NZ	40:R:9453:HOH:O	2.46	0.49
2:9:3049:G:O2'	2:9:3050:G:H5'	2.12	0.49
5:B:53:LEU:CD1	5:B:327:VAL:HG22	2.42	0.49
4:A:36:ASP:O	4:A:38:ILE:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1477:C:H2'	1:0:1478:U:C6	2.48	0.49
1:0:603:A:H4'	1:0:604:G:O5'	2.12	0.49
1:0:2712:G:H5'	40:K:4183:HOH:O	2.13	0.49
4:A:65:ARG:C	4:A:66:ARG:HG3	2.32	0.49
6:C:168:ARG:NH2	6:C:190:ALA:O	2.46	0.49
1:0:542:A:H2'	1:0:543:G:O4'	2.13	0.48
1:0:1466:C:N4	1:0:1476:A:H61	1.98	0.48
1:0:1175:G:H1'	1:0:1193:A:C2'	2.41	0.48
4:A:105:VAL:HG13	4:A:155:THR:O	2.13	0.48
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.43	0.48
24:V:64:GLY:O	24:V:65:ASP:CB	2.61	0.48
1:0:2453:G:H4'	14:L:50:GLY:C	2.33	0.48
1:0:666:A:H2'	1:0:667:C:O4'	2.13	0.48
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.95	0.48
1:0:1503:U:H2'	1:0:1504:A:O4'	2.13	0.48
1:0:1056:U:H2'	1:0:1057:A:O4'	2.13	0.48
1:0:247:A:H2'	40:0:4499:HOH:O	2.12	0.48
1:0:883:U:H2'	1:0:883:U:O2	2.12	0.48
1:0:2779:G:H21	8:E:143:GLN:NE2	2.11	0.48
2:9:3054:A:O2'	2:9:3055:U:H5'	2.13	0.48
1:0:2906:A:H5'	1:0:2907:C:O4'	2.13	0.48
6:C:154:VAL:O	6:C:158:GLU:HG3	2.13	0.48
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.94	0.48
8:E:81:GLU:HA	8:E:133:VAL:O	2.13	0.48
18:P:115:SER:N	18:P:118:GLN:HE21	2.04	0.48
7:D:154:LYS:HD2	7:D:154:LYS:N	2.22	0.48
27:Y:203:VAL:CG1	27:Y:228:VAL:HG22	2.43	0.48
30:2:36:ASN:HB3	30:2:39:ARG:NE	2.28	0.48
11:H:170:ASN:ND2	11:H:170:ASN:N	2.60	0.48
5:B:75:GLU:C	5:B:77:PRO:HD3	2.32	0.48
1:0:2237:G:H1'	1:0:2238:A:C8	2.48	0.48
1:0:2090:G:H2'	1:0:2091:G:C8	2.48	0.48
13:K:49:LEU:HD12	13:K:80:ILE:HD13	1.94	0.48
9:F:57:GLU:HB2	15:M:23:LEU:HD11	1.94	0.48
2:9:3044:A:O4'	7:D:76:ARG:NE	2.46	0.48
1:0:1878:G:O2'	1:0:1879:U:C5	2.62	0.48
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.48	0.48
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.49	0.48
40:0:7257:HOH:O	16:N:4:PRO:HD2	2.13	0.48
1:0:2545:U:OP2	5:B:2:GLN:NE2	2.47	0.48
1:0:2414:A:H2'	1:0:2415:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:236:THR:HA	40:C:9256:HOH:O	2.13	0.48
9:F:91:VAL:CG1	9:F:92:GLY:H	2.11	0.48
1:0:1552:G:N2	1:0:1634:G:H1'	2.29	0.48
1:0:185:G:O3'	1:0:186:A:H4'	2.14	0.48
18:P:89:ASN:OD1	18:P:92:GLU:HB2	2.13	0.48
1:0:1506:U:H6	1:0:1506:U:H5'	1.78	0.48
28:Z:36:ASP:HB3	28:Z:45:ASP:O	2.14	0.48
17:O:32:ARG:HB2	40:O:4656:HOH:O	2.14	0.48
1:0:1667:A:C8	1:0:1667:A:H5'	2.39	0.48
4:A:88:ILE:HG22	4:A:88:ILE:O	2.13	0.48
1:0:1249:U:H2'	1:0:1250:C:C6	2.49	0.48
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.44	0.48
1:0:1205:U:H2'	1:0:1206:U:H5''	1.96	0.48
24:V:39:ALA:O	24:V:41:GLU:N	2.42	0.48
1:0:1377:C:H5'	1:0:1377:C:C6	2.45	0.48
1:0:120:A:H5'	29:1:20:ARG:HH21	1.79	0.48
1:0:602:A:O2'	1:0:605:C:H4'	2.14	0.48
31:3:16:GLU:HG3	31:3:18:GLN:NE2	2.29	0.48
16:N:58:LEU:N	16:N:58:LEU:HD12	2.28	0.48
7:D:60:GLU:O	7:D:60:GLU:HG3	2.13	0.48
1:0:2072:G:C6	1:0:2533:C:H1'	2.49	0.48
1:0:1878:G:C1'	40:0:6632:HOH:O	2.56	0.48
25:W:108:ARG:CG	25:W:114:PRO:HG3	2.42	0.48
31:3:65:THR:CG2	31:3:88:LEU:HD22	2.44	0.48
28:Z:40:PRO:C	28:Z:42:CYS:H	2.17	0.48
5:B:321:PRO:HA	40:B:9650:HOH:O	2.12	0.48
1:0:2365:G:H5''	40:Q:6597:HOH:O	2.12	0.48
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.28	0.48
7:D:25:MET:SD	7:D:40:ILE:HD11	2.54	0.48
24:V:39:ALA:H	24:V:40:PRO:HD2	1.75	0.48
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.95	0.48
1:0:834:G:H3'	1:0:835:U:H4'	1.96	0.48
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.13	0.48
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.77	0.48
21:S:33:SER:O	21:S:37:VAL:HG23	2.13	0.48
21:S:37:VAL:O	21:S:41:VAL:HG23	2.13	0.48
12:J:80:LYS:NZ	40:J:7377:HOH:O	2.46	0.48
1:0:2415:A:O2'	16:N:29:SER:HB3	2.13	0.48
1:0:88:G:H2'	1:0:89:G:C8	2.49	0.48
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.29	0.47
24:V:1:THR:CG2	24:V:2:VAL:H	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2851:G:H4'	5:B:157:LYS:NZ	2.29	0.47
32:I:139:ILE:HG22	32:I:140:GLU:N	2.29	0.47
1:0:1163:G:H1	1:0:1184:C:N4	2.12	0.47
23:U:52:THR:HG22	23:U:54:THR:H	1.78	0.47
5:B:254:GLN:HG3	40:B:9530:HOH:O	2.13	0.47
1:0:396:U:OP2	31:3:38:ARG:HD2	2.13	0.47
1:0:830:G:O2'	1:0:831:U:H5'	2.14	0.47
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.13	0.47
17:O:73:ASP:HA	17:O:92:VAL:O	2.14	0.47
1:0:1789:G:O6	18:P:73:HIS:HE1	1.97	0.47
31:3:3:MET:O	31:3:90:PHE:HA	2.14	0.47
1:0:2338:G:OP1	7:D:97:GLN:HG2	2.14	0.47
5:B:91:PRO:O	12:J:144:THR:HG21	2.14	0.47
1:0:484:A:N1	1:0:506:G:H4'	2.28	0.47
1:0:2421:G:H4'	40:0:5325:HOH:O	2.13	0.47
16:N:69:TYR:HE2	16:N:184:ILE:HG13	1.79	0.47
1:0:2856:A:P	26:X:15:ARG:HH22	2.36	0.47
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.13	0.47
6:C:214:THR:HG23	40:C:9243:HOH:O	2.14	0.47
2:9:3064:C:C2'	2:9:3065:A:H5'	2.44	0.47
19:Q:75:ILE:HD13	19:Q:84:ILE:HD11	1.95	0.47
1:0:343:C:O2'	1:0:344:C:H5'	2.13	0.47
5:B:58:PRO:HA	5:B:63:GLU:OE2	2.14	0.47
13:K:87:ARG:NH1	40:K:4066:HOH:O	2.48	0.47
4:A:207:GLN:O	4:A:208:HIS:HB3	2.14	0.47
15:M:77:HIS:CD2	15:M:79:ALA:O	2.65	0.47
6:C:246:ARG:NH1	40:C:9177:HOH:O	2.46	0.47
12:J:142:ASN:O	12:J:144:THR:N	2.48	0.47
1:0:482:G:H4'	1:0:508:A:N1	2.29	0.47
18:P:141:ILE:C	18:P:143:ALA:H	2.17	0.47
17:O:42:GLU:HB2	40:O:2176:HOH:O	2.14	0.47
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.78	0.47
27:Y:155:ARG:NH1	40:Y:9357:HOH:O	2.46	0.47
5:B:205:VAL:O	5:B:307:ARG:NE	2.40	0.47
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.29	0.47
1:0:1086:A:C6	25:W:11:VAL:HG11	2.49	0.47
1:0:920:C:H4'	1:0:921:G:C2	2.50	0.47
1:0:1236:A:H2'	1:0:1237:U:O4'	2.14	0.47
1:0:952:G:N3	1:0:2302:A:H2'	2.29	0.47
17:O:15:LYS:HD3	17:O:19:ARG:NH2	2.29	0.47
40:0:5171:HOH:O	4:A:6:GLY:HA3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:132:ARG:NH2	40:R:9495:HOH:O	2.47	0.47
4:A:203:GLY:HA2	40:A:9535:HOH:O	2.14	0.47
2:9:3042:C:H5'	2:9:3043:G:OP2	2.14	0.47
5:B:41:PHE:CG	5:B:190:MET:HE3	2.50	0.47
4:A:53:ALA:HB3	40:A:9595:HOH:O	2.13	0.47
4:A:223:ARG:NE	40:A:9563:HOH:O	2.47	0.47
18:P:13:VAL:HG11	18:P:40:VAL:HG11	1.96	0.47
4:A:89:ALA:HB3	40:A:9614:HOH:O	2.14	0.47
22:T:71:VAL:HG13	22:T:91:LEU:O	2.14	0.47
1:0:622:G:P	27:Y:148:GLY:HA3	2.54	0.47
1:0:2670:G:H5'	5:B:112:THR:O	2.15	0.47
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.44	0.47
12:J:59:LYS:O	12:J:63:ILE:HG13	2.14	0.47
12:J:22:VAL:O	12:J:26:VAL:HG23	2.15	0.47
1:0:1853:C:OP1	4:A:231:LYS:HG3	2.15	0.47
1:0:1211:G:O2'	1:0:1212:C:H5'	2.14	0.47
1:0:697:G:H4'	1:0:730:G:O3'	2.15	0.47
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.15	0.47
25:W:48:VAL:CG1	25:W:48:VAL:O	2.62	0.47
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.96	0.47
14:L:143:THR:CG2	14:L:144:ASP:H	2.22	0.47
1:0:2747:C:H4'	40:0:8438:HOH:O	2.14	0.47
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.94	0.47
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.29	0.47
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.78	0.47
1:0:475:G:H5'	6:C:73:LEU:HD23	1.95	0.47
1:0:204:A:H2'	1:0:205:U:H5'	1.96	0.47
12:J:63:ILE:CG2	12:J:64:GLY:N	2.77	0.47
26:X:20:GLU:HG3	26:X:21:PRO:CD	2.45	0.47
14:L:57:VAL:O	14:L:57:VAL:HG12	2.14	0.47
8:E:86:VAL:HG12	8:E:129:GLU:O	2.15	0.47
5:B:277:GLU:N	5:B:278:PRO:HD2	2.29	0.47
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.49	0.47
1:0:1066:U:H2'	1:0:1067:A:C8	2.50	0.47
1:0:2820:A:H2'	1:0:2821:C:C6	2.50	0.47
1:0:1992:U:OP2	13:K:66:ARG:HD2	2.14	0.47
10:G:63:ARG:HB2	10:G:66:LEU:HG	1.96	0.47
14:L:119:THR:HG23	14:L:139:SER:OG	2.15	0.47
1:0:1242:A:C5'	12:J:82:THR:HG23	2.34	0.47
24:V:8:ILE:HG21	24:V:59:ILE:HG13	1.96	0.47
15:M:107:ARG:CG	15:M:107:ARG:NH1	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.55	0.47
4:A:69:LEU:HD23	4:A:107:ASN:CB	2.39	0.47
27:Y:144:ARG:CG	27:Y:144:ARG:NH1	2.67	0.47
1:0:447:A:O2'	1:0:448:G:H5'	2.15	0.47
22:T:78:THR:HG22	22:T:88:PRO:HA	1.96	0.47
1:0:2503:A:OP1	11:H:151:ARG:NH2	2.47	0.47
7:D:22:VAL:HG22	7:D:74:THR:HG22	1.97	0.47
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.35	0.47
15:M:60:VAL:C	15:M:61:ILE:HD12	2.35	0.47
1:0:196:G:H2'	40:0:7143:HOH:O	2.14	0.47
1:0:2717:C:O2'	1:0:2718:C:H5''	2.14	0.47
1:0:677:C:H4'	6:C:246:ARG:NH2	2.30	0.47
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.96	0.47
1:0:2333:G:P	7:D:56:ARG:HH22	2.38	0.47
1:0:1624:A:H4'	1:0:1625:U:H5'	1.96	0.47
9:F:5:ASP:O	9:F:119:ARG:NH1	2.48	0.47
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.31	0.47
1:0:1118:A:C8	1:0:1119:G:H5''	2.49	0.47
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.58	0.47
9:F:52:GLU:HG3	9:F:77:VAL:O	2.15	0.47
1:0:1328:A:C8	27:Y:169:ARG:HD3	2.49	0.47
32:I:87:THR:HG22	32:I:88:GLY:N	2.30	0.47
22:T:89:ARG:HG3	22:T:89:ARG:O	2.15	0.47
1:0:2456:A:H2'	1:0:2457:U:H6	1.80	0.47
1:0:1236:A:C8	12:J:63:ILE:HD11	2.50	0.47
1:0:737:A:H2'	1:0:738:G:O4'	2.15	0.47
1:0:820:G:O2'	1:0:856:G:H4'	2.15	0.47
8:E:77:THR:OG1	8:E:78:GLU:N	2.47	0.47
1:0:2296:C:H2'	1:0:2297:U:H6	1.80	0.47
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.15	0.47
6:C:127:ARG:HD3	6:C:129:HIS:CE1	2.48	0.46
2:9:3049:G:H5''	40:9:4707:HOH:O	2.14	0.46
26:X:30:MET:CE	26:X:58:ALA:HB3	2.42	0.46
23:U:39:ASN:ND2	23:U:44:ARG:NH1	2.63	0.46
1:0:664:U:O4	1:0:681:G:H5''	2.15	0.46
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.78	0.46
26:X:23:HIS:CD2	26:X:24:LYS:HG3	2.49	0.46
1:0:1755:A:H2'	1:0:1756:G:O4'	2.15	0.46
14:L:93:VAL:HG12	14:L:97:VAL:HG23	1.97	0.46
1:0:1422:U:H2'	1:0:1423:C:C6	2.50	0.46
1:0:2784:A:H1'	8:E:60:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2112:A:H2'	1:0:2113:G:C8	2.50	0.46
1:0:1180:U:O2'	32:I:92:PRO:HD2	2.15	0.46
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.98	0.46
12:J:42:GLU:O	12:J:131:THR:HG23	2.15	0.46
26:X:43:VAL:HG12	26:X:47:ALA:HB3	1.97	0.46
1:0:2326:U:H4'	1:0:2412:G:H4'	1.98	0.46
1:0:2372:A:H2'	1:0:2373:U:C6	2.51	0.46
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.30	0.46
1:0:812:A:H1'	40:0:4533:HOH:O	2.15	0.46
20:R:99:ALA:HB1	20:R:109:MET:HE3	1.95	0.46
5:B:36:PRO:CA	5:B:168:GLY:HA3	2.40	0.46
16:N:11:ARG:CG	16:N:14:ARG:HH12	2.25	0.46
1:0:1192:A:H3'	1:0:1193:A:H5'	1.97	0.46
2:9:3029:C:C2'	2:9:3030:C:H5'	2.45	0.46
18:P:135:ALA:HB1	18:P:139:ARG:HH12	1.79	0.46
16:N:89:GLY:O	16:N:92:ALA:HB3	2.15	0.46
5:B:88:GLU:HB3	5:B:97:LEU:HD12	1.98	0.46
1:0:177:A:H2'	1:0:178:U:O4'	2.15	0.46
2:9:3049:G:H2'	2:9:3050:G:O4'	2.16	0.46
2:9:3114:G:O6	16:N:11:ARG:HD3	2.15	0.46
40:0:5491:HOH:O	15:M:82:ARG:HD3	2.15	0.46
11:H:66:ARG:HD3	40:H:9544:HOH:O	2.15	0.46
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.46	0.46
14:L:10:SER:O	14:L:11:ARG:HB3	2.15	0.46
1:0:304:G:H1'	1:0:347:A:N6	2.31	0.46
15:M:59:GLY:HA3	15:M:141:ILE:HD12	1.96	0.46
12:J:76:ASP:HA	40:J:5907:HOH:O	2.16	0.46
1:0:903:U:O4	14:L:18:HIS:HB2	2.15	0.46
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.16	0.46
25:W:35:VAL:HA	25:W:36:PRO:HD3	1.86	0.46
7:D:172:VAL:CG1	7:D:173:GLU:H	2.20	0.46
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.16	0.46
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.80	0.46
11:H:29:ALA:C	11:H:30:GLN:HG3	2.35	0.46
1:0:1044:C:H5''	40:0:9648:HOH:O	2.15	0.46
1:0:107:U:H2'	1:0:108:U:H5'	1.98	0.46
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.49	0.46
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.15	0.46
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.98	0.46
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.45	0.46
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2346:C:O5'	1:0:2346:C:H6	1.97	0.46
5:B:254:GLN:HG2	5:B:255:GLY:H	1.81	0.46
7:D:49:PRO:HB3	40:D:5828:HOH:O	2.16	0.46
7:D:18:ILE:HG12	7:D:134:LEU:HD23	1.97	0.46
1:0:894:A:N1	6:C:87:ARG:NH2	2.63	0.46
15:M:22:GLU:HG2	15:M:26:GLN:NE2	2.31	0.46
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.96	0.46
9:F:65:GLU:O	9:F:69:GLU:HG2	2.15	0.46
5:B:185:GLY:HA2	40:B:9627:HOH:O	2.15	0.46
1:0:1829:A:H61	28:Z:18:TYR:H	1.64	0.46
32:I:75:THR:HA	32:I:112:LYS:NZ	2.31	0.46
16:N:154:LEU:O	16:N:155:GLU:CB	2.64	0.46
2:9:3024:U:H3'	2:9:3025:G:C5'	2.46	0.46
10:G:64:ASN:N	10:G:64:ASN:ND2	2.63	0.46
40:0:8006:HOH:O	31:3:61:PRO:HG2	2.16	0.46
5:B:321:PRO:HG3	40:B:9593:HOH:O	2.15	0.46
4:A:171:LYS:NZ	40:A:9513:HOH:O	2.48	0.46
1:0:1942:A:H3'	40:0:7801:HOH:O	2.16	0.46
40:0:4967:HOH:O	4:A:11:ARG:CZ	2.64	0.46
1:0:2642:G:H2'	1:0:2643:G:O4'	2.16	0.46
2:9:3091:C:H2'	2:9:3092:G:O4'	2.16	0.46
1:0:1441:G:O2'	1:0:1442:A:H5'	2.16	0.46
26:X:78:GLU:HG2	26:X:79:GLU:OE2	2.15	0.46
16:N:8:VAL:CG1	16:N:14:ARG:HE	2.29	0.46
6:C:218:VAL:HG12	40:C:9230:HOH:O	2.15	0.46
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.30	0.46
4:A:130:THR:HG22	4:A:131:HIS:O	2.15	0.46
8:E:114:ARG:HB3	8:E:151:LEU:HD11	1.97	0.46
14:L:80:ASP:HB2	14:L:90:ARG:HB3	1.98	0.46
11:H:9:ILE:HD12	11:H:54:THR:HG22	1.98	0.46
5:B:301:VAL:HG11	5:B:309:VAL:HG11	1.97	0.46
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.51	0.46
8:E:106:ASN:ND2	8:E:109:GLY:HA2	2.30	0.46
8:E:118:ILE:HG23	8:E:144:THR:HG21	1.98	0.46
17:O:38:ARG:NH1	40:O:7674:HOH:O	2.49	0.46
22:T:71:VAL:CG1	22:T:72:ILE:N	2.78	0.46
1:0:1666:C:C2'	1:0:1667:A:C5'	2.94	0.46
1:0:136:C:H2'	1:0:137:U:O4'	2.15	0.46
1:0:2904:U:H4'	26:X:8:ARG:HH12	1.80	0.46
40:0:7688:HOH:O	4:A:11:ARG:HA	2.16	0.46
1:0:1574:C:H2'	1:0:1575:C:C6	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:152:LYS:HB3	27:Y:160:LYS:HG3	1.98	0.46
1:0:1311:G:O6	6:C:173:LYS:HE3	2.15	0.46
1:0:2825:C:H4'	1:0:2826:G:O5'	2.17	0.46
1:0:1902:G:H2'	1:0:1903:U:O4'	2.16	0.46
17:O:24:ALA:O	17:O:28:ASP:HB2	2.16	0.46
7:D:10:PHE:CE1	7:D:11:HIS:HB3	2.51	0.46
5:B:36:PRO:HB3	5:B:174:ARG:CB	2.46	0.45
5:B:190:MET:CE	5:B:194:PHE:CD1	3.00	0.45
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.98	0.45
21:S:33:SER:OG	21:S:36:GLU:HG3	2.17	0.45
1:0:2824:C:H5''	1:0:2825:C:H5'	1.98	0.45
1:0:926:A:H5'	14:L:39:GLU:OE2	2.16	0.45
11:H:158:THR:HB	11:H:159:PRO:HD3	1.99	0.45
25:W:72:PRO:HB2	25:W:74:GLU:O	2.15	0.45
19:Q:31:GLU:CD	19:Q:93:ARG:HH12	2.19	0.45
27:Y:209:VAL:HG12	27:Y:214:ARG:HG3	1.97	0.45
6:C:115:LEU:O	6:C:118:THR:HB	2.16	0.45
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.28	0.45
1:0:1163:G:H5'	32:I:115:ASP:O	2.17	0.45
32:I:92:PRO:C	32:I:94:GLU:N	2.70	0.45
10:G:16:LYS:O	10:G:20:VAL:HG23	2.15	0.45
25:W:38:THR:CG2	25:W:39:ASP:N	2.78	0.45
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.31	0.45
15:M:74:LYS:HG3	40:M:9384:HOH:O	2.16	0.45
11:H:54:THR:HG23	11:H:128:GLN:HA	1.97	0.45
1:0:2821:C:H4'	5:B:116:PRO:HG3	1.97	0.45
11:H:146:VAL:HG22	40:H:9541:HOH:O	2.16	0.45
19:Q:3:SER:HB3	40:Q:5998:HOH:O	2.17	0.45
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.16	0.45
32:I:75:THR:HA	32:I:112:LYS:HZ3	1.81	0.45
40:O:7612:HOH:O	29:1:1:THR:HB	2.16	0.45
1:0:2769:C:H2'	1:0:2770:G:C5'	2.45	0.45
1:0:1741:U:O2'	1:0:2723:G:H4'	2.17	0.45
19:Q:75:ILE:HD13	19:Q:84:ILE:CD1	2.46	0.45
17:O:60:VAL:C	17:O:62:GLY:H	2.20	0.45
25:W:96:LEU:O	25:W:100:LEU:HG	2.16	0.45
1:0:1165:G:H1'	1:0:1174:A:H1'	1.98	0.45
16:N:154:LEU:HG	16:N:155:GLU:H	1.82	0.45
1:0:292:G:H2'	1:0:358:G:N2	2.32	0.45
5:B:24:PRO:HG3	5:B:204:GLY:HA2	1.97	0.45
1:0:1714:C:O2'	1:0:1715:C:H5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:134:GLU:HG3	40:L:9453:HOH:O	2.17	0.45
1:O:1881:A:OP1	4:A:199:HIS:HE1	1.99	0.45
4:A:94:LEU:N	4:A:94:LEU:HD23	2.32	0.45
32:I:99:ASP:O	32:I:100:LEU:HD23	2.17	0.45
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.45	0.45
23:U:9:CYS:HA	23:U:52:THR:HG23	1.99	0.45
1:O:1771:U:H5'	28:Z:20:ARG:NH2	2.31	0.45
1:O:396:U:H1'	40:O:8151:HOH:O	2.17	0.45
6:C:133:ARG:NH1	40:C:9218:HOH:O	2.49	0.45
5:B:58:PRO:HA	5:B:63:GLU:CD	2.36	0.45
1:O:2508:C:H2'	40:O:7239:HOH:O	2.17	0.45
1:O:1025:C:H5'	25:W:23:MET:O	2.17	0.45
1:O:1654:U:H2'	4:A:47:HIS:CD2	2.51	0.45
40:O:8228:HOH:O	6:C:94:THR:HG21	2.16	0.45
1:O:286:U:H2'	1:O:287:C:C6	2.52	0.45
15:M:107:ARG:NH2	40:M:9399:HOH:O	2.48	0.45
1:O:2072:G:H3'	1:O:2073:G:C5'	2.47	0.45
9:F:60:VAL:O	9:F:60:VAL:CG1	2.64	0.45
1:O:1878:G:O2'	1:O:1879:U:P	2.74	0.45
1:O:1299:G:N2	40:O:5228:HOH:O	2.49	0.45
10:G:64:ASN:O	10:G:68:GLU:HG3	2.17	0.45
1:O:818:A:O2'	28:Z:13:ARG:HD2	2.16	0.45
12:J:26:VAL:HG13	12:J:36:VAL:HG11	1.99	0.45
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.78	0.45
1:O:945:U:H2'	1:O:946:C:C6	2.51	0.45
1:O:1419:U:H2'	1:O:1685:A:C2	2.52	0.45
5:B:14:GLY:HA2	5:B:15:PRO:C	2.36	0.45
1:O:2312:G:H2'	1:O:2313:C:H5'	1.98	0.45
25:W:13:MET:CE	25:W:18:GLN:HA	2.37	0.45
25:W:80:ASP:HB2	40:W:3312:HOH:O	2.15	0.45
7:D:95:THR:OG1	7:D:174:VAL:HG22	2.16	0.45
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.32	0.45
22:T:38:ARG:NH1	22:T:38:ARG:HG3	2.32	0.45
9:F:38:LYS:NZ	15:M:3:SER:HA	2.32	0.45
7:D:49:PRO:HA	7:D:73:VAL:HG22	1.98	0.45
1:O:2626:C:H2'	1:O:2627:G:C8	2.52	0.45
1:O:2361:A:H2'	1:O:2362:A:C8	2.51	0.45
12:J:88:PRO:O	12:J:94:GLY:HA3	2.17	0.45
1:O:1717:A:H5''	18:P:54:LYS:HB2	1.97	0.45
31:3:91:GLN:O	31:3:92:GLU:HB2	2.17	0.45
7:D:25:MET:CE	7:D:37:ALA:HB1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.20	0.45
6:C:5:ILE:HG13	6:C:15:GLU:HA	1.99	0.45
1:0:2504:A:H2'	1:0:2505:G:O4'	2.17	0.45
25:W:122:ARG:HH22	25:W:154:ARG:HG2	1.75	0.45
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.52	0.45
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.70	0.45
11:H:151:ARG:HA	11:H:154:TYR:CE2	2.51	0.45
1:0:1200:A:H3'	40:0:6280:HOH:O	2.17	0.45
1:0:1773:G:C8	28:Z:16:ALA:HA	2.52	0.45
1:0:2568:A:C2'	1:0:2569:A:H5'	2.47	0.45
22:T:69:LYS:O	22:T:71:VAL:HG23	2.17	0.45
20:R:106:GLY:HA2	20:R:109:MET:CE	2.47	0.45
5:B:305:ASP:O	5:B:306:LYS:CB	2.63	0.45
8:E:22:VAL:HG12	8:E:76:VAL:HG11	1.99	0.45
12:J:39:VAL:HG21	12:J:107:ASN:ND2	2.32	0.45
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.47	0.45
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.52	0.45
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.17	0.45
1:0:958:G:H2'	1:0:959:C:C6	2.52	0.45
1:0:2250:G:OP1	4:A:31:LYS:HD3	2.16	0.45
1:0:702:G:O2'	1:0:703:G:H5'	2.17	0.45
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.38	0.45
1:0:371:U:H2'	1:0:372:A:H8	1.82	0.45
24:V:7:GLU:O	24:V:11:MET:HG3	2.17	0.45
2:9:3006:C:H5''	16:N:37:ARG:HE	1.82	0.45
32:I:96:PHE:HD2	32:I:136:GLY:HA2	1.82	0.45
29:1:28:HIS:HD2	29:1:31:LYS:H	1.63	0.45
1:0:2511:A:H2'	1:0:2512:U:O4'	2.17	0.45
5:B:265:LEU:CD2	5:B:316:ARG:HD3	2.47	0.45
1:0:526:U:H2'	1:0:527:U:C6	2.52	0.45
14:L:72:ASN:HB2	40:L:9477:HOH:O	2.16	0.45
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.17	0.45
30:2:41:HIS:N	30:2:45:ASN:HD22	1.97	0.44
15:M:164:THR:CG2	15:M:166:ALA:H	2.29	0.44
6:C:57:PRO:HG2	6:C:73:LEU:CD1	2.46	0.44
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.97	0.44
1:0:162:C:H2'	1:0:163:U:H5'	1.99	0.44
1:0:2011:A:H4'	1:0:2012:U:O5'	2.17	0.44
1:0:1369:A:H4'	20:R:64:SER:OG	2.17	0.44
1:0:317:A:OP1	22:T:52:ARG:O	2.35	0.44
15:M:98:GLN:O	15:M:102:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:57:THR:HG22	21:S:58:MET:N	2.32	0.44
1:0:1730:G:H5''	1:0:1731:C:H6	1.82	0.44
22:T:48:VAL:CG2	22:T:96:VAL:CG1	2.94	0.44
12:J:70:PHE:CG	12:J:70:PHE:O	2.70	0.44
12:J:71:TYR:CG	12:J:72:PRO:HD2	2.53	0.44
15:M:61:ILE:N	15:M:61:ILE:HD12	2.31	0.44
6:C:61:PHE:HB3	40:C:9250:HOH:O	2.17	0.44
1:0:1266:U:O2'	27:Y:119:GLN:NE2	2.41	0.44
7:D:128:LEU:HD23	7:D:128:LEU:C	2.38	0.44
1:0:2720:C:O2	13:K:87:ARG:NH2	2.49	0.44
1:0:1592:G:O2'	1:0:1593:C:O4'	2.34	0.44
14:L:145:LEU:C	14:L:145:LEU:HD23	2.37	0.44
1:0:470:U:O2'	29:1:16:HIS:CD2	2.60	0.44
1:0:1181:A:N1	1:0:1192:A:O2'	2.49	0.44
7:D:135:VAL:HG22	7:D:136:ARG:H	1.80	0.44
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.52	0.44
12:J:131:THR:HB	12:J:134:GLU:OE1	2.17	0.44
25:W:149:LEU:HG	25:W:153:MET:HE1	1.99	0.44
1:0:1198:U:H2'	1:0:1200:A:OP2	2.17	0.44
32:I:89:SER:HB3	32:I:97:VAL:CG2	2.48	0.44
1:0:1919:A:H4'	40:0:5395:HOH:O	2.17	0.44
11:H:1:LYS:N	40:H:9530:HOH:O	2.49	0.44
1:0:133:U:C3'	1:0:134:U:H5''	2.48	0.44
28:Z:36:ASP:CB	28:Z:45:ASP:HB3	2.34	0.44
27:Y:154:ARG:HH11	27:Y:154:ARG:CG	2.30	0.44
2:9:3042:C:O2	7:D:76:ARG:NH1	2.50	0.44
7:D:13:MET:HA	7:D:137:PRO:HG2	1.98	0.44
1:0:2542:C:H5''	1:0:2608:C:N4	2.33	0.44
1:0:1086:A:N6	25:W:11:VAL:HG11	2.33	0.44
1:0:92:G:H4'	24:V:44:GLY:HA3	2.00	0.44
1:0:1218:U:H2'	1:0:1219:U:C6	2.53	0.44
1:0:2102:G:H5''	1:0:2538:A:C2	2.52	0.44
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.52	0.44
1:0:2427:C:OP2	31:3:84:ARG:HD2	2.17	0.44
7:D:172:VAL:CG1	7:D:173:GLU:N	2.80	0.44
40:9:5851:HOH:O	16:N:115:VAL:HG13	2.17	0.44
6:C:194:PHE:HA	6:C:234:VAL:HG13	2.00	0.44
33:4:179:DA:H5''	33:4:180:C:H3'	2.00	0.44
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.52	0.44
1:0:2518:C:H2'	1:0:2519:C:O4'	2.17	0.44
1:0:2251:G:H2'	1:0:2252:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2531:U:O2'	1:0:2532:A:H5'	2.17	0.44
16:N:64:SER:C	16:N:66:LEU:H	2.20	0.44
6:C:31:ILE:HG23	6:C:220:THR:CG2	2.47	0.44
40:0:6242:HOH:O	13:K:87:ARG:CZ	2.64	0.44
7:D:60:GLU:O	7:D:61:PHE:C	2.55	0.44
1:0:1181:A:H2'	1:0:1182:C:H5'	2.00	0.44
16:N:24:LEU:HD13	19:Q:26:PRO:HB3	1.98	0.44
5:B:254:GLN:NE2	40:B:9585:HOH:O	2.48	0.44
11:H:21:THR:O	11:H:120:ILE:HD12	2.18	0.44
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.99	0.44
10:G:67:LEU:O	10:G:71:LEU:HG	2.18	0.44
11:H:169:GLY:C	11:H:170:ASN:HD22	2.21	0.44
5:B:178:ALA:O	5:B:182:VAL:HG23	2.18	0.44
5:B:8:LYS:HG3	5:B:220:VAL:HG12	1.99	0.44
1:0:125:U:H2'	40:0:4346:HOH:O	2.17	0.44
9:F:31:LYS:HE3	40:F:2623:HOH:O	2.17	0.44
1:0:2353:A:H4'	1:0:2354:A:O5'	2.17	0.44
1:0:2831:C:O3'	20:R:71:LYS:HE2	2.18	0.44
1:0:2314:G:C2'	1:0:2315:C:H5'	2.48	0.44
1:0:2857:C:H2'	1:0:2858:U:C6	2.53	0.44
1:0:821:U:H2'	1:0:822:C:H6	1.82	0.44
1:0:134:U:H5'	1:0:134:U:C6	2.47	0.44
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.38	0.44
1:0:2533:C:C6	1:0:2533:C:H5'	2.49	0.44
11:H:56:GLN:HE22	11:H:93:GLN:HG2	1.83	0.44
10:G:27:ILE:HD13	10:G:71:LEU:HD23	1.99	0.44
9:F:99:THR:O	9:F:100:ASP:HB2	2.17	0.44
1:0:497:A:H2'	1:0:498:A:C5'	2.48	0.44
1:0:1921:A:O2'	1:0:1922:A:H5'	2.18	0.44
1:0:333:G:O2'	1:0:334:G:H5'	2.18	0.44
2:9:3011:A:P	19:Q:19:ARG:HH21	2.40	0.44
13:K:49:LEU:CD1	13:K:80:ILE:HD13	2.48	0.44
1:0:1181:A:H5'	32:I:94:GLU:OE2	2.18	0.44
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.66	0.44
1:0:249:G:O2'	1:0:250:C:H5'	2.18	0.44
20:R:119:VAL:CG1	20:R:119:VAL:O	2.65	0.44
1:0:2767:C:OP1	5:B:318:ASN:ND2	2.51	0.44
27:Y:133:HIS:HD2	40:Y:9381:HOH:O	2.00	0.44
1:0:2101:A:H2'	6:C:63:SER:OG	2.18	0.44
1:0:629:A:H2'	1:0:630:A:O4'	2.18	0.44
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.83	0.44
1:0:1299:G:N7	14:L:6:ARG:NH1	2.65	0.44
2:9:3002:U:OP2	2:9:3003:A:H5'	2.18	0.44
6:C:194:PHE:CE2	6:C:234:VAL:HG11	2.53	0.44
1:0:603:A:H1'	1:0:605:C:C2	2.52	0.44
1:0:951:A:O2'	1:0:952:G:H5'	2.18	0.44
1:0:2362:A:H2'	1:0:2363:G:C8	2.53	0.44
1:0:1418:U:OP1	30:2:42:TRP:HB3	2.18	0.44
9:F:107:ASP:O	9:F:111:ILE:HG13	2.17	0.44
5:B:274:GLU:HA	5:B:292:GLY:O	2.18	0.44
30:2:41:HIS:CD2	30:2:44:ARG:H	2.36	0.43
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.80	0.43
4:A:201:PHE:HB3	40:A:9620:HOH:O	2.16	0.43
1:0:656:G:OP2	17:O:37:ARG:HD2	2.17	0.43
8:E:93:MET:HE1	8:E:165:GLY:N	2.33	0.43
14:L:94:ARG:NH1	14:L:143:THR:HG21	2.33	0.43
1:0:1205:U:C2'	1:0:1206:U:H5''	2.49	0.43
5:B:87:TYR:HD1	40:B:9575:HOH:O	2.01	0.43
1:0:1435:U:H5'	40:0:3204:HOH:O	2.16	0.43
12:J:131:THR:HG22	12:J:133:GLY:N	2.34	0.43
1:0:2568:A:H2'	1:0:2569:A:O4'	2.18	0.43
22:T:52:ARG:O	22:T:53:GLY:O	2.36	0.43
1:0:2809:G:H2'	1:0:2810:G:O4'	2.19	0.43
1:0:907:A:H2'	1:0:908:A:C8	2.52	0.43
6:C:21:VAL:HG13	40:C:9202:HOH:O	2.16	0.43
24:V:12:THR:OG1	24:V:13:PRO:HD2	2.18	0.43
1:0:283:U:H5''	1:0:284:C:OP2	2.19	0.43
4:A:132:ASP:OD1	4:A:133:ARG:N	2.42	0.43
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.15	0.43
5:B:175:LEU:C	5:B:175:LEU:HD23	2.38	0.43
1:0:1829:A:N6	28:Z:18:TYR:HA	2.33	0.43
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.18	0.43
1:0:2898:G:H4'	5:B:288:GLY:HA2	2.00	0.43
1:0:1657:A:H2'	1:0:1658:A:C8	2.54	0.43
8:E:112:ALA:HA	8:E:113:PRO:HD3	1.83	0.43
1:0:2016:U:H2'	1:0:2017:U:O4'	2.17	0.43
23:U:38:ASN:O	23:U:42:LEU:HG	2.18	0.43
30:2:41:HIS:HB3	30:2:44:ARG:HB2	2.00	0.43
25:W:122:ARG:CG	25:W:152:ALA:O	2.66	0.43
1:0:506:G:H22	1:0:509:A:H5'	1.80	0.43
4:A:211:LYS:HB2	40:A:9576:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1641:A:C2'	1:0:1642:A:H5'	2.47	0.43
1:0:2568:A:H2'	1:0:2569:A:H5'	2.01	0.43
1:0:1132:A:N6	1:0:1229:C:H2'	2.34	0.43
1:0:245:C:H2'	1:0:246:G:H5'	2.01	0.43
5:B:40:GLY:HA3	40:B:9640:HOH:O	2.17	0.43
1:0:1160:G:HO2'	1:0:1190:G:H8	1.62	0.43
7:D:173:GLU:HG3	7:D:174:VAL:H	1.82	0.43
16:N:110:THR:HB	16:N:113:SER:HG	1.84	0.43
5:B:307:ARG:HD2	40:B:9645:HOH:O	2.18	0.43
32:I:92:PRO:O	32:I:94:GLU:HG3	2.19	0.43
12:J:74:ARG:NH1	12:J:76:ASP:CB	2.80	0.43
1:0:338:C:H4'	6:C:174:ILE:HD11	2.00	0.43
24:V:56:ILE:HG22	24:V:60:GLN:NE2	2.33	0.43
6:C:72:LYS:HA	6:C:76:ARG:O	2.19	0.43
1:0:1067:A:H5'	40:0:4907:HOH:O	2.17	0.43
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.48	0.43
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.99	0.43
20:R:82:GLU:O	20:R:86:LYS:HG3	2.19	0.43
5:B:280:VAL:HG13	5:B:333:GLU:O	2.18	0.43
5:B:84:LEU:HD13	5:B:84:LEU:C	2.39	0.43
13:K:14:LYS:HG3	13:K:32:ILE:O	2.18	0.43
24:V:8:ILE:HA	24:V:11:MET:HE2	2.00	0.43
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.82	0.43
23:U:9:CYS:O	23:U:52:THR:HG23	2.18	0.43
7:D:103:ASN:OD1	7:D:133:ASN:ND2	2.52	0.43
5:B:102:THR:HG21	5:B:182:VAL:O	2.19	0.43
1:0:699:C:H2'	1:0:744:G:O4'	2.18	0.43
16:N:170:GLU:O	16:N:174:GLU:HG3	2.18	0.43
25:W:142:ASP:O	25:W:145:GLY:N	2.52	0.43
1:0:1415:G:H5'	29:1:12:ASN:O	2.19	0.43
1:0:2717:C:OP1	5:B:207:LYS:HG3	2.18	0.43
1:0:1119:G:C8	12:J:52:GLN:NE2	2.83	0.43
22:T:75:GLU:O	22:T:76:ASP:HB2	2.18	0.43
1:0:1667:A:H2'	1:0:1668:U:C6	2.53	0.43
4:A:65:ARG:HH11	4:A:65:ARG:HG2	1.84	0.43
1:0:2421:G:H2'	40:0:4649:HOH:O	2.18	0.43
12:J:130:VAL:HG12	12:J:131:THR:H	1.84	0.43
5:B:85:ARG:HB2	5:B:99:GLU:HG2	2.00	0.43
1:0:816:G:C6	1:0:817:G:N1	2.87	0.43
19:Q:46:SER:O	19:Q:48:PRO:HD3	2.19	0.43
1:0:962:C:H1'	16:N:5:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:297:U:H1'	40:0:4511:HOH:O	2.17	0.43
1:0:2039:A:H4'	1:0:2760:C:O2'	2.18	0.43
1:0:2506:A:O2'	1:0:2507:G:P	2.77	0.43
26:X:73:ARG:HB2	26:X:88:GLU:OE2	2.18	0.43
16:N:86:LEU:HD21	16:N:180:LEU:HD12	2.01	0.43
6:C:138:VAL:HG11	6:C:160:LEU:HD13	2.01	0.43
5:B:243:ASN:HA	5:B:244:PRO:C	2.38	0.43
1:0:820:G:C6	4:A:171:LYS:HB2	2.54	0.43
1:0:1573:A:H2'	1:0:1574:C:O4'	2.18	0.43
7:D:96:SER:C	7:D:98:PHE:H	2.22	0.43
1:0:1759:A:N3	1:0:1818:C:H2'	2.34	0.43
27:Y:216:ARG:HD2	40:Y:9369:HOH:O	2.19	0.43
5:B:56:ASP:CG	5:B:322:ARG:HB3	2.38	0.43
21:S:53:ASN:ND2	40:S:9480:HOH:O	2.51	0.43
1:0:2506:A:O2'	1:0:2507:G:O5'	2.37	0.43
22:T:23:VAL:HG23	22:T:41:ARG:HG3	2.00	0.43
23:U:14:GLU:OE1	23:U:15:PRO:HD2	2.19	0.43
25:W:3:ALA:O	25:W:54:PHE:HA	2.19	0.43
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.53	0.43
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.83	0.43
1:0:1130:U:H2'	1:0:1131:G:O4'	2.19	0.43
27:Y:184:GLU:HG2	27:Y:229:LEU:HD11	2.00	0.43
1:0:1456:C:H2'	1:0:1457:U:C6	2.54	0.43
13:K:80:ILE:O	13:K:87:ARG:HA	2.19	0.43
22:T:40:VAL:HG22	22:T:41:ARG:H	1.82	0.43
2:9:3050:G:H5''	16:N:159:TYR:HE1	1.83	0.43
5:B:18:ARG:HE	5:B:256:GLN:NE2	2.17	0.43
1:0:2726:U:O2	1:0:2749:U:O5'	2.37	0.43
7:D:135:VAL:HG21	7:D:139:TYR:CG	2.54	0.43
18:P:13:VAL:HG11	18:P:40:VAL:HG12	2.00	0.43
28:Z:39:CYS:HB3	28:Z:42:CYS:SG	2.59	0.43
1:0:2831:C:H2'	1:0:2832:C:H5'	2.01	0.43
1:0:2699:A:H2'	1:0:2700:G:O4'	2.18	0.43
1:0:64:G:H2'	1:0:65:C:O4'	2.19	0.43
1:0:2356:A:H2'	1:0:2357:G:O4'	2.18	0.43
5:B:279:THR:HA	5:B:284:PHE:HE1	1.84	0.43
13:K:4:LEU:HD23	13:K:4:LEU:HA	1.85	0.42
32:I:113:HIS:CE1	32:I:121:LEU:HD22	2.53	0.42
32:I:132:CYS:C	32:I:134:SER:N	2.72	0.42
32:I:102:VAL:CG1	32:I:106:LYS:HE3	2.44	0.42
1:0:1298:U:H2'	1:0:1299:G:C8	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:97:SER:OG	17:O:100:GLN:HG3	2.19	0.42
1:O:2064:U:H4'	1:O:2653:A:OP1	2.18	0.42
1:O:1095:U:O2	25:W:120:PRO:HG2	2.19	0.42
28:Z:41:ASN:O	28:Z:42:CYS:HB3	2.19	0.42
22:T:55:PHE:CE1	22:T:89:ARG:HG2	2.54	0.42
1:O:65:C:O2'	1:O:66:G:H5'	2.18	0.42
16:N:137:ALA:HB1	16:N:141:ARG:HD3	2.00	0.42
7:D:51:ARG:HD3	40:D:7636:HOH:O	2.19	0.42
1:O:2088:C:H1'	1:O:2841:A:N1	2.35	0.42
15:M:115:LEU:HD13	15:M:116:ASN:HB2	2.01	0.42
23:U:4:ARG:HH11	23:U:4:ARG:HG2	1.84	0.42
25:W:52:VAL:HG13	25:W:53:ALA:N	2.33	0.42
31:3:70:ARG:HB3	40:3:9502:HOH:O	2.18	0.42
15:M:82:ARG:O	15:M:83:SER:C	2.57	0.42
1:O:553:G:O4'	1:O:1325:G:H5'	2.19	0.42
4:A:36:ASP:CG	4:A:36:ASP:O	2.57	0.42
16:N:152:GLU:HA	16:N:152:GLU:OE1	2.19	0.42
29:1:21:ARG:HD3	29:1:45:ARG:NE	2.34	0.42
26:X:20:GLU:CG	26:X:21:PRO:HD2	2.48	0.42
5:B:146:THR:C	5:B:148:PRO:HD3	2.40	0.42
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.49	0.42
1:O:2239:C:H2'	1:O:2240:U:C6	2.54	0.42
8:E:6:GLU:HA	8:E:46:THR:HG22	2.01	0.42
1:O:2724:U:H2'	1:O:2725:G:O4'	2.19	0.42
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.01	0.42
1:O:27:U:H2'	1:O:28:G:O4'	2.19	0.42
1:O:366:U:H2'	1:O:367:G:O4'	2.19	0.42
20:R:84:ALA:O	20:R:88:PHE:HD1	2.02	0.42
20:R:114:VAL:HG13	20:R:114:VAL:O	2.19	0.42
1:O:1603:A:H5''	1:O:1604:G:H3'	2.00	0.42
28:Z:26:VAL:HG12	28:Z:30:GLU:OE1	2.18	0.42
6:C:46:TYR:CE1	6:C:92:PRO:HB3	2.54	0.42
1:O:2676:C:H4'	12:J:70:PHE:HE1	1.84	0.42
1:O:2541:U:O2	3:4:76:PPU:HA	2.20	0.42
27:Y:187:VAL:HB	27:Y:203:VAL:CG2	2.50	0.42
8:E:7:ILE:HD11	8:E:11:VAL:C	2.39	0.42
5:B:62:ARG:CB	5:B:65:MET:HE3	2.49	0.42
1:O:2807:U:OP2	5:B:27:ASN:ND2	2.50	0.42
15:M:34:GLU:HB3	15:M:38:GLU:HG3	2.01	0.42
1:O:1940:C:H4'	40:O:7801:HOH:O	2.18	0.42
1:O:308:U:C4	1:O:342:C:H1'	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:415:A:O2'	1:0:416:G:H5'	2.19	0.42
1:0:912:A:C4	1:0:1294:A:C2	3.06	0.42
1:0:2911:C:O2'	1:0:2912:C:H5'	2.19	0.42
1:0:188:C:H5''	15:M:163:LEU:HD21	2.02	0.42
1:0:1099:G:H2'	1:0:1100:G:O4'	2.19	0.42
8:E:166:VAL:HG12	40:E:3134:HOH:O	2.18	0.42
12:J:132:LEU:HA	12:J:132:LEU:HD23	1.84	0.42
40:0:5821:HOH:O	25:W:122:ARG:NH2	2.51	0.42
1:0:1159:G:H1	1:0:1208:C:N4	2.15	0.42
2:9:3039:U:HO2'	2:9:3042:C:H5	1.57	0.42
7:D:76:ARG:O	7:D:77:ASP:HB2	2.20	0.42
1:0:1342:C:O2'	1:0:1343:C:H5'	2.19	0.42
16:N:173:ASP:O	16:N:177:GLU:HB2	2.19	0.42
26:X:66:THR:HG23	26:X:67:PRO:HD2	2.01	0.42
2:9:3107:C:H5	40:9:3167:HOH:O	2.01	0.42
2:9:3039:U:O2'	2:9:3042:C:H5	2.02	0.42
1:0:1181:A:C2'	1:0:1182:C:H5'	2.49	0.42
7:D:136:ARG:HB3	7:D:137:PRO:HD2	2.01	0.42
4:A:130:THR:HB	4:A:137:VAL:HB	2.02	0.42
12:J:39:VAL:HG11	12:J:107:ASN:CB	2.50	0.42
11:H:154:TYR:CD1	11:H:154:TYR:C	2.93	0.42
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.48	0.42
1:0:793:A:C5'	18:P:83:LYS:HG2	2.49	0.42
9:F:111:ILE:O	9:F:115:VAL:HG23	2.20	0.42
1:0:87:C:H2'	30:2:28:LYS:O	2.19	0.42
1:0:1226:G:H5'	40:0:5084:HOH:O	2.19	0.42
1:0:2263:G:O2'	15:M:70:GLY:HA2	2.20	0.42
5:B:294:TYR:HE2	40:B:9642:HOH:O	2.01	0.42
16:N:108:SER:HA	16:N:109:PRO:HD3	1.80	0.42
1:0:588:G:O6	25:W:154:ARG:NH1	2.53	0.42
6:C:119:ALA:HA	6:C:137:PRO:HD3	2.01	0.42
27:Y:154:ARG:HH11	27:Y:154:ARG:CB	2.33	0.42
5:B:41:PHE:HA	5:B:79:MET:CE	2.49	0.42
7:D:99:ASP:N	7:D:103:ASN:O	2.47	0.42
1:0:945:U:H2'	1:0:946:C:H6	1.84	0.42
1:0:497:A:H2'	1:0:498:A:H5'	2.01	0.42
26:X:45:GLU:HG3	40:X:6178:HOH:O	2.19	0.42
4:A:93:THR:C	4:A:94:LEU:HD23	2.40	0.42
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.49	0.42
5:B:41:PHE:HA	5:B:79:MET:HE2	2.02	0.42
20:R:39:THR:CG2	20:R:107:GLU:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:167:ASP:C	16:N:168:LEU:HG	2.39	0.42
5:B:86:ALA:HA	40:B:9575:HOH:O	2.19	0.42
22:T:85:GLU:CG	22:T:86:GLU:N	2.80	0.42
5:B:62:ARG:HA	5:B:65:MET:HE3	2.02	0.42
23:U:20:MET:CG	23:U:28:THR:HG23	2.50	0.42
1:0:2436:U:H5'	31:3:68:LYS:HE2	2.01	0.42
1:0:1314:U:H2'	40:0:6398:HOH:O	2.20	0.42
1:0:2449:G:H2'	1:0:2450:C:O4'	2.19	0.42
7:D:88:LEU:N	7:D:89:PRO:CD	2.82	0.42
1:0:1616:A:H5''	1:0:1617:C:OP1	2.20	0.42
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.79	0.42
18:P:18:LYS:O	18:P:21:VAL:HG13	2.20	0.42
1:0:362:G:H2'	1:0:363:A:C8	2.54	0.42
1:0:1119:G:N2	1:0:1246:A:H2	2.08	0.42
23:U:17:THR:HG23	23:U:18:GLY:N	2.34	0.42
1:0:960:G:N3	1:0:960:G:H2'	2.34	0.42
4:A:100:PRO:HG2	4:A:103:VAL:CG2	2.45	0.42
10:G:12:ILE:HG13	40:G:6833:HOH:O	2.19	0.42
12:J:74:ARG:CB	12:J:74:ARG:HH11	2.28	0.42
1:0:835:U:P	5:B:229:ARG:HH12	2.43	0.42
40:0:3167:HOH:O	25:W:119:HIS:HE1	2.03	0.42
1:0:2769:C:H2'	1:0:2770:G:H5'	2.01	0.42
1:0:1778:A:H2'	1:0:1779:A:H5'	2.01	0.42
16:N:43:VAL:CG1	16:N:118:ILE:HD11	2.49	0.42
1:0:2649:A:O4'	1:0:2650:U:H5	2.02	0.42
1:0:820:G:C5	4:A:171:LYS:HB2	2.55	0.42
1:0:1218:U:H2'	1:0:1219:U:H6	1.84	0.42
1:0:220:C:H1'	40:0:6282:HOH:O	2.18	0.42
1:0:426:G:H2'	1:0:427:C:O4'	2.20	0.42
1:0:1065:G:H5'	40:0:4138:HOH:O	2.19	0.42
1:0:612:U:H2'	1:0:613:C:C6	2.55	0.42
15:M:48:LYS:O	15:M:52:GLN:HG3	2.20	0.42
11:H:51:VAL:CG1	11:H:53:GLU:O	2.67	0.42
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.49	0.42
1:0:932:U:H2'	1:0:933:C:C6	2.55	0.42
1:0:2787:C:H5	40:0:5181:HOH:O	2.02	0.42
6:C:129:HIS:HD2	6:C:165:ASP:OD2	2.03	0.42
15:M:164:THR:CG2	15:M:165:GLY:N	2.81	0.42
14:L:91:VAL:CG1	14:L:120:LEU:HD23	2.43	0.42
14:L:144:ASP:O	14:L:147:GLU:HB2	2.19	0.42
5:B:51:VAL:HG23	5:B:327:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:92:PRO:HB3	40:I:6825:HOH:O	2.19	0.42
4:A:122:SER:O	4:A:124:VAL:HG13	2.19	0.42
1:0:2269:C:H2'	1:0:2270:G:O4'	2.19	0.42
6:C:162:VAL:CG2	6:C:232:LEU:HD21	2.50	0.42
4:A:52:SER:HB2	4:A:164:ARG:HH11	1.85	0.42
31:3:17:HIS:O	31:3:18:GLN:HG3	2.20	0.42
16:N:82:TYR:HE1	16:N:120:GLU:HG2	1.84	0.42
8:E:20:ILE:HD12	8:E:33:LEU:HD12	2.02	0.42
2:9:3003:A:H2	2:9:3021:G:N3	2.18	0.42
27:Y:115:ARG:NE	40:Y:9355:HOH:O	2.52	0.42
18:P:14:LEU:O	18:P:16:VAL:HG23	2.19	0.42
1:0:40:C:H6	1:0:40:C:O5'	2.03	0.42
1:0:2338:G:H2'	7:D:129:ASP:OD1	2.20	0.42
1:0:2296:C:H2'	1:0:2297:U:C6	2.55	0.42
1:0:1849:G:H1'	1:0:2011:A:N1	2.34	0.42
24:V:42:ASN:O	24:V:44:GLY:N	2.53	0.42
9:F:16:ALA:HA	9:F:111:ILE:HD13	2.02	0.42
1:0:2015:A:H2'	1:0:2016:U:O4'	2.20	0.42
1:0:1398:G:H5'	18:P:23:PHE:O	2.19	0.42
1:0:1400:C:H4'	26:X:56:GLU:HG2	2.01	0.42
1:0:2837:U:H2'	40:0:7320:HOH:O	2.20	0.42
9:F:113:ASP:O	9:F:117:GLU:HG3	2.19	0.42
8:E:10:ASP:HA	40:E:3707:HOH:O	2.20	0.42
1:0:2505:G:C2'	1:0:2506:A:H5'	2.50	0.41
25:W:108:ARG:HE	25:W:114:PRO:HG2	1.85	0.41
22:T:48:VAL:O	22:T:59:GLU:HA	2.20	0.41
2:9:3041:C:C6	7:D:50:VAL:HG21	2.54	0.41
26:X:8:ARG:HB3	26:X:8:ARG:HE	1.63	0.41
1:0:449:A:C8	6:C:43:LYS:HG2	2.55	0.41
1:0:2819:C:H2'	1:0:2820:A:C8	2.55	0.41
40:0:6789:HOH:O	27:Y:158:LYS:HD3	2.19	0.41
4:A:43:VAL:O	4:A:44:ASP:HB2	2.20	0.41
40:0:3827:HOH:O	32:I:92:PRO:HD3	2.19	0.41
5:B:41:PHE:CD1	5:B:79:MET:CE	3.03	0.41
16:N:24:LEU:HD22	40:Q:2847:HOH:O	2.19	0.41
5:B:115:VAL:HA	5:B:116:PRO:HD3	1.94	0.41
1:0:907:A:H2'	1:0:908:A:H8	1.85	0.41
1:0:1203:G:O2'	1:0:1204:C:H5'	2.20	0.41
1:0:1603:A:H5''	1:0:1605:G:H5'	2.01	0.41
32:I:112:LYS:C	32:I:114:PRO:HD2	2.40	0.41
14:L:6:ARG:NH2	40:L:9445:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:82:ARG:HA	40:M:9339:HOH:O	2.19	0.41
1:0:538:C:H5''	1:0:539:G:C8	2.55	0.41
14:L:80:ASP:CB	14:L:90:ARG:HB3	2.50	0.41
1:0:926:A:O2'	14:L:41:HIS:HD2	2.03	0.41
23:U:4:ARG:NH1	23:U:4:ARG:HG2	2.35	0.41
1:0:522:U:O2'	1:0:1366:C:H5'	2.20	0.41
1:0:451:C:O2'	1:0:452:G:H5'	2.20	0.41
6:C:120:ASP:OD1	6:C:120:ASP:C	2.58	0.41
2:9:3050:G:H5''	16:N:159:TYR:CE1	2.55	0.41
4:A:192:VAL:HG13	40:A:9546:HOH:O	2.20	0.41
32:I:103:ASP:HA	32:I:106:LYS:HD2	2.02	0.41
1:0:82:C:OP1	22:T:67:LEU:HB2	2.20	0.41
28:Z:41:ASN:O	28:Z:41:ASN:ND2	2.53	0.41
11:H:76:GLU:C	11:H:77:LEU:HD23	2.41	0.41
6:C:133:ARG:HG3	6:C:133:ARG:HH11	1.84	0.41
1:0:2323:G:H5'	40:0:7497:HOH:O	2.19	0.41
26:X:18:ARG:NH1	40:X:4132:HOH:O	2.41	0.41
1:0:2886:C:O2'	1:0:2887:G:H5'	2.20	0.41
1:0:407:A:H2'	1:0:408:A:C8	2.55	0.41
16:N:33:ARG:NH1	16:N:103:ASP:OD2	2.51	0.41
4:A:30:ARG:HB3	4:A:30:ARG:HE	1.72	0.41
4:A:192:VAL:HG12	4:A:192:VAL:O	2.19	0.41
1:0:2748:G:H4'	1:0:2749:U:H5'	2.02	0.41
5:B:183:GLU:O	5:B:184:ASP:C	2.58	0.41
5:B:16:ARG:NH2	40:B:9552:HOH:O	2.44	0.41
1:0:2676:C:H4'	12:J:70:PHE:HD1	1.82	0.41
4:A:186:TRP:CG	4:A:187:PRO:HA	2.56	0.41
14:L:66:VAL:HG23	14:L:67:ARG:N	2.35	0.41
12:J:15:ARG:NH1	12:J:43:ARG:HH11	2.17	0.41
1:0:2415:A:N3	16:N:26:LEU:HD13	2.35	0.41
11:H:47:ILE:HG21	40:H:9541:HOH:O	2.19	0.41
1:0:1131:G:C6	1:0:1230:A:C4	3.08	0.41
1:0:1098:A:O3'	25:W:129:LYS:HE2	2.20	0.41
7:D:88:LEU:HB2	7:D:89:PRO:HD3	2.02	0.41
1:0:1139:U:H2'	1:0:1140:C:C6	2.56	0.41
1:0:1797:A:H2'	1:0:1799:G:O5'	2.21	0.41
40:C:9165:HOH:O	17:O:3:THR:HG21	2.19	0.41
24:V:8:ILE:CG2	24:V:59:ILE:HG13	2.50	0.41
1:0:2717:C:H2'	1:0:2718:C:C5'	2.37	0.41
25:W:122:ARG:NH1	25:W:152:ALA:O	2.54	0.41
29:1:28:HIS:O	29:1:32:LYS:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3088:G:OP1	25:W:130:HIS:NE2	2.47	0.41
13:K:23:ASN:HD21	13:K:107:THR:HB	1.84	0.41
1:0:1552:G:H2'	1:0:1553:C:C6	2.56	0.41
1:0:1829:A:H2'	1:0:1830:C:H5'	2.03	0.41
1:0:517:U:H1'	40:0:8071:HOH:O	2.19	0.41
1:0:1335:C:H2'	1:0:1336:U:C6	2.56	0.41
1:0:29:C:C2'	1:0:30:U:H5'	2.49	0.41
8:E:133:VAL:HG12	8:E:141:VAL:HG13	2.03	0.41
32:I:102:VAL:HG23	32:I:140:GLU:O	2.20	0.41
1:0:1182:C:H1'	1:0:1192:A:C8	2.45	0.41
1:0:1183:C:H5	1:0:1192:A:OP1	2.03	0.41
1:0:1044:C:H3'	1:0:1045:G:H5''	2.02	0.41
1:0:255:A:H2'	1:0:256:C:C6	2.55	0.41
1:0:892:G:H5''	29:1:54:ALA:HB2	2.02	0.41
1:0:329:A:OP2	6:C:206:ASN:HB2	2.20	0.41
1:0:2379:G:N3	1:0:2418:G:H2'	2.35	0.41
15:M:49:ALA:C	15:M:54:TYR:HB3	2.40	0.41
28:Z:30:GLU:HB2	40:Z:9215:HOH:O	2.20	0.41
5:B:312:ARG:HG2	5:B:313:PRO:N	2.35	0.41
1:0:1943:C:O4'	4:A:212:PRO:HA	2.20	0.41
1:0:2346:C:H4'	7:D:52:THR:CG2	2.51	0.41
40:0:7990:HOH:O	15:M:91:ILE:HG12	2.19	0.41
30:2:19:SER:O	30:2:36:ASN:ND2	2.53	0.41
1:0:441:A:H8	1:0:441:A:O5'	2.03	0.41
1:0:1867:G:O2'	1:0:1868:G:H5'	2.21	0.41
5:B:43:GLY:O	5:B:308:LEU:HD12	2.20	0.41
1:0:1495:C:H2'	1:0:1496:G:C8	2.56	0.41
1:0:1795:G:H2'	1:0:1796:A:O4'	2.20	0.41
7:D:75:LEU:HD22	7:D:79:MET:HB3	2.02	0.41
27:Y:122:ARG:NH2	40:Y:9335:HOH:O	2.53	0.41
1:0:2690:U:H4'	8:E:111:LYS:HE3	2.03	0.41
25:W:26:ILE:O	25:W:26:ILE:CG1	2.68	0.41
6:C:236:THR:HG22	6:C:239:ALA:HB2	2.03	0.41
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.50	0.41
8:E:80:TRP:O	8:E:134:SER:HA	2.19	0.41
20:R:9:ASP:O	20:R:13:THR:HB	2.20	0.41
14:L:73:VAL:HG23	14:L:74:THR:N	2.31	0.41
1:0:1268:C:O2'	1:0:1269:G:H5'	2.20	0.41
27:Y:189:ASN:ND2	27:Y:189:ASN:C	2.73	0.41
1:0:2032:U:H2'	1:0:2033:G:H5'	2.02	0.41
14:L:67:ARG:HB2	14:L:112:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:16:VAL:HG12	18:P:17:GLY:H	1.84	0.41
8:E:7:ILE:HA	8:E:8:PRO:HD3	1.95	0.41
26:X:43:VAL:CG1	26:X:44:ASP:N	2.83	0.41
1:0:2453:G:H5'	40:0:5235:HOH:O	2.21	0.41
1:0:499:G:O2'	1:0:500:G:H5'	2.20	0.41
23:U:19:THR:HG22	23:U:20:MET:N	2.35	0.41
1:0:2456:A:H5'	40:0:6223:HOH:O	2.21	0.41
2:9:3092:G:H2'	2:9:3093:A:C8	2.56	0.41
15:M:90:ARG:HB2	31:3:46:ILE:HD11	2.03	0.41
32:I:101:SER:OG	32:I:104:GLN:HG3	2.21	0.41
1:0:2053:G:H4'	20:R:136:TRP:CE2	2.56	0.41
13:K:9:THR:HG21	13:K:78:LYS:HE2	2.03	0.41
1:0:2134:G:C6	1:0:2258:A:C8	3.09	0.41
1:0:210:U:H2'	1:0:211:U:C6	2.55	0.41
2:9:3052:A:H2'	2:9:3053:G:O4'	2.21	0.41
1:0:101:C:H2'	1:0:102:A:C8	2.56	0.41
7:D:37:ALA:O	7:D:40:ILE:HG12	2.21	0.41
14:L:145:LEU:C	14:L:147:GLU:N	2.74	0.41
1:0:1555:G:H4'	1:0:1630:A:C2	2.50	0.41
4:A:130:THR:HG22	4:A:131:HIS:N	2.36	0.41
11:H:20:ILE:HG23	11:H:120:ILE:CD1	2.50	0.41
15:M:74:LYS:HA	40:M:9375:HOH:O	2.20	0.41
16:N:69:TYR:CE2	16:N:184:ILE:HG13	2.55	0.41
1:0:1235:G:O4'	12:J:63:ILE:HG23	2.20	0.41
1:0:2044:G:OP1	26:X:23:HIS:HE1	2.04	0.41
2:9:3054:A:H2	40:9:3535:HOH:O	2.04	0.41
1:0:2698:G:H2'	1:0:2699:A:C8	2.56	0.41
1:0:1929:G:H1'	40:0:5691:HOH:O	2.20	0.41
1:0:2597:U:H2'	1:0:2598:U:H5'	2.02	0.41
1:0:2115:U:H2'	1:0:2116:U:C6	2.56	0.41
4:A:103:VAL:O	4:A:105:VAL:HG23	2.21	0.40
11:H:29:ALA:H	11:H:66:ARG:HH12	1.69	0.40
4:A:179:MET:HG2	4:A:186:TRP:HB2	2.02	0.40
1:0:2523:U:O2'	1:0:2524:G:H5'	2.21	0.40
12:J:45:VAL:HG22	12:J:46:ILE:N	2.35	0.40
2:9:3023:U:O2'	2:9:3024:U:H4'	2.21	0.40
16:N:112:GLY:HA2	16:N:137:ALA:N	2.36	0.40
1:0:1098:A:H2'	1:0:1099:G:O4'	2.21	0.40
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	2.02	0.40
5:B:195:ARG:NH1	5:B:324:ASP:OD1	2.55	0.40
40:0:4099:HOH:O	6:C:81:PRO:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:162:ARG:HD3	40:H:9548:HOH:O	2.20	0.40
1:0:646:G:H2'	1:0:647:U:C6	2.56	0.40
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.53	0.40
20:R:25:PHE:CZ	20:R:29:LYS:HE2	2.55	0.40
2:9:3014:G:H2'	2:9:3015:C:H5'	2.03	0.40
20:R:39:THR:HG22	20:R:107:GLU:O	2.21	0.40
16:N:167:ASP:O	16:N:168:LEU:HG	2.21	0.40
31:3:20:HIS:HA	31:3:70:ARG:O	2.21	0.40
1:0:2032:U:C2'	1:0:2033:G:C5'	2.97	0.40
1:0:1333:U:H2'	1:0:1334:C:H6	1.85	0.40
1:0:2672:C:H1'	40:B:9628:HOH:O	2.20	0.40
16:N:67:ALA:C	16:N:69:TYR:H	2.24	0.40
9:F:99:THR:HG23	9:F:99:THR:O	2.22	0.40
5:B:144:THR:HG22	5:B:145:HIS:N	2.36	0.40
1:0:2101:A:OP2	6:C:66:GLY:HA2	2.21	0.40
1:0:2442:G:H3'	40:0:7117:HOH:O	2.20	0.40
1:0:23:G:C6	1:0:24:G:N1	2.89	0.40
15:M:58:GLN:HG3	40:M:9408:HOH:O	2.21	0.40
1:0:2782:G:O6	1:0:2790:C:H5''	2.21	0.40
1:0:2072:G:H3'	1:0:2073:G:H5''	2.03	0.40
14:L:114:VAL:HB	40:L:9469:HOH:O	2.21	0.40
1:0:999:C:H2'	1:0:1000:C:O4'	2.21	0.40
15:M:82:ARG:O	15:M:84:LYS:N	2.55	0.40
28:Z:39:CYS:O	28:Z:42:CYS:O	2.39	0.40
1:0:1462:C:H2'	1:0:1463:A:H8	1.85	0.40
1:0:87:C:C2	30:2:30:ASP:OD2	2.74	0.40
1:0:1314:U:H5''	1:0:1316:G:O4'	2.21	0.40
7:D:35:ALA:O	7:D:38:GLU:HG3	2.21	0.40
26:X:10:VAL:HG12	26:X:11:THR:N	2.36	0.40
1:0:669:G:O2'	1:0:670:G:H5'	2.21	0.40
1:0:1304:U:H2'	1:0:1305:C:C6	2.56	0.40
4:A:17:ARG:HD2	40:A:9532:HOH:O	2.20	0.40
1:0:791:A:H2'	1:0:792:G:O4'	2.22	0.40
23:U:49:LEU:HG	40:U:3805:HOH:O	2.22	0.40
5:B:36:PRO:HA	5:B:167:GLY:O	2.22	0.40
22:T:20:HIS:HB3	22:T:41:ARG:HD2	2.03	0.40
17:O:32:ARG:HD3	17:O:32:ARG:C	2.41	0.40
16:N:110:THR:HG22	40:N:9349:HOH:O	2.20	0.40
2:9:3114:G:H2'	2:9:3115:C:C6	2.57	0.40
5:B:217:ARG:CG	5:B:257:THR:HG22	2.43	0.40
1:0:710:G:H5'	17:O:25:VAL:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:57:THR:HA	40:D:5728:HOH:O	2.22	0.40
1:0:949:U:C4'	19:Q:95:GLU:HA	2.52	0.40
1:0:2238:A:O2'	1:0:2239:C:H5'	2.21	0.40
9:F:118:LEU:O	9:F:119:ARG:HB3	2.21	0.40
31:3:25:VAL:HB	31:3:66:ASP:OD2	2.21	0.40
1:0:2912:C:H2'	1:0:2913:A:O4'	2.21	0.40
4:A:135:VAL:HG21	4:A:147:ARG:NH1	2.37	0.40
4:A:173:GLY:O	4:A:176:HIS:HB3	2.22	0.40
1:0:1525:G:H5'	1:0:1526:A:OP2	2.21	0.40
15:M:42:ARG:HA	15:M:43:PRO:HD3	1.90	0.40
1:0:1636:G:O2'	1:0:1637:A:H5'	2.20	0.40
29:1:53:LYS:HD3	29:1:53:LYS:HA	1.89	0.40
16:N:143:ARG:HE	16:N:143:ARG:HB3	1.70	0.40
1:0:876:A:H2'	1:0:876:A:N3	2.37	0.40
26:X:70:ILE:O	26:X:70:ILE:HG23	2.22	0.40
1:0:1602:C:OP2	28:Z:46:ARG:NH2	2.54	0.40
1:0:1834:C:H2'	1:0:1840:A:N6	2.37	0.40
31:3:48:ASN:ND2	31:3:50:GLY:H	2.20	0.40
25:W:38:THR:HG22	25:W:40:ALA:H	1.87	0.40
1:0:2408:A:H4'	31:3:15:ASN:O	2.22	0.40
9:F:26:THR:HG21	9:F:102:GLY:C	2.42	0.40
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.21	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%)	213 (91%)	17 (7%)	5 (2%)	9	7
5	B	335/338 (99%)	312 (93%)	18 (5%)	5 (2%)	13	12
6	C	244/246 (99%)	226 (93%)	18 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	D	134/177 (76%)	104 (78%)	18 (13%)	12 (9%)	1	0
8	E	170/178 (96%)	164 (96%)	6 (4%)	0	100	100
9	F	117/120 (98%)	104 (89%)	11 (9%)	2 (2%)	11	10
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	141 (90%)	13 (8%)	2 (1%)	15	15
12	J	140/145 (97%)	132 (94%)	5 (4%)	3 (2%)	9	7
13	K	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	24	27
14	L	141/165 (86%)	120 (85%)	20 (14%)	1 (1%)	26	31
15	M	192/195 (98%)	180 (94%)	11 (6%)	1 (0%)	34	41
16	N	184/187 (98%)	162 (88%)	15 (8%)	7 (4%)	4	2
17	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
18	P	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
19	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
21	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
22	T	117/120 (98%)	108 (92%)	8 (7%)	1 (1%)	21	24
23	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	V	63/71 (89%)	55 (87%)	7 (11%)	1 (2%)	12	11
25	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
26	X	80/92 (87%)	71 (89%)	9 (11%)	0	100	100
27	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
28	Z	71/83 (86%)	58 (82%)	10 (14%)	3 (4%)	3	1
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
31	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	17	18
32	I	68/162 (42%)	52 (76%)	14 (21%)	2 (3%)	6	3
All	All	3705/4431 (84%)	3409 (92%)	249 (7%)	47 (1%)	15	15

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	37	VAL
7	D	137	PRO

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Mol	Chain	Res	Type
9	F	101	ALA
11	H	166	SER
12	J	143	LYS
14	L	80	ASP
16	N	154	LEU
16	N	183	ASP
16	N	184	ILE
28	Z	42	CYS
28	Z	81	ARG
4	A	34	ASP
5	B	169	GLY
7	D	60	GLU
7	D	171	ASP
11	H	168	ALA
22	T	53	GLY
28	Z	20	ARG
32	I	129	VAL
4	A	132	ASP
5	B	34	GLY
7	D	16	PRO
7	D	56	ARG
7	D	138	GLY
7	D	147	ALA
12	J	65	ASN
15	M	83	SER
16	N	162	ASP
4	A	27	LEU
5	B	185	GLY
7	D	61	PHE
12	J	5	GLU
13	K	126	SER
16	N	68	GLU
24	V	43	PRO
31	3	56	PRO
7	D	65	GLU
7	D	97	GLN
16	N	65	ASP
16	N	164	ASP
5	B	107	SER
9	F	100	ASP
4	A	112	PRO
7	D	27	ILE

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Mol	Chain	Res	Type
7	D	69	ILE
32	I	114	PRO
5	B	2	GLN

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%)	26	35
5	B	282/283 (100%)	268 (95%)	14 (5%)	30	41
6	C	193/193 (100%)	174 (90%)	19 (10%)	10	11
7	D	117/148 (79%)	110 (94%)	7 (6%)	24	31
8	E	152/156 (97%)	145 (95%)	7 (5%)	33	44
9	F	93/94 (99%)	90 (97%)	3 (3%)	46	62
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	130 (98%)	2 (2%)	72	85
12	J	118/121 (98%)	110 (93%)	8 (7%)	20	25
13	K	106/106 (100%)	102 (96%)	4 (4%)	40	54
14	L	113/127 (89%)	109 (96%)	4 (4%)	43	58
15	M	158/159 (99%)	153 (97%)	5 (3%)	46	62
16	N	149/150 (99%)	142 (95%)	7 (5%)	32	43
17	O	93/94 (99%)	91 (98%)	2 (2%)	60	77
18	P	113/117 (97%)	110 (97%)	3 (3%)	52	70
19	Q	79/80 (99%)	75 (95%)	4 (5%)	29	39
20	R	117/122 (96%)	117 (100%)	0	100	100
21	S	71/74 (96%)	71 (100%)	0	100	100
22	T	105/106 (99%)	101 (96%)	4 (4%)	40	54
23	U	44/52 (85%)	43 (98%)	1 (2%)	58	75
24	V	51/57 (90%)	50 (98%)	1 (2%)	63	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	W	130/130 (100%)	126 (97%)	4 (3%)	47	64
26	X	66/74 (89%)	62 (94%)	4 (6%)	23	30
27	Y	120/196 (61%)	109 (91%)	11 (9%)	11	13
28	Z	60/68 (88%)	59 (98%)	1 (2%)	68	83
29	1	46/47 (98%)	45 (98%)	1 (2%)	60	77
30	2	42/46 (91%)	41 (98%)	1 (2%)	57	74
31	3	79/79 (100%)	77 (98%)	2 (2%)	55	73
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2964 (96%)	129 (4%)	36	49

All (129) 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	78	ASP
4	A	94	LEU
4	A	131	HIS
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	28	SER
5	B	82	VAL
5	B	98	THR
5	B	113	LEU
5	B	149	ASP
5	B	162	MET
5	B	195	ARG
5	B	251	VAL
5	B	254	GLN
5	B	277	GLU
5	B	279	THR
5	B	312	ARG
6	C	16	VAL
6	C	27	ARG

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Mol	Chain	Res	Type
6	C	67	GLN
6	C	76	ARG
6	C	78	ARG
6	C	91	PRO
6	C	94	THR
6	C	95	GLU
6	C	101	ASP
6	C	136	VAL
6	C	162	VAL
6	C	187	ARG
6	C	214	THR
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
6	C	243	VAL
6	C	246	ARG
7	D	24	HIS
7	D	50	VAL
7	D	61	PHE
7	D	99	ASP
7	D	100	ASP
7	D	133	ASN
7	D	137	PRO
8	E	15	GLN
8	E	16	ASP
8	E	102	VAL
8	E	131	LEU
8	E	155	ASN
8	E	156	ASP
8	E	164	ASP
9	F	12	LEU
9	F	46	GLU
9	F	99	THR
11	H	84	LYS
11	H	154	TYR
12	J	46	ILE
12	J	52	GLN
12	J	70	PHE
12	J	74	ARG
12	J	79	PHE
12	J	107	ASN

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Mol	Chain	Res	Type
12	J	127	ILE
12	J	131	THR
13	K	4	LEU
13	K	10	GLN
13	K	84	ASP
13	K	100	GLU
14	L	35	ARG
14	L	43	HIS
14	L	89	PHE
14	L	140	VAL
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
16	N	12	ARG
16	N	23	ARG
16	N	26	LEU
16	N	37	ARG
16	N	49	THR
16	N	127	LEU
16	N	139	TRP
17	O	3	THR
17	O	111	VAL
18	P	81	LYS
18	P	98	ILE
18	P	117	SER
19	Q	16	ASN
19	Q	18	PRO
19	Q	57	ASP
19	Q	95	GLU
22	T	26	THR
22	T	39	ASN
22	T	48	VAL
22	T	89	ARG
23	U	17	THR
24	V	65	ASP
25	W	35	VAL
25	W	52	VAL
25	W	122	ARG
25	W	146	ILE
26	X	27	ASP

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Mol	Chain	Res	Type
26	X	72	VAL
26	X	79	GLU
26	X	82	GLU
27	Y	103	THR
27	Y	115	ARG
27	Y	141	THR
27	Y	144	ARG
27	Y	154	ARG
27	Y	163	THR
27	Y	189	ASN
27	Y	200	THR
27	Y	203	VAL
27	Y	204	ARG
27	Y	235	GLU
28	Z	22	SER
29	1	47	ASP
30	2	18	ASN
31	3	56	PRO
31	3	65	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	29	HIS
4	A	199	HIS
5	B	27	ASN
5	B	145	HIS
5	B	221	GLN
5	B	238	ASN
5	B	256	GLN
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	39	GLN
6	C	129	HIS
7	D	47	GLN
7	D	103	ASN
7	D	133	ASN
8	E	106	ASN
8	E	143	GLN
10	G	64	ASN
11	H	31	HIS

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Mol	Chain	Res	Type
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	170	ASN
12	J	52	GLN
12	J	107	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
14	L	43	HIS
14	L	116	HIS
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	77	HIS
15	M	143	ASN
15	M	170	ASN
16	N	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	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
23	U	39	ASN
23	U	48	ASN
24	V	29	ASN
24	V	60	GLN

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Mol	Chain	Res	Type
25	W	27	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	22	ASN
27	Y	119	GLN
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
28	Z	41	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	30	GLN
31	3	48	ASN
32	I	113	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	235 (8%)	36 (1%)
2	9	121/122 (99%)	14 (11%)	1 (0%)
3	4	1/7 (14%)	0	0
All	All	2867/3051 (93%)	249 (8%)	37 (1%)

All (249) 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

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Mol	Chain	Res	Type
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	134	U
1	0	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	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	497	A
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

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Mol	Chain	Res	Type
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	702	G
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	1087	G
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G

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Mol	Chain	Res	Type
1	0	1130	U
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1331	A
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	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

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Mol	Chain	Res	Type
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1732	A
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	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	2103	A
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A

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Mol	Chain	Res	Type
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2467	A
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2542	C
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2637	A
1	0	2644	C
1	0	2645	U
1	0	2648	U
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2727	A
1	0	2747	C

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Mol	Chain	Res	Type
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2852	A
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	644	G
1	0	699	C

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Mol	Chain	Res	Type
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1506	U
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1730	G
1	0	1819	G
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2536	C
1	0	2541	U
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
1	0	2791	U
1	0	2852	A
2	9	3065	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	0	2587	1	12,22,23	1.01	1 (8%)	19,31,34	3.12	2 (10%)
1	OMG	0	2588	1,3	17,26,27	1.02	1 (5%)	21,38,41	2.54	3 (14%)
1	UR3	0	2619	1	12,22,23	0.91	1 (8%)	16,32,35	0.74	0
1	PSU	0	2621	1	13,21,22	1.66	2 (15%)	18,30,33	6.08	3 (16%)
1	1MA	0	628	1	14,25,26	1.00	1 (7%)	15,37,40	1.13	1 (6%)
3	PPU	4	76	33,1,3	30,40,41	1.18	1 (3%)	37,57,60	1.05	3 (8%)

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	-	0/3/25/26	0/3/3/3
3	PPU	4	76	33,1,3	-	0/21/43/44	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	76	PPU	OC-CM	-5.41	1.26	1.42
1	0	2621	PSU	C5-C1'	-4.85	1.48	1.52
1	0	2619	UR3	C6-C5	-2.19	1.33	1.38
1	0	2587	OMU	C4-N3	2.42	1.37	1.33
1	0	628	1MA	C6-N6	2.75	1.34	1.29
1	0	2621	PSU	C4-N3	2.80	1.38	1.33
1	0	2588	OMG	C6-N1	3.04	1.38	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	-21.33	114.72	128.33
1	0	2588	OMG	C5-C6-N1	-8.73	111.65	123.59
1	0	628	1MA	C2-N3-C4	-3.62	110.79	116.40
1	0	2587	OMU	C5-C4-N3	-3.23	114.84	123.12
3	4	76	PPU	C4'-C3'-N3'	-2.71	107.96	113.61
1	0	2588	OMG	N3-C2-N1	-2.28	123.97	127.44
3	4	76	PPU	C3'-N3'-C	-2.07	119.92	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-N1-C2	2.51	119.51	115.47
3	4	76	PPU	C2-N1-C6	3.49	118.86	111.43
1	0	2588	OMG	C6-N1-C2	6.68	125.22	115.94
1	0	2587	OMU	C4-N3-C2	12.95	126.96	114.14
1	0	2621	PSU	C4-N3-C2	13.86	127.23	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
3	4	76	PPU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 316 ligands modelled in this entry, 312 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
33	PO2	4	178	33,3	0,2,2	0.00	-	0,1,1	0.00	-
33	DA	4	179	33,1,34	15,23,24	0.60	0	17,33,36	0.74	0
33	C	4	180	33,34	12,21,22	0.77	0	16,30,33	0.89	1 (6%)
33	C	4	181	33	13,18,22	0.78	0	16,26,33	0.87	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PO2	4	178	33,3	-	0/0/0/0	0/0/0/0
33	DA	4	179	33,1,34	-	0/3/21/22	0/3/3/3
33	C	4	180	33,34	-	0/3/25/26	0/2/2/2
33	C	4	181	33	-	0/2/22/26	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	4	180	C	C2-N3-C4	3.06	119.93	115.61
33	4	181	C	C2-N3-C4	3.08	119.96	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	4	179	DA	2	0
33	4	180	C	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.07	81 (2%) 55 64	26, 50, 94, 154	0
2	9	122/122 (100%)	0.18	6 (4%) 33 42	45, 70, 97, 154	0
3	4	2/7 (28%)	-0.84	0 100 100	46, 46, 46, 54	0
4	A	237/240 (98%)	0.61	21 (8%) 12 17	31, 55, 88, 108	0
5	B	337/338 (99%)	0.47	18 (5%) 30 39	32, 57, 83, 94	0
6	C	246/246 (100%)	0.25	7 (2%) 56 66	29, 51, 76, 90	0
7	D	140/177 (79%)	2.51	69 (49%) 0 0	64, 100, 128, 135	0
8	E	172/178 (96%)	1.22	43 (25%) 1 1	47, 71, 89, 96	0
9	F	119/120 (99%)	1.55	41 (34%) 0 0	51, 77, 106, 112	0
10	G	29/348 (8%)	2.90	19 (65%) 0 0	75, 97, 105, 106	0
11	H	160/171 (93%)	0.97	28 (17%) 2 3	49, 66, 97, 105	0
12	J	142/145 (97%)	0.34	5 (3%) 48 56	40, 55, 76, 95	0
13	K	132/132 (100%)	0.13	2 (1%) 76 81	36, 52, 74, 83	0
14	L	145/165 (87%)	1.08	32 (22%) 1 1	29, 70, 114, 125	0
15	M	194/195 (99%)	1.07	24 (12%) 5 8	36, 49, 90, 98	0
16	N	186/187 (99%)	1.36	48 (25%) 1 1	48, 70, 117, 121	0
17	O	115/116 (99%)	0.45	4 (3%) 48 56	42, 60, 75, 81	0
18	P	143/149 (95%)	0.36	4 (2%) 56 66	41, 56, 69, 81	0
19	Q	95/96 (98%)	0.44	6 (6%) 23 31	42, 54, 70, 78	0
20	R	150/155 (96%)	0.17	3 (2%) 68 75	33, 49, 69, 77	0
21	S	81/85 (95%)	0.50	8 (9%) 9 14	42, 60, 81, 98	0
22	T	119/120 (99%)	0.97	16 (13%) 4 7	46, 59, 89, 113	0
23	U	53/66 (80%)	0.44	3 (5%) 27 36	46, 57, 77, 84	0
24	V	65/71 (91%)	1.92	18 (27%) 1 1	55, 80, 116, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.40	4 (2%) 59 68	42, 56, 79, 88	0
26	X	82/92 (89%)	0.99	12 (14%) 3 5	46, 60, 88, 105	0
27	Y	142/241 (58%)	0.46	13 (9%) 11 16	32, 49, 70, 90	0
28	Z	73/83 (87%)	2.29	30 (41%) 0 0	51, 83, 99, 106	0
29	1	56/57 (98%)	-0.24	0 100 100	30, 36, 45, 54	0
30	2	46/50 (92%)	1.13	10 (21%) 1 2	39, 63, 88, 100	0
31	3	92/92 (100%)	0.68	11 (11%) 6 9	39, 61, 76, 90	0
32	I	70/162 (43%)	6.25	68 (97%) 0 0	114, 127, 144, 146	0
All	All	6648/7482 (88%)	0.49	654 (9%) 10 14	26, 56, 102, 154	0

All (654) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	21.5
24	V	1	THR	16.5
7	D	63	ILE	15.2
15	M	70	GLY	14.4
32	I	133	THR	13.9
16	N	166	ALA	13.0
7	D	57	THR	13.0
32	I	79	ILE	12.0
24	V	39	ALA	12.0
15	M	80	GLY	11.7
22	T	119	ALA	11.6
28	Z	11	SER	11.5
32	I	109	ALA	11.5
28	Z	22	SER	11.3
32	I	105	VAL	10.8
15	M	79	ALA	10.8
32	I	75	THR	10.7
32	I	137	VAL	10.6
32	I	76	ALA	10.5
24	V	40	PRO	10.4
32	I	96	PHE	10.1
32	I	121	LEU	9.6
32	I	102	VAL	9.5
32	I	118	SER	9.4
26	X	88	GLU	9.1
32	I	85	PHE	8.9

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Mol	Chain	Res	Type	RSRZ
32	I	116	LEU	8.9
15	M	74	LYS	8.8
30	2	49	GLU	8.6
2	9	3001	U	8.5
32	I	125	ALA	8.4
32	I	81	ASP	8.3
28	Z	21	VAL	8.1
32	I	126	LYS	8.1
32	I	108	ILE	8.0
32	I	107	GLN	8.0
15	M	87	GLY	8.0
32	I	129	VAL	8.0
28	Z	20	ARG	8.0
32	I	77	GLU	7.9
32	I	111	GLN	7.9
32	I	114	PRO	7.8
32	I	93	GLN	7.7
32	I	113	HIS	7.7
15	M	86	GLN	7.6
32	I	104	GLN	7.6
32	I	132	CYS	7.5
15	M	71	SER	7.5
32	I	78	LEU	7.5
28	Z	19	GLY	7.4
15	M	77	HIS	7.4
24	V	38	GLY	7.3
7	D	61	PHE	7.2
32	I	91	GLU	7.1
10	G	23	ILE	7.1
10	G	26	MET	7.1
4	A	37	VAL	7.0
32	I	87	THR	6.9
32	I	138	THR	6.9
1	0	282	C	6.9
1	0	1951	G	6.8
7	D	88	LEU	6.8
32	I	88	GLY	6.8
15	M	78	LYS	6.8
8	E	45	ASP	6.7
28	Z	29	ILE	6.7
4	A	237	GLY	6.5
32	I	83	ALA	6.5

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Mol	Chain	Res	Type	RSRZ
28	Z	18	TYR	6.4
7	D	166	ILE	6.4
15	M	76	ARG	6.3
7	D	90	LEU	6.3
32	I	97	VAL	6.2
32	I	117	LEU	6.2
28	Z	24	ARG	6.2
10	G	27	ILE	6.2
15	M	83	SER	6.2
30	2	35	ARG	6.1
16	N	175	LEU	6.1
7	D	170	TYR	6.1
7	D	134	LEU	6.1
28	Z	25	ARG	6.1
1	0	1199	A	6.1
16	N	147	ILE	5.9
28	Z	23	ARG	5.9
7	D	64	ARG	5.9
16	N	165	ALA	5.8
32	I	74	PRO	5.8
28	Z	12	GLY	5.8
32	I	136	GLY	5.8
9	F	16	ALA	5.7
7	D	27	ILE	5.7
21	S	81	ILE	5.7
28	Z	31	SER	5.6
32	I	89	SER	5.6
28	Z	34	ASN	5.6
1	0	497	A	5.6
28	Z	45	ASP	5.5
16	N	163	PHE	5.5
7	D	104	PHE	5.5
7	D	44	ILE	5.5
1	0	2004	U	5.5
2	9	3024	U	5.4
15	M	75	ARG	5.4
24	V	36	ALA	5.4
7	D	135	VAL	5.3
32	I	86	GLU	5.3
1	0	1177	A	5.3
14	L	93	VAL	5.2
7	D	69	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
15	M	73	ARG	5.2
1	0	1173	A	5.2
28	Z	33	MET	5.1
28	Z	32	GLU	5.1
22	T	118	SER	5.1
9	F	106	ALA	5.1
9	F	119	ARG	5.0
32	I	103	ASP	5.0
1	0	1172	G	5.0
14	L	75	LEU	5.0
16	N	155	GLU	5.0
4	A	133	ARG	4.9
1	0	272	A	4.9
8	E	86	VAL	4.9
7	D	10	PHE	4.9
16	N	95	ALA	4.9
7	D	62	ASP	4.9
1	0	1198	U	4.9
15	M	81	ARG	4.8
2	9	3023	U	4.8
32	I	123	ASN	4.8
7	D	40	ILE	4.8
14	L	91	VAL	4.8
16	N	68	GLU	4.8
1	0	970	U	4.8
9	F	22	VAL	4.8
22	T	116	ASP	4.8
1	0	280	C	4.8
11	H	171	ALA	4.7
7	D	81	GLU	4.7
7	D	73	VAL	4.7
14	L	76	LEU	4.7
7	D	92	GLU	4.7
14	L	106	VAL	4.7
1	0	960	G	4.7
11	H	73	LEU	4.7
7	D	26	GLY	4.7
24	V	41	GLU	4.6
32	I	99	ASP	4.6
1	0	735	C	4.6
8	E	4	GLU	4.6
9	F	118	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
7	D	93	LEU	4.6
24	V	37	GLY	4.6
13	K	132	VAL	4.6
26	X	80	GLU	4.5
1	0	285	A	4.5
1	0	999	C	4.5
6	C	61	PHE	4.5
9	F	110	ASP	4.5
28	Z	30	GLU	4.5
11	H	74	ILE	4.4
25	W	86	GLU	4.4
9	F	49	PHE	4.4
12	J	70	PHE	4.4
7	D	85	GLN	4.4
17	O	22	GLY	4.4
1	0	1202	A	4.4
32	I	122	THR	4.4
7	D	18	ILE	4.3
28	Z	14	PHE	4.3
14	L	105	TYR	4.3
15	M	84	LYS	4.3
30	2	39	ARG	4.3
1	0	1525	G	4.3
16	N	159	TYR	4.3
4	A	36	ASP	4.2
9	F	28	ALA	4.2
15	M	82	ARG	4.2
10	G	24	VAL	4.2
32	I	72	VAL	4.2
8	E	108	LEU	4.2
1	0	2238	A	4.2
9	F	117	GLU	4.2
16	N	184	ILE	4.2
14	L	102	ASP	4.2
31	3	92	GLU	4.1
8	E	10	ASP	4.1
7	D	11	HIS	4.1
32	I	112	LYS	4.1
1	0	1965	C	4.1
7	D	172	VAL	4.1
1	0	2645	U	4.1
1	0	2237	G	4.1

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Mol	Chain	Res	Type	RSRZ
15	M	88	VAL	4.1
9	F	17	LEU	4.1
14	L	80	ASP	4.1
10	G	73	ASP	4.0
7	D	56	ARG	4.0
8	E	87	PHE	4.0
1	0	514	G	4.0
32	I	134	SER	4.0
1	0	1948	G	4.0
27	Y	235	GLU	4.0
2	9	3002	U	4.0
8	E	6	GLU	4.0
31	3	62	THR	3.9
11	H	37	GLN	3.9
24	V	8	ILE	3.9
26	X	85	VAL	3.9
28	Z	36	ASP	3.9
7	D	41	LEU	3.9
10	G	71	LEU	3.9
7	D	130	VAL	3.9
28	Z	26	VAL	3.9
9	F	25	ASP	3.8
9	F	100	ASP	3.8
22	T	117	ASP	3.8
7	D	89	PRO	3.8
24	V	43	PRO	3.8
10	G	69	ARG	3.8
32	I	115	ASP	3.8
9	F	108	VAL	3.8
27	Y	216	ARG	3.8
11	H	146	VAL	3.8
16	N	152	GLU	3.8
1	0	2769	C	3.8
1	0	288	A	3.8
1	0	284	C	3.8
32	I	110	GLU	3.7
11	H	78	GLY	3.7
32	I	98	ALA	3.7
1	0	1200	A	3.7
16	N	161	GLY	3.7
32	I	80	LYS	3.7
10	G	67	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
16	N	181	ASP	3.7
26	X	10	VAL	3.7
1	0	1169	U	3.7
1	0	2508	C	3.7
9	F	99	THR	3.7
22	T	82	THR	3.7
15	M	72	ALA	3.7
7	D	84	LEU	3.7
32	I	106	LYS	3.7
15	M	85	ARG	3.7
14	L	81	VAL	3.7
10	G	25	GLU	3.7
19	Q	95	GLU	3.7
24	V	63	GLU	3.7
16	N	158	LEU	3.6
28	Z	37	HIS	3.6
7	D	23	VAL	3.6
4	A	145	MET	3.6
14	L	120	LEU	3.6
30	2	27	LEU	3.6
7	D	167	GLU	3.6
14	L	104	ASP	3.6
10	G	22	ALA	3.6
16	N	154	LEU	3.6
14	L	60	GLU	3.6
14	L	62	ALA	3.6
32	I	120	ASP	3.6
1	0	1163	G	3.6
9	F	19	ALA	3.6
9	F	98	VAL	3.6
11	H	35	ARG	3.6
26	X	7	GLU	3.5
28	Z	28	GLU	3.5
14	L	145	LEU	3.5
8	E	88	TYR	3.5
32	I	119	TYR	3.5
16	N	178	THR	3.5
32	I	95	ASP	3.5
13	K	118	ALA	3.5
8	E	76	VAL	3.5
14	L	148	GLU	3.5
26	X	77	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	0	10	U	3.5
8	E	11	VAL	3.5
8	E	42	VAL	3.5
7	D	68	PRO	3.5
14	L	121	ILE	3.5
27	Y	108	ASP	3.4
1	0	969	G	3.4
14	L	97	VAL	3.4
1	0	1000	C	3.4
23	U	47	ARG	3.4
26	X	71	ARG	3.4
16	N	185	GLU	3.4
1	0	1171	A	3.4
1	0	1168	C	3.4
27	Y	236	VAL	3.4
1	0	2748	G	3.4
7	D	106	PHE	3.4
7	D	157	LEU	3.4
9	F	12	LEU	3.4
1	0	2511	A	3.4
8	E	100	ASP	3.4
27	Y	96	GLU	3.4
8	E	160	ARG	3.4
5	B	108	GLU	3.4
9	F	21	GLU	3.3
16	N	183	ASP	3.3
28	Z	16	ALA	3.3
30	2	48	ASP	3.3
8	E	94	GLN	3.3
14	L	79	ASP	3.3
4	A	35	GLY	3.3
4	A	85	SER	3.3
9	F	107	ASP	3.3
6	C	1	MET	3.3
7	D	66	GLY	3.3
16	N	134	ASP	3.3
28	Z	10	ARG	3.3
16	N	180	LEU	3.3
5	B	57	GLU	3.2
32	I	94	GLU	3.2
10	G	66	LEU	3.2
9	F	101	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
12	J	4	ALA	3.2
9	F	15	ASP	3.2
8	E	1	PRO	3.2
26	X	72	VAL	3.2
9	F	11	ASP	3.2
8	E	118	ILE	3.2
32	I	124	ALA	3.2
9	F	72	VAL	3.2
4	A	31	LYS	3.2
21	S	45	TYR	3.1
8	E	43	ASP	3.1
14	L	99	GLU	3.1
30	2	44	ARG	3.1
11	H	143	ALA	3.1
16	N	137	ALA	3.1
14	L	142	LEU	3.1
1	0	1966	U	3.1
16	N	71	TRP	3.1
11	H	138	CYS	3.1
1	0	138	U	3.1
27	Y	95	THR	3.1
7	D	58	VAL	3.1
1	0	281	U	3.1
16	N	139	TRP	3.1
8	E	127	ASP	3.1
16	N	143	ARG	3.0
32	I	92	PRO	3.0
9	F	69	GLU	3.0
7	D	160	ALA	3.0
7	D	65	GLU	3.0
19	Q	76	VAL	3.0
1	0	1950	G	3.0
8	E	98	GLU	3.0
16	N	156	GLU	3.0
14	L	100	ALA	3.0
14	L	44	GLU	3.0
11	H	82	ASP	3.0
7	D	53	LYS	3.0
16	N	172	PHE	3.0
24	V	10	ASP	3.0
1	0	1178	G	3.0
7	D	75	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
22	T	112	LEU	3.0
22	T	115	GLU	3.0
8	E	7	ILE	3.0
31	3	41	GLU	2.9
9	F	44	SER	2.9
2	9	3122	C	2.9
4	A	91	GLY	2.9
11	H	141	GLU	2.9
22	T	42	VAL	2.9
28	Z	59	TYR	2.9
25	W	76	ASP	2.9
7	D	154	LYS	2.9
15	M	1	ALA	2.9
8	E	89	SER	2.9
5	B	104	GLU	2.9
4	A	38	ILE	2.9
14	L	130	ARG	2.9
8	E	154	ILE	2.9
21	S	20	PHE	2.9
10	G	21	ASP	2.9
10	G	72	ASP	2.9
16	N	138	ASP	2.9
11	H	149	ALA	2.9
7	D	51	ARG	2.9
16	N	179	LEU	2.9
1	0	2344	G	2.8
24	V	5	VAL	2.8
8	E	93	MET	2.8
16	N	94	GLU	2.8
32	I	127	GLU	2.8
12	J	7	ASP	2.8
1	0	1170	U	2.8
16	N	16	ALA	2.8
7	D	77	ASP	2.8
27	Y	196	VAL	2.8
9	F	18	GLU	2.8
11	H	79	GLU	2.8
27	Y	234	VAL	2.8
5	B	2	GLN	2.8
22	T	35	TYR	2.8
16	N	72	GLU	2.8
18	P	108	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
18	P	114	LEU	2.8
32	I	135	LEU	2.8
14	L	61	ALA	2.8
21	S	78	ALA	2.8
24	V	32	ALA	2.8
18	P	111	GLU	2.8
32	I	128	VAL	2.7
16	N	106	LEU	2.7
24	V	59	ILE	2.7
31	3	1	MET	2.7
32	I	100	LEU	2.7
16	N	2	THR	2.7
7	D	129	ASP	2.7
8	E	90	HIS	2.7
25	W	91	ASP	2.7
11	H	83	TYR	2.7
31	3	20	HIS	2.7
4	A	99	ILE	2.7
32	I	73	PRO	2.7
1	0	362	G	2.7
1	0	1929	G	2.7
7	D	171	ASP	2.7
8	E	121	ASP	2.7
15	M	89	THR	2.7
4	A	236	GLY	2.7
8	E	124	VAL	2.7
32	I	82	GLU	2.7
11	H	139	ASN	2.7
7	D	107	GLY	2.7
1	0	1279	U	2.7
26	X	73	ARG	2.7
30	2	20	ARG	2.7
7	D	132	VAL	2.7
19	Q	18	PRO	2.7
9	F	75	ILE	2.7
18	P	141	ILE	2.7
7	D	91	ALA	2.7
14	L	149	ARG	2.7
1	0	283	U	2.7
7	D	173	GLU	2.7
1	0	372	A	2.7
5	B	105	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	0	1208	C	2.6
27	Y	98	GLN	2.6
5	B	109	LEU	2.6
9	F	45	ALA	2.6
10	G	28	GLU	2.6
9	F	111	ILE	2.6
5	B	117	GLU	2.6
7	D	38	GLU	2.6
8	E	44	GLY	2.6
8	E	162	PHE	2.6
12	J	5	GLU	2.6
28	Z	13	ARG	2.6
8	E	99	GLY	2.6
1	0	279	C	2.6
27	Y	187	VAL	2.6
27	Y	193	LEU	2.6
1	0	736	A	2.6
7	D	12	GLU	2.6
5	B	1	PRO	2.6
28	Z	27	ALA	2.6
8	E	126	ILE	2.6
1	0	1181	A	2.6
6	C	246	ARG	2.6
16	N	92	ALA	2.6
16	N	149	GLU	2.5
4	A	64	ASP	2.5
8	E	123	ASP	2.5
4	A	65	ARG	2.5
1	0	1625	U	2.5
1	0	358	G	2.5
4	A	59	GLU	2.5
9	F	29	VAL	2.5
31	3	22	VAL	2.5
11	H	34	GLY	2.5
1	0	1967	U	2.5
10	G	15	TRP	2.5
1	0	370	G	2.5
11	H	67	LEU	2.5
7	D	70	GLY	2.5
5	B	134	ALA	2.5
5	B	119	HIS	2.5
10	G	12	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
11	H	47	ILE	2.5
22	T	59	GLU	2.5
8	E	105	GLU	2.5
16	N	177	GLU	2.5
7	D	50	VAL	2.5
11	H	24	PRO	2.5
16	N	37	ARG	2.5
7	D	43	GLU	2.5
15	M	164	THR	2.5
20	R	150	PRO	2.5
20	R	96	VAL	2.5
1	0	369	G	2.5
6	C	135	GLU	2.5
9	F	24	ARG	2.5
1	0	1189	A	2.4
16	N	73	ALA	2.4
9	F	37	THR	2.4
11	H	140	VAL	2.4
1	0	295	C	2.4
7	D	95	THR	2.4
8	E	129	GLU	2.4
19	Q	92	ARG	2.4
7	D	128	LEU	2.4
8	E	169	THR	2.4
28	Z	44	GLU	2.4
9	F	23	ALA	2.4
16	N	145	ALA	2.4
1	0	1192	A	2.4
5	B	33	ASP	2.4
9	F	115	VAL	2.4
22	T	36	GLY	2.4
32	I	90	GLY	2.4
4	A	206	ARG	2.4
10	G	63	ARG	2.4
1	0	441	A	2.4
17	O	98	LEU	2.4
19	Q	84	ILE	2.4
22	T	77	VAL	2.4
1	0	1196	C	2.4
1	0	716	G	2.4
16	N	182	GLY	2.3
8	E	48	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
22	T	13	ARG	2.3
23	U	52	THR	2.3
16	N	170	GLU	2.3
1	0	1947	G	2.3
7	D	86	THR	2.3
8	E	46	THR	2.3
11	H	66	ARG	2.3
6	C	237	GLU	2.3
22	T	103	LEU	2.3
19	Q	17	LYS	2.3
24	V	33	VAL	2.3
9	F	47	LEU	2.3
21	S	2	TRP	2.3
1	0	1981	A	2.3
1	0	2345	A	2.3
4	A	135	VAL	2.3
5	B	115	VAL	2.3
5	B	186	GLY	2.3
1	0	1164	U	2.3
1	0	1180	U	2.3
26	X	41	PHE	2.3
4	A	128	LEU	2.3
28	Z	35	GLU	2.3
17	O	23	GLY	2.2
7	D	71	ALA	2.2
11	H	50	ILE	2.2
1	0	129	A	2.2
9	F	70	LYS	2.2
1	0	1184	C	2.2
22	T	109	GLU	2.2
32	I	140	GLU	2.2
11	H	162	ARG	2.2
9	F	20	LEU	2.2
32	I	84	GLY	2.2
1	0	1203	G	2.2
5	B	133	GLU	2.2
8	E	81	GLU	2.2
10	G	68	GLU	2.2
1	0	1174	A	2.2
31	3	26	ARG	2.2
9	F	113	ASP	2.2
9	F	26	THR	2.2

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Mol	Chain	Res	Type	RSRZ
5	B	181	ILE	2.2
26	X	12	ILE	2.2
9	F	60	VAL	2.2
20	R	104	PHE	2.2
15	M	97	ILE	2.2
7	D	163	VAL	2.2
10	G	19	GLU	2.2
14	L	147	GLU	2.2
31	3	73	GLU	2.2
16	N	81	ALA	2.2
12	J	39	VAL	2.2
14	L	96	VAL	2.2
14	L	150	GLN	2.2
9	F	103	GLU	2.2
11	H	70	ASN	2.2
14	L	59	GLU	2.2
7	D	169	THR	2.2
27	Y	106	THR	2.2
8	E	16	ASP	2.1
7	D	83	PHE	2.1
16	N	74	PRO	2.1
6	C	63	SER	2.1
11	H	142	ASP	2.1
24	V	14	ALA	2.1
30	2	30	ASP	2.1
7	D	47	GLN	2.1
2	9	3072	C	2.1
23	U	4	ARG	2.1
25	W	78	ASP	2.1
17	O	31	GLU	2.1
8	E	109	GLY	2.1
1	0	1206	U	2.1
8	E	159	VAL	2.1
8	E	161	VAL	2.1
31	3	13	HIS	2.1
8	E	39	ASP	2.1
21	S	71	ASP	2.1
24	V	9	ARG	2.1
1	0	130	C	2.1
1	0	717	C	2.1
14	L	77	ALA	2.1
11	H	23	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
14	L	144	ASP	2.1
16	N	153	GLN	2.1
7	D	45	THR	2.1
30	2	47	THR	2.1
1	0	1527	A	2.1
15	M	49	ALA	2.1
32	I	130	GLY	2.1
4	A	61	GLU	2.1
7	D	100	ASP	2.1
16	N	128	ASP	2.1
7	D	72	LYS	2.1
4	A	60	PHE	2.1
8	E	5	LEU	2.1
11	H	39	ASP	2.1
22	T	58	GLU	2.0
16	N	186	LEU	2.0
11	H	111	ASP	2.0
16	N	69	TYR	2.0
32	I	139	ILE	2.0
7	D	67	ASP	2.0
4	A	97	ALA	2.0
7	D	87	ALA	2.0
26	X	74	ALA	2.0
28	Z	38	ALA	2.0
30	2	26	MET	2.0
5	B	183	GLU	2.0
16	N	160	SER	2.0
24	V	62	GLU	2.0
31	3	23	GLU	2.0
1	0	1197	G	2.0
31	3	29	ARG	2.0
21	S	21	GLN	2.0
5	B	100	VAL	2.0
5	B	149	ASP	2.0
6	C	16	VAL	2.0
21	S	52	VAL	2.0
14	L	89	PHE	2.0
27	Y	102	LEU	2.0
1	0	361	C	2.0
1	0	1201	C	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	PSU	0	2621	20/21	0.98	0.13	-	35,39,43,44	0
3	PPU	4	76	37/38	0.98	0.12	-	38,43,49,54	0
1	UR3	0	2619	21/22	0.98	0.14	-	39,40,43,47	0
1	OMG	0	2588	24/25	0.97	0.12	-	34,37,42,43	0
1	1MA	0	628	23/24	0.98	0.15	-	35,37,40,44	0
1	OMU	0	2587	21/22	0.98	0.12	-	35,40,43,43	0

6.3 Carbohydrates ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
34	MG	0	8022	1/1	0.76	1.05	46.55	123,123,123,123	0
36	NA	0	9174	1/1	0.83	0.52	43.26	71,71,71,71	0
34	MG	0	8014	1/1	0.77	0.84	40.08	94,94,94,94	0
36	NA	0	9125	1/1	0.85	0.56	32.83	87,87,87,87	0
35	K	0	9001	1/1	0.88	0.73	32.52	92,92,92,92	0
34	MG	0	8001	1/1	0.99	0.24	22.70	19,19,19,19	0
36	NA	0	9173	1/1	0.89	0.38	18.89	69,69,69,69	0
36	NA	0	9156	1/1	0.89	0.34	18.76	59,59,59,59	0
36	NA	0	9185	1/1	0.67	0.47	15.26	62,62,62,62	0
36	NA	0	9120	1/1	0.96	0.26	15.22	61,61,61,61	0
38	SR	0	9482	1/1	0.97	0.26	12.49	122,122,122,122	0
34	MG	0	8013	1/1	0.96	0.37	12.31	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	9172	1/1	0.88	0.36	10.50	78,78,78,78	0
36	NA	0	9171	1/1	0.81	0.25	8.76	66,66,66,66	0
34	MG	0	8008	1/1	0.98	0.19	8.60	22,22,22,22	0
34	MG	0	8038	1/1	0.99	0.26	8.47	27,27,27,27	0
34	MG	0	8065	1/1	0.74	0.48	8.43	90,90,90,90	0
38	SR	B	9521	1/1	0.89	0.41	8.34	184,184,184,184	0
34	MG	0	8097	1/1	0.94	0.23	8.22	63,63,63,63	0
36	NA	0	9161	1/1	0.88	0.20	7.93	61,61,61,61	0
36	NA	0	9131	1/1	0.91	0.21	7.63	52,52,52,52	0
36	NA	0	9167	1/1	0.91	0.16	7.27	57,57,57,57	0
34	MG	0	8027	1/1	0.95	0.25	6.06	40,40,40,40	0
36	NA	0	9178	1/1	0.75	0.26	6.02	57,57,57,57	0
34	MG	0	8080	1/1	0.93	0.20	5.51	58,58,58,58	0
37	CL	B	9319	1/1	0.91	0.22	5.13	62,62,62,62	0
34	MG	0	8012	1/1	0.96	0.22	5.04	46,46,46,46	0
36	NA	0	9168	1/1	0.83	0.15	4.98	68,68,68,68	0
38	SR	0	9406	1/1	1.00	0.17	4.93	36,36,36,36	0
38	SR	0	9407	1/1	0.99	0.15	4.70	46,46,46,46	0
36	NA	0	9162	1/1	0.95	0.19	4.61	50,50,50,50	0
34	MG	0	8021	1/1	0.92	0.19	4.39	58,58,58,58	0
34	MG	0	8057	1/1	0.95	0.35	4.37	68,68,68,68	0
36	NA	0	9135	1/1	0.97	0.18	3.91	54,54,54,54	0
36	NA	0	9115	1/1	0.97	0.16	3.76	47,47,47,47	0
36	NA	0	9159	1/1	0.94	0.20	3.50	54,54,54,54	0
36	NA	0	9127	1/1	0.94	0.18	3.25	71,71,71,71	0
37	CL	0	9316	1/1	0.78	0.23	2.74	86,86,86,86	0
36	NA	R	9186	1/1	0.96	0.19	2.56	71,71,71,71	0
36	NA	0	9150	1/1	0.96	0.17	2.44	52,52,52,52	0
36	NA	0	9165	1/1	0.96	0.22	2.29	46,46,46,46	0
34	MG	0	8020	1/1	0.98	0.19	2.26	38,38,38,38	0
34	MG	0	8060	1/1	0.94	0.17	2.16	97,97,97,97	0
34	MG	0	8054	1/1	0.85	0.14	2.15	60,60,60,60	0
38	SR	0	9515	1/1	0.96	0.15	1.49	94,94,94,94	0
38	SR	H	9486	1/1	0.97	0.21	1.49	114,114,114,114	0
34	MG	0	8101	1/1	0.85	0.15	1.42	68,68,68,68	0
38	SR	0	9534	1/1	0.96	0.17	1.40	108,108,108,108	0
36	NA	0	9110	1/1	0.90	0.15	1.26	49,49,49,49	0
36	NA	0	9132	1/1	0.94	0.15	1.18	57,57,57,57	0
33	DA	4	179	21/22	0.98	0.14	1.18	44,47,51,52	0
36	NA	M	9147	1/1	0.96	0.18	1.06	45,45,45,45	0
34	MG	0	8074	1/1	0.96	0.20	0.90	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	9182	1/1	0.83	0.14	0.63	81,81,81,81	0
34	MG	0	8056	1/1	0.98	0.18	0.61	47,47,47,47	0
33	C	4	181	17/21	0.96	0.11	0.57	51,53,55,56	0
34	MG	0	8017	1/1	0.98	0.12	0.47	30,30,30,30	0
37	CL	M	9318	1/1	0.99	0.18	0.44	43,43,43,43	0
34	MG	0	8107	1/1	0.82	0.16	0.41	67,67,67,67	0
38	SR	0	9475	1/1	0.95	0.12	0.09	84,84,84,84	0
38	SR	L	9409	1/1	1.00	0.13	-0.01	44,44,44,44	0
36	NA	0	9124	1/1	0.94	0.12	-0.24	54,54,54,54	0
39	CD	Z	9203	1/1	0.48	0.19	-0.25	93,93,93,93	0
34	MG	0	8004	1/1	0.99	0.11	-0.28	36,36,36,36	0
36	NA	9	9183	1/1	0.87	0.14	-0.29	80,80,80,80	0
38	SR	F	9595	1/1	0.96	0.15	-0.40	104,104,104,104	0
38	SR	0	9451	1/1	1.00	0.11	-0.47	60,60,60,60	0
36	NA	0	9114	1/1	0.97	0.13	-0.47	46,46,46,46	0
37	CL	J	9321	1/1	0.95	0.13	-0.52	68,68,68,68	0
35	K	0	9002	1/1	0.88	0.12	-0.52	90,90,90,90	0
38	SR	1	9419	1/1	0.99	0.11	-0.60	42,42,42,42	0
34	MG	0	8096	1/1	0.94	0.12	-0.62	51,51,51,51	0
36	NA	R	9138	1/1	0.96	0.11	-0.68	76,76,76,76	0
38	SR	0	9504	1/1	0.87	0.12	-0.72	107,107,107,107	0
34	MG	0	8003	1/1	0.98	0.16	-0.75	38,38,38,38	0
34	MG	A	8066	1/1	0.96	0.13	-0.78	53,53,53,53	0
37	CL	0	9315	1/1	0.95	0.11	-0.82	59,59,59,59	0
36	NA	J	9146	1/1	0.94	0.12	-0.87	58,58,58,58	0
38	SR	0	9509	1/1	0.97	0.12	-0.91	91,91,91,91	0
36	NA	0	9139	1/1	0.96	0.08	-0.99	50,50,50,50	0
33	C	4	180	20/21	0.98	0.10	-1.10	47,50,51,52	0
36	NA	0	9117	1/1	0.97	0.12	-1.16	44,44,44,44	0
36	NA	R	9137	1/1	0.89	0.11	-1.23	43,43,43,43	0
39	CD	U	9201	1/1	0.99	0.09	-1.27	60,60,60,60	0
36	NA	C	9104	1/1	0.93	0.11	-1.30	33,33,33,33	0
38	SR	0	9590	1/1	0.94	0.10	-1.32	98,98,98,98	0
38	SR	0	9457	1/1	0.99	0.10	-1.33	54,54,54,54	0
36	NA	Q	9148	1/1	0.95	0.12	-1.35	48,48,48,48	0
38	SR	0	9545	1/1	0.99	0.05	-1.46	79,79,79,79	0
38	SR	0	9490	1/1	0.98	0.09	-1.50	108,108,108,108	0
37	CL	0	9312	1/1	0.99	0.09	-1.56	60,60,60,60	0
34	MG	T	8073	1/1	0.93	0.12	-1.60	52,52,52,52	0
36	NA	0	9166	1/1	0.96	0.08	-1.62	68,68,68,68	0
34	MG	Y	8109	1/1	0.94	0.12	-1.65	47,47,47,47	0
37	CL	O	9308	1/1	0.98	0.08	-1.67	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	MG	0	8015	1/1	0.95	0.10	-1.79	33,33,33,33	0
39	CD	3	9204	1/1	0.99	0.05	-1.80	63,63,63,63	0
38	SR	0	9450	1/1	0.98	0.07	-1.81	76,76,76,76	0
34	MG	0	8002	1/1	0.95	0.10	-1.97	37,37,37,37	0
38	SR	0	9424	1/1	1.00	0.14	-2.11	47,47,47,47	0
38	SR	A	9436	1/1	0.99	0.07	-2.13	57,57,57,57	0
36	NA	0	9143	1/1	0.98	0.08	-2.28	46,46,46,46	0
38	SR	3	9439	1/1	0.99	0.03	-2.33	74,74,74,74	0
34	MG	0	8067	1/1	0.96	0.10	-2.51	44,44,44,44	0
36	NA	0	9105	1/1	0.98	0.10	-2.54	45,45,45,45	0
39	CD	1	9202	1/1	1.00	0.05	-2.60	55,55,55,55	0
34	MG	0	8032	1/1	0.78	0.10	-2.61	47,47,47,47	0
38	SR	0	9456	1/1	0.99	0.09	-2.69	64,64,64,64	0
34	MG	0	8039	1/1	0.93	0.09	-2.71	66,66,66,66	0
38	SR	0	9428	1/1	1.00	0.07	-2.72	55,55,55,55	0
34	MG	0	8112	1/1	0.99	0.07	-2.74	43,43,43,43	0
38	SR	0	9455	1/1	0.97	0.07	-2.85	77,77,77,77	0
38	SR	0	9483	1/1	0.98	0.07	-2.86	80,80,80,80	0
34	MG	0	8044	1/1	0.98	0.06	-2.87	44,44,44,44	0
37	CL	3	9304	1/1	0.99	0.10	-3.14	65,65,65,65	0
38	SR	0	9416	1/1	0.99	0.10	-3.15	47,47,47,47	0
38	SR	0	9444	1/1	1.00	0.09	-3.17	56,56,56,56	0
38	SR	0	9468	1/1	0.95	0.03	-3.41	120,120,120,120	0
38	SR	0	9532	1/1	0.93	0.05	-3.59	127,127,127,127	0
34	MG	0	8110	1/1	0.99	0.10	-3.74	46,46,46,46	0
38	SR	0	9442	1/1	0.97	0.11	-3.94	65,65,65,65	0
38	SR	0	9498	1/1	0.99	0.05	-4.04	66,66,66,66	0
37	CL	0	9305	1/1	0.98	0.07	-4.20	58,58,58,58	0
38	SR	0	9453	1/1	0.99	0.07	-4.29	71,71,71,71	0
38	SR	0	9410	1/1	0.99	0.12	-4.66	41,41,41,41	0
38	SR	0	9506	1/1	0.99	0.04	-4.66	71,71,71,71	0
36	NA	0	9123	1/1	0.98	0.09	-5.74	42,42,42,42	0
34	MG	0	8091	1/1	0.78	0.08	-6.14	58,58,58,58	0
34	MG	0	8019	1/1	0.96	0.05	-6.27	51,51,51,51	0
38	SR	0	9473	1/1	0.97	0.02	-12.35	79,79,79,79	0
38	SR	0	9601	1/1	0.99	0.04	-	95,95,95,95	0
34	MG	0	8024	1/1	0.90	0.42	-	76,76,76,76	0
36	NA	9	9151	1/1	0.71	0.23	-	83,83,83,83	0
36	NA	0	9118	1/1	0.88	0.31	-	71,71,71,71	0
34	MG	0	8063	1/1	0.89	0.11	-	67,67,67,67	0
39	CD	O	9205	1/1	0.90	0.04	-	138,138,138,138	0
37	CL	0	9303	1/1	0.99	0.10	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
38	SR	0	9522	1/1	0.96	0.07	-	118,118,118,118	0
38	SR	0	9426	1/1	0.98	0.08	-	72,72,72,72	0
36	NA	0	9106	1/1	0.97	0.39	-	44,44,44,44	0
38	SR	0	9539	1/1	0.93	0.50	-	162,162,162,162	0
34	MG	0	8090	1/1	0.89	0.18	-	67,67,67,67	0
38	SR	0	9469	1/1	0.97	0.03	-	91,91,91,91	0
36	NA	0	9163	1/1	0.83	0.18	-	65,65,65,65	0
34	MG	0	8102	1/1	0.44	0.16	-	76,76,76,76	0
36	NA	0	9149	1/1	0.91	0.21	-	52,52,52,52	0
34	MG	0	8094	1/1	0.50	0.70	-	93,93,93,93	0
38	SR	0	9462	1/1	0.99	0.12	-	73,73,73,73	0
36	NA	0	9140	1/1	0.80	0.55	-	67,67,67,67	0
36	NA	0	9116	1/1	0.95	0.44	-	55,55,55,55	0
36	NA	0	9184	1/1	0.55	0.22	-	83,83,83,83	0
37	CL	L	9310	1/1	0.97	0.09	-	58,58,58,58	0
36	NA	0	9179	1/1	0.70	1.23	-	96,96,96,96	0
38	SR	9	9481	1/1	1.00	0.07	-	88,88,88,88	0
34	MG	0	8031	1/1	0.97	0.10	-	55,55,55,55	0
38	SR	0	9411	1/1	0.99	0.18	-	46,46,46,46	0
34	MG	0	8088	1/1	0.95	0.08	-	39,39,39,39	0
37	CL	0	9322	1/1	0.93	0.20	-	58,58,58,58	0
34	MG	0	8028	1/1	0.96	0.12	-	37,37,37,37	0
34	MG	0	8118	1/1	0.98	0.15	-	30,30,30,30	0
36	NA	0	9158	1/1	0.84	0.24	-	62,62,62,62	0
38	SR	0	9566	1/1	0.97	0.07	-	80,80,80,80	0
34	MG	0	8030	1/1	0.97	0.05	-	37,37,37,37	0
38	SR	0	9448	1/1	0.99	0.06	-	63,63,63,63	0
38	SR	0	9560	1/1	0.95	0.07	-	98,98,98,98	0
38	SR	0	9454	1/1	0.99	0.07	-	83,83,83,83	0
37	CL	A	9309	1/1	0.96	0.11	-	60,60,60,60	0
36	NA	0	9129	1/1	0.30	0.31	-	82,82,82,82	0
38	SR	0	9488	1/1	0.98	0.12	-	84,84,84,84	0
34	MG	0	8079	1/1	0.91	0.14	-	33,33,33,33	0
38	SR	1	9460	1/1	0.99	0.11	-	53,53,53,53	0
34	MG	B	8055	1/1	0.91	0.27	-	94,94,94,94	0
34	MG	0	8072	1/1	0.79	0.33	-	78,78,78,78	0
38	SR	S	9470	1/1	0.98	0.13	-	99,99,99,99	0
38	SR	A	9497	1/1	0.99	0.10	-	91,91,91,91	0
38	SR	0	9415	1/1	0.99	0.11	-	58,58,58,58	0
36	NA	3	9169	1/1	0.89	0.40	-	98,98,98,98	0
38	SR	0	9408	1/1	1.00	0.16	-	41,41,41,41	0
36	NA	0	9128	1/1	0.95	0.08	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	MG	0	8075	1/1	0.93	0.05	-	41,41,41,41	0
36	NA	0	9108	1/1	0.98	0.15	-	35,35,35,35	0
38	SR	0	9441	1/1	0.99	0.07	-	68,68,68,68	0
38	SR	0	9432	1/1	0.99	0.13	-	67,67,67,67	0
36	NA	0	9113	1/1	0.91	0.11	-	74,74,74,74	0
36	NA	0	9154	1/1	0.92	0.27	-	57,57,57,57	0
34	MG	0	8043	1/1	0.93	0.06	-	57,57,57,57	0
34	MG	0	8070	1/1	0.98	0.16	-	28,28,28,28	0
36	NA	H	9122	1/1	0.81	0.18	-	78,78,78,78	0
38	SR	0	9440	1/1	0.99	0.04	-	73,73,73,73	0
34	MG	0	8099	1/1	0.84	0.19	-	74,74,74,74	0
34	MG	0	8061	1/1	0.97	0.12	-	81,81,81,81	0
38	SR	0	9412	1/1	0.99	0.12	-	46,46,46,46	0
34	MG	0	8009	1/1	0.99	0.13	-	26,26,26,26	0
38	SR	0	9629	1/1	0.97	0.08	-	77,77,77,77	0
38	SR	0	9465	1/1	0.96	0.09	-	101,101,101,101	0
38	SR	0	9423	1/1	0.99	0.09	-	58,58,58,58	0
34	MG	0	8052	1/1	0.76	0.40	-	87,87,87,87	0
34	MG	9	8095	1/1	0.91	0.26	-	61,61,61,61	0
34	MG	0	8115	1/1	0.92	0.17	-	61,61,61,61	0
38	SR	0	9435	1/1	0.98	0.08	-	75,75,75,75	0
36	NA	0	9107	1/1	0.89	0.26	-	59,59,59,59	0
34	MG	0	8084	1/1	0.83	0.33	-	84,84,84,84	0
34	MG	0	8082	1/1	0.92	0.41	-	89,89,89,89	0
38	SR	0	9466	1/1	0.98	0.04	-	101,101,101,101	0
34	MG	0	8108	1/1	0.47	0.13	-	107,107,107,107	0
34	MG	2	8076	1/1	0.94	0.20	-	64,64,64,64	0
34	MG	0	8036	1/1	0.98	0.10	-	60,60,60,60	0
33	PO2	4	178	3/3	0.98	0.13	-	41,41,42,44	0
37	CL	0	9313	1/1	0.99	0.07	-	57,57,57,57	0
37	CL	N	9307	1/1	0.95	0.14	-	65,65,65,65	0
38	SR	0	9443	1/1	0.99	0.09	-	59,59,59,59	0
34	MG	K	8069	1/1	0.98	0.19	-	26,26,26,26	0
34	MG	0	8103	1/1	0.93	0.20	-	74,74,74,74	0
36	NA	0	9101	1/1	0.99	0.17	-	50,50,50,50	0
34	MG	0	8045	1/1	0.90	0.33	-	82,82,82,82	0
34	MG	0	8040	1/1	0.79	0.44	-	100,100,100,100	0
38	SR	0	9474	1/1	0.99	0.11	-	61,61,61,61	0
36	NA	0	9130	1/1	0.90	0.14	-	53,53,53,53	0
38	SR	0	9422	1/1	0.99	0.12	-	59,59,59,59	0
34	MG	0	8068	1/1	0.95	0.13	-	55,55,55,55	0
36	NA	0	9175	1/1	0.91	0.19	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	CL	0	9311	1/1	0.96	0.10	-	64,64,64,64	0
38	SR	0	9585	1/1	0.96	0.10	-	94,94,94,94	0
38	SR	0	9452	1/1	0.96	0.11	-	107,107,107,107	0
34	MG	0	8047	1/1	0.17	1.14	-	111,111,111,111	0
38	SR	0	9581	1/1	0.94	0.10	-	136,136,136,136	0
38	SR	0	9430	1/1	1.00	0.10	-	50,50,50,50	0
34	MG	0	8116	1/1	0.84	0.08	-	59,59,59,59	0
38	SR	0	9420	1/1	0.98	0.15	-	73,73,73,73	0
38	SR	0	9530	1/1	0.97	0.14	-	73,73,73,73	0
38	SR	0	9413	1/1	0.99	0.12	-	50,50,50,50	0
38	SR	9	9588	1/1	0.78	0.14	-	141,141,141,141	0
38	SR	0	9447	1/1	0.98	0.11	-	69,69,69,69	0
38	SR	0	9517	1/1	0.92	0.04	-	117,117,117,117	0
38	SR	0	9478	1/1	1.00	0.06	-	76,76,76,76	0
38	SR	0	9570	1/1	0.98	0.04	-	105,105,105,105	0
38	SR	A	9437	1/1	0.97	0.12	-	73,73,73,73	0
34	MG	0	8104	1/1	0.95	0.10	-	59,59,59,59	0
34	MG	0	8029	1/1	0.98	0.31	-	37,37,37,37	0
38	SR	0	9484	1/1	0.76	0.08	-	139,139,139,139	0
34	MG	0	8025	1/1	0.98	0.40	-	33,33,33,33	0
34	MG	0	8042	1/1	0.76	0.09	-	58,58,58,58	0
38	SR	0	9626	1/1	0.88	0.39	-	147,147,147,147	0
38	SR	0	9508	1/1	0.97	0.07	-	91,91,91,91	0
38	SR	0	9417	1/1	0.97	0.13	-	61,61,61,61	0
34	MG	0	8098	1/1	0.96	0.07	-	47,47,47,47	0
38	SR	0	9405	1/1	0.98	0.15	-	59,59,59,59	0
34	MG	0	8059	1/1	0.73	0.39	-	71,71,71,71	0
38	SR	0	9434	1/1	0.99	0.13	-	68,68,68,68	0
38	SR	0	9467	1/1	0.92	0.10	-	91,91,91,91	0
36	NA	9	9152	1/1	0.87	0.49	-	76,76,76,76	0
34	MG	0	8005	1/1	0.99	0.11	-	34,34,34,34	0
34	MG	0	8093	1/1	0.86	0.17	-	52,52,52,52	0
34	MG	0	8058	1/1	0.95	0.56	-	92,92,92,92	0
34	MG	0	8114	1/1	0.86	0.40	-	79,79,79,79	0
37	CL	0	9314	1/1	0.97	0.09	-	55,55,55,55	0
38	SR	0	9449	1/1	0.98	0.07	-	66,66,66,66	0
34	MG	0	8085	1/1	0.94	0.32	-	68,68,68,68	0
38	SR	0	9429	1/1	0.97	0.11	-	71,71,71,71	0
36	NA	S	9112	1/1	0.73	0.30	-	85,85,85,85	0
38	SR	0	9431	1/1	0.98	0.15	-	66,66,66,66	0
34	MG	0	8089	1/1	0.81	0.23	-	64,64,64,64	0
38	SR	0	9537	1/1	0.12	0.21	-	159,159,159,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
38	SR	0	9480	1/1	0.99	0.05	-	95,95,95,95	0
36	NA	0	9141	1/1	0.94	0.09	-	64,64,64,64	0
38	SR	0	9461	1/1	0.99	0.04	-	80,80,80,80	0
38	SR	0	9489	1/1	0.96	0.08	-	92,92,92,92	0
36	NA	0	9136	1/1	0.97	0.14	-	38,38,38,38	0
34	MG	0	8050	1/1	0.72	0.18	-	86,86,86,86	0
38	SR	0	9477	1/1	0.97	0.07	-	83,83,83,83	0
36	NA	0	9134	1/1	0.95	0.06	-	52,52,52,52	0
38	SR	0	9433	1/1	0.98	0.13	-	75,75,75,75	0
38	SR	0	9547	1/1	0.38	0.28	-	184,184,184,184	0
36	NA	0	9160	1/1	0.95	0.16	-	45,45,45,45	0
36	NA	0	9102	1/1	0.82	0.24	-	64,64,64,64	0
34	MG	0	8026	1/1	0.98	0.18	-	35,35,35,35	0
38	SR	0	9505	1/1	0.95	0.08	-	91,91,91,91	0
36	NA	0	9177	1/1	0.93	0.35	-	78,78,78,78	0
38	SR	0	9427	1/1	0.98	0.13	-	58,58,58,58	0
38	SR	0	9529	1/1	0.92	0.09	-	120,120,120,120	0
34	MG	0	8051	1/1	0.91	0.29	-	33,33,33,33	0
34	MG	0	8092	1/1	0.84	0.49	-	79,79,79,79	0
38	SR	0	9446	1/1	0.98	0.10	-	93,93,93,93	0
37	CL	Y	9320	1/1	0.97	0.10	-	49,49,49,49	0
37	CL	J	9302	1/1	0.95	0.08	-	63,63,63,63	0
34	MG	0	8083	1/1	0.94	0.08	-	59,59,59,59	0
37	CL	0	9317	1/1	0.96	0.07	-	57,57,57,57	0
37	CL	R	9306	1/1	0.99	0.07	-	48,48,48,48	0
36	NA	0	9170	1/1	0.84	0.38	-	87,87,87,87	0
38	SR	0	9421	1/1	1.00	0.11	-	74,74,74,74	0
38	SR	0	9438	1/1	0.99	0.10	-	68,68,68,68	0
38	SR	0	9568	1/1	0.98	0.07	-	77,77,77,77	0
34	MG	0	8113	1/1	0.87	0.13	-	49,49,49,49	0
37	CL	J	9301	1/1	0.96	0.10	-	59,59,59,59	0
38	SR	0	9501	1/1	0.99	0.11	-	76,76,76,76	0
36	NA	0	9157	1/1	0.86	0.17	-	52,52,52,52	0
38	SR	B	9458	1/1	0.98	0.08	-	83,83,83,83	0
34	MG	0	8041	1/1	0.85	0.12	-	56,56,56,56	0
36	NA	0	9155	1/1	0.92	0.30	-	62,62,62,62	0
38	SR	0	9425	1/1	0.99	0.12	-	59,59,59,59	0
38	SR	0	9464	1/1	0.97	0.05	-	83,83,83,83	0
38	SR	0	9500	1/1	0.79	1.26	-	200,200,200,200	0
34	MG	0	8046	1/1	0.90	0.10	-	47,47,47,47	0
38	SR	9	9503	1/1	0.96	0.04	-	116,116,116,116	0
36	NA	0	9126	1/1	0.91	0.11	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
38	SR	0	9445	1/1	0.99	0.10	-	59,59,59,59	0
38	SR	0	9414	1/1	0.98	0.11	-	58,58,58,58	0
38	SR	R	9418	1/1	0.99	0.14	-	59,59,59,59	0
36	NA	0	9181	1/1	0.94	0.20	-	55,55,55,55	0
38	SR	0	9459	1/1	0.91	0.07	-	107,107,107,107	0
34	MG	0	8117	1/1	0.89	0.15	-	48,48,48,48	0
38	SR	0	9495	1/1	0.98	0.10	-	102,102,102,102	0
36	NA	0	9164	1/1	0.85	0.34	-	62,62,62,62	0
34	MG	0	8106	1/1	0.93	0.09	-	50,50,50,50	0
34	MG	0	8037	1/1	0.98	0.07	-	42,42,42,42	0
36	NA	0	9111	1/1	0.67	0.26	-	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.