



# Full wwPDB X-ray Structure Validation Report

May 8, 2014 – 03:22 AM EDT

PDB ID : 3CC7  
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation C2487U  
Authors : Blaha, G.; Gurel, G.  
Deposited on : 2008-02-25  
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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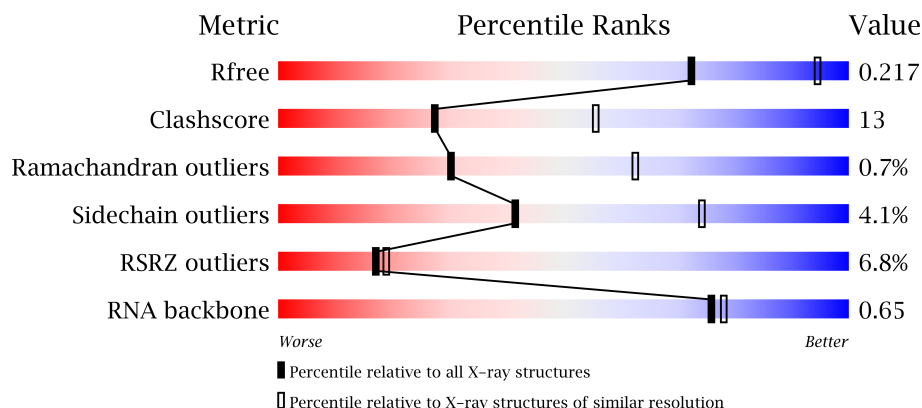
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)
RNA backbone	1838	1042 (3.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	240	
2	B	338	
3	C	246	
4	D	177	
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	

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Mol	Chain	Length	Quality of chain
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	
30	0	2923	
31	9	122	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8001	-	X
32	MG	0	8009	-	X
32	MG	0	8017	-	X
32	MG	0	8018	-	X
32	MG	0	8024	-	X
32	MG	0	8030	-	X
32	MG	0	8031	-	X
32	MG	0	8037	-	X
32	MG	0	8039	-	X
32	MG	0	8040	-	X
32	MG	0	8041	-	X
32	MG	0	8047	-	X
32	MG	0	8049	-	X
32	MG	0	8061	-	X
32	MG	0	8062	-	X
32	MG	0	8063	-	X
32	MG	0	8069	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8071	-	X
32	MG	0	8078	-	X
32	MG	0	8079	-	X
32	MG	0	8081	-	X
32	MG	0	8083	-	X
32	MG	0	8090	-	X
32	MG	A	8051	-	X
33	K	0	8401	-	X
34	NA	0	8502	-	X
34	NA	0	8505	-	X
34	NA	0	8506	-	X
34	NA	0	8511	-	X
34	NA	0	8512	-	X
34	NA	0	8513	-	X
34	NA	0	8514	-	X
34	NA	0	8517	-	X
34	NA	0	8519	-	X
34	NA	0	8521	-	X
34	NA	0	8522	-	X
34	NA	0	8524	-	X
34	NA	0	8525	-	X
34	NA	0	8526	-	X
34	NA	0	8527	-	X
34	NA	0	8535	-	X
34	NA	0	8541	-	X
34	NA	0	8542	-	X
34	NA	0	8544	-	X
34	NA	0	8545	-	X
34	NA	0	8546	-	X
34	NA	0	8547	-	X
34	NA	0	8548	-	X
34	NA	0	8549	-	X
34	NA	0	8550	-	X
34	NA	0	8551	-	X
34	NA	0	8552	-	X
34	NA	0	8553	-	X
34	NA	0	8554	-	X
34	NA	0	8555	-	X
34	NA	0	8556	-	X
34	NA	0	8558	-	X
34	NA	0	8559	-	X
34	NA	0	8560	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	NA	0	8561	-	X
34	NA	0	8562	-	X
34	NA	0	8563	-	X
34	NA	0	8564	-	X
34	NA	0	8565	-	X
34	NA	0	8566	-	X
34	NA	0	8567	-	X
34	NA	0	8568	-	X
34	NA	0	8569	-	X
34	NA	0	8571	-	X
34	NA	0	8574	-	X
34	NA	9	8572	-	X
34	NA	R	8575	-	X
35	CL	0	8822	-	X
36	SR	0	8905	-	X
36	SR	0	8906	-	X
36	SR	0	8907	-	X
36	SR	0	8914	-	X
36	SR	0	8919	-	X
36	SR	0	8922	-	X
36	SR	0	8934	-	X
36	SR	0	8947	-	X
36	SR	0	8955	-	X
36	SR	0	8959	-	X
36	SR	0	8962	-	X
36	SR	0	8974	-	X
36	SR	0	8976	-	X
36	SR	0	8979	-	X
36	SR	0	8982	-	X
36	SR	0	8985	-	X
36	SR	0	8989	-	X
36	SR	0	8991	-	X
36	SR	0	8992	-	X
36	SR	0	8994	-	X
36	SR	0	8996	-	X
36	SR	0	8997	-	X
36	SR	0	8998	-	X
36	SR	0	9004	-	X
36	SR	0	9006	-	X
36	SR	0	9007	-	X
36	SR	9	8980	-	X
36	SR	B	8987	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	SR	J	8986	-	X

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99122 atoms, of which 0 are hydrogen and 0 are deuterium.

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 protein called 50S ribosomal protein L2P.

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

- Molecule 2 is a protein called 50S ribosomal protein L3P.

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

- Molecule 3 is a protein called 50S ribosomal protein L4P.

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

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

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

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

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

- Molecule 9 is a protein called 50S ribosomal protein L11P.

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

- Molecule 10 is a protein called 50S ribosomal protein L13P.

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

- Molecule 11 is a protein called 50S ribosomal protein L14P.

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

- Molecule 12 is a protein called 50S ribosomal protein L15P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15e.

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

- Molecule 14 is a protein called 50S ribosomal protein L18P.



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

- Molecule 15 is a protein called 50S ribosomal protein L18e.

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

- Molecule 16 is a protein called 50S ribosomal protein L19e.

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

- Molecule 17 is a protein called 50S ribosomal protein L21e.

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

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

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

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59020	26349	10872	19054	2745			

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	85	Total	Mg	0	0
			85	85		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	2	Total	Mg	0	0
			2	2		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	2	Total K 2 2	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	66	Total Na 66 66	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	R	2	Total Na 2 2	0	0
34	9	2	Total Na 2 2	0	0
34	S	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0
35	L	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	93	Total 93	Sr 93	0	0
36	J	1	Total 1	Sr 1	0	0
36	1	2	Total 2	Sr 2	0	0
36	B	2	Total 2	Sr 2	0	0
36	3	2	Total 2	Sr 2	0	0
36	A	3	Total 3	Sr 3	0	0
36	R	1	Total 1	Sr 1	0	0
36	9	2	Total 2	Sr 2	0	0
36	S	1	Total 1	Sr 1	0	0
36	F	1	Total 1	Sr 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5951	Total O 5951 5951	0	0
38	A	111	Total O 111 111	0	0
38	B	153	Total O 153 153	0	0
38	C	165	Total O 165 165	0	0
38	D	46	Total O 46 46	0	0
38	E	44	Total O 44 44	0	0
38	F	23	Total O 23 23	0	0
38	G	19	Total O 19 19	0	0
38	H	71	Total O 71 71	0	0
38	I	10	Total O 10 10	0	0
38	J	54	Total O 54 54	0	0
38	K	56	Total O 56 56	0	0
38	L	80	Total O 80 80	0	0
38	M	130	Total O 130 130	0	0
38	N	59	Total O 59 59	0	0
38	O	41	Total O 41 41	0	0
38	P	61	Total O 61 61	0	0
38	Q	51	Total O 51 51	0	0
38	R	78	Total O 78 78	0	0
38	S	33	Total O 33 33	0	0
38	T	37	Total O 37 37	0	0

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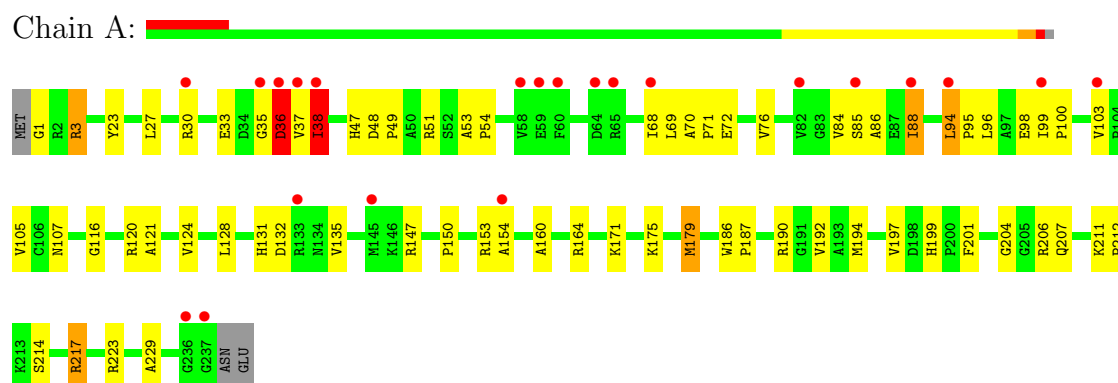
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	U	25	Total 25	O 25	0	0
38	V	11	Total 11	O 11	0	0
38	W	63	Total 63	O 63	0	0
38	X	28	Total 28	O 28	0	0
38	Y	91	Total 91	O 91	0	0
38	Z	28	Total 28	O 28	0	0
38	1	52	Total 52	O 52	0	0
38	2	37	Total 37	O 37	0	0
38	3	68	Total 68	O 68	0	0
38	9	147	Total 147	O 147	0	0

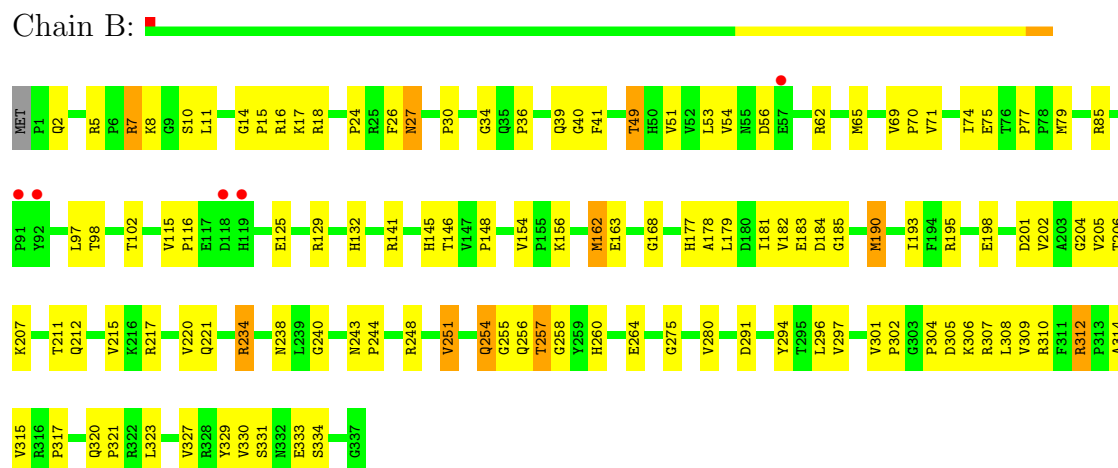
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

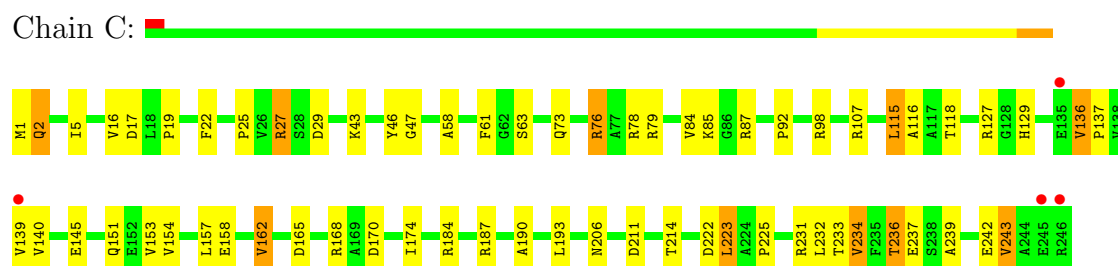
#### • Molecule 1: 50S ribosomal protein L2P



#### • Molecule 2: 50S ribosomal protein L3P



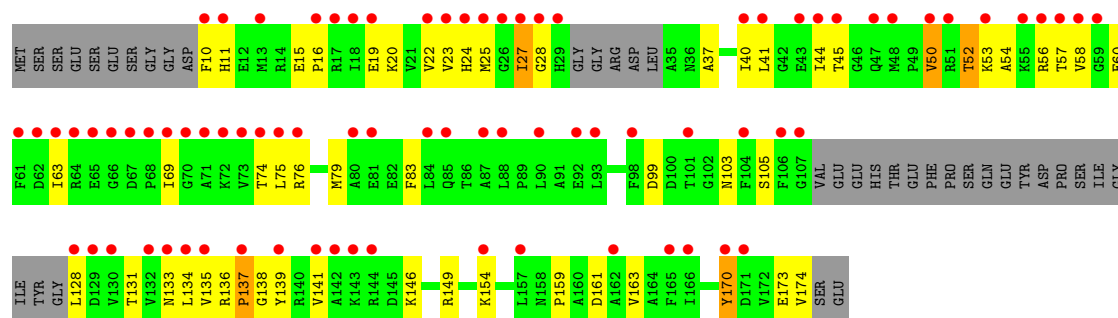
#### • Molecule 3: 50S ribosomal protein L4P





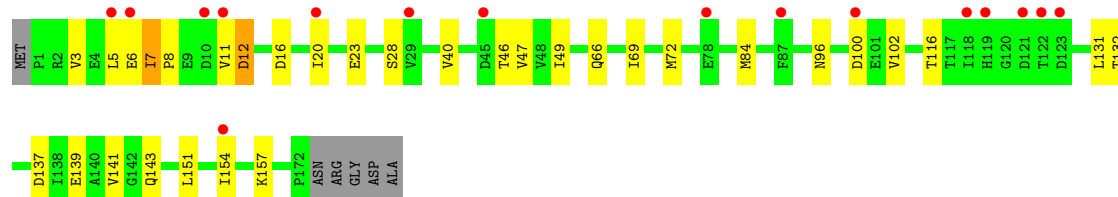
- Molecule 4: 50S ribosomal protein L5P

Chain D:



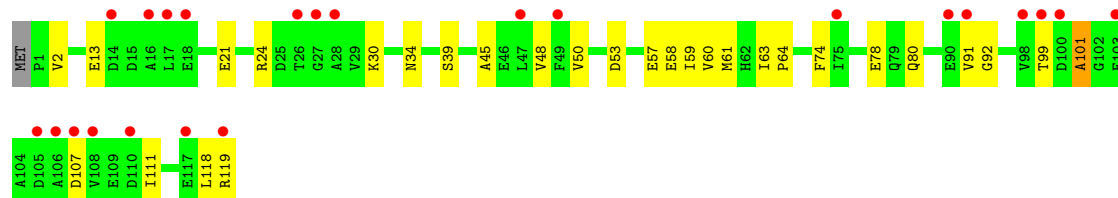
- Molecule 5: 50S ribosomal protein L6P

Chain E:



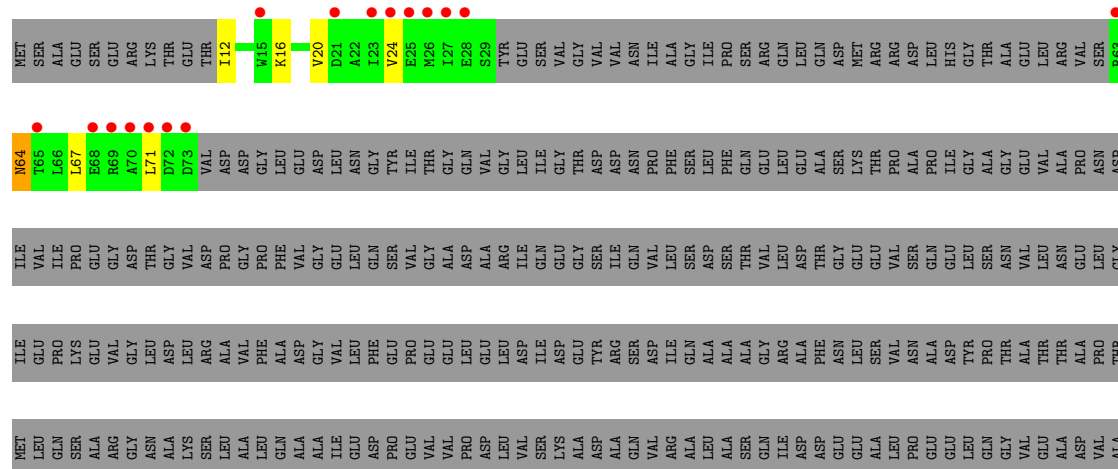
- Molecule 6: 50S ribosomal protein L7Ae

Chain F:



- Molecule 7: 50S ribosomal protein L10E

Chain G:



THR  
GLU  
GLU  
PRO  
THR  
ASP  
ASP  
GLN  
ASP  
ASP  
THR  
ALA  
SER  
GLU  
ASP  
ASP  
ALA  
ASP  
ALA  
ASP  
ALA  
ALA  
ASP  
GLU  
GLU  
ALA  
ASP  
ASP  
ASP  
ASP  
ASP  
ALA  
GLY  
ASP  
ALA  
LEU  
GLY  
MET  
PHE

- Molecule 8: 50S ribosomal protein L10e

Chain H:

MET SER ASP K4 P5 A6 P15 R19 Y22 S29 K30 I31 A32 Q33 H34 K35 K39 Q40 V43 Q49 Q59 L60 R61 H62 G63 S64 L65 E66 R69 K72 N73 R74 H75 L76 E82 Y86 X87 L90 R91 R99 K102 G103 ALA THR GLY ALA

GLY ALA ASP ARG VAL SER D114 K122 I123 R129 A139 Y140 V149 Q155 A156 Y157 V168 E169 R170 G171 E172 E173 L174 ILE ALA

- Molecule 9: 50S ribosomal protein L11P

Chain I:

MET ALA GLY THR ILE GLU VAL LEU VAL VAL PRO GLY GLY ALA ASN PRO GLY PRO PRO PRO LEU LEU PRO THR VAL ASP VAL GLN ALA VAL VAL VAL GLN ILE ASN GLN THR ALA PHE ASP GLY THR VAL PRO VAL THR VAL LYS TYR ASP ASP GLY

SER PHE GLU ILE GLU VAL G66 G67 P68 P69 T70 A71 E72 L73 I74 K75 D76 E77 A78 G79 F80 E81 T82 G83 S84 G85 E86 P87 Q88 F91 Y92 A93 D94 L95 S96 V97 D98 Q99 V100 Q101 I103 A104 E105 Q106 K107 H108 P109 D110 L111 L112 S113 Y114 D115 T117 N118 A119 A120

K121 E122 V123 V124 T125 G126 G127 T128 S129 G131 V132 T133 I134 E135 GLY ASN ARG GLU GLU PHE LYS ARG ILE ASP ALA GLY TYR ASP VAL PHE ALA ALA GLN ALA

- Molecule 10: 50S ribosomal protein L13P

Chain J:

MET SER VAL I18 M19 V36 A37 A41 E42 V45 I46 Q52 I63 Y69 F70 R74 P75 F79 T82 R93 L105 G106 N107 P108 Y109 L121 V130 T131 L132 G133 E134 S136 T144 W145

- Molecule 11: 50S ribosomal protein L14P

Chain K:

H1 V8 T9 Q10 K14 C20 R27 L29 K30 V31 I32 S33 V34 G39 N42 P45 K46 A47 G48 L49 V55 S56 M64 R65 R66 Q67 V74 R75 K78 P79 T80 R81 R87 V88 R89 Y98 E102 L109 I113 A114 A118 Q119

A125 S126 A127 A128 T129 M130 I131 V132

- Molecule 12: 50S ribosomal protein L15P

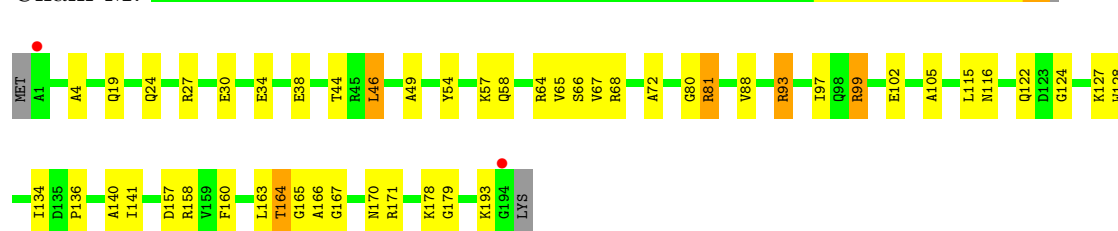
Chain L:

MET T1 K4 K5 R6 G14 H18 R35 H41 Q50 K56 V57 E60 A61 A62 R67 E71 N72 V73 T74 L75 L76 A77 A78 D79 D80 V81 A82 VAL ASP ASP ASP GLY F89 R90 V91 D95 V96 V97 E98 E99 A100 D101 D104 Y105 V106 K107

V108 V114 L118 T119 L120 I121 D122 D123 D124 F125 R130 V133 I134 G135 A136 S139 V140 E141 L142 T143 D144 L145 E147 E148 R149 Q150 ALA GLU ALA GLU THR GLU ASP VAL ASP ASP ASP ASP GLU

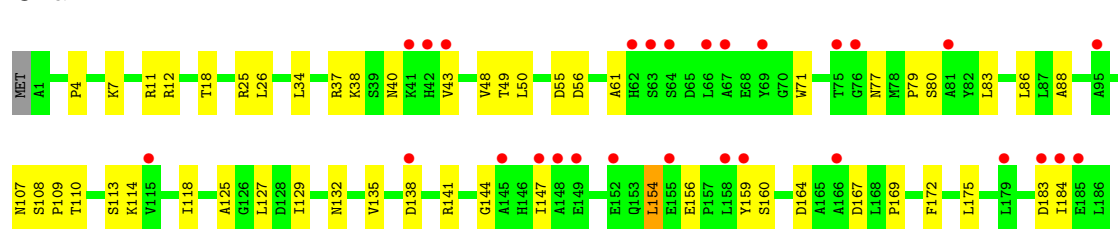
- Molecule 13: 50S ribosomal protein L15e

Chain M:



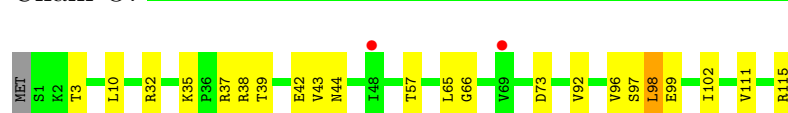
- Molecule 14: 50S ribosomal protein L18P

Chain N:



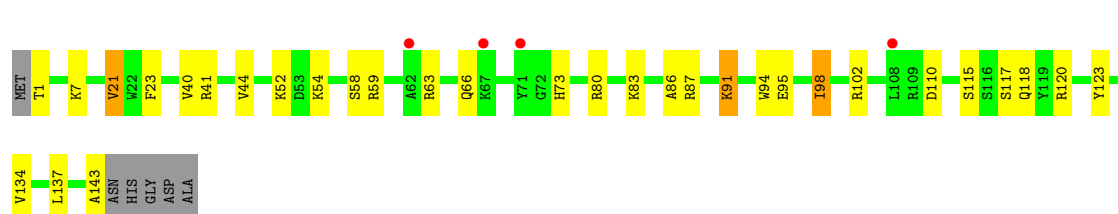
- Molecule 15: 50S ribosomal protein L18e

Chain O:



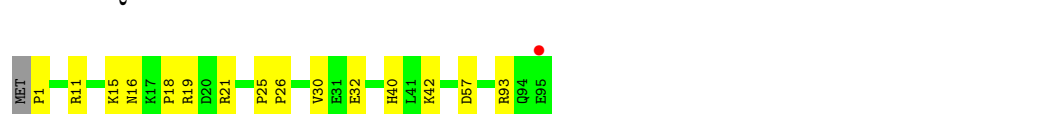
- Molecule 16: 50S ribosomal protein L19e

Chain P:



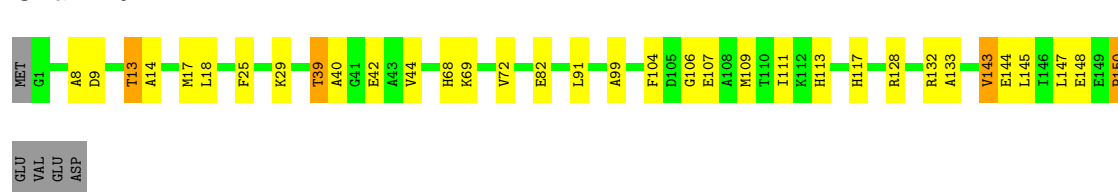
- Molecule 17: 50S ribosomal protein L21e

Chain Q:



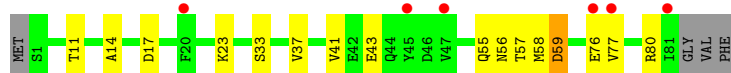
- Molecule 18: 50S ribosomal protein L22P

Chain R:



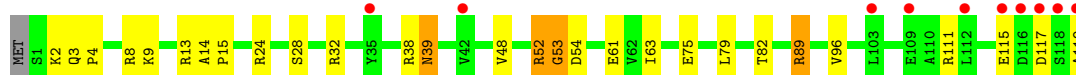
- Molecule 19: 50S ribosomal protein L23P

Chain S:



- Molecule 20: 50S ribosomal protein L24P

Chain T:



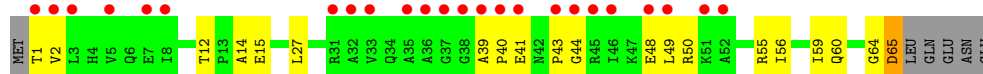
- Molecule 21: 50S ribosomal protein L24e

Chain U:



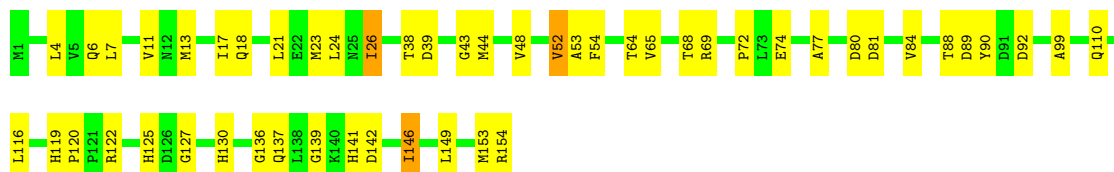
- Molecule 22: 50S ribosomal protein L29P

Chain V:



- Molecule 23: 50S ribosomal protein L30P

Chain W:



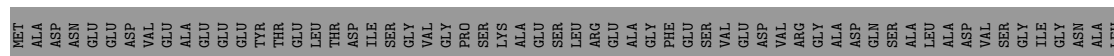
- Molecule 24: 50S ribosomal protein L31e

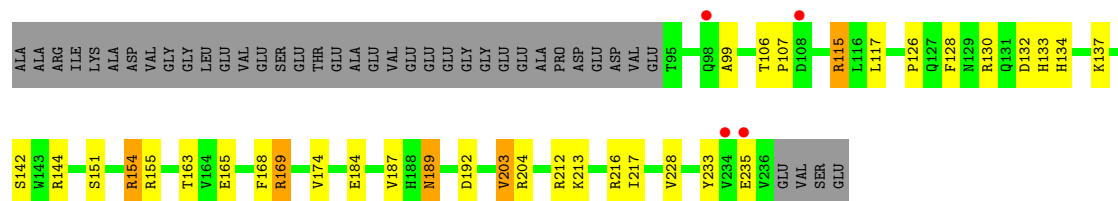
Chain X:



- Molecule 25: 50S ribosomal protein L32e

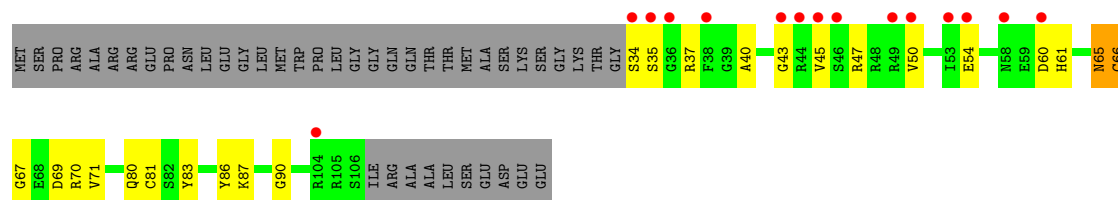
Chain Y:





- Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



- Molecule 27: 50S ribosomal protein L37e

Chain 1:



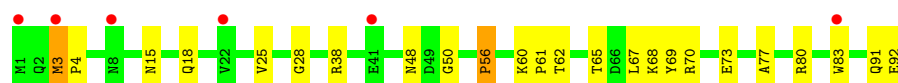
- Molecule 28: 50S ribosomal protein L39e

Chain 2:



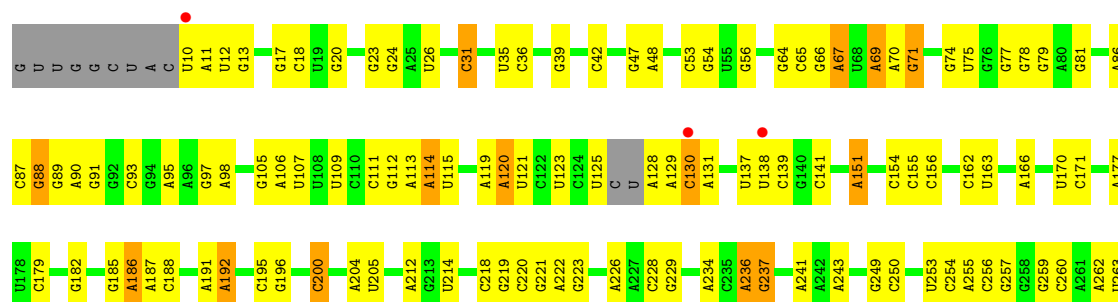
- Molecule 29: 50S ribosomal protein L44E

Chain 3:

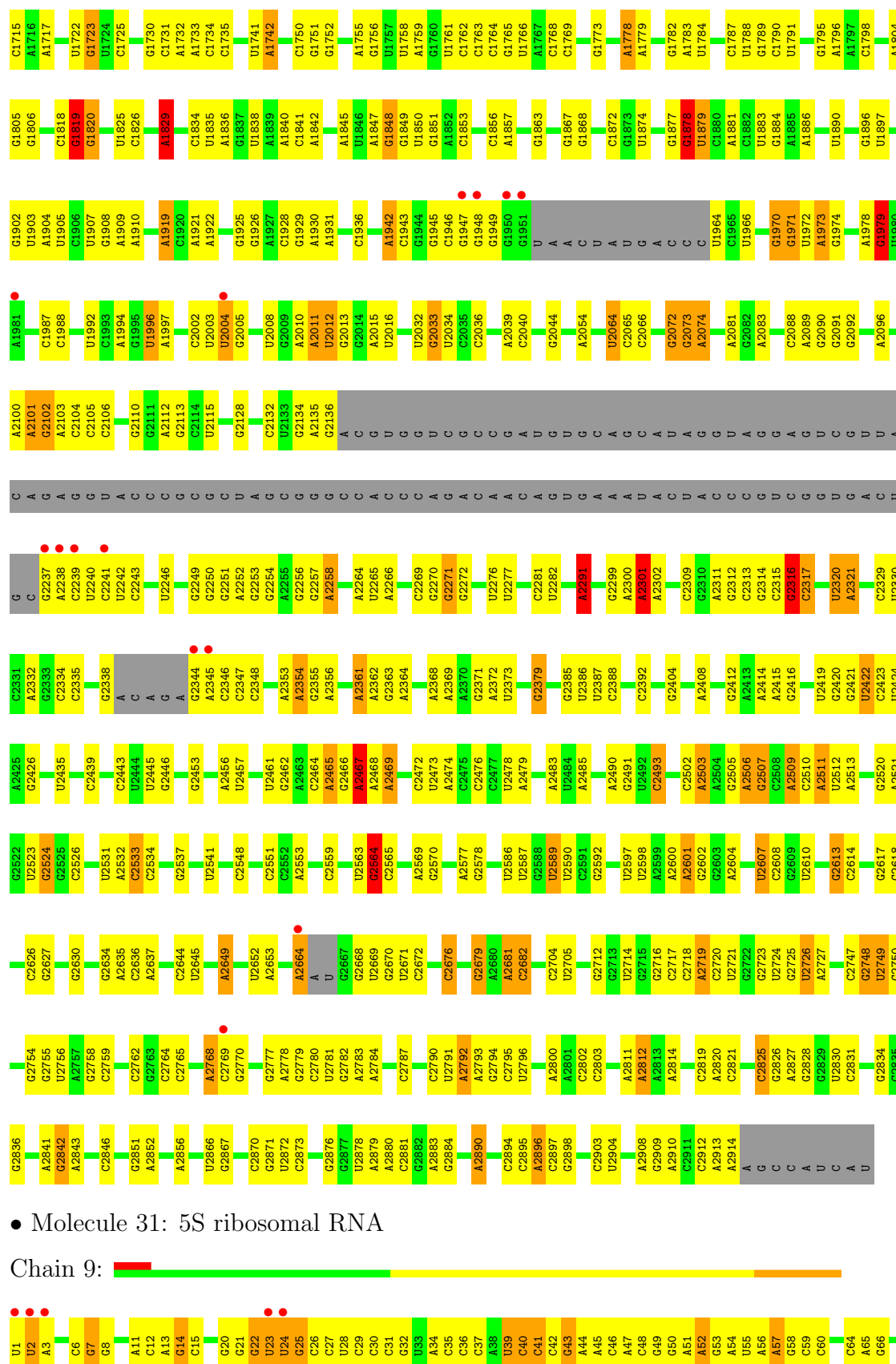


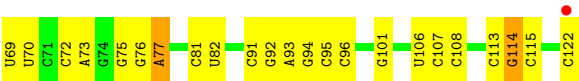
- Molecule 30: 23S ribosomal RNA

Chain 0:



C1613	G1512	A1308	G1214	G1151	C1044	A961	G869	C764	A441	G345	G264
G1614	A1515	G1311	A1215	C1156	G1045	C962	G870	G765	A442	U346	U265
A1615	G1416	G1312	G1216	C1157	G1045	C963	U872	G775	C443	A347	G269
C1617	C1517	A1313	C1229	G1158	C1051	G968	A875	U777	U445	G350	U270
U1625	G1520	A1314	A1230	G1159	G1052	G969	A876	A790	U446	G358	A271
A1626	U1419	U1311	U1234	G1160	G1053	U970	G877	A791	A447	A272	G273
A1627	G1420	A1321	G1235	A1161	G1054	G	A877	G792	C383	C378	A278
A1628	C1421	G1322	A1236	G1162	G1055	U	G878	G793	U364	C384	C279
A1629	U1524	G1323	A1237	G1163	U1056	U	A882	U794	G365	U366	C280
A1630	C1423	G1324	C1238	G1164	A1057	G	U883	G795	C367	U281	U281
A1631	U1525	A1328	G1239	G1165	A1058	C	U886	A796	C388	C282	C282
A1632	G1526	G1329	U1239	A1166	G1059	C	A886	U797	G389	U283	U283
A1633	A1527	A1330	U1242	G1167	C1060	G	A886	A797	C370	A284	A284
A1634	U1427	A1331	A1243	G1168	C1061	C	G892	U797	U371	A285	A285
A1635	U1432	C1332	C1243	U1169	G1063	C	G892	U797	A372	U286	U286
A1641	G1433	G1333	U1244	C1170	U1066	U	G898	U800	G373	G373	G373
A1642	U1434	C1334	C1245	A1171	A1067	C	G902	A806	A461	A462	A462
A1643	U1435	C1335	A1246	G1172	A1067	C	U903	A807	A466	A467	A467
A1644	C1436	U1336	U1249	A1173	G1071	G	U904	A808	A467	A468	A468
A1645	U1440	G1339	C1250	G1174	G1072	A	C905	A809	A468	A469	A469
U1654	G1441	G1340	A1251	G1175	A1073	A	C906	A812	U382	U382	U382
U1655	A1442	A1341	A1252	C1176	G1074	G	U907	C813	A383	A383	A383
A1656	G1443	C1342	C1253	G1177	G1074	G	A908	C814	G384	G384	G384
A1657	G1444	C1343	G1260	C1178	A1078	A	U908	U815	U392	U392	U392
A1658	U1445	U1343	A1261	C1179	A1079	G	A912	U816	U393	U393	U393
U1659	U1446	G1344	C1262	U1180	A1080	U	C920	U817	U394	U394	U394
U1660	G1447	G1345	C1263	A1181	A1081	C	C921	U818	U395	U395	U395
U1661	U1448	C1346	U1264	G1182	A1082	C	C922	U819	U396	U396	U396
U1662	U1449	U1347	C1265	C1183	A1083	C	C923	U820	A397	A397	A397
U1663	U1450	C1348	C1266	G1184	A1084	C	C924	U821	U398	U398	U398
U1664	G1451	G1349	C1267	U1185	A1085	C	C925	U822	C400	C400	C400
U1665	U1452	U1350	C1268	C1186	A1086	C	C926	U823	A401	A401	A401
U1666	U1453	C1351	C1269	U1187	A1087	C	C927	U824	A402	A402	A402
U1667	U1454	U1352	C1270	C1188	A1088	C	C928	U825	A403	A403	A403
U1668	U1455	C1353	A1271	U1189	A1089	C	C929	U826	A404	A404	A404
U1669	U1456	G1354	U1272	G1190	A1090	A	C930	U827	A405	A405	A405
U1670	U1457	C1355	C1273	C1191	A1091	C	C931	U828	A406	A406	A406
U1671	U1458	U1356	A1274	U1192	A1092	C	C932	U829	A407	A407	A407
U1672	U1459	C1357	C1275	A1193	A1093	C	C933	U830	A408	A408	A408
U1673	U1460	G1358	U1276	U1194	A1094	C	C934	U831	A409	A409	A409
U1674	U1461	C1359	C1277	G1195	A1095	C	C935	U832	A410	A410	A410
U1675	U1462	U1360	U1278	C1196	A1096	C	C936	U833	A411	A411	A411
U1676	U1463	C1361	C1279	U1197	A1097	C	C937	U834	A412	A412	A412
U1677	U1464	G1362	U1280	G1198	A1098	C	C938	U835	A413	A413	A413
U1678	U1465	U1363	A1281	U1199	A1099	C	C939	U836	A414	A414	A414
U1679	U1466	C1364	C1282	U1200	A1100	C	C940	U837	A415	A415	A415
U1680	U1467	G1365	U1283	A1201	A1101	C	C941	U838	A416	A416	A416
U1681	U1468	U1366	U1284	C1202	A1102	C	C942	U839	A417	A417	A417
U1682	U1469	C1367	C1285	G1203	A1103	C	C943	U840	A418	A418	A418
U1683	U1470	G1368	U1286	U1204	A1104	C	C944	U841	A419	A419	A419
U1684	U1471	C1369	C1287	C1205	A1105	C	C945	U842	A420	A420	A420
U1685	U1472	U1370	U1288	U1206	A1106	C	C946	U843	A421	A421	A421
U1686	U1473	G1371	C1289	U1207	A1107	C	C947	U844	A422	A422	A422
U1687	U1474	C1372	A1290	G1208	A1108	C	C948	U845	A423	A423	A423
U1688	U1475	U1373	U1291	C1209	A1109	C	C949	U846	A424	A424	A424
U1689	U1476	G1374	C1292	U1210	A1110	C	C950	U847	A425	A425	A425
U1690	U1477	C1375	U1293	G1211	A1111	C	C951	U848	A426	A426	A426
U1691	U1478	U1376	A1294	C1212	A1112	C	C952	U849	A427	A427	A427
U1692	U1479	C1377	C1295	U1213	A1113	C	C953	U850	A428	A428	A428
U1693	U1480	G1378	U1296	U1214	A1114	C	C954	U851	A429	A429	A429
U1694	U1481	C1379	U1297	C1215	A1115	C	C955	U852	A430	A430	A430
U1695	U1482	U1380	U1298	U1216	A1116	C	C956	U853	A431	A431	A431
U1696	U1483	G1381	U1299	G1217	A1117	C	C957	U854	A432	A432	A432
U1697	U1484	C1382	U1300	C1218	A1118	C	C958	U855	A433	A433	A433
U1698	U1485	U1383	U1301	U1219	A1119	C	C959	U856	A434	A434	A434
U1699	U1486	G1384	U1302	U1220	A1120	C	C960	U857	A435	A435	A435
U1700	U1487	C1385	U1303	C1221	U1121	C	C961	U858	A436	A436	A436
U1701	U1488	U1386	U1304	U1222	U1122	C	C962	U859	A437	A437	A437
U1702	U1489	G1387	U1305	U1223	U1123	C	C963	U860	A438	A438	A438
U1703	U1490	C1388	U1306	C1224	U1124	C	C964	U861	A439	A439	A439
U1704	U1491	U1389	U1307	U1225	U1125	C	C965	U862	A440	A440	A440
U1705	U1492	G1390	U1308	U1226	U1126	C	C966	U863	A441	A441	A441
U1706	U1493	C1391	U1309	U1227	U1127	C	C967	U864	A442	A442	A442
U1707	U1494	U1392	U1310	U1228	U1128	C	C968	U865	A443	A443	A443
U1708	U1495	G1393	U1311	U1229	U1129	C	C969	U866	A444	A444	A444
U1709	U1496	C1394	U1312	U1230	U1130	C	C970	U867	A445	A445	A445
U1710	U1497	U1395	U1313	U1231	U1131	C	C971	U868	A446	A446	A446
U1711	U1498	G1396	U1314	U1232	U1132	C	C972	U869	A447	A447	A447
U1712	U1499	C1397	U1315	U1233	U1133	C	C973	U870	A448	A448	A448
U1713	U1500	U1398	U1316	U1234	U1134	C	C974	U871	A449	A449	A449
U1714	U1501	G1399	U1317	U1235	U1135	C	C975	U872	A450	A450	A450
U1715	U1502	C1399	U1318	U1236	U1136	C	C976	U873	A451	A451	A451
U1716	U1503	U1400	U1319	U1237	U1137	C	C977	U874	A452	A452	A452
U1717	U1504	G1401	U1320	U1238	U1138	C	C978	U875	A453	A453	A453
U1718	U1505	C1402	U1321	U1239	U1139	C	C979	U876	A454	A454	A454
U1719	U1506	U1403	U1322	U1240	U1140	C	C980	U877	A455	A455	A455
U1720	U1507	C1404	U1323	U1241	U1141	C	C981	U878	A456	A456	A456
U1721	U1508	U1405	U1324	U1242	U1142	C	C982	U879	A457	A457	A457
U1722	U1509	C1406	U1325	U1243	U1143	C	C983	U880	A458	A458	A458
U1723	U1510	U1407	U1326	U1244	U1144	C	C984	U881	A459	A459	A459
U1724	U1511	C1408	U1327	U1245	U1145	C	C985	U882	A460	A460	A460
U1725	U1512	U1409	U1328	U1246	U1146	C	C986	U883	A461	A461	A461
U1726	U1513	C1409	U1329	U1247	U1147	C	C987	U884	A462	A462	A462
U1727	U1514	U1410	U1330	U1248	U1148	C	C988	U885	A463	A463	A463
U1728	U1515	G1411	U1331	U1249	U1149	C	C989	U886	A464	A464	A464
U1729	U1516	C1412	U1332	U1250	U1150	C	C990	U887	A465	A465	A465
U1730	U1517	U1412	U1333	U1251	U1151	C	C991	U888	A466	A466	A466
U1731	U1518	C1413	U1334	U1252	U1152	C	C992	U889	A467	A467	A467
U1732	U1519	U1413	U1335	U1253	U1153	C	C993	U890	A468	A468	A468
U1733	U1520	G1414	U1336	U1254	U1154	C	C994	U891	A469	A469	A469
U1734	U1521	C1415	U1337	U1255	U1155	C	C995	U892	A470	A470	A470
U1735	U1522	U1414	U1338	U1256	U1156	C	C996	U893	A471	A471	A471
U1736	U1523	G1415	U1339	U1257	U1157	C	C997	U894	A472	A472	A472
U1737	U1524	C1416	U1340	U1258	U1158	C	C998	U895	A473	A473	A473
U1738	U1525	U1415	U1341	U1259	U1159	C	C999	U896	A474	A474	A474
U1739	U1526	G1416	U1342	U1260	U1160	C	C1000	U897	A475	A475	A475
U1740	U1527	C1417	U1343	U1261	U1161	C	C1001	U898	A476	A476	A476
U1741	U1528	U1416	U1344	U1262	U1162	C	C1002	U899	A477	A477	A477
U1742	U1529	G1417	U1345	U1263	U1163	C	C1003	U900	A478	A478	A478
U1743	U1530	C1418	U1346	U1264	U1164	C	C1004	U901	A479	A479	A479
U1744	U1531	U1417	U1347	U1265	U1165	C	C1005	U902	A480	A480	A480
U1745	U1532	G1418	U1348</								







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.83Å 299.90Å 576.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 2.70 85.81 – 2.41	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.83-2.70) 90.8 (85.81-2.41)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.184 , 0.226 0.175 , 0.217	Depositor DCC
$R_{free}$ test set	4705 reflections (0.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 667281 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99122	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, 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	A	0.32	0/1786	0.64	0/2408
2	B	0.32	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.62	0/2552
4	D	0.31	0/1111	0.55	0/1498
5	E	0.32	0/1382	0.56	0/1880
6	F	0.32	0/901	0.57	0/1224
7	G	0.31	0/241	0.48	0/324
8	H	0.32	0/1302	0.63	0/1743
9	I	0.29	0/526	0.51	0/716
10	J	0.35	0/1136	0.59	0/1530
11	K	0.33	0/1004	0.65	0/1351
12	L	0.33	0/1130	0.63	0/1509
13	M	0.34	0/1582	0.62	0/2116
14	N	0.29	0/1474	0.61	0/1999
15	O	0.34	0/874	0.59	1/1181 (0.1%)
16	P	0.32	0/1147	0.52	0/1528
17	Q	0.35	0/749	0.68	0/1005
18	R	1.26	7/1172 (0.6%)	1.11	6/1578 (0.4%)
19	S	0.31	0/648	0.57	0/875
20	T	0.33	0/958	0.62	1/1289 (0.1%)
21	U	0.34	0/417	0.55	0/562
22	V	0.31	0/502	0.52	0/675
23	W	0.34	0/1219	0.64	0/1655
24	X	0.34	0/664	0.58	0/895
25	Y	0.36	0/1146	0.60	0/1536
26	Z	0.35	0/584	0.60	0/781
27	1	0.37	0/438	0.61	0/578
28	2	0.34	0/401	0.55	0/529
29	3	0.36	0/771	0.57	0/1024
30	0	0.36	0/65957	0.68	17/102867 (0.0%)
31	9	0.32	0/2904	0.68	1/4526 (0.0%)
All	All	0.38	7/98701 (0.0%)	0.67	26/147586 (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
18	R	1	0
30	0	0	42
31	9	0	1
All	All	1	43

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.34	2.86	1.50
18	R	150	PRO	CA-C	-18.21	1.16	1.52
18	R	150	PRO	CG-CD	13.97	1.96	1.50
18	R	150	PRO	C-O	11.88	1.47	1.23
18	R	150	PRO	N-CA	11.28	1.66	1.47
18	R	150	PRO	N-CD	10.80	1.62	1.47
18	R	150	PRO	CA-CB	7.58	1.68	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.47	55.83	112.00
18	R	150	PRO	N-CA-C	-19.39	61.69	112.10
18	R	150	PRO	CA-N-CD	12.31	128.94	111.70
18	R	150	PRO	N-CA-CB	10.98	116.48	103.30
18	R	150	PRO	CA-C-O	-8.51	99.77	120.20
30	0	1878	G	N9-C1'-C2'	-6.59	104.75	112.00
18	R	150	PRO	CA-CB-CG	-6.10	92.41	104.00
30	0	1504	A	C1'-O4'-C4'	-6.07	105.04	109.90
30	0	871	G	C5'-C4'-O4'	-5.99	101.91	109.10
30	0	2291	A	N9-C1'-C2'	5.57	121.24	114.00
31	9	39	U	N1-C1'-C2'	5.48	121.12	114.00
30	0	2467	A	C1'-O4'-C4'	-5.41	105.57	109.90
30	0	1829	A	N9-C1'-C2'	-5.40	106.06	112.00
30	0	1819	G	C5'-C4'-C3'	5.26	124.42	116.00
30	0	2313	C	C5'-C4'-O4'	5.24	115.39	109.10
30	0	1504	A	N9-C1'-C2'	5.23	120.80	114.00
20	T	52	ARG	N-CA-C	5.18	124.97	111.00
30	0	2607	U	N1-C1'-C2'	5.17	120.72	114.00
30	0	2301	A	N9-C1'-C2'	5.15	120.69	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2313	C	C1'-O4'-C4'	-5.12	105.80	109.90
15	O	66	GLY	N-CA-C	5.08	125.81	113.10
30	0	699	C	C1'-O4'-C4'	-5.07	105.85	109.90
30	0	2316	G	C5'-C4'-C3'	-5.02	107.96	116.00
30	0	841	A	C1'-O4'-C4'	-5.02	105.88	109.90
30	0	777	U	O4'-C1'-N1	5.02	112.21	108.20
30	0	1120	U	C5'-C4'-C3'	-5.00	107.99	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1078	A	Sidechain
30	0	1262	C	Sidechain
30	0	1342	C	Sidechain
30	0	1417	G	Sidechain
30	0	1432	U	Sidechain
30	0	1681	G	Sidechain
30	0	1829	A	Sidechain
30	0	1848	G	Sidechain
30	0	1863	G	Sidechain
30	0	1867	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1970	G	Sidechain
30	0	1979	G	Sidechain
30	0	2036	C	Sidechain
30	0	2115	U	Sidechain
30	0	221	G	Sidechain
30	0	2301	A	Sidechain
30	0	2312	G	Sidechain
30	0	2316	G	Sidechain
30	0	2412	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain

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Mol	Chain	Res	Type	Group
30	0	2524	G	Sidechain
30	0	2551	C	Sidechain
30	0	2564	G	Sidechain
30	0	26	U	Sidechain
30	0	2607	U	Sidechain
30	0	2679	G	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	48	A	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	686	A	Sidechain
30	0	817	G	Sidechain
30	0	903	U	Sidechain
31	9	94	G	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	75	0
2	B	2625	0	2533	92	0
3	C	1860	0	1813	57	0
4	D	1094	0	1085	40	0
5	E	1357	0	1266	23	0
6	F	890	0	843	26	0
7	G	240	0	231	7	0
8	H	1282	0	1292	37	0
9	I	519	0	500	15	0
10	J	1120	0	1098	30	0
11	K	994	0	1027	36	0
12	L	1118	0	1076	22	0
13	M	1558	0	1573	42	0
14	N	1445	0	1401	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	865	0	873	15	0
16	P	1136	0	1123	28	0
17	Q	735	0	729	14	0
18	R	1149	0	1122	34	0
19	S	641	0	605	11	0
20	T	950	0	924	19	0
21	U	410	0	364	19	0
22	V	499	0	511	17	0
23	W	1196	0	1137	55	0
24	X	654	0	653	24	0
25	Y	1130	0	1133	36	0
26	Z	573	0	531	16	0
27	1	431	0	426	22	0
28	2	396	0	413	19	0
29	3	755	0	728	20	0
30	0	59020	0	29806	1142	0
31	9	2599	0	1325	101	0
32	0	85	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	2	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	66	0	0	0	0
34	9	2	0	0	0	0
34	C	1	0	0	0	0
34	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	2	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	93	0	0	0	0
36	1	2	0	0	0	0
36	3	2	0	0	0	0
36	9	2	0	0	0	0
36	A	3	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	J	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5951	0	0	153	0
38	1	52	0	0	3	0
38	2	37	0	0	2	0
38	3	68	0	0	5	0
38	9	147	0	0	8	0
38	A	111	0	0	5	0
38	B	153	0	0	14	0
38	C	165	0	0	11	0
38	D	46	0	0	2	0
38	E	44	0	0	2	0
38	F	23	0	0	1	0
38	G	19	0	0	0	0
38	H	71	0	0	6	0
38	I	10	0	0	2	0
38	J	54	0	0	1	0
38	K	56	0	0	3	0
38	L	80	0	0	6	0
38	M	130	0	0	5	0
38	N	59	0	0	5	0
38	O	41	0	0	3	0
38	P	61	0	0	1	0
38	Q	51	0	0	2	0
38	R	78	0	0	3	0
38	S	33	0	0	2	0
38	T	37	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	U	25	0	0	3	0
38	V	11	0	0	0	0
38	W	63	0	0	4	0
38	X	28	0	0	1	0
38	Y	91	0	0	6	0
38	Z	28	0	0	3	0
All	All	99122	0	59907	1937	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (1937) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.44
30:0:1160:G:C5'	30:0:1161:A:H5'	1.81	1.10
31:9:56:A:H2'	31:9:57:A:H5''	1.33	1.08
30:0:871:G:C8	30:0:871:G:H5'	1.87	1.07
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.07
14:N:37:ARG:NH1	31:9:6:C:H5''	1.71	1.05
30:0:1160:G:H5'	30:0:1161:A:C5'	1.88	1.03
30:0:381:G:H5''	38:0:4345:HOH:O	1.58	1.02
30:0:1160:G:H5'	30:0:1161:A:H5'	1.02	1.02
30:0:2812:A:H2	30:0:2814:A:H62	1.03	1.02
13:M:171:ARG:HD3	30:0:156:C:H5''	1.40	1.00
10:J:82:THR:HG23	30:0:1242:A:H5'	1.44	1.00
30:0:2717:C:C2'	30:0:2718:C:H5''	1.92	0.99
11:K:10:GLN:H	11:K:10:GLN:HE21	1.06	0.99
31:9:76:G:H3'	31:9:77:A:H5''	1.42	0.99
30:0:182:G:H5'	38:0:5188:HOH:O	1.63	0.98
30:0:871:G:H8	30:0:871:G:H5'	1.23	0.98
30:0:1666:C:O2'	30:0:1667:A:H5''	1.61	0.98
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.44	0.98
30:0:1118:A:H3'	30:0:1118:A:H8	1.29	0.97
30:0:2717:C:H2'	30:0:2718:C:H5''	1.46	0.97
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.47	0.96
30:0:1474:C:H6	30:0:1474:C:H5'	1.29	0.96
15:O:3:THR:HG22	30:0:656:G:H5'	1.46	0.96
30:0:1243:C:H3'	38:0:4869:HOH:O	1.65	0.95
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.12	0.94
30:0:1187:U:HO2'	30:0:1189:A:H2	1.07	0.94
3:C:236:THR:HG22	3:C:239:ALA:H	1.31	0.94
30:0:282:C:O2'	30:0:283:U:H5'	1.68	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:P:115:SER:H	16:P:118:GLN:HE21	0.95	0.92
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.84	0.92
30:0:69:A:H5'	30:0:69:A:H8	1.33	0.92
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.14	0.92
30:0:871:G:H8	30:0:871:G:C5'	1.83	0.91
30:0:1205:U:H2'	30:0:1206:U:C5'	2.00	0.91
30:0:2491:G:H1'	38:0:6910:HOH:O	1.70	0.91
30:0:69:A:H5'	30:0:69:A:C8	2.06	0.91
30:0:1118:A:H3'	30:0:1118:A:C8	2.04	0.91
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.51	0.91
30:0:2533:C:H5'	30:0:2533:C:H6	1.35	0.90
8:H:49:GLN:HE21	8:H:140:TYR:HE2	1.15	0.90
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.53	0.90
4:D:154:LYS:HD2	4:D:154:LYS:H	1.37	0.89
30:0:1603:A:H5'	30:0:1605:G:O4'	1.72	0.89
30:0:870:G:H2'	30:0:871:G:H5''	1.53	0.89
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.37	0.89
30:0:1474:C:C6	30:0:1474:C:H5'	2.08	0.89
30:0:1701:A:H5'	38:0:6316:HOH:O	1.73	0.89
30:0:1183:C:H2'	38:0:6276:HOH:O	1.73	0.89
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.19	0.89
30:0:1184:C:H1'	38:0:7504:HOH:O	1.71	0.88
30:0:542:A:H5'	30:0:542:A:H8	1.38	0.88
30:0:282:C:H1'	30:0:368:C:N4	1.88	0.88
30:0:1666:C:C2'	30:0:1667:A:H5''	2.03	0.88
30:0:1835:U:H5	30:0:1840:A:N7	1.72	0.88
30:0:877:G:H5'	30:0:878:G:OP1	1.74	0.88
30:0:2251:G:H2'	30:0:2252:A:C8	2.09	0.87
30:0:558:C:C2'	30:0:559:U:H5''	2.04	0.87
2:B:238:ASN:HD22	2:B:240:GLY:H	1.20	0.87
30:0:1206:U:H6	30:0:1206:U:H5'	1.40	0.87
31:9:56:A:C2'	31:9:57:A:H5''	2.05	0.86
31:9:14:G:H5'	31:9:14:G:H8	1.39	0.86
30:0:10:U:H6	30:0:10:U:H3'	1.40	0.86
14:N:37:ARG:HH12	31:9:6:C:H5''	1.37	0.86
30:0:1372:A:H3'	38:0:7227:HOH:O	1.76	0.85
30:0:1701:A:H4'	30:0:1702:U:H5''	1.56	0.85
16:P:117:SER:HB3	30:0:1593:C:OP1	1.77	0.85
30:0:506:G:H22	30:0:509:A:C5'	1.88	0.85
30:0:871:G:C8	30:0:871:G:C5'	2.59	0.85
2:B:162:MET:HE3	2:B:308:LEU:HD21	1.57	0.85
30:0:1205:U:H2'	30:0:1206:U:H5'	1.56	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1118:A:H62	30:0:1244:U:H3	1.25	0.84
30:0:545:G:H8	30:0:545:G:H5'	1.39	0.84
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.59	0.84
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.60	0.84
30:0:1667:A:H8	30:0:1667:A:H5'	1.41	0.84
30:0:1116:U:H3	30:0:1246:A:H62	1.26	0.84
30:0:2502:C:C2'	30:0:2503:A:H5'	2.08	0.83
30:0:2506:A:HO2'	30:0:2507:G:H8	0.88	0.83
30:0:541:C:C2'	30:0:542:A:H5''	2.08	0.83
30:0:2769:C:C2'	30:0:2770:G:H5'	2.07	0.83
30:0:1300:G:H1'	38:0:4714:HOH:O	1.78	0.83
30:0:214:U:H5'	38:0:6173:HOH:O	1.77	0.83
30:0:1189:A:H1'	30:0:1209:C:O4'	1.79	0.82
30:0:506:G:H22	30:0:509:A:H5'	1.42	0.82
30:0:541:C:H2'	30:0:542:A:H5''	1.60	0.82
30:0:396:U:H1'	38:0:7666:HOH:O	1.77	0.82
28:2:41:HIS:H	28:2:45:ASN:HD22	1.25	0.82
30:0:1878:G:H1'	38:0:6153:HOH:O	1.79	0.82
30:0:2502:C:H2'	30:0:2503:A:H5'	1.60	0.82
30:0:2506:A:O2'	30:0:2507:G:H8	1.61	0.82
23:W:88:THR:HB	38:W:6679:HOH:O	1.80	0.82
30:0:1183:C:N4	30:0:1184:C:H41	1.78	0.81
30:0:236:A:H4'	30:0:237:G:H5'	1.62	0.81
30:0:1116:U:HO2'	30:0:1118:A:H2	0.82	0.81
30:0:1116:U:O2'	30:0:1118:A:H2	1.63	0.81
30:0:544:G:H2'	30:0:545:G:H5''	1.63	0.81
30:0:2783:A:H3'	38:0:5262:HOH:O	1.80	0.81
11:K:39:GLY:HA2	38:0:5251:HOH:O	1.79	0.81
30:0:559:U:H5'	30:0:559:U:H6	1.43	0.81
30:0:558:C:O2'	30:0:559:U:H5''	1.79	0.81
30:0:1632:A:H2'	30:0:1633:C:H5'	1.63	0.80
30:0:380:A:H2'	38:0:7266:HOH:O	1.81	0.80
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.28	0.80
30:0:1189:A:H3'	38:0:7718:HOH:O	1.80	0.80
30:0:2291:A:C8	30:0:2309:C:H5'	2.16	0.80
30:0:2586:U:H3	30:0:2592:G:H22	1.26	0.80
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.78	0.80
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.64	0.80
30:0:2426:G:H1'	38:0:6125:HOH:O	1.82	0.80
30:0:1603:A:H5''	30:0:1605:G:H5'	1.63	0.80
30:0:1741:U:H5'	30:0:1742:A:OP1	1.82	0.80
16:P:115:SER:H	16:P:118:GLN:NE2	1.77	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1119:G:N2	30:0:1246:A:C2	2.49	0.79
30:0:2533:C:C6	30:0:2533:C:H5'	2.15	0.79
3:C:139:VAL:HG13	38:C:8641:HOH:O	1.82	0.79
15:O:3:THR:CG2	30:0:656:G:H5'	2.11	0.79
30:0:541:C:H2'	30:0:542:A:C5'	2.12	0.79
30:0:2851:G:O2'	30:0:2852:A:H5'	1.83	0.79
20:T:9:LYS:HE3	20:T:13:ARG:NH1	1.98	0.79
30:0:2896:A:H5''	38:0:6132:HOH:O	1.81	0.78
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.65	0.78
30:0:2827:A:H2'	30:0:2828:G:O4'	1.83	0.78
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.48	0.78
35:0:8813:CL:CL	38:0:4714:HOH:O	2.39	0.78
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.13	0.78
30:0:1634:G:H3'	38:0:3915:HOH:O	1.84	0.77
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.49	0.77
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.99	0.77
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.67	0.77
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.33	0.77
30:0:2769:C:O2'	30:0:2770:G:H5'	1.85	0.77
30:0:1666:C:H2'	30:0:1667:A:C5'	2.14	0.77
13:M:164:THR:HG22	13:M:167:GLY:H	1.50	0.77
2:B:179:LEU:O	2:B:183:GLU:HG2	1.84	0.76
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.50	0.76
22:V:50:ARG:HH12	30:0:56:G:H5''	1.48	0.76
30:0:1209:C:H2'	30:0:1210:G:H8	1.50	0.76
5:E:143:GLN:NE2	30:0:2779:G:H21	1.82	0.76
30:0:2908:A:H2'	30:0:2909:G:O4'	1.85	0.76
30:0:282:C:H1'	30:0:368:C:H42	1.50	0.76
30:0:1080:C:H4'	30:0:1081:A:OP1	1.85	0.76
30:0:558:C:H2'	30:0:559:U:C5'	2.15	0.76
31:9:2:U:OP2	31:9:3:A:H5'	1.86	0.76
3:C:174:ILE:HD11	30:0:338:C:H4'	1.66	0.76
30:0:2768:A:O2'	30:0:2769:C:H5'	1.86	0.76
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.68	0.76
30:0:2004:U:H4'	38:0:5338:HOH:O	1.86	0.76
30:0:31:C:H4'	38:0:7463:HOH:O	1.87	0.75
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.68	0.75
30:0:2637:A:H5'	38:0:4961:HOH:O	1.85	0.75
30:0:2717:C:O2'	30:0:2718:C:H5''	1.86	0.75
30:0:1973:A:H5'	30:0:1973:A:H8	1.52	0.74
30:0:2239:C:H2'	30:0:2240:U:H6	1.52	0.74
30:0:283:U:H5	30:0:284:C:C4	2.05	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:603:A:H5''	30:0:604:G:OP1	1.87	0.74
28:2:41:HIS:HD2	28:2:44:ARG:H	1.35	0.74
30:0:2748:G:H5'	38:0:7579:HOH:O	1.85	0.74
30:0:2851:G:C2'	30:0:2852:A:H5'	2.17	0.74
30:0:179:C:H5''	38:0:9320:HOH:O	1.86	0.74
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.69	0.74
30:0:1118:A:C8	30:0:1118:A:C3'	2.69	0.74
30:0:2559:C:H4'	38:0:7294:HOH:O	1.86	0.74
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.69	0.74
14:N:113:SER:HB2	38:N:8854:HOH:O	1.87	0.74
30:0:272:A:H5'	30:0:273:G:OP2	1.88	0.74
31:9:14:G:H5'	31:9:14:G:C8	2.23	0.74
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.69	0.73
30:0:1942:A:H3'	38:0:7386:HOH:O	1.88	0.73
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.69	0.73
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.71	0.73
30:0:1180:U:H2'	30:0:1181:A:O4'	1.89	0.73
16:P:115:SER:N	16:P:118:GLN:HE21	1.79	0.73
30:0:10:U:C6	30:0:10:U:H3'	2.23	0.73
30:0:1183:C:H42	30:0:1184:C:H41	1.35	0.73
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.88	0.73
30:0:2717:C:H2'	30:0:2718:C:C5'	2.19	0.73
30:0:1205:U:H2'	30:0:1206:U:H5''	1.70	0.72
30:0:338:C:H5''	38:0:3821:HOH:O	1.89	0.72
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.71	0.72
11:K:10:GLN:H	11:K:10:GLN:NE2	1.83	0.72
31:9:49:G:O2'	31:9:50:G:H5'	1.88	0.72
30:0:1279:U:O2	30:0:1279:U:H2'	1.88	0.72
30:0:2256:G:O2'	30:0:2257:G:H5'	1.88	0.72
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.87	0.72
18:R:39:THR:HG22	18:R:42:GLU:H	1.53	0.72
30:0:2420:G:O2'	30:0:2421:G:H5'	1.90	0.72
30:0:1666:C:H2'	30:0:1667:A:H5'	1.72	0.71
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.70	0.71
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.73	0.71
30:0:1666:C:C2'	30:0:1667:A:C5'	2.68	0.71
30:0:544:G:C2'	30:0:545:G:H5''	2.20	0.71
30:0:1632:A:C2'	30:0:1633:C:H5'	2.19	0.71
30:0:558:C:H2'	30:0:559:U:H5''	1.70	0.71
18:R:9:ASP:O	18:R:13:THR:HB	1.89	0.71
30:0:2679:G:H2'	30:0:2681:A:OP2	1.91	0.71
30:0:2010:A:H2'	38:0:5990:HOH:O	1.90	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2578:G:H5'	30:0:2578:G:H8	1.54	0.71
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.37	0.71
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.72	0.71
30:0:1964:U:O2	30:0:1964:U:H2'	1.91	0.71
31:9:92:G:H2'	31:9:93:A:C8	2.26	0.71
30:0:1157:C:H2'	30:0:1158:G:H8	1.56	0.70
30:0:2635:A:O2'	30:0:2636:C:H5'	1.90	0.70
30:0:2769:C:H2'	30:0:2770:G:O4'	1.91	0.70
31:9:39:U:H1'	31:9:44:A:H61	1.55	0.70
30:0:1527:A:H1'	30:0:1528:A:C8	2.27	0.70
18:R:25:PHE:CE2	18:R:29:LYS:HE2	2.27	0.70
30:0:1174:A:C5	30:0:1201:C:H4'	2.26	0.70
3:C:174:ILE:CD1	30:0:338:C:H4'	2.21	0.70
30:0:1701:A:H4'	30:0:1702:U:C5'	2.20	0.70
30:0:31:C:H2'	38:0:7726:HOH:O	1.89	0.70
22:V:1:THR:HG23	22:V:2:VAL:H	1.56	0.70
30:0:2852:A:H5''	38:0:5264:HOH:O	1.91	0.70
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.05	0.69
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.07	0.69
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.74	0.69
30:0:1165:G:O2'	30:0:1174:A:H1'	1.92	0.69
30:0:308:U:H5'	30:0:309:C:OP1	1.91	0.69
12:L:148:GLU:HA	38:L:8870:HOH:O	1.92	0.69
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.73	0.69
30:0:2507:G:H2'	30:0:2510:C:H42	1.57	0.69
31:9:29:C:H2'	31:9:30:C:H5'	1.73	0.69
30:0:814:G:H4'	38:0:3155:HOH:O	1.91	0.69
3:C:1:MET:HG2	3:C:2:GLN:H	1.55	0.69
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.92	0.69
30:0:1603:A:C5'	30:0:1605:G:H5'	2.22	0.69
31:9:1:U:H4'	31:9:3:A:OP1	1.92	0.69
30:0:545:G:C8	30:0:545:G:H5'	2.25	0.69
12:L:133:VAL:HA	38:L:8871:HOH:O	1.92	0.69
2:B:217:ARG:HG3	2:B:257:THR:HB	1.75	0.68
30:0:281:U:H2'	30:0:282:C:O4'	1.94	0.68
31:9:7:G:H5'	38:9:9099:HOH:O	1.93	0.68
38:Y:8852:HOH:O	35:0:8817:CL:CL	2.49	0.68
14:N:37:ARG:NH1	31:9:6:C:C5'	2.53	0.68
2:B:258:GLY:H	2:B:260:HIS:CE1	2.12	0.68
30:0:1120:U:H5''	30:0:1120:U:C6	2.29	0.68
30:0:1819:G:H2'	30:0:1820:G:H4'	1.74	0.68
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.07	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2256:G:C2'	30:0:2257:G:H5'	2.23	0.68
30:0:870:G:C2'	30:0:871:G:H5''	2.23	0.68
13:M:171:ARG:CD	30:0:156:C:H5''	2.20	0.67
2:B:244:PRO:HB3	30:0:1234:U:N3	2.09	0.67
10:J:70:PHE:HD1	30:0:2676:C:HO2'	1.40	0.67
30:0:292:G:H2'	30:0:358:G:N2	2.08	0.67
14:N:144:GLY:O	14:N:147:ILE:HG22	1.94	0.67
18:R:150:PRO:CG	18:R:150:PRO:O	2.41	0.67
27:1:42:SER:HB2	38:1:354:HOH:O	1.93	0.67
14:N:11:ARG:HD3	31:9:114:G:O6	1.94	0.67
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.94	0.67
30:0:297:U:H2'	30:0:298:C:C6	2.28	0.67
30:0:2812:A:C2	30:0:2814:A:N6	2.58	0.67
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.76	0.67
20:T:24:ARG:HH21	20:T:39:ASN:ND2	1.93	0.67
31:9:39:U:H1'	31:9:44:A:N6	2.08	0.67
30:0:1667:A:C8	30:0:1667:A:H5'	2.27	0.67
30:0:564:G:H1'	38:0:6342:HOH:O	1.94	0.67
30:0:1060:C:H6	30:0:1060:C:H5'	1.60	0.66
30:0:1474:C:C5'	30:0:1474:C:H6	2.07	0.66
3:C:27:ARG:NH2	30:0:657:G:OP1	2.28	0.66
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.58	0.66
12:L:6:ARG:HD3	30:0:1299:G:O6	1.95	0.66
30:0:2681:A:H4'	30:0:2682:C:H5'	1.75	0.66
30:0:1116:U:O2'	30:0:1118:A:C2	2.44	0.66
30:0:1205:U:C2'	30:0:1206:U:C5'	2.72	0.66
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.26	0.66
12:L:136:ALA:HB3	38:L:8871:HOH:O	1.96	0.66
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.78	0.66
30:0:1289:C:H3'	38:0:6443:HOH:O	1.95	0.66
30:0:2239:C:H2'	30:0:2240:U:C6	2.30	0.66
22:V:50:ARG:NH1	30:0:56:G:H5''	2.10	0.66
30:0:1016:U:H1'	38:0:3678:HOH:O	1.96	0.66
30:0:1159:G:H21	30:0:1189:A:H8	1.44	0.66
30:0:960:G:H2'	30:0:960:G:N3	2.11	0.66
3:C:236:THR:HG22	3:C:239:ALA:N	2.09	0.66
30:0:125:U:H2'	38:0:3785:HOH:O	1.96	0.65
30:0:2769:C:H2'	30:0:2770:G:H5'	1.77	0.65
30:0:2836:G:H1'	38:0:6880:HOH:O	1.95	0.65
1:A:199:HIS:HD2	1:A:201:PHE:H	1.44	0.65
15:O:42:GLU:HB2	38:O:2176:HOH:O	1.96	0.65
30:0:2795:C:O2'	30:0:2796:U:H5'	1.95	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:283:U:C5	30:0:284:C:C4	2.85	0.65
30:0:960:G:N3	30:0:960:G:C2'	2.59	0.65
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.37	0.65
30:0:1183:C:N3	30:0:1184:C:C5	2.65	0.65
30:0:1189:A:O2'	30:0:1208:C:H2'	1.96	0.65
2:B:212:GLN:HA	30:0:1733:A:H4'	1.79	0.65
16:P:59:ARG:HH22	16:P:66:GLN:NE2	1.94	0.65
30:0:1451:C:H5'	30:0:1505:U:C5	2.32	0.65
30:0:704:C:O2'	30:0:705:C:H5'	1.97	0.65
30:0:1058:A:H2'	30:0:1060:C:H5''	1.78	0.64
30:0:1925:G:O2'	30:0:1926:G:H5'	1.97	0.64
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.32	0.64
30:0:363:C:H1'	38:0:5312:HOH:O	1.97	0.64
4:D:103:ASN:ND2	4:D:134:LEU:H	1.95	0.64
30:0:2414:A:H2'	30:0:2415:A:C8	2.32	0.64
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.62	0.64
30:0:2505:G:O2'	30:0:2506:A:H5'	1.97	0.64
30:0:256:C:H2'	30:0:257:G:O4'	1.96	0.64
2:B:206:THR:HG21	30:0:2716:G:H5''	1.80	0.64
30:0:1189:A:H1'	30:0:1209:C:C1'	2.28	0.64
30:0:1441:G:O2'	30:0:1442:A:H5'	1.97	0.64
30:0:1741:U:O2'	30:0:2723:G:H4'	1.97	0.64
30:0:280:C:H2'	30:0:281:U:O4'	1.97	0.64
30:0:558:C:C2'	30:0:559:U:C5'	2.74	0.64
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.63	0.64
25:Y:204:ARG:HH22	30:0:553:G:P	2.21	0.64
3:C:184:ARG:NH2	30:0:450:C:OP1	2.30	0.64
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.78	0.64
23:W:125:HIS:HD2	23:W:127:GLY:H	1.46	0.64
30:0:297:U:H2'	30:0:298:C:H6	1.63	0.64
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.26	0.64
30:0:2769:C:H2'	30:0:2770:G:C5'	2.28	0.64
30:0:10:U:C3'	30:0:10:U:C6	2.80	0.63
30:0:1205:U:C2'	30:0:1206:U:H5''	2.28	0.63
30:0:2256:G:H2'	30:0:2257:G:C5'	2.27	0.63
1:A:199:HIS:CD2	1:A:201:PHE:H	2.15	0.63
30:0:1187:U:H2'	38:0:6939:HOH:O	1.98	0.63
29:3:65:THR:HG23	29:3:67:LEU:HG	1.79	0.63
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.81	0.63
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.79	0.63
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.64	0.63
18:R:128:ARG:NH2	30:0:2054:A:N3	2.46	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2533:C:H6	30:0:2533:C:C5'	2.09	0.63
21:U:46:ALA:O	21:U:52:THR:HG21	1.98	0.63
24:X:71:ARG:HD3	38:X:2171:HOH:O	1.98	0.63
30:0:1120:U:H6	30:0:1120:U:H5''	1.63	0.63
30:0:1278:A:H4'	30:0:1279:U:C4	2.33	0.63
30:0:1878:G:O2'	30:0:1879:U:C6	2.49	0.63
31:9:75:G:H1	31:9:106:U:H3	1.47	0.63
13:M:27:ARG:NH2	13:M:44:THR:HG23	2.13	0.63
9:I:110:ASP:O	30:0:1163:G:H5'	1.99	0.63
30:0:2524:G:H21	30:0:2526:C:N4	1.96	0.63
30:0:317:A:H4'	38:0:3791:HOH:O	1.98	0.63
30:0:1835:U:C5	30:0:1840:A:N7	2.60	0.63
30:0:2509:A:H2'	30:0:2510:C:O4'	1.99	0.63
30:0:2649:A:H5'	30:0:2649:A:H8	1.64	0.63
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.81	0.63
2:B:162:MET:CE	2:B:308:LEU:HD21	2.27	0.63
2:B:264:GLU:HG3	2:B:302:PRO:HD3	1.79	0.63
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.64	0.63
30:0:2604:A:H5'	38:0:5822:HOH:O	1.99	0.62
31:9:54:A:O2'	31:9:55:U:H5'	1.98	0.62
30:0:2250:G:C2	30:0:2251:G:H1'	2.34	0.62
30:0:2256:G:H2'	30:0:2257:G:H5'	1.81	0.62
30:0:853:C:H3'	38:0:4580:HOH:O	2.00	0.62
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.96	0.62
23:W:13:MET:HE1	23:W:18:GLN:HA	1.81	0.62
15:O:73:ASP:HA	15:O:92:VAL:O	2.00	0.62
30:0:2421:G:H1'	38:0:7060:HOH:O	1.98	0.62
13:M:178:LYS:HB2	38:0:6916:HOH:O	1.99	0.62
8:H:168:VAL:HG13	38:H:211:HOH:O	1.98	0.62
30:0:1701:A:H5''	30:0:1702:U:H3'	1.82	0.62
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.81	0.62
30:0:1198:U:H1'	30:0:1201:C:H5	1.63	0.62
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.81	0.62
30:0:567:U:H5''	38:0:6435:HOH:O	1.99	0.62
27:1:16:HIS:HD2	30:0:470:U:O2'	1.83	0.62
27:1:20:ARG:HG2	30:0:111:C:O2'	2.00	0.62
31:9:2:U:P	31:9:3:A:H5'	2.40	0.62
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.82	0.62
7:G:64:ASN:N	7:G:64:ASN:HD22	1.96	0.62
30:0:1166:A:H61	30:0:1180:U:H3	1.46	0.62
30:0:2404:G:H5''	38:0:5241:HOH:O	2.00	0.62
30:0:2670:G:O2'	30:0:2671:U:H5'	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:960:G:H3'	30:0:960:G:N3	2.14	0.62
29:3:48:ASN:HD21	30:0:2468:A:H61	1.47	0.62
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.80	0.62
11:K:10:GLN:N	11:K:10:GLN:HE21	1.87	0.62
30:0:1170:U:H2'	30:0:1172:G:OP2	2.00	0.61
30:0:1314:U:H2'	38:0:5904:HOH:O	2.00	0.61
6:F:91:VAL:HG12	6:F:92:GLY:N	2.14	0.61
13:M:65:VAL:HG21	13:M:105:ALA:HB2	1.82	0.61
25:Y:216:ARG:HD2	38:Y:8865:HOH:O	2.00	0.61
30:0:848:C:H5'	38:0:7311:HOH:O	2.00	0.61
11:K:32:ILE:HD11	11:K:56:SER:HB2	1.82	0.61
30:0:958:G:O2'	30:0:959:C:H5'	2.00	0.61
30:0:2083:A:H3'	38:0:7616:HOH:O	1.99	0.61
30:0:2613:G:O2'	30:0:2614:C:H5'	2.00	0.61
30:0:506:G:H22	30:0:509:A:H5''	1.63	0.61
31:9:20:G:O2'	31:9:21:G:H5'	2.00	0.61
13:M:157:ASP:HB3	13:M:160:PHE:HD1	1.65	0.61
2:B:162:MET:HG3	2:B:310:ARG:HD3	1.83	0.61
14:N:4:PRO:HG3	31:9:69:U:OP1	2.00	0.61
23:W:88:THR:HG22	23:W:89:ASP:H	1.65	0.61
30:0:1679:C:H5'	38:0:9334:HOH:O	2.00	0.61
30:0:1759:A:N3	30:0:1818:C:H2'	2.16	0.61
31:9:64:C:C2'	31:9:65:A:H5'	2.30	0.61
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.82	0.61
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.83	0.61
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.81	0.61
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.83	0.61
30:0:1506:U:H6	30:0:1506:U:H5'	1.66	0.61
30:0:1641:A:H2'	30:0:1642:A:H5'	1.83	0.61
30:0:1948:G:H2'	30:0:1949:G:O4'	2.01	0.61
22:V:1:THR:HB	30:0:93:C:H5''	1.82	0.61
30:0:2787:C:H5	38:0:4664:HOH:O	1.83	0.61
27:1:10:LYS:HG3	38:1:2979:HOH:O	2.00	0.61
30:0:558:C:H2'	30:0:559:U:H5'	1.82	0.61
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.16	0.61
3:C:16:VAL:HG12	3:C:17:ASP:H	1.66	0.61
3:C:236:THR:HG21	38:C:8569:HOH:O	2.00	0.61
14:N:141:ARG:HH21	31:9:48:C:H4'	1.66	0.60
1:A:36:ASP:CB	1:A:85:SER:H	2.14	0.60
30:0:2505:G:C2'	30:0:2506:A:H5'	2.31	0.60
23:W:84:VAL:HG12	38:W:6679:HOH:O	2.01	0.60
30:0:2637:A:H4'	38:0:6094:HOH:O	2.00	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:936:C:H5	38:0:5991:HOH:O	1.82	0.60
14:N:40:ASN:ND2	31:9:28:U:H5''	2.16	0.60
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.82	0.60
30:0:1515:A:H2'	30:0:1516:U:C6	2.37	0.60
30:0:236:A:H4'	30:0:237:G:OP1	2.01	0.60
38:B:9109:HOH:O	30:0:2672:C:H1'	2.02	0.60
30:0:542:A:H5'	30:0:542:A:C8	2.28	0.60
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.84	0.60
30:0:836:G:H5''	38:0:9288:HOH:O	1.99	0.60
23:W:88:THR:HG22	23:W:89:ASP:N	2.17	0.60
4:D:57:THR:HG23	4:D:63:ILE:HA	1.82	0.60
11:K:27:ARG:HD2	38:K:4747:HOH:O	2.01	0.60
30:0:1080:C:O5'	30:0:1080:C:H6	1.85	0.60
30:0:2563:U:H2'	30:0:2565:C:O5'	2.01	0.60
30:0:702:G:O2'	30:0:703:G:H5'	2.02	0.60
10:J:41:ALA:HB3	38:J:5907:HOH:O	2.00	0.60
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.84	0.60
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.84	0.60
25:Y:117:LEU:HA	25:Y:174:VAL:HG11	1.84	0.60
30:0:2089:A:O2'	30:0:2090:G:H5'	2.02	0.60
31:9:3:A:N6	31:9:22:G:H1'	2.16	0.60
30:0:2419:U:H5''	30:0:2420:G:H5'	1.83	0.59
6:F:101:ALA:HA	38:F:5413:HOH:O	2.02	0.59
8:H:102:LYS:HD3	8:H:122:LYS:HD3	1.83	0.59
30:0:368:C:H2'	30:0:369:G:H5'	1.84	0.59
9:I:87:PRO:HB3	38:I:6825:HOH:O	2.02	0.59
30:0:567:U:H5''	38:0:5320:HOH:O	2.02	0.59
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.83	0.59
13:M:80:GLY:O	13:M:81:ARG:HD3	2.01	0.59
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.32	0.59
30:0:1132:A:N6	30:0:1229:C:H2'	2.17	0.59
30:0:1790:C:H2'	30:0:1791:U:H6	1.67	0.59
30:0:2329:C:O2'	30:0:2330:U:H5'	2.01	0.59
30:0:271:C:H41	30:0:378:A:H2	1.47	0.59
38:Z:8706:HOH:O	30:0:1886:A:H4'	2.03	0.59
30:0:2237:G:H1'	38:0:4887:HOH:O	2.02	0.59
2:B:254:GLN:HG3	38:0:9714:HOH:O	2.01	0.59
8:H:49:GLN:NE2	8:H:140:TYR:HE2	1.95	0.59
8:H:29:SER:HA	8:H:62:HIS:HD2	1.68	0.59
30:0:2718:C:H6	30:0:2718:C:H5'	1.68	0.59
30:0:119:A:H2'	30:0:120:A:H5''	1.83	0.59
30:0:1377:C:H6	30:0:1377:C:H5'	1.68	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1595:G:O2'	30:0:1596:U:H5'	2.03	0.59
1:A:33:GLU:CD	1:A:33:GLU:H	2.04	0.59
3:C:236:THR:CG2	3:C:239:ALA:H	2.11	0.59
8:H:174:LEU:HA	38:H:222:HOH:O	2.02	0.59
9:I:108:HIS:H	9:I:109:PRO:HD2	1.66	0.59
18:R:39:THR:HG23	18:R:107:GLU:O	2.02	0.59
30:0:2344:G:N3	30:0:2344:G:H2'	2.17	0.59
30:0:2756:U:H3	30:0:2896:A:H2	1.43	0.59
30:0:308:U:C4	30:0:342:C:H1'	2.38	0.59
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.32	0.59
13:M:66:SER:HB3	13:M:128:TRP:CD1	2.37	0.59
1:A:48:ASP:HB3	38:A:9060:HOH:O	2.03	0.59
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.85	0.59
7:G:16:LYS:O	7:G:20:VAL:HG23	2.03	0.59
23:W:125:HIS:CD2	23:W:127:GLY:H	2.21	0.59
31:9:64:C:H2'	31:9:65:A:H5'	1.84	0.59
7:G:12:ILE:HG23	38:0:5490:HOH:O	2.03	0.59
38:C:8655:HOH:O	30:0:2100:A:H5'	2.03	0.58
30:0:2812:A:H2	30:0:2814:A:N6	1.87	0.58
30:0:468:U:H3'	38:0:7607:HOH:O	2.03	0.58
31:9:24:U:H3'	31:9:25:G:C5'	2.32	0.58
2:B:248:ARG:O	2:B:251:VAL:HG13	2.03	0.58
2:B:51:VAL:HG23	2:B:330:VAL:HG22	1.85	0.58
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.04	0.58
30:0:2534:C:H1'	38:0:3513:HOH:O	2.01	0.58
1:A:171:LYS:HB2	30:0:820:G:C6	2.37	0.58
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.67	0.58
28:2:38:LYS:HE3	38:0:4254:HOH:O	2.01	0.58
6:F:48:VAL:HG23	6:F:74:PHE:HB3	1.85	0.58
30:0:1603:A:H5'	30:0:1605:G:C4'	2.33	0.58
30:0:1972:U:H2'	30:0:1973:A:C5'	2.32	0.58
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.03	0.58
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.19	0.58
30:0:1304:U:H2'	30:0:1305:C:C6	2.39	0.58
30:0:2252:A:C5	30:0:2253:G:H1'	2.38	0.58
30:0:2649:A:H5'	30:0:2649:A:C8	2.39	0.58
1:A:36:ASP:HB2	1:A:85:SER:H	1.68	0.58
16:P:115:SER:OG	16:P:118:GLN:HG3	2.03	0.58
28:2:10:ARG:NH2	30:0:121:U:OP2	2.32	0.58
30:0:407:A:H5'	38:0:6057:HOH:O	2.04	0.58
4:D:103:ASN:HD22	4:D:134:LEU:H	1.49	0.58
30:0:660:A:H4'	30:0:661:G:O5'	2.04	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.34	0.58
30:0:2346:C:O5'	30:0:2346:C:H6	1.86	0.58
30:0:441:A:H1'	30:0:442:A:N7	2.19	0.58
2:B:238:ASN:HD22	2:B:240:GLY:N	1.96	0.58
23:W:139:GLY:O	23:W:141:HIS:HD2	1.87	0.58
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.85	0.58
30:0:1819:G:H5'	38:0:5847:HOH:O	2.04	0.57
12:L:145:LEU:O	12:L:148:GLU:HG3	2.03	0.57
17:Q:11:ARG:HG3	30:0:2363:G:O2'	2.04	0.57
30:0:1477:C:H5'	30:0:1868:G:C5'	2.34	0.57
30:0:192:A:H5'	38:0:7682:HOH:O	2.03	0.57
30:0:567:U:C5'	38:0:6435:HOH:O	2.52	0.57
30:0:947:U:H2'	30:0:948:G:C8	2.39	0.57
30:0:228:C:H2'	30:0:229:G:H5'	1.86	0.57
30:0:644:G:N3	30:0:644:G:H5'	2.19	0.57
30:0:88:G:H2'	30:0:89:G:C8	2.39	0.57
3:C:79:ARG:O	3:C:87:ARG:HG2	2.04	0.57
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.86	0.57
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.03	0.57
22:V:39:ALA:N	22:V:40:PRO:HD2	2.19	0.57
30:0:711:G:C2	30:0:718:C:C2	2.92	0.57
31:9:1:U:O3'	31:9:3:A:H5'	2.03	0.57
30:0:2894:C:O2'	30:0:2895:C:H5'	2.05	0.57
30:0:1183:C:C2	30:0:1184:C:C5	2.93	0.57
30:0:1592:G:H2'	30:0:1593:C:H6	1.69	0.57
30:0:1714:C:O2'	30:0:1715:C:H5'	2.05	0.57
30:0:512:G:O3'	30:0:513:A:H8	1.87	0.57
1:A:51:ARG:HB2	38:A:9060:HOH:O	2.04	0.57
24:X:25:ARG:HD3	24:X:64:ALA:O	2.05	0.57
30:0:2372:A:H2'	30:0:2373:U:C6	2.39	0.57
18:R:68:HIS:O	30:0:2842:G:H5'	2.05	0.57
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.86	0.57
12:L:41:HIS:HD2	30:0:926:A:O2'	1.88	0.57
30:0:1768:C:H2'	30:0:1769:C:O4'	2.05	0.57
30:0:1942:A:H5'	38:0:7386:HOH:O	2.05	0.57
30:0:396:U:O2'	30:0:418:C:H4'	2.04	0.57
30:0:541:C:H2'	30:0:542:A:H5'	1.87	0.57
30:0:1477:C:O2'	30:0:1478:U:H5'	2.05	0.56
31:9:49:G:H5''	38:9:9090:HOH:O	2.05	0.56
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.87	0.56
10:J:74:ARG:NH1	10:J:144:THR:HG21	2.20	0.56
18:R:117:HIS:HD2	30:0:20:G:H21	1.53	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2269:C:H2'	30:0:2270:G:H5'	1.86	0.56
30:0:2320:U:H4'	30:0:2321:A:O4'	2.04	0.56
30:0:283:U:C5	30:0:284:C:N3	2.73	0.56
30:0:366:U:H2'	30:0:367:G:O4'	2.05	0.56
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.87	0.56
30:0:2005:G:H3'	30:0:2005:G:OP2	2.06	0.56
30:0:2668:G:H2'	30:0:2669:U:C6	2.40	0.56
30:0:485:A:N3	30:0:487:G:H5''	2.20	0.56
31:9:1:U:O3'	31:9:3:A:C5'	2.53	0.56
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.87	0.56
30:0:255:A:H2'	30:0:256:C:H6	1.71	0.56
30:0:542:A:H2'	30:0:543:G:O4'	2.05	0.56
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.86	0.56
31:9:12:C:H5'	31:9:70:U:O4'	2.04	0.56
2:B:71:VAL:HG21	2:B:296:LEU:HB3	1.87	0.56
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.70	0.56
30:0:319:A:H4'	30:0:338:C:C4	2.40	0.56
12:L:134:GLU:HG3	38:L:8854:HOH:O	2.06	0.56
23:W:44:MET:CE	30:0:944:G:H21	2.19	0.56
30:0:1206:U:C5'	30:0:1206:U:H6	2.15	0.56
3:C:63:SER:OG	30:0:2101:A:H2'	2.05	0.56
10:J:74:ARG:HH12	10:J:144:THR:HG21	1.71	0.56
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.71	0.56
30:0:2472:C:O2'	30:0:2634:G:H4'	2.05	0.56
30:0:2880:A:H2'	30:0:2881:C:H5'	1.88	0.56
30:0:363:C:H2'	30:0:364:U:H6	1.69	0.56
31:9:114:G:H2'	31:9:115:C:C6	2.41	0.56
31:9:76:G:C3'	31:9:77:A:H5''	2.28	0.56
2:B:145:HIS:HD2	2:B:146:THR:O	1.89	0.56
12:L:143:THR:HG22	12:L:144:ASP:H	1.71	0.56
26:Z:66:CYS:SG	26:Z:67:GLY:N	2.79	0.56
30:0:2002:C:H2'	30:0:2003:U:H5'	1.87	0.56
29:3:70:ARG:HB3	38:3:9064:HOH:O	2.06	0.56
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.41	0.56
30:0:1213:C:O2'	30:0:1214:G:H5'	2.06	0.56
27:1:9:GLY:HA2	30:0:1687:C:O2	2.05	0.56
30:0:2064:U:H5'	30:0:2652:U:H4'	1.87	0.56
27:1:28:HIS:HE1	30:0:776:A:OP1	1.89	0.56
2:B:17:LYS:O	2:B:260:HIS:HD2	1.88	0.56
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.41	0.56
30:0:583:C:H2'	30:0:584:U:H6	1.70	0.56
7:G:20:VAL:O	7:G:24:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1209:C:H2'	30:0:1210:G:C8	2.36	0.55
30:0:681:G:N3	30:0:681:G:H5'	2.21	0.55
30:0:834:G:H4'	30:0:835:U:OP2	2.05	0.55
14:N:164:ASP:CG	14:N:167:ASP:HA	2.26	0.55
30:0:1766:U:O2	30:0:1778:A:H5'	2.06	0.55
30:0:2316:G:H4'	38:0:6125:HOH:O	2.05	0.55
30:0:1904:A:H2'	30:0:1905:U:O4'	2.05	0.55
30:0:2269:C:C2'	30:0:2270:G:H5'	2.36	0.55
30:0:281:U:O2'	30:0:282:C:H5'	2.06	0.55
30:0:283:U:H5	30:0:284:C:N3	2.04	0.55
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.89	0.55
30:0:1676:G:O2'	30:0:1677:U:H5'	2.06	0.55
30:0:1834:C:H2'	30:0:1840:A:N6	2.20	0.55
30:0:236:A:C4'	30:0:237:G:H5'	2.36	0.55
30:0:65:C:O2'	30:0:66:G:H5'	2.06	0.55
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.07	0.55
30:0:1973:A:H5'	30:0:1973:A:C8	2.39	0.55
2:B:125:GLU:O	2:B:129:ARG:HG3	2.06	0.55
30:0:249:G:H2'	30:0:250:C:H6	1.71	0.55
30:0:2748:G:H1'	38:0:7936:HOH:O	2.05	0.55
30:0:2756:U:N3	30:0:2896:A:C2	2.71	0.55
12:L:18:HIS:HD2	30:0:902:G:N7	2.05	0.55
31:9:22:G:H5'	31:9:23:U:OP1	2.06	0.55
14:N:80:SER:HB2	38:N:8833:HOH:O	2.07	0.55
25:Y:203:VAL:HG12	25:Y:228:VAL:HG22	1.89	0.55
30:0:1592:G:H2'	30:0:1593:C:C6	2.42	0.55
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.89	0.55
5:E:11:VAL:HG12	5:E:12:ASP:N	2.22	0.55
26:Z:40:ALA:HA	30:0:1773:G:C8	2.41	0.55
30:0:2748:G:H2'	38:0:7579:HOH:O	2.06	0.55
30:0:282:C:C2'	30:0:283:U:H5'	2.35	0.55
15:O:37:ARG:HD2	30:0:656:G:OP2	2.07	0.55
31:9:49:G:C2'	31:9:50:G:H5'	2.37	0.55
30:0:1200:A:H3'	38:0:5786:HOH:O	2.06	0.55
12:L:41:HIS:CD2	30:0:926:A:O2'	2.60	0.55
14:N:37:ARG:NH1	31:9:6:C:OP1	2.39	0.55
30:0:2768:A:H5''	38:0:4453:HOH:O	2.07	0.55
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.89	0.55
15:O:35:LYS:HD3	38:0:4645:HOH:O	2.06	0.55
13:M:163:LEU:HD21	30:0:188:C:H5''	1.89	0.54
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.37	0.54
30:0:1157:C:H2'	30:0:1158:G:C8	2.40	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2064:U:H5'	30:0:2652:U:O3'	2.08	0.54
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.05	0.54
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.07	0.54
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.42	0.54
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.89	0.54
30:0:1165:G:O2'	30:0:1174:A:C1'	2.54	0.54
30:0:1681:G:H5''	30:0:1682:A:H5'	1.88	0.54
30:0:1819:G:H2'	30:0:1820:G:C4'	2.38	0.54
30:0:1878:G:O2'	30:0:1879:U:P	2.66	0.54
14:N:110:THR:HB	14:N:113:SER:OG	2.08	0.54
38:I:1549:HOH:O	30:0:1180:U:H1'	2.07	0.54
30:0:350:G:H1'	38:0:5705:HOH:O	2.06	0.54
31:9:47:A:C2	31:9:48:C:C2	2.94	0.54
2:B:177:HIS:O	2:B:181:ILE:HG13	2.07	0.54
5:E:132:THR:HB	38:E:2227:HOH:O	2.07	0.54
30:0:363:C:O2'	30:0:364:U:H5'	2.07	0.54
29:3:73:GLU:HB3	38:3:9053:HOH:O	2.08	0.54
31:9:23:U:O2'	31:9:24:U:H4'	2.07	0.54
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.89	0.54
18:R:99:ALA:HB1	18:R:109:MET:CE	2.37	0.54
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.90	0.54
30:0:1947:G:H2'	30:0:1948:G:H8	1.73	0.54
30:0:661:G:C5	30:0:686:A:C2	2.96	0.54
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.08	0.54
8:H:69:ARG:HD3	38:H:231:HOH:O	2.07	0.54
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.73	0.54
30:0:1193:A:H2	30:0:1194:A:N6	2.06	0.54
30:0:1559:A:H4'	38:0:5895:HOH:O	2.07	0.54
30:0:1594:C:O2'	30:0:1607:A:H4'	2.08	0.54
30:0:1755:A:H2'	30:0:1756:G:O4'	2.07	0.54
30:0:1842:A:C4	30:0:1979:G:C6	2.95	0.54
30:0:2135:A:O2'	30:0:2136:G:H5'	2.06	0.54
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.89	0.54
31:9:3:A:H2	31:9:21:G:N3	2.06	0.54
9:I:126:THR:O	9:I:130:LEU:HG	2.08	0.54
23:W:130:HIS:O	23:W:136:GLY:HA3	2.08	0.54
30:0:2415:A:H2'	30:0:2416:G:H5'	1.88	0.54
30:0:2505:G:H2'	30:0:2506:A:H5'	1.89	0.54
30:0:2507:G:H2'	30:0:2510:C:N4	2.23	0.54
30:0:2781:U:C2'	30:0:2782:G:H5'	2.37	0.54
4:D:138:GLY:HA2	31:9:29:C:O3'	2.08	0.54
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1878:G:O2'	30:0:1879:U:H6	1.89	0.54
30:0:877:G:C5'	30:0:878:G:OP1	2.53	0.54
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.90	0.54
16:P:58:SER:HB3	38:0:5659:HOH:O	2.08	0.54
22:V:64:GLY:O	22:V:65:ASP:HB2	2.08	0.54
30:0:10:U:O4	30:0:531:G:H2'	2.08	0.54
30:0:1535:G:H2'	30:0:1536:C:C6	2.43	0.54
30:0:2073:G:OP2	30:0:2490:A:H5'	2.08	0.53
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.73	0.53
14:N:160:SER:HB2	31:9:51:A:H5'	1.90	0.53
30:0:407:A:H3'	38:0:4486:HOH:O	2.08	0.53
31:9:49:G:H2'	31:9:50:G:O4'	2.09	0.53
2:B:198:GLU:HA	38:B:9133:HOH:O	2.07	0.53
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.90	0.53
30:0:1130:U:H2'	30:0:1131:G:O4'	2.08	0.53
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.38	0.53
30:0:2371:G:H5'	38:0:5041:HOH:O	2.08	0.53
30:0:2502:C:H2'	30:0:2503:A:C5'	2.37	0.53
30:0:24:G:N2	30:0:518:G:H1'	2.23	0.53
10:J:19:MET:CE	10:J:132:LEU:HD11	2.39	0.53
20:T:2:LYS:HG2	30:0:447:A:OP1	2.08	0.53
20:T:61:GLU:HG2	38:T:3851:HOH:O	2.09	0.53
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.39	0.53
30:0:1819:G:H2'	30:0:1820:G:C5'	2.38	0.53
30:0:1850:U:H2'	30:0:1851:G:H8	1.73	0.53
30:0:2756:U:N3	30:0:2896:A:H2	2.06	0.53
30:0:953:G:H4'	30:0:954:U:OP1	2.08	0.53
5:E:137:ASP:O	5:E:141:VAL:HG23	2.08	0.53
17:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.08	0.53
30:0:2783:A:H2'	30:0:2784:A:C8	2.44	0.53
2:B:294:TYR:HE2	38:B:9124:HOH:O	1.89	0.53
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.09	0.53
30:0:1333:U:H2'	30:0:1334:C:C6	2.44	0.53
30:0:138:U:OP2	30:0:139:C:H5	1.91	0.53
30:0:1523:G:C6	30:0:1524:U:C4	2.96	0.53
30:0:1787:C:H4'	30:0:2883:A:O4'	2.08	0.53
30:0:368:C:C2'	30:0:369:G:H5'	2.39	0.53
31:9:2:U:H4'	38:9:9103:HOH:O	2.08	0.53
21:U:17:THR:HG22	21:U:18:GLY:N	2.24	0.53
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.91	0.53
30:0:2249:G:C2	30:0:2253:G:C6	2.96	0.53
30:0:67:A:H5''	30:0:69:A:C8	2.44	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:947:U:H2'	30:0:948:G:H8	1.72	0.53
31:9:39:U:O2'	31:9:42:C:C5	2.61	0.53
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.90	0.53
11:K:113:ILE:HD12	11:K:128:ALA:HB2	1.90	0.53
21:U:14:GLU:O	21:U:17:THR:HB	2.08	0.53
30:0:1206:U:H2'	30:0:1207:A:O4'	2.09	0.53
30:0:123:U:H5'	38:0:6694:HOH:O	2.09	0.53
30:0:1556:G:O2'	30:0:1557:G:H5'	2.09	0.53
30:0:2597:U:H2'	30:0:2598:U:H5'	1.90	0.53
5:E:154:ILE:HD11	5:E:157:LYS:HE2	1.90	0.53
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.39	0.53
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.88	0.53
30:0:2897:C:O2'	30:0:2898:G:H5'	2.09	0.53
30:0:960:G:C3'	30:0:960:G:N3	2.72	0.53
3:C:5:ILE:HD11	3:C:16:VAL:CG2	2.39	0.53
13:M:57:LYS:HE2	13:M:140:ALA:O	2.09	0.53
30:0:1206:U:C6	30:0:1206:U:H5'	2.32	0.53
30:0:876:A:N3	30:0:876:A:H2'	2.23	0.53
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.23	0.53
6:F:48:VAL:CG2	6:F:74:PHE:HB3	2.39	0.53
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.23	0.53
30:0:1524:U:OP1	30:0:1524:U:H4'	2.09	0.52
30:0:2781:U:O2'	30:0:2782:G:H5'	2.07	0.52
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.91	0.52
23:W:80:ASP:O	23:W:84:VAL:HG23	2.09	0.52
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	1.91	0.52
30:0:1702:U:H1'	38:0:5805:HOH:O	2.08	0.52
30:0:2314:G:C2'	30:0:2315:C:H5'	2.39	0.52
30:0:241:A:C2	30:0:378:A:H4'	2.44	0.52
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.90	0.52
12:L:4:LYS:HE2	30:0:645:U:OP2	2.09	0.52
25:Y:235:GLU:H	25:Y:235:GLU:CD	2.12	0.52
18:R:150:PRO:CG	18:R:150:PRO:CB	2.86	0.52
30:0:1174:A:C6	30:0:1201:C:H4'	2.45	0.52
30:0:1377:C:H5'	30:0:1377:C:C6	2.45	0.52
30:0:1972:U:H2'	30:0:1973:A:H5'	1.90	0.52
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.92	0.52
4:D:159:PRO:O	4:D:163:VAL:HG23	2.09	0.52
13:M:30:GLU:O	13:M:34:GLU:HG3	2.10	0.52
30:0:113:A:OP2	30:0:114:A:H2'	2.09	0.52
30:0:2478:U:O2'	30:0:2479:A:H5'	2.08	0.52
3:C:153:VAL:O	3:C:157:LEU:HG	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:50:VAL:HG13	31:9:41:C:O4'	2.10	0.52
17:Q:25:PRO:HB2	38:9:9082:HOH:O	2.10	0.52
19:S:43:GLU:HB3	38:S:8991:HOH:O	2.10	0.52
30:0:1135:G:H5'	38:0:5960:HOH:O	2.09	0.52
28:2:39:ARG:HG2	38:2:3143:HOH:O	2.08	0.52
12:L:143:THR:HG22	12:L:144:ASP:N	2.25	0.52
20:T:38:ARG:NH1	38:0:6725:HOH:O	2.42	0.52
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.45	0.52
30:0:2105:C:H2'	30:0:2106:C:C6	2.44	0.52
30:0:2250:G:H2'	30:0:2251:G:O4'	2.09	0.52
30:0:2664:A:OP1	30:0:2664:A:H8	1.93	0.52
30:0:2681:A:H4'	30:0:2682:C:C5'	2.39	0.52
30:0:602:A:O2'	30:0:605:C:H4'	2.09	0.52
1:A:36:ASP:HB2	1:A:84:VAL:N	2.25	0.52
4:D:138:GLY:N	38:D:7597:HOH:O	2.42	0.52
8:H:48:VAL:HA	8:H:170:ARG:O	2.10	0.52
30:0:2509:A:OP2	30:0:2510:C:H5	1.93	0.52
30:0:1444:G:O2'	30:0:1445:G:H5'	2.09	0.52
30:0:1921:A:C6	30:0:1922:A:C2	2.98	0.52
30:0:1930:A:H2'	30:0:1931:A:C8	2.45	0.52
30:0:968:G:O2'	30:0:969:G:H5'	2.10	0.52
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.91	0.52
30:0:1279:U:O2	30:0:1279:U:C2'	2.58	0.52
30:0:1289:C:O2'	30:0:1290:G:H5'	2.10	0.52
30:0:12:U:H2'	30:0:13:G:H5'	1.91	0.52
30:0:1805:G:O2'	30:0:1806:G:H5'	2.10	0.52
30:0:2237:G:O2'	30:0:2238:A:C8	2.62	0.52
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.10	0.52
30:0:2878:U:H2'	30:0:2879:A:O4'	2.10	0.52
30:0:704:C:H2'	30:0:705:C:H6	1.75	0.52
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.10	0.52
30:0:1130:U:H5'	38:0:7710:HOH:O	2.10	0.51
30:0:1188:A:C6	30:0:1189:A:C6	2.99	0.51
30:0:185:G:H4'	30:0:186:A:OP1	2.10	0.51
30:0:200:C:H2'	38:0:3463:HOH:O	2.09	0.51
30:0:2531:U:O2'	30:0:2532:A:H5'	2.10	0.51
31:9:24:U:H3'	31:9:25:G:H5'	1.91	0.51
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.91	0.51
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.92	0.51
13:M:179:GLY:O	30:0:399:C:H5'	2.10	0.51
23:W:64:THR:O	23:W:68:THR:HG22	2.10	0.51
30:0:2250:G:N2	30:0:2251:G:H1'	2.25	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2830:U:O2'	30:0:2831:C:H5'	2.09	0.51
30:0:299:U:H5'	38:0:7375:HOH:O	2.09	0.51
2:B:148:PRO:HD2	38:B:9049:HOH:O	2.10	0.51
6:F:57:GLU:O	6:F:61:MET:HG3	2.10	0.51
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.26	0.51
22:V:12:THR:HG23	22:V:14:ALA:H	1.75	0.51
23:W:119:HIS:HD2	23:W:120:PRO:O	1.92	0.51
30:0:1762:C:O2'	30:0:1763:C:H5'	2.10	0.51
30:0:363:C:H2'	30:0:364:U:C6	2.46	0.51
30:0:10:U:O4	30:0:532:A:OP2	2.28	0.51
30:0:541:C:O2'	30:0:542:A:H5''	2.11	0.51
31:9:39:U:O2'	31:9:42:C:H5	1.92	0.51
3:C:145:GLU:HG3	38:C:8569:HOH:O	2.09	0.51
23:W:24:LEU:O	23:W:26:ILE:HG22	2.10	0.51
30:0:2252:A:H2'	30:0:2253:G:H5'	1.92	0.51
30:0:228:C:C2'	30:0:229:G:H5'	2.41	0.51
30:0:2825:C:H4'	30:0:2826:G:O5'	2.10	0.51
30:0:285:A:H2'	30:0:286:U:O4'	2.10	0.51
31:9:1:U:C4'	31:9:3:A:OP1	2.59	0.51
2:B:211:THR:HG21	38:0:7492:HOH:O	2.11	0.51
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.92	0.51
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.92	0.51
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.41	0.51
30:0:1386:G:O2'	30:0:1387:G:H5'	2.11	0.51
30:0:414:C:H5'	38:0:9667:HOH:O	2.11	0.51
30:0:958:G:H2'	30:0:959:C:C6	2.45	0.51
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.44	0.51
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.93	0.51
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.93	0.51
30:0:1205:U:O2'	30:0:1206:U:H5''	2.11	0.51
30:0:2421:G:H3'	30:0:2422:U:H5''	1.92	0.51
30:0:2781:U:H2'	30:0:2782:G:C5'	2.40	0.51
30:0:2826:G:C6	30:0:2913:A:N6	2.78	0.51
30:0:69:A:H8	30:0:69:A:C5'	2.15	0.51
14:N:77:ASN:OD1	14:N:79:PRO:HD2	2.11	0.51
25:Y:189:ASN:HD22	25:Y:189:ASN:C	2.14	0.51
30:0:1398:G:O2'	30:0:1399:A:H5'	2.11	0.51
30:0:2241:C:O2'	30:0:2242:U:H5'	2.11	0.51
30:0:541:C:C2'	30:0:542:A:C5'	2.79	0.51
30:0:790:A:H2'	30:0:791:A:O4'	2.10	0.51
31:9:91:C:H2'	31:9:92:G:O4'	2.10	0.51
3:C:46:TYR:CE2	3:C:98:ARG:NH1	2.79	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:X:23:HIS:HD2	38:0:9973:HOH:O	1.93	0.51
12:L:14:GLY:O	30:0:1295:G:H5''	2.11	0.51
30:0:2764:C:O2'	30:0:2765:C:H5'	2.10	0.51
30:0:2781:U:H2'	30:0:2782:G:H5'	1.92	0.51
30:0:282:C:O2'	30:0:283:U:C5'	2.50	0.51
30:0:346:U:H4'	38:0:6884:HOH:O	2.11	0.51
2:B:256:GLN:HG2	38:B:9132:HOH:O	2.11	0.51
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.59	0.51
16:P:7:LYS:HD3	16:P:21:VAL:CG2	2.41	0.51
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.93	0.51
19:S:33:SER:O	19:S:37:VAL:HG23	2.11	0.51
30:0:2251:G:H2'	30:0:2252:A:H8	1.72	0.51
30:0:952:G:N3	30:0:2302:A:H2'	2.26	0.51
29:3:15:ASN:O	30:0:2408:A:H4'	2.11	0.51
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.93	0.51
30:0:1419:U:H2'	30:0:1685:A:C2	2.46	0.51
2:B:41:PHE:HA	2:B:79:MET:HE2	1.92	0.51
3:C:233:THR:HG22	3:C:234:VAL:N	2.26	0.51
25:Y:184:GLU:OE2	25:Y:204:ARG:HD2	2.11	0.51
30:0:120:A:H2'	30:0:120:A:N3	2.27	0.50
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.76	0.50
30:0:1167:G:H2'	30:0:1168:C:C6	2.46	0.50
30:0:1186:C:N4	30:0:1187:U:C4	2.79	0.50
30:0:249:G:H2'	30:0:250:C:C6	2.46	0.50
30:0:289:G:O2'	30:0:290:C:H5'	2.12	0.50
30:0:383:A:H4'	38:0:5359:HOH:O	2.10	0.50
30:0:683:G:O2'	30:0:684:G:H5'	2.11	0.50
2:B:85:ARG:NH1	38:B:9109:HOH:O	2.44	0.50
22:V:56:ILE:O	22:V:60:GLN:HG3	2.11	0.50
30:0:1183:C:O2	30:0:1183:C:H2'	2.10	0.50
30:0:1202:A:C2'	30:0:1203:G:H5'	2.40	0.50
30:0:1494:A:H1'	30:0:1495:C:C6	2.47	0.50
30:0:1557:G:O2'	30:0:1558:C:H5'	2.11	0.50
30:0:1972:U:C2'	30:0:1973:A:H5''	2.41	0.50
2:B:41:PHE:CD2	2:B:190:MET:HE3	2.45	0.50
5:E:8:PRO:HB2	5:E:11:VAL:HG23	1.94	0.50
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.94	0.50
30:0:1183:C:H42	30:0:1184:C:N4	2.05	0.50
30:0:559:U:C5'	30:0:559:U:H6	2.20	0.50
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.27	0.50
2:B:314:ALA:HB3	2:B:317:PRO:HG3	1.94	0.50
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.12	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:O:39:THR:O	15:O:115:ARG:NH2	2.44	0.50
22:V:44:GLY:O	22:V:48:GLU:HG2	2.12	0.50
30:0:2610:U:H4'	38:0:9491:HOH:O	2.12	0.50
30:0:69:A:C8	30:0:69:A:C5'	2.89	0.50
30:0:858:U:H5	38:0:5459:HOH:O	1.93	0.50
30:0:95:A:H5''	30:0:97:G:O4'	2.11	0.50
1:A:135:VAL:HA	1:A:150:PRO:HD3	1.93	0.50
5:E:7:ILE:HG13	5:E:11:VAL:HB	1.93	0.50
8:H:66:GLU:HA	38:H:231:HOH:O	2.11	0.50
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.94	0.50
11:K:66:ARG:HH22	30:0:1994:A:P	2.35	0.50
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.95	0.50
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.11	0.50
30:0:1588:G:C6	30:0:1589:G:N1	2.80	0.50
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.47	0.50
30:0:1795:G:H2'	30:0:1796:A:O4'	2.12	0.50
30:0:1878:G:C1'	38:0:6153:HOH:O	2.47	0.50
27:1:16:HIS:HE1	30:0:775:G:OP1	1.94	0.50
31:9:13:A:O2'	31:9:14:G:H5''	2.12	0.50
10:J:42:GLU:O	10:J:131:THR:HG23	2.12	0.50
24:X:61:ARG:NH1	24:X:67:PRO:HD3	2.27	0.50
30:0:1118:A:H8	30:0:1119:G:H5''	1.76	0.50
30:0:2421:G:H3'	30:0:2422:U:C5'	2.42	0.50
5:E:143:GLN:HE22	30:0:2779:G:H21	1.55	0.50
30:0:2793:A:N6	38:0:5912:HOH:O	2.44	0.50
30:0:2883:A:H2'	30:0:2884:G:O4'	2.12	0.50
3:C:19:PRO:HG2	3:C:22:PHE:CE1	2.47	0.50
18:R:111:ILE:HG23	18:R:145:LEU:CD1	2.41	0.50
23:W:149:LEU:HG	23:W:153:MET:CE	2.41	0.50
23:W:65:VAL:HG12	23:W:116:LEU:HD13	1.94	0.50
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.30	0.50
30:0:912:A:C4	30:0:1294:A:C2	2.99	0.50
30:0:154:C:H2'	30:0:155:C:H6	1.76	0.50
30:0:1667:A:H2'	30:0:1668:U:C6	2.47	0.50
30:0:264:G:H1'	30:0:265:U:H5	1.77	0.50
31:9:36:C:C5	31:9:37:C:C5	3.00	0.50
2:B:310:ARG:HD2	38:B:9122:HOH:O	2.12	0.50
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.93	0.50
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.93	0.50
14:N:132:ASN:O	14:N:135:VAL:HG12	2.12	0.50
23:W:139:GLY:O	23:W:141:HIS:CD2	2.64	0.50
30:0:968:G:C2	30:0:1001:U:O2	2.65	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2820:A:H2'	30:0:2821:C:C6	2.47	0.50
30:0:2896:A:N3	30:0:2896:A:H2'	2.27	0.50
30:0:79:G:N2	30:0:97:G:H1'	2.27	0.50
30:0:79:G:H22	30:0:97:G:H1'	1.77	0.50
30:0:969:G:H1	30:0:999:C:N4	2.10	0.50
1:A:35:GLY:O	1:A:36:ASP:HB3	2.12	0.50
5:E:69:ILE:HA	5:E:72:MET:CE	2.41	0.50
5:E:84:MET:HB2	5:E:131:LEU:HB2	1.94	0.50
8:H:123:ILE:HD12	8:H:123:ILE:N	2.27	0.50
30:0:1149:U:H5''	30:0:1151:G:O4'	2.12	0.49
30:0:1644:C:H2'	30:0:1645:U:H6	1.77	0.49
30:0:1848:G:O2'	30:0:1849:G:H5'	2.12	0.49
30:0:2010:A:C2'	38:0:5990:HOH:O	2.56	0.49
4:D:52:THR:HG21	30:0:2347:C:H5'	1.94	0.49
30:0:2577:A:H8	38:0:9613:HOH:O	1.95	0.49
30:0:886:A:OP2	30:0:2113:G:H5'	2.11	0.49
30:0:941:G:C5	30:0:942:U:C4	3.00	0.49
31:9:95:C:O2'	31:9:96:C:H5'	2.12	0.49
19:S:76:GLU:HB3	38:S:8992:HOH:O	2.11	0.49
22:V:39:ALA:H	22:V:40:PRO:HD2	1.76	0.49
30:0:2256:G:C2'	30:0:2257:G:C5'	2.89	0.49
30:0:2793:A:H2'	30:0:2794:G:H5'	1.94	0.49
29:3:60:LYS:HG3	38:0:7595:HOH:O	2.12	0.49
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.77	0.49
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.94	0.49
2:B:254:GLN:HG2	2:B:255:GLY:N	2.27	0.49
3:C:236:THR:HA	38:C:8644:HOH:O	2.12	0.49
4:D:103:ASN:ND2	4:D:133:ASN:HD22	2.10	0.49
14:N:37:ARG:NH2	38:N:8831:HOH:O	2.45	0.49
30:0:2092:G:H2'	30:0:2613:G:OP1	2.13	0.49
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.11	0.49
10:J:131:THR:HB	10:J:134:GLU:HG3	1.95	0.49
13:M:122:GLN:OE1	13:M:127:LYS:HE2	2.13	0.49
16:P:41:ARG:HH22	30:0:1500:U:P	2.35	0.49
25:Y:154:ARG:NH1	25:Y:155:ARG:HG3	2.28	0.49
30:0:1972:U:H2'	30:0:1973:A:H5''	1.92	0.49
30:0:2724:U:H2'	30:0:2725:G:O4'	2.12	0.49
30:0:2851:G:H2'	30:0:2852:A:H5'	1.91	0.49
30:0:301:C:O2'	30:0:302:A:H5'	2.13	0.49
1:A:51:ARG:NH1	1:A:120:ARG:O	2.46	0.49
2:B:54:VAL:HB	38:B:9087:HOH:O	2.11	0.49
3:C:43:LYS:HG2	30:0:449:A:N7	2.28	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1198:U:C6	30:0:1200:A:OP2	2.65	0.49
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.93	0.49
13:M:193:LYS:HB3	30:0:392:U:H4'	1.94	0.49
30:0:671:A:O2'	30:0:672:G:H2'	2.13	0.49
31:9:39:U:HO2'	31:9:42:C:H5	1.52	0.49
2:B:26:PHE:HE1	38:B:9122:HOH:O	1.96	0.49
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.93	0.49
5:E:69:ILE:HA	5:E:72:MET:HE3	1.95	0.49
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.95	0.49
20:T:54:ASP:OD2	30:0:316:A:H5'	2.12	0.49
21:U:33:SER:O	21:U:37:GLU:HG3	2.13	0.49
30:0:1666:C:HO2'	30:0:1667:A:H5''	1.70	0.49
30:0:2265:U:H2'	30:0:2266:A:C8	2.48	0.49
30:0:2356:A:H5'	38:0:5666:HOH:O	2.12	0.49
30:0:2467:A:H2'	38:0:5488:HOH:O	2.12	0.49
30:0:255:A:C4	30:0:256:C:C6	3.00	0.49
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.42	0.49
30:0:1008:C:O2'	30:0:1009:U:H5'	2.13	0.49
30:0:1552:G:H2'	30:0:1553:C:C6	2.47	0.49
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.95	0.49
20:T:52:ARG:O	30:0:317:A:OP1	2.29	0.49
25:Y:154:ARG:HH21	30:0:1293:U:H5'	1.78	0.49
30:0:790:A:H1'	30:0:1710:A:H2'	1.95	0.49
30:0:2453:G:H5''	38:0:4755:HOH:O	2.13	0.49
30:0:255:A:H2'	30:0:256:C:C6	2.47	0.49
30:0:2717:C:C2'	30:0:2718:C:C5'	2.79	0.49
30:0:2769:C:C2'	30:0:2770:G:C5'	2.84	0.49
30:0:304:G:H1'	30:0:347:A:N6	2.28	0.49
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.94	0.49
8:H:30:LYS:H	8:H:62:HIS:CD2	2.30	0.49
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.93	0.49
30:0:154:C:H2'	30:0:155:C:C6	2.48	0.49
30:0:1857:A:H5''	38:0:6744:HOH:O	2.12	0.49
30:0:2002:C:C2'	30:0:2003:U:H5'	2.42	0.49
30:0:2316:G:OP1	30:0:2317:C:H1'	2.13	0.49
30:0:513:A:N3	38:0:3679:HOH:O	2.35	0.49
30:0:1158:G:O2'	30:0:1159:G:H5'	2.13	0.48
30:0:1391:G:H2'	30:0:1392:A:H5'	1.95	0.48
30:0:1562:C:O2	30:0:1562:C:H2'	2.12	0.48
30:0:282:C:O2	30:0:282:C:H2'	2.13	0.48
3:C:115:LEU:HD21	3:C:243:VAL:HG13	1.94	0.48
5:E:47:VAL:HG11	5:E:69:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:67:LEU:O	7:G:71:LEU:HG	2.12	0.48
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.42	0.48
21:U:37:GLU:HB3	38:U:408:HOH:O	2.11	0.48
22:V:1:THR:HG23	22:V:2:VAL:HG23	1.94	0.48
30:0:1159:G:H1	30:0:1208:C:H42	1.58	0.48
30:0:1825:U:O2'	30:0:1826:C:H5'	2.12	0.48
27:1:1:THR:O	30:0:1836:A:H1'	2.13	0.48
30:0:195:C:H2'	30:0:196:G:H5'	1.95	0.48
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.45	0.48
10:J:75:PRO:HB3	10:J:132:LEU:HB3	1.95	0.48
12:L:6:ARG:NH1	30:0:1299:G:N7	2.62	0.48
16:P:83:LYS:HG2	30:0:793:A:H5''	1.94	0.48
24:X:43:VAL:HG12	24:X:44:ASP:N	2.28	0.48
23:W:23:MET:O	30:0:1025:C:H5'	2.12	0.48
30:0:1087:G:H4'	30:0:1088:A:OP1	2.13	0.48
30:0:137:U:H2'	30:0:139:C:C5	2.47	0.48
30:0:1528:A:H2'	30:0:1529:G:O4'	2.13	0.48
30:0:1632:A:C3'	30:0:1633:C:H5'	2.43	0.48
2:B:205:VAL:O	2:B:307:ARG:NE	2.47	0.48
3:C:136:VAL:HG22	3:C:137:PRO:HA	1.95	0.48
15:O:32:ARG:HD3	15:O:32:ARG:O	2.12	0.48
19:S:37:VAL:O	19:S:41:VAL:HG23	2.13	0.48
25:Y:212:ARG:HD2	38:Y:8896:HOH:O	2.12	0.48
26:Z:80:GLN:HA	26:Z:86:TYR:O	2.12	0.48
30:0:1321:A:H2'	30:0:1322:G:C8	2.48	0.48
24:X:30:MET:HG2	30:0:1384:C:H5'	1.94	0.48
30:0:2300:A:H4'	30:0:2301:A:O5'	2.13	0.48
1:A:121:ALA:O	1:A:124:VAL:HG22	2.13	0.48
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.95	0.48
20:T:8:ARG:HD2	30:0:31:C:OP2	2.13	0.48
30:0:1883:U:O2'	30:0:1884:G:H5'	2.13	0.48
30:0:2301:A:H5''	30:0:2302:A:H5'	1.95	0.48
1:A:171:LYS:HB2	30:0:820:G:C5	2.47	0.48
30:0:961:A:H4'	38:0:6814:HOH:O	2.12	0.48
2:B:255:GLY:O	2:B:257:THR:HG22	2.14	0.48
2:B:49:THR:HG21	2:B:331:SER:O	2.14	0.48
3:C:236:THR:H	3:C:239:ALA:HB3	1.78	0.48
6:F:48:VAL:HG23	6:F:74:PHE:CB	2.42	0.48
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.95	0.48
30:0:1165:G:H4'	30:0:1174:A:O2'	2.13	0.48
30:0:2269:C:H2'	30:0:2270:G:C5'	2.44	0.48
30:0:447:A:O2'	30:0:448:G:H5'	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.96	0.48
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.95	0.48
30:0:222:A:H2'	30:0:223:G:O4'	2.14	0.48
30:0:2564:G:OP2	30:0:2565:C:H5''	2.14	0.48
10:J:107:ASN:C	10:J:107:ASN:HD22	2.17	0.48
30:0:1130:U:H4'	38:0:6158:HOH:O	2.13	0.48
30:0:484:A:N1	30:0:506:G:H4'	2.28	0.48
30:0:920:C:H5'	30:0:921:G:C4	2.49	0.48
31:9:45:A:H2'	31:9:46:C:H6	1.79	0.48
6:F:21:GLU:O	6:F:24:ARG:HG2	2.14	0.48
18:R:104:PHE:HB3	18:R:109:MET:HE1	1.96	0.48
30:0:1051:C:H2'	30:0:1052:G:O4'	2.14	0.48
30:0:1131:G:C6	30:0:1230:A:C4	3.02	0.48
30:0:1545:C:H2'	30:0:1546:G:O4'	2.14	0.48
2:B:156:LYS:HB3	30:0:2846:C:H4'	1.94	0.48
30:0:2912:C:H2'	30:0:2913:A:O4'	2.14	0.48
30:0:960:G:H3'	30:0:960:G:C4	2.49	0.48
29:3:48:ASN:ND2	29:3:50:GLY:H	2.11	0.48
3:C:140:VAL:HB	38:C:8644:HOH:O	2.13	0.48
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.46	0.48
15:O:57:THR:HB	15:O:111:VAL:HG23	1.95	0.48
30:0:1625:U:H5''	38:0:6053:HOH:O	2.13	0.48
30:0:1477:C:H5'	30:0:1868:G:H5''	1.96	0.48
30:0:2439:C:H5'	38:0:5518:HOH:O	2.12	0.48
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.44	0.48
2:B:275:GLY:O	2:B:291:ASP:HA	2.14	0.48
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.79	0.48
12:L:121:ILE:HG12	12:L:141:GLU:HB2	1.96	0.48
30:0:2314:G:H2'	30:0:2315:C:H5'	1.96	0.47
30:0:90:A:H2'	30:0:91:G:O4'	2.14	0.47
27:1:28:HIS:HD2	27:1:30:LYS:H	1.60	0.47
1:A:3:ARG:HD3	30:0:870:G:OP2	2.14	0.47
3:C:22:PHE:HA	3:C:116:ALA:HA	1.94	0.47
13:M:64:ARG:HD2	38:M:8881:HOH:O	2.14	0.47
14:N:114:LYS:O	14:N:118:ILE:HG13	2.14	0.47
14:N:169:PRO:O	14:N:172:PHE:HB3	2.14	0.47
14:N:43:VAL:HG13	14:N:118:ILE:HD11	1.96	0.47
23:W:65:VAL:HA	23:W:68:THR:HG22	1.95	0.47
30:0:1666:C:H2'	30:0:1667:A:H5''	1.78	0.47
30:0:1850:U:H2'	30:0:1851:G:C8	2.48	0.47
30:0:1838:U:O2'	30:0:2644:C:H5'	2.14	0.47
30:0:398:U:H2'	30:0:399:C:C6	2.49	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:76:ARG:NE	31:9:44:A:O4'	2.47	0.47
21:U:9:CYS:HA	21:U:52:THR:OG1	2.14	0.47
30:0:1422:U:H2'	30:0:1423:C:C6	2.50	0.47
30:0:1641:A:C2'	30:0:1642:A:H5'	2.44	0.47
30:0:1788:U:O2'	30:0:1789:G:H5'	2.14	0.47
30:0:2264:A:H2'	30:0:2265:U:C6	2.48	0.47
30:0:2506:A:H1'	38:0:3766:HOH:O	2.13	0.47
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.47
27:1:25:LYS:HD2	28:2:48:ASP:HA	1.96	0.47
1:A:217:ARG:CG	1:A:217:ARG:HH11	2.27	0.47
8:H:61:ARG:NH1	8:H:61:ARG:HG3	2.29	0.47
30:0:1268:C:O2'	30:0:1269:G:H5'	2.14	0.47
30:0:1280:A:H3'	30:0:1280:A:OP1	2.15	0.47
30:0:2064:U:H4'	30:0:2653:A:OP1	2.13	0.47
30:0:955:A:C2	30:0:1013:A:C4	3.03	0.47
1:A:30:ARG:NH2	1:A:38:ILE:HG13	2.28	0.47
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.79	0.47
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.50	0.47
6:F:107:ASP:O	6:F:111:ILE:HG13	2.14	0.47
16:P:143:ALA:HA	38:P:184:HOH:O	2.13	0.47
23:W:154:ARG:NH1	30:0:588:G:O6	2.47	0.47
30:0:1193:A:C2	30:0:1194:A:N6	2.78	0.47
30:0:1252:A:H2'	30:0:1253:C:O4'	2.14	0.47
30:0:137:U:OP1	30:0:259:G:O2'	2.33	0.47
14:N:40:ASN:HD21	31:9:28:U:H5''	1.80	0.47
31:9:56:A:C3'	31:9:57:A:H5''	2.44	0.47
8:H:39:LYS:HA	8:H:87:LYS:NZ	2.30	0.47
11:K:87:ARG:NH2	30:0:2720:C:O2	2.47	0.47
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.49	0.47
30:0:1393:A:H2'	30:0:1394:C:C6	2.49	0.47
30:0:2271:G:H5'	38:0:4783:HOH:O	2.14	0.47
30:0:2469:A:H2'	38:0:7512:HOH:O	2.15	0.47
30:0:407:A:H2'	30:0:408:A:C8	2.50	0.47
1:A:105:VAL:HG11	1:A:154:ALA:HB1	1.97	0.47
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.48	0.47
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.15	0.47
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.45	0.47
16:P:120:ARG:NH1	30:0:1594:C:C5	2.82	0.47
24:X:85:VAL:HG12	24:X:86:GLU:N	2.30	0.47
25:Y:151:SER:HB3	25:Y:154:ARG:HB3	1.97	0.47
30:0:1118:A:C8	30:0:1119:G:H5''	2.49	0.47
30:0:1762:C:H2'	30:0:1763:C:H6	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.47	0.47
30:0:2353:A:H4'	30:0:2354:A:O5'	2.14	0.47
30:0:440:C:H2'	30:0:441:A:C8	2.50	0.47
4:D:10:PHE:CG	4:D:11:HIS:N	2.81	0.47
12:L:149:ARG:O	12:L:150:GLN:HB2	2.14	0.47
30:0:1176:C:N4	38:0:5775:HOH:O	2.48	0.47
30:0:283:U:H5	30:0:284:C:N4	2.12	0.47
17:Q:32:GLU:O	17:Q:93:ARG:NH2	2.48	0.47
30:0:2791:U:H1'	30:0:2792:A:H5''	1.97	0.47
30:0:426:G:H2'	30:0:427:C:O4'	2.15	0.47
30:0:483:C:C4	30:0:484:A:C6	3.03	0.47
27:1:22:CYS:SG	27:1:24:GLU:HB2	2.55	0.47
29:3:65:THR:HB	29:3:83:TRP:H	1.79	0.47
31:9:52:A:H2'	31:9:53:G:O4'	2.15	0.47
13:M:164:THR:HG22	13:M:166:ALA:N	2.29	0.47
23:W:11:VAL:HG11	30:0:1086:A:C6	2.49	0.47
30:0:1682:A:H2'	38:0:9820:HOH:O	2.14	0.47
30:0:2533:C:C6	30:0:2533:C:C5'	2.92	0.47
31:9:55:U:H4'	31:9:56:A:C8	2.49	0.47
6:F:91:VAL:HG12	6:F:92:GLY:H	1.78	0.47
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.45	0.47
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.44	0.47
30:0:1249:U:H2'	30:0:1250:C:C6	2.50	0.47
30:0:1477:C:C5'	30:0:1868:G:H5''	2.44	0.47
30:0:1928:C:H2'	30:0:1929:G:H5'	1.96	0.47
30:0:2281:C:H2'	30:0:2282:U:H5'	1.97	0.47
30:0:2372:A:H2'	30:0:2373:U:H6	1.78	0.47
30:0:816:G:C6	30:0:817:G:N1	2.83	0.47
2:B:297:VAL:HB	38:B:9080:HOH:O	2.15	0.47
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.97	0.47
30:0:170:U:H2'	30:0:171:C:H5'	1.95	0.46
30:0:2011:A:H4'	30:0:2012:U:O5'	2.15	0.46
30:0:2238:A:H3'	38:0:6711:HOH:O	2.15	0.46
30:0:2589:U:H2'	30:0:2590:U:C6	2.50	0.46
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.30	0.46
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.15	0.46
23:W:4:LEU:CD2	23:W:54:PHE:HB3	2.35	0.46
26:Z:34:SER:HB3	30:0:797:A:H4'	1.96	0.46
1:A:175:LYS:HG3	30:0:1847:A:OP1	2.16	0.46
27:1:11:LYS:HG2	30:0:777:U:O2'	2.15	0.46
31:9:28:U:H2'	31:9:29:C:C6	2.50	0.46
2:B:307:ARG:NH1	2:B:307:ARG:HG3	2.19	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:172:GLU:HB3	38:H:243:HOH:O	2.15	0.46
21:U:50:GLU:HB2	30:0:2866:U:C5	2.50	0.46
24:X:43:VAL:HG12	24:X:47:ALA:HB3	1.97	0.46
25:Y:165:GLU:HB3	38:0:6747:HOH:O	2.15	0.46
16:P:1:THR:O	30:0:1396:C:H1'	2.15	0.46
30:0:1907:U:O2'	30:0:1908:G:H5'	2.15	0.46
30:0:304:G:H1'	30:0:347:A:H61	1.80	0.46
30:0:559:U:C5	30:0:560:U:C5	3.03	0.46
30:0:800:G:H2'	30:0:801:U:C6	2.50	0.46
30:0:969:G:H1	30:0:999:C:H42	1.62	0.46
14:N:141:ARG:NH2	31:9:48:C:H4'	2.30	0.46
30:0:105:G:O2'	30:0:106:A:H5'	2.15	0.46
25:Y:115:ARG:NH2	30:0:1266:U:H4'	2.30	0.46
30:0:2103:A:H2'	30:0:2104:C:H5'	1.96	0.46
30:0:699:C:C2	30:0:744:G:C2	3.03	0.46
30:0:690:G:H4'	30:0:741:C:O2	2.15	0.46
1:A:132:ASP:HB3	1:A:135:VAL:H	1.80	0.46
1:A:88:ILE:HG22	1:A:88:ILE:O	2.14	0.46
3:C:129:HIS:HD2	3:C:165:ASP:OD2	1.99	0.46
17:Q:42:LYS:HE2	30:0:952:G:OP1	2.15	0.46
23:W:122:ARG:NH2	38:0:5320:HOH:O	2.48	0.46
10:J:82:THR:CG2	30:0:1242:A:H5'	2.30	0.46
30:0:1117:A:C2	30:0:1244:U:C2	3.04	0.46
30:0:1657:A:H2'	30:0:1658:A:C8	2.51	0.46
30:0:343:C:O2'	30:0:344:C:H5'	2.15	0.46
30:0:638:C:H2'	30:0:639:A:C8	2.51	0.46
30:0:920:C:H5''	30:0:921:G:O5'	2.15	0.46
31:9:101:G:H5''	38:9:9140:HOH:O	2.15	0.46
2:B:320:GLN:HE21	2:B:321:PRO:CD	2.24	0.46
8:H:139:ALA:HB3	8:H:149:VAL:HG21	1.97	0.46
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.31	0.46
10:J:107:ASN:HD22	10:J:109:TYR:H	1.64	0.46
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.51	0.46
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.96	0.46
30:0:11:A:H5'	30:0:12:U:OP2	2.15	0.46
30:0:1503:U:H2'	30:0:1504:A:O4'	2.15	0.46
30:0:1596:U:H2'	30:0:1598:A:OP2	2.15	0.46
30:0:2712:G:H5'	38:0:5251:HOH:O	2.15	0.46
30:0:583:C:C2	30:0:584:U:C5	3.03	0.46
1:A:51:ARG:HD2	30:0:1874:U:OP1	2.15	0.46
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.95	0.46
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.82	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:T:28:SER:O	20:T:32:ARG:HG3	2.15	0.46
30:0:1883:U:C2'	30:0:1884:G:H5'	2.46	0.46
30:0:613:C:H2'	30:0:614:U:H6	1.80	0.46
30:0:812:A:H2'	30:0:813:C:O4'	2.16	0.46
27:1:1:THR:HA	38:0:9368:HOH:O	2.16	0.46
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.54	0.46
31:9:39:U:C2'	31:9:40:C:OP1	2.63	0.46
18:R:104:PHE:CB	18:R:109:MET:HE1	2.46	0.46
24:X:30:MET:CE	24:X:58:ALA:HB3	2.45	0.46
30:0:1202:A:O2'	30:0:1203:G:H5'	2.16	0.46
30:0:1928:C:C2'	30:0:1929:G:H5'	2.46	0.46
1:A:214:SER:HB2	38:0:4392:HOH:O	2.15	0.46
3:C:206:ASN:HB2	30:0:329:A:OP2	2.15	0.46
4:D:27:ILE:HB	4:D:69:ILE:O	2.15	0.46
8:H:61:ARG:HG3	38:0:5004:HOH:O	2.15	0.46
18:R:132:ARG:NH1	38:R:8984:HOH:O	2.48	0.46
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.98	0.46
10:J:63:ILE:CD1	30:0:1236:A:C8	2.99	0.46
30:0:2065:C:O2'	30:0:2066:C:H5'	2.16	0.46
30:0:2445:U:H2'	30:0:2446:G:C8	2.51	0.46
30:0:2758:G:H2'	30:0:2759:C:C6	2.51	0.46
18:R:29:LYS:HD3	30:0:524:A:H5''	1.98	0.46
30:0:622:G:O2'	30:0:623:U:H5'	2.16	0.46
30:0:711:G:H1'	38:0:7133:HOH:O	2.14	0.46
30:0:71:G:H5''	38:0:3932:HOH:O	2.16	0.46
28:2:20:ARG:HD3	38:0:6163:HOH:O	2.16	0.46
31:9:29:C:C2'	31:9:30:C:H5'	2.42	0.46
6:F:91:VAL:HG11	30:0:262:A:OP2	2.16	0.46
11:K:74:VAL:HG13	11:K:113:ILE:HG23	1.97	0.46
30:0:1311:G:C2	30:0:1312:G:C8	3.04	0.46
30:0:1790:C:H2'	30:0:1791:U:C6	2.50	0.46
30:0:2241:C:H2'	30:0:2242:U:C6	2.51	0.46
30:0:2379:G:N7	30:0:2408:A:N1	2.63	0.46
1:A:206:ARG:NH2	30:0:2630:G:O6	2.49	0.46
2:B:141:ARG:N	38:B:9048:HOH:O	2.48	0.46
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.98	0.46
30:0:1511:U:O2'	30:0:1512:G:H5'	2.16	0.45
30:0:1522:A:C2	30:0:1665:G:C6	3.04	0.45
30:0:162:C:H2'	30:0:163:U:H5'	1.98	0.45
30:0:2415:A:C2'	30:0:2416:G:H5'	2.46	0.45
30:0:278:A:H2'	30:0:279:C:O4'	2.16	0.45
30:0:2872:U:H2'	30:0:2873:C:H6	1.81	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2880:A:C2'	30:0:2881:C:H5'	2.46	0.45
30:0:2831:C:H42	30:0:2909:G:H1	1.64	0.45
30:0:372:A:H2'	30:0:373:G:C8	2.51	0.45
30:0:78:G:C6	30:0:79:G:C6	3.04	0.45
1:A:194:MET:HG2	30:0:875:A:C2	2.52	0.45
30:0:876:A:N3	30:0:876:A:C2'	2.80	0.45
29:3:62:THR:HB	38:3:9044:HOH:O	2.15	0.45
2:B:62:ARG:HA	2:B:65:MET:CE	2.46	0.45
30:0:1194:A:O2'	30:0:1195:G:H5'	2.16	0.45
30:0:1074:G:H4'	30:0:1260:G:C6	2.51	0.45
30:0:1339:G:C6	30:0:1340:G:N1	2.85	0.45
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.31	0.45
30:0:1778:A:H2'	30:0:1779:A:H5'	1.97	0.45
30:0:412:C:O2'	30:0:413:G:H5'	2.16	0.45
30:0:53:C:H2'	30:0:54:G:O4'	2.16	0.45
30:0:669:G:O2'	30:0:670:G:H5'	2.16	0.45
30:0:758:A:H2'	30:0:759:C:O4'	2.17	0.45
10:J:75:PRO:HD3	10:J:136:SER:OG	2.16	0.45
20:T:63:ILE:HD11	20:T:75:GLU:HB2	1.99	0.45
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.98	0.45
30:0:2456:A:H2'	30:0:2457:U:C6	2.51	0.45
30:0:407:A:H8	38:0:4486:HOH:O	2.00	0.45
30:0:445:U:H2'	30:0:446:G:H8	1.81	0.45
3:C:19:PRO:HG2	3:C:22:PHE:CD1	2.51	0.45
7:G:64:ASN:N	7:G:64:ASN:ND2	2.63	0.45
23:W:38:THR:HG22	23:W:39:ASP:N	2.31	0.45
30:0:1333:U:H2'	30:0:1334:C:H6	1.82	0.45
30:0:2271:G:N3	30:0:2271:G:H2'	2.31	0.45
30:0:253:U:H1'	30:0:256:C:H41	1.82	0.45
30:0:281:U:H2'	30:0:282:C:H6	1.82	0.45
30:0:506:G:N2	30:0:509:A:H5'	2.22	0.45
30:0:522:U:O2'	30:0:1366:C:H5'	2.16	0.45
31:9:3:A:OP2	31:9:25:G:N2	2.49	0.45
31:9:53:G:O2'	31:9:54:A:H5'	2.16	0.45
6:F:91:VAL:CG1	6:F:92:GLY:N	2.80	0.45
10:J:19:MET:HE1	10:J:79:PHE:HA	1.99	0.45
13:M:49:ALA:C	13:M:54:TYR:HB3	2.37	0.45
30:0:1919:A:H4'	38:0:4883:HOH:O	2.15	0.45
30:0:2493:C:O2	30:0:2493:C:H2'	2.15	0.45
31:9:40:C:H2'	31:9:41:C:OP1	2.17	0.45
31:9:57:A:N6	38:9:9066:HOH:O	2.47	0.45
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.35	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:113:ILE:HG22	11:K:114:ALA:N	2.32	0.45
15:O:10:LEU:HD13	15:O:99:GLU:HG3	1.99	0.45
30:0:1202:A:H2'	30:0:1203:G:H5'	1.99	0.45
30:0:1588:G:C6	30:0:1589:G:C6	3.05	0.45
30:0:1947:G:H2'	30:0:1948:G:C8	2.52	0.45
30:0:2598:U:O2	30:0:2600:A:H8	2.00	0.45
30:0:603:A:H1'	30:0:605:C:C2	2.52	0.45
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.51	0.45
4:D:20:LYS:HG2	4:D:133:ASN:HB3	1.97	0.45
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.51	0.45
11:K:125:ALA:C	11:K:127:ALA:H	2.20	0.45
18:R:132:ARG:HG2	18:R:133:ALA:N	2.31	0.45
24:X:78:GLU:HG2	24:X:79:GLU:H	1.81	0.45
30:0:1183:C:N3	30:0:1184:C:H5	2.15	0.45
30:0:2090:G:H2'	30:0:2091:G:C8	2.51	0.45
30:0:2281:C:C2'	30:0:2282:U:H5'	2.47	0.45
17:Q:1:PRO:HA	30:0:2299:G:O6	2.16	0.45
30:0:2812:A:N7	38:0:7555:HOH:O	2.36	0.45
30:0:42:C:H1'	38:0:4707:HOH:O	2.15	0.45
30:0:821:U:H3'	38:0:3789:HOH:O	2.15	0.45
1:A:164:ARG:NE	38:A:9043:HOH:O	2.49	0.45
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.99	0.45
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.99	0.45
13:M:99:ARG:HG3	38:M:8855:HOH:O	2.16	0.45
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.99	0.45
16:P:134:VAL:O	16:P:137:LEU:HB3	2.17	0.45
30:0:1987:C:H2'	30:0:1988:C:C6	2.51	0.45
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.52	0.45
1:A:96:LEU:HD22	1:A:128:LEU:HD13	1.99	0.45
1:A:186:TRP:CG	1:A:187:PRO:HA	2.52	0.45
1:A:99:ILE:O	1:A:131:HIS:HE1	2.00	0.45
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.99	0.45
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.98	0.45
8:H:34:HIS:HD2	8:H:90:LEU:O	2.00	0.45
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.97	0.45
23:W:149:LEU:HG	23:W:153:MET:HE2	1.99	0.45
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.32	0.45
30:0:128:A:H3'	30:0:128:A:C8	2.52	0.45
30:0:1902:G:N2	30:0:1936:C:C2	2.85	0.45
12:L:50:GLY:C	30:0:2453:G:H4'	2.37	0.45
30:0:2506:A:O2'	30:0:2507:G:P	2.75	0.45
31:9:81:C:O2'	31:9:82:U:H5'	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:84:VAL:O	3:C:85:LYS:HB2	2.17	0.45
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.99	0.45
18:R:113:HIS:O	18:R:145:LEU:HD12	2.17	0.45
19:S:77:VAL:O	19:S:80:ARG:HG2	2.16	0.45
23:W:119:HIS:HE1	38:0:9565:HOH:O	2.00	0.45
30:0:1615:A:H5'	38:0:4210:HOH:O	2.16	0.45
30:0:1626:A:H2'	30:0:1627:G:O4'	2.17	0.45
30:0:77:G:C2'	30:0:78:G:H5'	2.47	0.45
30:0:951:A:O2'	30:0:952:G:H5'	2.17	0.45
30:0:969:G:N2	30:0:1000:C:C2	2.84	0.45
27:1:2:GLY:O	27:1:6:PRO:HG2	2.17	0.45
31:9:1:U:O3'	31:9:3:A:OP1	2.35	0.45
3:C:168:ARG:NH2	3:C:190:ALA:O	2.50	0.45
23:W:74:GLU:OE1	30:0:1285:U:H4'	2.17	0.45
25:Y:137:LYS:HD2	30:0:521:A:H5''	1.99	0.45
30:0:1783:A:O2'	30:0:1784:U:H5'	2.16	0.44
30:0:1896:G:C6	30:0:1897:U:C4	3.05	0.44
30:0:1942:A:O2'	30:0:1943:C:H5'	2.17	0.44
30:0:2754:G:H2'	30:0:2755:G:O4'	2.17	0.44
30:0:542:A:O2'	30:0:543:G:H5'	2.16	0.44
1:A:199:HIS:HE1	30:0:1881:A:OP1	2.00	0.44
2:B:62:ARG:HA	2:B:65:MET:HE2	1.99	0.44
13:M:164:THR:HB	38:M:8819:HOH:O	2.15	0.44
30:0:1406:A:H4'	30:0:1407:A:H5''	1.99	0.44
30:0:291:C:H2'	30:0:292:G:O4'	2.17	0.44
30:0:812:A:H2'	30:0:813:C:C6	2.52	0.44
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.64	0.44
29:3:65:THR:CG2	29:3:67:LEU:HG	2.46	0.44
1:A:53:ALA:HB3	38:A:9060:HOH:O	2.16	0.44
4:D:135:VAL:HG22	4:D:136:ARG:N	2.32	0.44
16:P:7:LYS:HD3	16:P:21:VAL:HG22	1.98	0.44
26:Z:37:ARG:HD2	38:Z:8719:HOH:O	2.17	0.44
30:0:1182:C:HO2'	30:0:1183:C:H5	1.64	0.44
30:0:187:A:H3'	30:0:188:C:H6	1.82	0.44
30:0:2032:U:H2'	30:0:2033:G:C5'	2.47	0.44
30:0:204:A:H2'	30:0:205:U:H5'	1.98	0.44
30:0:582:U:H2'	30:0:583:C:C6	2.53	0.44
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.38	0.44
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.76	0.44
11:K:14:LYS:HG3	11:K:32:ILE:O	2.18	0.44
14:N:108:SER:HA	14:N:109:PRO:HD3	1.81	0.44
30:0:2385:G:H2'	30:0:2386:U:C6	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2464:C:H5''	30:0:2465:A:OP1	2.17	0.44
30:0:2473:U:O3'	30:0:2474:A:H3'	2.17	0.44
30:0:451:C:O2'	30:0:452:G:H5'	2.18	0.44
30:0:453:A:H4'	30:0:455:A:N7	2.32	0.44
27:1:16:HIS:CD2	30:0:470:U:O2'	2.67	0.44
13:M:58:GLN:HG3	38:M:8906:HOH:O	2.18	0.44
25:Y:144:ARG:NH2	38:Y:8907:HOH:O	2.51	0.44
30:0:1342:C:C2'	30:0:1343:C:H5'	2.47	0.44
30:0:815:U:O2'	30:0:1598:A:H4'	2.17	0.44
30:0:185:G:H4'	30:0:186:A:H4'	1.99	0.44
30:0:1973:A:H2'	30:0:1974:G:O4'	2.18	0.44
30:0:2635:A:C2'	30:0:2636:C:H5'	2.46	0.44
30:0:558:C:HO2'	30:0:559:U:H5''	1.80	0.44
30:0:825:U:H5''	30:0:826:U:OP1	2.18	0.44
30:0:947:U:O2'	30:0:948:G:H5'	2.16	0.44
2:B:102:THR:CG2	2:B:182:VAL:HG12	2.47	0.44
16:P:120:ARG:NH2	16:P:123:TYR:CD2	2.85	0.44
30:0:1427:A:H61	30:0:1440:U:C1'	2.30	0.44
30:0:1592:G:C4	30:0:1593:C:C5	3.06	0.44
30:0:1592:G:O2'	30:0:1593:C:O5'	2.35	0.44
30:0:218:C:C5	30:0:220:C:C4	3.06	0.44
30:0:2276:U:H2'	30:0:2277:U:C6	2.53	0.44
30:0:2636:C:H4'	38:0:6666:HOH:O	2.18	0.44
30:0:77:G:H2'	30:0:78:G:H5'	1.99	0.44
30:0:816:G:H5'	30:0:1598:A:H4'	1.99	0.44
28:2:2:LYS:HG3	30:0:1486:A:C5	2.52	0.44
31:9:76:G:H3'	31:9:77:A:C5'	2.31	0.44
2:B:74:ILE:HG13	38:B:9080:HOH:O	2.17	0.44
4:D:53:LYS:HE3	31:9:40:C:H42	1.82	0.44
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.17	0.44
13:M:46:LEU:HG	38:M:8922:HOH:O	2.18	0.44
30:0:1603:A:C5'	30:0:1605:G:C5'	2.94	0.44
30:0:1878:G:O2'	30:0:1879:U:OP2	2.36	0.44
30:0:204:A:C2'	30:0:205:U:H5'	2.47	0.44
30:0:764:C:H2'	30:0:765:G:O4'	2.17	0.44
30:0:794:U:C2'	30:0:795:G:H5'	2.48	0.44
2:B:79:MET:HE1	38:B:9100:HOH:O	2.17	0.44
14:N:11:ARG:NH1	31:9:8:G:O6	2.50	0.44
16:P:91:LYS:O	16:P:95:GLU:HG3	2.17	0.44
30:0:1006:A:N1	30:0:2311:A:H1'	2.33	0.44
30:0:1044:C:H5''	38:0:9028:HOH:O	2.18	0.44
4:D:131:THR:HG21	30:0:2348:C:H1'	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2461:U:O2	30:0:2466:G:H1'	2.18	0.44
30:0:2511:A:H2'	30:0:2512:U:O4'	2.17	0.44
30:0:2565:C:H4'	38:0:4868:HOH:O	2.18	0.44
30:0:441:A:H8	30:0:441:A:O5'	1.99	0.44
30:0:497:A:H2'	30:0:498:A:C5'	2.48	0.44
30:0:807:A:O2'	30:0:808:A:H5'	2.17	0.44
31:9:107:C:O2'	31:9:108:C:H5'	2.18	0.44
1:A:204:GLY:N	30:0:2634:G:OP2	2.48	0.44
2:B:280:VAL:HG13	2:B:333:GLU:O	2.17	0.44
4:D:135:VAL:HG22	4:D:136:ARG:H	1.82	0.44
5:E:6:GLU:HG2	5:E:46:THR:HG22	1.99	0.44
6:F:60:VAL:HG13	6:F:63:ILE:HG13	1.99	0.44
8:H:30:LYS:H	8:H:62:HIS:HD2	1.65	0.44
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.83	0.44
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.53	0.44
30:0:1066:U:H2'	30:0:1067:A:C8	2.52	0.44
30:0:66:G:C2	30:0:109:U:C4	3.06	0.44
30:0:1189:A:H1'	30:0:1209:C:H1'	1.99	0.44
30:0:1375:A:C2'	30:0:1376:G:H5'	2.47	0.44
30:0:1588:G:C5	30:0:1589:G:C6	3.06	0.44
30:0:1903:U:O2'	30:0:1904:A:N7	2.50	0.44
30:0:2015:A:H2'	30:0:2016:U:O4'	2.18	0.44
30:0:2238:A:O2'	30:0:2239:C:H5'	2.18	0.44
30:0:2506:A:O2'	30:0:2507:G:O5'	2.36	0.44
30:0:2569:A:H2'	30:0:2570:G:O5'	2.18	0.44
30:0:383:A:H2'	30:0:384:G:O4'	2.18	0.44
30:0:629:A:C2	30:0:2074:A:C2	3.06	0.44
30:0:88:G:H2'	30:0:89:G:H8	1.83	0.44
4:D:146:LYS:NZ	14:N:107:ASN:ND2	2.66	0.44
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.49	0.44
11:K:89:LYS:HE2	21:U:19:THR:HG21	2.00	0.44
21:U:49:LEU:HG	38:U:3805:HOH:O	2.17	0.44
1:A:76:VAL:HG23	26:Z:87:LYS:HB3	2.00	0.44
30:0:1632:A:H2'	30:0:1633:C:C5'	2.42	0.43
1:A:190:ARG:HH11	30:0:1845:A:P	2.41	0.43
30:0:2842:G:H2'	30:0:2843:A:H5'	2.00	0.43
30:0:499:G:O2'	30:0:500:G:H5'	2.16	0.43
30:0:594:C:C4	30:0:595:U:C4	3.06	0.43
30:0:177:A:O2'	30:0:892:G:H4'	2.17	0.43
31:9:55:U:H4'	31:9:56:A:H8	1.83	0.43
2:B:53:LEU:HD11	2:B:327:VAL:HG22	1.99	0.43
3:C:170:ASP:OD2	30:0:330:C:H5	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.99	0.43
10:J:70:PHE:HD1	30:0:2676:C:O2'	2.00	0.43
14:N:37:ARG:HH12	31:9:6:C:C5'	2.21	0.43
14:N:37:ARG:NE	38:N:8831:HOH:O	2.51	0.43
16:P:73:HIS:HE1	30:0:1789:G:O6	2.01	0.43
17:Q:19:ARG:HH21	31:9:11:A:P	2.41	0.43
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.51	0.43
30:0:1119:G:N2	30:0:1246:A:H2	2.13	0.43
30:0:963:C:O2	30:0:1005:A:N1	2.51	0.43
29:3:91:GLN:O	29:3:92:GLU:HB2	2.18	0.43
31:9:114:G:H2'	31:9:115:C:H6	1.81	0.43
31:9:31:C:H2'	31:9:32:G:O4'	2.18	0.43
2:B:10:SER:HB2	30:0:2714:U:H4'	1.99	0.43
13:M:134:ILE:O	13:M:136:PRO:HD3	2.19	0.43
14:N:50:LEU:HA	14:N:50:LEU:HD12	1.86	0.43
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.53	0.43
30:0:1056:U:H2'	30:0:1057:A:O4'	2.18	0.43
30:0:1156:C:O5'	30:0:1156:C:H6	2.01	0.43
30:0:1565:C:H2'	30:0:1566:C:H6	1.83	0.43
30:0:1517:C:O2	30:0:1670:A:C2	2.71	0.43
30:0:271:C:C2	30:0:273:G:O4'	2.70	0.43
30:0:2870:C:O2'	30:0:2871:G:H5'	2.19	0.43
28:2:16:ASN:HB2	38:2:5203:HOH:O	2.17	0.43
31:9:3:A:C2	31:9:21:G:N3	2.85	0.43
1:A:1:GLY:HA2	1:A:197:VAL:HG23	1.99	0.43
1:A:95:PRO:O	1:A:99:ILE:HG12	2.19	0.43
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.84	0.43
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.16	0.43
18:R:40:ALA:O	18:R:44:VAL:HG23	2.18	0.43
30:0:1434:A:H2'	30:0:1436:C:C5	2.53	0.43
30:0:1456:C:H2'	30:0:1457:U:C6	2.54	0.43
30:0:1789:G:H2'	30:0:1790:C:O5'	2.18	0.43
30:0:17:G:H2'	30:0:18:C:C6	2.53	0.43
30:0:1972:U:C2'	30:0:1973:A:C5'	2.96	0.43
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.51	0.43
30:0:212:A:O4'	30:0:214:U:C6	2.72	0.43
30:0:294:C:H2'	30:0:295:C:O4'	2.18	0.43
30:0:559:U:H2'	30:0:560:U:O4'	2.18	0.43
30:0:677:C:O2'	30:0:678:G:H5'	2.18	0.43
30:0:960:G:C3'	30:0:960:G:C4	3.01	0.43
3:C:61:PHE:HB3	38:C:8639:HOH:O	2.18	0.43
7:G:12:ILE:HG12	38:0:5490:HOH:O	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1946:C:H2'	30:0:1971:G:C8	2.53	0.43
30:0:365:G:C6	30:0:366:U:C4	3.06	0.43
30:0:424:C:H2'	30:0:425:U:C6	2.53	0.43
30:0:951:A:C2'	30:0:952:G:H5'	2.48	0.43
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.48	0.43
28:2:41:HIS:CD2	28:2:44:ARG:H	2.26	0.43
2:B:305:ASP:O	2:B:306:LYS:HB2	2.19	0.43
3:C:242:GLU:HB2	38:C:8577:HOH:O	2.17	0.43
11:K:8:VAL:HG13	11:K:80:ILE:HG22	2.00	0.43
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.89	0.43
22:V:1:THR:HG23	22:V:2:VAL:N	2.30	0.43
30:0:226:A:H1'	30:0:393:G:C5	2.54	0.43
30:0:35:U:H2'	30:0:36:C:C6	2.53	0.43
31:9:42:C:H5'	31:9:43:G:OP2	2.19	0.43
31:9:58:G:H3'	31:9:59:C:C6	2.54	0.43
20:T:3:GLN:HA	20:T:4:PRO:HD3	1.82	0.43
30:0:130:C:H5'	38:0:5243:HOH:O	2.19	0.43
30:0:1764:C:H2'	30:0:1765:G:O4'	2.18	0.43
30:0:1970:G:H2'	30:0:1970:G:N3	2.33	0.43
30:0:1992:U:H2'	30:0:1994:A:OP2	2.18	0.43
30:0:2523:U:O2'	30:0:2524:G:H5'	2.19	0.43
6:F:59:ILE:CD1	30:0:263:U:C2	3.01	0.43
30:0:2088:C:H1'	30:0:2841:A:N1	2.34	0.43
30:0:512:G:O3'	30:0:513:A:C8	2.71	0.43
30:0:794:U:H3	30:0:819:A:H61	1.65	0.43
30:0:794:U:H2'	30:0:795:G:H5'	2.01	0.43
30:0:844:A:C6	30:0:882:A:C5	3.06	0.43
1:A:94:LEU:HG	1:A:99:ILE:HD13	2.01	0.43
8:H:64:SER:OG	30:0:2520:G:H5'	2.17	0.43
30:0:1250:C:O2'	30:0:1251:C:H5'	2.19	0.43
30:0:1589:G:N2	30:0:1605:G:H1'	2.34	0.43
30:0:2387:U:H2'	30:0:2388:C:C6	2.54	0.43
6:F:59:ILE:HD13	30:0:263:U:O4'	2.19	0.43
3:C:98:ARG:NH1	38:C:8554:HOH:O	2.51	0.43
6:F:99:THR:HG23	6:F:99:THR:O	2.19	0.43
11:K:130:MET:SD	21:U:25:ASP:O	2.77	0.43
19:S:57:THR:HG22	19:S:58:MET:N	2.33	0.43
22:V:55:ARG:O	22:V:59:ILE:HG12	2.19	0.43
25:Y:168:PHE:CE2	30:0:1090:A:H4'	2.54	0.43
30:0:1245:C:O5'	30:0:1245:C:H6	2.02	0.43
30:0:1421:C:O2'	30:0:1422:U:H5'	2.18	0.43
30:0:1616:A:H5"	30:0:1617:C:OP1	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:537:G:O4'	30:0:538:C:C5	2.71	0.43
30:0:941:G:C6	30:0:942:U:C4	3.07	0.43
31:9:59:C:H2'	31:9:60:C:C6	2.54	0.43
3:C:151:GLN:HG3	30:0:327:A:OP2	2.19	0.43
4:D:128:LEU:HB2	38:D:6007:HOH:O	2.19	0.43
10:J:36:VAL:HG12	10:J:37:ALA:N	2.34	0.43
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.49	0.43
11:K:64:MET:HA	11:K:67:GLN:HE21	1.84	0.43
16:P:40:VAL:O	16:P:44:VAL:HG23	2.19	0.43
21:U:49:LEU:O	21:U:52:THR:HG22	2.17	0.43
25:Y:133:HIS:HD2	38:Y:8877:HOH:O	2.02	0.43
30:0:1032:A:N3	30:0:1032:A:H2'	2.33	0.43
30:0:1160:G:H5'	30:0:1161:A:C4'	2.46	0.43
30:0:1187:U:O2'	30:0:1189:A:H2	1.85	0.43
30:0:1555:G:O2'	30:0:1556:G:H5'	2.19	0.43
30:0:1644:C:C2	30:0:1645:U:C6	3.07	0.43
30:0:1996:U:O2'	30:0:1997:A:H5'	2.18	0.43
30:0:2524:G:N2	30:0:2526:C:H41	2.17	0.43
30:0:488:U:H2'	38:0:4031:HOH:O	2.18	0.43
27:1:25:LYS:O	27:1:25:LYS:HG2	2.19	0.43
31:9:52:A:O2'	31:9:53:G:H5'	2.19	0.43
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.90	0.43
4:D:99:ASP:HB3	4:D:103:ASN:H	1.84	0.43
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.99	0.43
14:N:38:LYS:HB2	14:N:38:LYS:HE3	1.77	0.43
18:R:109:MET:HG2	18:R:148:GLU:C	2.40	0.43
20:T:53:GLY:HA3	38:T:6384:HOH:O	2.19	0.43
9:I:86:GLU:HG2	30:0:1180:U:H4'	2.01	0.42
30:0:1202:A:H2'	30:0:1203:G:C5'	2.48	0.42
30:0:1788:U:C2	30:0:1805:G:N2	2.87	0.42
30:0:2252:A:C6	30:0:2253:G:H1'	2.53	0.42
30:0:2435:U:H1'	38:0:5462:HOH:O	2.19	0.42
30:0:332:G:O2'	30:0:333:G:H5'	2.19	0.42
30:0:39:G:N2	30:0:444:C:C2	2.87	0.42
31:9:45:A:H2'	31:9:46:C:C6	2.54	0.42
2:B:30:PRO:HB2	2:B:39:GLN:NE2	2.34	0.42
2:B:5:ARG:NH1	2:B:8:LYS:HE2	2.34	0.42
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.18	0.42
30:0:1015:C:O5'	30:0:1015:C:H6	2.02	0.42
30:0:1761:U:H2'	30:0:1762:C:C6	2.54	0.42
1:A:190:ARG:HD2	30:0:1884:G:O6	2.18	0.42
31:9:14:G:H2'	31:9:15:C:H5'	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:9:2:U:C4'	38:9:9103:HOH:O	2.67	0.42
31:9:2:U:OP2	31:9:2:U:H4'	2.19	0.42
31:9:72:C:O2'	31:9:73:A:H5'	2.19	0.42
1:A:99:ILE:O	1:A:131:HIS:CE1	2.72	0.42
3:C:25:PRO:HG2	38:C:8520:HOH:O	2.18	0.42
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.20	0.42
18:R:113:HIS:HE1	18:R:144:GLU:CD	2.22	0.42
30:0:1058:A:H2'	30:0:1060:C:C5'	2.46	0.42
30:0:1634:G:C6	30:0:1635:U:C4	3.07	0.42
30:0:1762:C:H2'	30:0:1763:C:C6	2.54	0.42
30:0:2004:U:H2'	30:0:2005:G:OP1	2.19	0.42
38:Q:2875:HOH:O	30:0:2392:C:H4'	2.20	0.42
30:0:2423:C:H2'	30:0:2424:U:C6	2.54	0.42
30:0:2819:C:H2'	30:0:2820:A:C8	2.54	0.42
29:3:3:MET:HG3	29:3:4:PRO:HD2	2.01	0.42
1:A:179:MET:HG2	1:A:186:TRP:CG	2.55	0.42
6:F:58:GLU:OE1	13:M:27:ARG:NH2	2.51	0.42
8:H:31:ILE:HG23	38:H:231:HOH:O	2.18	0.42
12:L:67:ARG:O	12:L:71:GLU:HG3	2.20	0.42
30:0:1175:G:H1'	30:0:1193:A:H2'	2.02	0.42
30:0:1416:G:C2'	30:0:1417:G:H5'	2.49	0.42
30:0:1561:U:H2'	30:0:1561:U:O2	2.18	0.42
30:0:2104:C:O2	30:0:2485:A:N1	2.53	0.42
30:0:254:C:O2	30:0:254:C:H2'	2.19	0.42
1:A:179:MET:HG2	1:A:186:TRP:CB	2.49	0.42
2:B:178:ALA:O	2:B:182:VAL:HG23	2.20	0.42
6:F:118:LEU:O	6:F:119:ARG:HB3	2.19	0.42
9:I:111:LEU:HD23	30:0:1163:G:H4'	2.01	0.42
9:I:73:LEU:HD12	9:I:107:LYS:HZ1	1.84	0.42
16:P:59:ARG:NH2	16:P:66:GLN:HE22	2.10	0.42
23:W:43:GLY:HA3	30:0:945:U:O2'	2.19	0.42
24:X:15:ARG:HH22	30:0:2856:A:P	2.42	0.42
30:0:1634:G:H2'	30:0:1635:U:C6	2.54	0.42
30:0:2134:G:N2	30:0:2242:U:C2	2.87	0.42
30:0:2414:A:N1	30:0:2415:A:C6	2.88	0.42
30:0:2719:A:H5''	38:0:3702:HOH:O	2.19	0.42
30:0:344:C:H2'	30:0:345:G:O4'	2.20	0.42
10:J:93:ARG:HH11	10:J:93:ARG:HB3	1.83	0.42
20:T:32:ARG:NH1	20:T:38:ARG:HH12	2.17	0.42
23:W:13:MET:CE	23:W:17:ILE:HG22	2.49	0.42
23:W:80:ASP:HB2	38:W:3312:HOH:O	2.18	0.42
30:0:1206:U:C6	30:0:1206:U:C3'	3.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1211:G:O2'	30:0:1212:C:H5'	2.19	0.42
30:0:1451:C:H5'	30:0:1505:U:C4	2.54	0.42
30:0:1987:C:H2'	30:0:1988:C:H6	1.85	0.42
30:0:2134:G:C6	30:0:2258:A:C8	3.08	0.42
30:0:2361:A:H2'	30:0:2362:A:O4'	2.19	0.42
30:0:2578:G:C8	30:0:2578:G:H5'	2.44	0.42
30:0:243:A:H61	30:0:269:G:H1'	1.84	0.42
30:0:2754:G:C2'	30:0:2755:G:H5'	2.49	0.42
30:0:284:C:H4'	30:0:285:A:H8	1.84	0.42
30:0:544:G:C3'	30:0:545:G:H5''	2.48	0.42
30:0:603:A:H4'	30:0:604:G:O5'	2.20	0.42
30:0:843:A:C2	30:0:846:A:C8	3.08	0.42
31:9:14:G:H2'	31:9:15:C:C5'	2.50	0.42
2:B:14:GLY:HA2	2:B:15:PRO:C	2.39	0.42
4:D:23:VAL:HG11	4:D:83:PHE:CZ	2.55	0.42
14:N:34:LEU:HD22	14:N:129:ILE:HD13	2.01	0.42
21:U:17:THR:CG2	21:U:18:GLY:N	2.83	0.42
30:0:1307:A:H2'	30:0:1308:A:C8	2.55	0.42
30:0:2505:G:H2'	30:0:2506:A:C5'	2.50	0.42
30:0:369:G:C2	30:0:370:G:C8	3.08	0.42
30:0:466:A:H2'	30:0:467:G:O4'	2.20	0.42
2:B:314:ALA:CB	2:B:317:PRO:HG3	2.50	0.42
14:N:25:ARG:HB3	30:0:2415:A:C2	2.54	0.42
23:W:7:LEU:HD12	23:W:53:ALA:HB2	2.00	0.42
26:Z:45:VAL:HG12	38:Z:8713:HOH:O	2.19	0.42
30:0:1023:C:H2'	30:0:1024:G:O4'	2.20	0.42
30:0:1244:U:H4'	30:0:1246:A:O4'	2.20	0.42
30:0:1298:U:H2'	30:0:1299:G:C8	2.54	0.42
30:0:1782:G:O2'	30:0:1783:A:H5'	2.19	0.42
30:0:2252:A:C2'	30:0:2253:G:H5'	2.49	0.42
30:0:2756:U:C2	30:0:2896:A:H2	2.38	0.42
30:0:2909:G:H2'	30:0:2910:A:H8	1.84	0.42
30:0:539:G:H2'	30:0:540:A:C8	2.54	0.42
30:0:790:A:H8	38:0:6134:HOH:O	2.01	0.42
1:A:38:ILE:HD13	1:A:38:ILE:HA	1.85	0.42
3:C:85:LYS:HA	3:C:85:LYS:HD2	1.90	0.42
4:D:170:TYR:CD1	4:D:170:TYR:N	2.87	0.42
8:H:4:LYS:HA	8:H:5:PRO:HD3	1.86	0.42
8:H:87:LYS:NZ	8:H:87:LYS:HB2	2.35	0.42
13:M:124:GLY:HA3	30:0:2132:C:H1'	2.02	0.42
15:O:96:VAL:HG12	15:O:97:SER:O	2.20	0.42
18:R:69:LYS:HB2	18:R:72:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:12:THR:HG22	22:V:15:GLU:CG	2.47	0.42
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.30	0.42
24:X:37:LEU:O	24:X:41:PHE:HB2	2.19	0.42
30:0:1198:U:H1'	30:0:1201:C:C5	2.50	0.42
30:0:1433:G:O2'	30:0:1434:A:H5'	2.20	0.42
30:0:1676:G:C2'	30:0:1677:U:H5'	2.50	0.42
30:0:2783:A:O2'	30:0:2784:A:H5'	2.19	0.42
30:0:417:G:P	38:0:7457:HOH:O	2.77	0.42
1:A:23:TYR:HD1	30:0:1872:C:H2'	1.85	0.42
1:A:94:LEU:N	1:A:94:LEU:HD23	2.34	0.42
2:B:27:ASN:H	2:B:27:ASN:HD22	1.67	0.42
14:N:159:TYR:HE1	31:9:50:G:H5''	1.85	0.42
15:O:44:ASN:OD1	15:O:65:LEU:HB2	2.19	0.42
19:S:56:ASN:O	28:2:8:LYS:NZ	2.51	0.42
24:X:37:LEU:HD21	24:X:72:VAL:HG11	2.02	0.42
24:X:8:ARG:NH1	30:0:2904:U:H4'	2.35	0.42
30:0:128:A:C8	30:0:128:A:C3'	3.03	0.42
30:0:1334:C:H2'	30:0:1335:C:H6	1.85	0.42
30:0:2509:A:OP2	30:0:2510:C:C5	2.72	0.42
30:0:2712:G:P	38:0:5251:HOH:O	2.77	0.42
30:0:2718:C:H5'	30:0:2718:C:C6	2.53	0.42
30:0:2908:A:C2'	30:0:2909:G:H5'	2.49	0.42
1:A:107:ASN:OD1	1:A:116:GLY:HA3	2.20	0.42
1:A:211:LYS:HB2	38:A:9075:HOH:O	2.19	0.42
1:A:54:PRO:HG2	1:A:160:ALA:HB3	2.02	0.42
2:B:243:ASN:HA	2:B:244:PRO:C	2.40	0.42
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.85	0.42
3:C:5:ILE:HD11	3:C:16:VAL:HG23	2.01	0.42
10:J:45:VAL:HG11	10:J:121:LEU:HD22	2.02	0.42
18:R:29:LYS:NZ	38:R:8944:HOH:O	2.53	0.42
25:Y:154:ARG:HH22	30:0:1071:G:H4'	1.85	0.41
30:0:129:A:O2'	30:0:131:A:OP1	2.36	0.41
30:0:1335:C:H2'	30:0:1336:U:C6	2.55	0.41
30:0:1406:A:H4'	30:0:1407:A:C5'	2.50	0.41
30:0:1562:C:N4	38:0:5895:HOH:O	2.53	0.41
30:0:1789:G:C2'	30:0:1790:C:O5'	2.68	0.41
30:0:259:G:O2'	30:0:260:C:H5'	2.20	0.41
30:0:2600:A:H2'	30:0:2601:A:O4'	2.20	0.41
30:0:2727:A:C6	30:0:2756:U:C2	3.08	0.41
30:0:821:U:H2'	30:0:822:C:H6	1.84	0.41
30:0:883:U:C2'	30:0:883:U:O2	2.67	0.41
30:0:960:G:H2'	30:0:961:A:OP2	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:3:18:GLN:HG3	38:3:9009:HOH:O	2.20	0.41
4:D:105:SER:OG	30:0:2338:G:H1'	2.20	0.41
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.20	0.41
6:F:39:SER:HB3	6:F:45:ALA:HB2	2.02	0.41
10:J:131:THR:HG22	10:J:134:GLU:H	1.85	0.41
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.17	0.41
14:N:147:ILE:HB	38:9:9090:HOH:O	2.19	0.41
30:0:1052:G:C5	30:0:1063:G:C6	3.09	0.41
25:Y:142:SER:OG	30:0:1331:G:OP2	2.34	0.41
30:0:420:U:H2'	30:0:421:C:C6	2.55	0.41
30:0:64:G:H2'	30:0:65:C:O4'	2.20	0.41
31:9:47:A:H2'	31:9:48:C:O4'	2.20	0.41
2:B:40:GLY:O	2:B:193:ILE:HD13	2.20	0.41
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.51	0.41
3:C:193:LEU:HD12	3:C:211:ASP:O	2.20	0.41
4:D:22:VAL:HG22	4:D:74:THR:HG22	2.00	0.41
4:D:37:ALA:O	4:D:40:ILE:HG12	2.20	0.41
12:L:150:GLN:HB3	38:L:8868:HOH:O	2.20	0.41
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.44	0.41
19:S:11:THR:H	19:S:14:ALA:HB3	1.84	0.41
9:I:69:PRO:HA	30:0:1164:U:OP1	2.21	0.41
30:0:1167:G:C2	30:0:1168:C:C2	3.08	0.41
30:0:1185:U:H5'	38:0:7504:HOH:O	2.20	0.41
30:0:1840:A:H4'	30:0:1841:C:O5'	2.20	0.41
30:0:1890:U:H4'	30:0:2010:A:C6	2.55	0.41
30:0:506:G:N2	30:0:509:A:H5''	2.32	0.41
27:1:45:ARG:HB3	38:1:988:HOH:O	2.20	0.41
28:2:41:HIS:CD2	28:2:43:ARG:H	2.39	0.41
2:B:248:ARG:NH1	38:B:9090:HOH:O	2.53	0.41
2:B:75:GLU:C	2:B:77:PRO:HD3	2.40	0.41
4:D:141:VAL:HG21	31:9:57:A:H8	1.85	0.41
14:N:37:ARG:HD3	35:N:8807:CL:CL	2.57	0.41
30:0:1422:U:O2'	30:0:1423:C:H5'	2.20	0.41
30:0:1474:C:C5'	30:0:1474:C:C6	2.89	0.41
30:0:151:A:C2	30:0:442:A:C8	3.09	0.41
30:0:1909:A:H2'	30:0:1910:A:C8	2.54	0.41
30:0:635:A:H2'	30:0:636:G:H5''	2.02	0.41
30:0:729:C:C2	30:0:743:G:C2	3.08	0.41
28:2:41:HIS:N	28:2:45:ASN:HD22	2.03	0.41
31:9:45:A:C5	31:9:46:C:C5	3.08	0.41
9:I:101:LYS:O	9:I:105:GLU:HG3	2.21	0.41
13:M:158:ARG:HB2	13:M:163:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1138:G:H4'	38:0:5739:HOH:O	2.18	0.41
30:0:1342:C:O2'	30:0:1343:C:H5'	2.20	0.41
30:0:1667:A:C2	30:0:1668:U:C2	3.08	0.41
30:0:1903:U:O2'	30:0:1904:A:C8	2.68	0.41
30:0:2421:G:H4'	38:0:4814:HOH:O	2.20	0.41
30:0:2704:C:H2'	30:0:2705:U:O4'	2.20	0.41
30:0:834:G:H3'	30:0:835:U:H4'	2.01	0.41
28:2:37:HIS:CE1	30:0:462:A:C8	3.08	0.41
1:A:36:ASP:O	1:A:38:ILE:N	2.53	0.41
3:C:223:LEU:HA	3:C:223:LEU:HD12	1.91	0.41
16:P:7:LYS:HG2	16:P:23:PHE:CE2	2.55	0.41
24:X:39:LYS:HE2	30:0:2834:G:OP1	2.20	0.41
30:0:2102:G:C2	30:0:2104:C:C4	3.08	0.41
30:0:2361:A:H8	30:0:2361:A:H5'	1.86	0.41
30:0:2419:U:H5''	30:0:2420:G:C5'	2.50	0.41
30:0:243:A:H61	30:0:269:G:C1'	2.34	0.41
30:0:2637:A:C5'	38:0:4961:HOH:O	2.59	0.41
30:0:2791:U:H4'	30:0:2792:A:OP1	2.20	0.41
30:0:2802:C:H2'	30:0:2803:C:C6	2.55	0.41
30:0:290:C:H1'	38:0:6136:HOH:O	2.21	0.41
30:0:318:U:H5'	30:0:339:A:C2	2.56	0.41
29:3:38:ARG:HD2	30:0:396:U:OP2	2.21	0.41
30:0:482:G:H4'	30:0:508:A:N1	2.36	0.41
2:B:215:VAL:HA	2:B:220:VAL:HG22	2.02	0.41
3:C:154:VAL:O	3:C:158:GLU:HG3	2.21	0.41
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.20	0.41
10:J:52:GLN:HE22	30:0:1119:G:H8	1.69	0.41
16:P:59:ARG:O	16:P:63:ARG:HG3	2.21	0.41
19:S:57:THR:C	19:S:59:ASP:H	2.24	0.41
24:X:43:VAL:HG11	24:X:82:GLU:HA	2.01	0.41
30:0:1377:C:C5'	30:0:1377:C:H6	2.33	0.41
30:0:1481:G:H2'	30:0:1482:A:O4'	2.20	0.41
30:0:1548:U:H1'	38:0:6897:HOH:O	2.19	0.41
27:1:5:THR:HG23	30:0:1688:G:O2'	2.20	0.41
30:0:2089:A:C2'	30:0:2090:G:H5'	2.49	0.41
30:0:2777:G:O2'	30:0:2778:A:H5'	2.20	0.41
30:0:290:C:O2'	30:0:291:C:H5'	2.20	0.41
30:0:559:U:H5'	30:0:559:U:C6	2.35	0.41
29:3:69:TYR:CZ	29:3:80:ARG:HD2	2.56	0.41
1:A:212:PRO:HB2	38:0:4392:HOH:O	2.20	0.41
1:A:217:ARG:HG2	1:A:229:ALA:HB2	2.03	0.41
2:B:280:VAL:CG1	2:B:334:SER:HA	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:67:VAL:HB	13:M:97:ILE:HG23	2.03	0.41
16:P:94:TRP:CZ2	16:P:98:ILE:HG13	2.56	0.41
25:Y:213:LYS:HE3	25:Y:213:LYS:HB2	1.90	0.41
30:0:1544:U:O2'	30:0:1545:C:H5'	2.20	0.41
30:0:1714:C:C2'	30:0:1715:C:H5'	2.51	0.41
30:0:1804:A:H2'	30:0:1805:G:C8	2.56	0.41
30:0:2617:G:C2	30:0:2618:G:C8	3.08	0.41
30:0:2802:C:H2'	30:0:2803:C:H6	1.84	0.41
30:0:667:C:H2'	30:0:668:C:H6	1.85	0.41
30:0:81:G:N3	30:0:98:A:C2	2.88	0.41
31:9:13:A:OP1	31:9:113:C:H5'	2.21	0.41
14:N:160:SER:CB	31:9:51:A:H5'	2.50	0.41
1:A:95:PRO:HA	1:A:153:ARG:HA	2.03	0.41
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.48	0.41
11:K:30:LYS:HB3	11:K:56:SER:HB3	2.03	0.41
13:M:167:GLY:O	13:M:171:ARG:HG3	2.21	0.41
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.21	0.41
14:N:71:TRP:CE3	14:N:175:LEU:HD22	2.56	0.41
15:O:98:LEU:O	15:O:102:ILE:HG13	2.21	0.41
16:P:83:LYS:O	16:P:86:ALA:HB3	2.21	0.41
18:R:17:MET:SD	38:R:8951:HOH:O	2.62	0.41
22:V:27:LEU:HA	22:V:49:LEU:HD13	2.02	0.41
23:W:48:VAL:HG12	23:W:48:VAL:O	2.19	0.41
30:0:1166:A:N3	30:0:1166:A:H2'	2.35	0.41
30:0:1184:C:O2'	30:0:1185:U:OP2	2.36	0.41
30:0:130:C:H2'	38:0:3183:HOH:O	2.20	0.41
30:0:969:G:H2'	30:0:970:U:C6	2.56	0.41
31:9:34:A:H2'	31:9:35:C:O4'	2.21	0.41
3:C:76:ARG:NH1	3:C:76:ARG:HB3	2.36	0.41
4:D:25:MET:HE1	4:D:37:ALA:O	2.21	0.41
13:M:164:THR:CG2	13:M:165:GLY:N	2.83	0.41
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.49	0.41
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.51	0.41
15:O:115:ARG:NH1	38:O:6194:HOH:O	2.54	0.41
26:Z:50:VAL:O	26:Z:54:GLU:HG3	2.20	0.41
30:0:1634:G:C5	30:0:1635:U:C4	3.08	0.41
30:0:1909:A:N1	30:0:2128:G:H1'	2.35	0.41
30:0:1945:G:O2'	30:0:1946:C:H5'	2.20	0.41
30:0:2039:A:H2'	30:0:2040:C:C6	2.56	0.41
30:0:2246:U:N3	30:0:2256:G:C2	2.89	0.41
38:N:8830:HOH:O	30:0:2368:A:H8	2.04	0.41
30:0:23:G:C6	30:0:24:G:N1	2.89	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.85	0.41
2:B:154:VAL:CG1	2:B:156:LYS:HG2	2.51	0.41
20:T:79:LEU:HG	20:T:89:ARG:HB2	2.03	0.41
38:K:7438:HOH:O	21:U:20:MET:HE2	2.21	0.41
22:V:39:ALA:C	22:V:41:GLU:H	2.23	0.41
30:0:1119:G:N2	30:0:1246:A:N1	2.69	0.41
30:0:1163:G:N2	38:0:6078:HOH:O	2.54	0.41
30:0:1271:A:C2	30:0:1286:A:C2	3.09	0.41
30:0:1522:A:C2'	30:0:1523:G:H5'	2.51	0.41
30:0:1574:C:H6	30:0:1574:C:O5'	2.04	0.41
30:0:1613:C:H2'	30:0:1614:G:O4'	2.21	0.41
30:0:2072:G:N2	38:0:6910:HOH:O	2.54	0.41
30:0:2251:G:C6	30:0:2252:A:C6	3.09	0.41
30:0:595:U:O2'	30:0:596:C:H5'	2.21	0.41
29:3:70:ARG:HD3	38:3:9064:HOH:O	2.21	0.41
2:B:102:THR:HG23	2:B:182:VAL:HG12	2.02	0.41
30:0:106:A:H2'	30:0:107:U:O4'	2.21	0.40
30:0:1098:A:H2'	30:0:1099:G:O4'	2.21	0.40
30:0:1182:C:O2'	30:0:1183:C:H5	2.04	0.40
30:0:1515:A:H2'	30:0:1516:U:H6	1.82	0.40
30:0:1520:G:C6	30:0:1521:C:C4	3.09	0.40
30:0:1536:C:H6	30:0:1536:C:O5'	2.03	0.40
30:0:1750:C:N4	30:0:1751:G:C6	2.89	0.40
30:0:1758:U:H2'	30:0:1759:A:O4'	2.22	0.40
30:0:2334:C:O2'	30:0:2335:C:H5'	2.21	0.40
30:0:2332:A:C2	30:0:2355:G:C5	3.09	0.40
30:0:369:G:O2'	30:0:370:G:H5'	2.21	0.40
30:0:401:C:H2'	30:0:402:U:C6	2.56	0.40
30:0:745:G:H5''	30:0:746:A:OP1	2.21	0.40
31:9:64:C:O2'	31:9:65:A:H5'	2.21	0.40
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.86	0.40
2:B:154:VAL:HG12	2:B:156:LYS:HG2	2.02	0.40
4:D:25:MET:HE3	4:D:37:ALA:HB1	2.04	0.40
6:F:34:ASN:HA	13:M:4:ALA:HB2	2.03	0.40
25:Y:106:THR:HG23	25:Y:107:PRO:HD2	2.03	0.40
25:Y:189:ASN:ND2	25:Y:192:ASP:H	2.19	0.40
30:0:1192:A:H3'	30:0:1193:A:H5'	2.02	0.40
30:0:1327:G:N1	30:0:1330:A:OP2	2.52	0.40
30:0:1617:C:C4	30:0:1643:C:H4'	2.56	0.40
30:0:1700:C:H5''	30:0:1701:A:OP2	2.22	0.40
30:0:1377:C:H2'	30:0:1723:G:O6	2.21	0.40
30:0:1947:G:C8	30:0:1970:G:C8	3.09	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2253:G:C2	30:0:2254:G:C8	3.09	0.40
30:0:2524:G:H21	30:0:2526:C:H41	1.67	0.40
30:0:278:A:C6	30:0:279:C:C4	3.09	0.40
30:0:74:G:H2'	30:0:75:U:C6	2.56	0.40
2:B:234:ARG:HD3	30:0:1734:C:OP1	2.21	0.40
12:L:143:THR:HG21	38:L:8837:HOH:O	2.21	0.40
14:N:154:LEU:C	14:N:156:GLU:H	2.24	0.40
30:0:111:C:O2'	30:0:112:G:H5'	2.21	0.40
30:0:1163:G:C4	30:0:1164:U:C5	3.09	0.40
30:0:1183:C:O2	30:0:1183:C:C2'	2.69	0.40
30:0:1409:G:C2	30:0:1410:G:C8	3.10	0.40
30:0:1896:G:H1'	38:0:4284:HOH:O	2.21	0.40
30:0:1947:G:N2	30:0:1966:U:C2	2.90	0.40
30:0:200:C:H6	38:0:3463:HOH:O	2.03	0.40
30:0:255:A:C5	30:0:256:C:C5	3.09	0.40
30:0:2626:C:H2'	30:0:2627:G:C8	2.56	0.40
30:0:2727:A:N1	30:0:2756:U:C2	2.90	0.40
30:0:2782:G:O6	30:0:2790:C:H5''	2.21	0.40
30:0:932:U:H2'	30:0:933:C:C6	2.57	0.40
31:9:26:C:H2'	31:9:27:C:C6	2.57	0.40
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.80	0.40
8:H:76:LEU:HD21	8:H:149:VAL:HA	2.02	0.40
8:H:91:ARG:HG2	8:H:91:ARG:H	1.59	0.40
20:T:24:ARG:NH2	20:T:39:ASN:HD22	2.07	0.40
25:Y:154:ARG:NH2	30:0:1071:G:H4'	2.37	0.40
30:0:1149:U:C5	30:0:1215:A:C5	3.09	0.40
30:0:1414:A:H2'	30:0:1415:G:O4'	2.21	0.40
30:0:1503:U:H3'	30:0:1503:U:H6	1.86	0.40
30:0:1741:U:C5'	30:0:1742:A:OP1	2.63	0.40
30:0:2112:A:H2'	30:0:2113:G:C8	2.56	0.40
30:0:2726:U:O2	30:0:2749:U:O5'	2.40	0.40
30:0:2842:G:C2'	30:0:2843:A:H5'	2.51	0.40
30:0:445:U:H2'	30:0:446:G:C8	2.56	0.40
30:0:724:G:O2'	30:0:725:C:H5'	2.22	0.40
30:0:806:A:H2'	30:0:807:A:O4'	2.22	0.40
30:0:853:C:H2'	30:0:854:G:O4'	2.21	0.40
31:9:39:U:H3'	31:9:40:C:H5''	2.02	0.40
1:A:86:ALA:HB3	1:A:94:LEU:HD22	2.03	0.40
2:B:202:VAL:HG11	2:B:301:VAL:HG13	2.04	0.40
3:C:107:ARG:NH1	3:C:107:ARG:HB3	2.37	0.40
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.95	0.40
23:W:90:TYR:CE2	23:W:99:ALA:HB2	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.21	0.40
30:0:47:G:N3	30:0:114:A:C2	2.90	0.40
30:0:138:U:OP2	30:0:139:C:C5	2.73	0.40
30:0:1705:C:H2'	30:0:1706:G:O4'	2.20	0.40
30:0:1878:G:H2'	38:0:3278:HOH:O	2.21	0.40
30:0:2016:U:H6	30:0:2016:U:O5'	2.05	0.40
30:0:234:A:H4'	30:0:437:A:O4'	2.22	0.40
8:H:155:ARG:NH1	30:0:2503:A:H5''	2.36	0.40
30:0:517:U:H1'	38:0:7614:HOH:O	2.21	0.40
30:0:907:A:H2'	30:0:908:A:H8	1.85	0.40
28:2:5:LYS:O	28:2:9:LYS:HG3	2.22	0.40
3:C:118:THR:O	3:C:136:VAL:HG13	2.22	0.40
3:C:16:VAL:HG12	3:C:17:ASP:N	2.36	0.40
3:C:236:THR:HG22	3:C:239:ALA:CB	2.51	0.40
3:C:2:GLN:HB3	38:C:8530:HOH:O	2.21	0.40
20:T:82:THR:HG21	30:0:488:U:O2'	2.21	0.40
23:W:149:LEU:HG	23:W:153:MET:HE1	2.03	0.40
25:Y:144:ARG:NH1	38:Y:8871:HOH:O	2.53	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	212 (90%)	18 (8%)	5 (2%)	11	27
2	B	335/338 (99%)	306 (91%)	26 (8%)	3 (1%)	25	55
3	C	244/246 (99%)	228 (93%)	16 (7%)	0	100	100
4	D	134/177 (76%)	112 (84%)	19 (14%)	3 (2%)	10	25
5	E	170/178 (96%)	161 (95%)	9 (5%)	0	100	100
6	F	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	25	55
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	149 (96%)	6 (4%)	1 (1%)	33	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	68/162 (42%)	55 (81%)	10 (15%)	3 (4%)	4	8
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
11	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
12	L	141/165 (86%)	127 (90%)	13 (9%)	1 (1%)	30	62
13	M	192/196 (98%)	182 (95%)	9 (5%)	1 (0%)	38	70
14	N	184/187 (98%)	168 (91%)	13 (7%)	3 (2%)	14	35
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	141 (100%)	0	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
19	S	79/85 (93%)	78 (99%)	1 (1%)	0	100	100
20	T	117/120 (98%)	110 (94%)	6 (5%)	1 (1%)	25	55
21	U	51/67 (76%)	47 (92%)	4 (8%)	0	100	100
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	14	35
23	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
24	X	80/92 (87%)	73 (91%)	6 (8%)	1 (1%)	18	43
25	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
26	Z	71/116 (61%)	61 (86%)	8 (11%)	2 (3%)	8	18
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	21	49
All	All	3705/4472 (83%)	3458 (93%)	220 (6%)	27 (1%)	30	62

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	37	VAL
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
2	B	34	GLY
6	F	101	ALA
12	L	149	ARG
20	T	53	GLY

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Mol	Chain	Res	Type
26	Z	66	CYS
2	B	185	GLY
4	D	27	ILE
4	D	137	PRO
8	H	19	ARG
2	B	2	GLN
22	V	43	PRO
1	A	36	ASP
4	D	56	ARG
9	I	108	HIS
29	3	56	PRO
26	Z	65	ASN
9	I	83	GLY
24	X	70	ILE
1	A	88	ILE
9	I	125	GLY
1	A	38	ILE
13	M	88	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	171 (96%)	8 (4%)	38	70
2	B	282/283 (100%)	265 (94%)	17 (6%)	27	56
3	C	193/193 (100%)	178 (92%)	15 (8%)	18	40
4	D	117/148 (79%)	109 (93%)	8 (7%)	22	48
5	E	152/156 (97%)	147 (97%)	5 (3%)	50	81
6	F	93/94 (99%)	93 (100%)	0	100	100
7	G	27/282 (10%)	26 (96%)	1 (4%)	45	78
8	H	134/145 (92%)	127 (95%)	7 (5%)	32	63
9	I	58/130 (45%)	57 (98%)	1 (2%)	73	94
10	J	118/121 (98%)	112 (95%)	6 (5%)	33	64
11	K	106/106 (100%)	103 (97%)	3 (3%)	56	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	113/127 (89%)	111 (98%)	2 (2%)	71	93
13	M	158/160 (99%)	150 (95%)	8 (5%)	33	64
14	N	149/150 (99%)	144 (97%)	5 (3%)	49	81
15	O	93/94 (99%)	91 (98%)	2 (2%)	64	90
16	P	113/117 (97%)	108 (96%)	5 (4%)	39	71
17	Q	79/80 (99%)	77 (98%)	2 (2%)	60	89
18	R	117/122 (96%)	113 (97%)	4 (3%)	49	81
19	S	71/74 (96%)	70 (99%)	1 (1%)	78	95
20	T	105/106 (99%)	99 (94%)	6 (6%)	29	58
21	U	44/53 (83%)	43 (98%)	1 (2%)	63	90
22	V	51/57 (90%)	50 (98%)	1 (2%)	68	92
23	W	130/130 (100%)	126 (97%)	4 (3%)	52	83
24	X	66/74 (89%)	60 (91%)	6 (9%)	14	30
25	Y	120/196 (61%)	114 (95%)	6 (5%)	34	66
26	Z	60/94 (64%)	59 (98%)	1 (2%)	73	94
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	61	89
29	3	79/79 (100%)	77 (98%)	2 (2%)	60	89
All	All	3095/3646 (85%)	2967 (96%)	128 (4%)	41	74

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	36	ASP
1	A	38	ILE
1	A	68	ILE
1	A	69	LEU
1	A	94	LEU
1	A	179	MET
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	16	ARG
2	B	27	ASN
2	B	49	THR

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Mol	Chain	Res	Type
2	B	56	ASP
2	B	97	LEU
2	B	98	THR
2	B	132	HIS
2	B	162	MET
2	B	184	ASP
2	B	190	MET
2	B	234	ARG
2	B	251	VAL
2	B	254	GLN
2	B	257	THR
2	B	312	ARG
3	C	2	GLN
3	C	27	ARG
3	C	76	ARG
3	C	78	ARG
3	C	115	LEU
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	214	THR
3	C	222	ASP
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	237	GLU
3	C	243	VAL
4	D	19	GLU
4	D	24	HIS
4	D	50	VAL
4	D	52	THR
4	D	137	PRO
4	D	149	ARG
4	D	161	ASP
4	D	170	TYR
5	E	7	ILE
5	E	12	ASP
5	E	16	ASP
5	E	96	ASN
5	E	102	VAL
7	G	64	ASN
8	H	33	GLN

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Mol	Chain	Res	Type
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
8	H	169	GLU
8	H	173	GLU
9	I	94	ASP
10	J	46	ILE
10	J	52	GLN
10	J	79	PHE
10	J	107	ASN
10	J	130	VAL
10	J	131	THR
11	K	10	GLN
11	K	55	VAL
11	K	119	GLN
12	L	35	ARG
12	L	101	ASP
13	M	46	LEU
13	M	68	ARG
13	M	81	ARG
13	M	93	ARG
13	M	99	ARG
13	M	115	LEU
13	M	116	ASN
13	M	164	THR
14	N	26	LEU
14	N	49	THR
14	N	56	ASP
14	N	127	LEU
14	N	138	ASP
15	O	43	VAL
15	O	98	LEU
16	P	21	VAL
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE
16	P	110	ASP
17	Q	16	ASN
17	Q	57	ASP
18	R	13	THR
18	R	39	THR

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Mol	Chain	Res	Type
18	R	82	GLU
18	R	143	VAL
19	S	59	ASP
20	T	39	ASN
20	T	48	VAL
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
20	T	117	ASP
21	U	52	THR
22	V	65	ASP
23	W	26	ILE
23	W	52	VAL
23	W	142	ASP
23	W	146	ILE
24	X	46	ASP
24	X	49	ARG
24	X	52	PRO
24	X	72	VAL
24	X	82	GLU
24	X	88	GLU
25	Y	115	ARG
25	Y	154	ARG
25	Y	163	THR
25	Y	169	ARG
25	Y	189	ASN
25	Y	203	VAL
26	Z	65	ASN
28	2	18	ASN
29	3	3	MET
29	3	56	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	256	GLN

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Mol	Chain	Res	Type
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN
3	C	2	GLN
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
3	C	163	HIS
4	D	85	GLN
4	D	103	ASN
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
8	H	73	ASN
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	44	HIS
11	K	67	GLN
12	L	18	HIS
12	L	41	HIS
12	L	116	HIS
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	170	ASN
14	N	40	ASN
14	N	93	GLN
14	N	107	ASN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	40	HIS
18	R	22	GLN
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN

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Mol	Chain	Res	Type
18	R	113	HIS
18	R	117	HIS
18	R	122	GLN
19	S	44	GLN
20	T	39	ASN
21	U	39	ASN
22	V	60	GLN
23	W	2	HIS
23	W	28	HIS
23	W	87	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	119	GLN
25	Y	133	HIS
25	Y	134	HIS
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	41	HIS
28	2	45	ASN
29	3	20	HIS
29	3	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	239 (8%)	0
31	9	121/122 (99%)	16 (13%)	0
All	All	2866/3045 (94%)	255 (8%)	0

All (255) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A

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Mol	Chain	Res	Type
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	219	G
30	0	236	A
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A

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Mol	Chain	Res	Type
30	0	545	G
30	0	553	G
30	0	559	U
30	0	588	G
30	0	604	G
30	0	605	C
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	698	A
30	0	701	U
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	898	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C

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Mol	Chain	Res	Type
30	0	1072	G
30	0	1081	A
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1137	G
30	0	1151	G
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1279	U
30	0	1287	A
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1460	G
30	0	1474	C
30	0	1485	A
30	0	1488	U
30	0	1505	U
30	0	1506	U
30	0	1507	C
30	0	1524	U
30	0	1525	G
30	0	1526	A

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Mol	Chain	Res	Type
30	0	1528	A
30	0	1562	C
30	0	1592	G
30	0	1603	A
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1730	G
30	0	1731	C
30	0	1732	A
30	0	1742	A
30	0	1752	G
30	0	1778	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1996	U
30	0	2004	U
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G

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Mol	Chain	Res	Type
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2110	G
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2320	U
30	0	2321	A
30	0	2345	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2467	A
30	0	2469	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2513	A
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G

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Mol	Chain	Res	Type
30	0	2645	U
30	0	2649	A
30	0	2664	A
30	0	2676	C
30	0	2681	A
30	0	2682	C
30	0	2719	A
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2867	G
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
30	OMU	0	2587	30	20,22,23	1.46	2 (10%)	24,31,34	0.75	0
30	OMG	0	2588	30	24,26,27	0.90	0	33,38,41	5.31	4 (12%)
30	UR3	0	2619	30	20,22,23	1.49	1 (5%)	23,32,35	0.79	0
30	PSU	0	2621	30	19,21,22	1.50	2 (10%)	23,30,33	0.99	0
30	1MA	0	628	30,34	23,25,26	0.95	2 (8%)	32,37,40	0.97	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/8/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/10/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/6/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/8/25/26	0/2/2/2
30	1MA	0	628	30,34	-	1/8/25/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2619	UR3	C5-C4	5.81	1.43	1.37
30	0	2587	OMU	C5-C4	5.50	1.43	1.37
30	0	2621	PSU	C5-C1'	-4.98	1.47	1.52
30	0	628	1MA	C6-N6	2.23	1.33	1.29
30	0	2587	OMU	P-OP1	2.16	1.49	1.46
30	0	628	1MA	C6-N1	-2.06	1.35	1.37
30	0	2621	PSU	C2-N1	2.03	1.43	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-C5-N7	-28.81	130.26	134.14
30	0	2588	OMG	C6-N1-C2	8.53	125.02	120.20
30	0	628	1MA	C2-N3-C4	-3.46	110.60	116.23
30	0	2588	OMG	C2-N3-C4	-2.89	111.84	115.30
30	0	2588	OMG	C5-C4-N3	2.11	128.50	126.07

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	237/240 (98%)	0.39	22 (9%) 9 9	26, 50, 86, 109	0
2	B	337/338 (99%)	0.00	5 (1%) 70 75	28, 51, 79, 93	0
3	C	246/246 (100%)	0.17	4 (1%) 68 74	21, 43, 69, 77	0
4	D	140/177 (79%)	2.42	80 (57%) 0 0	56, 98, 124, 134	0
5	E	172/178 (96%)	0.75	16 (9%) 9 9	43, 66, 87, 91	0
6	F	119/120 (99%)	0.92	23 (19%) 2 2	47, 70, 99, 114	0
7	G	29/348 (8%)	2.09	16 (55%) 0 0	75, 93, 103, 106	0
8	H	160/177 (90%)	0.35	7 (4%) 33 37	34, 54, 92, 100	0
9	I	70/162 (43%)	4.57	61 (87%) 0 0	129, 145, 162, 163	0
10	J	142/145 (97%)	0.00	1 (0%) 84 89	34, 48, 70, 91	0
11	K	132/132 (100%)	0.26	3 (2%) 57 64	31, 49, 72, 78	0
12	L	145/165 (87%)	1.21	40 (27%) 1 1	24, 63, 111, 125	0
13	M	194/196 (98%)	-0.07	2 (1%) 79 83	28, 40, 55, 64	0
14	N	186/187 (99%)	0.79	28 (15%) 3 3	39, 61, 111, 121	0
15	O	115/116 (99%)	0.24	2 (1%) 67 73	36, 51, 69, 79	0
16	P	143/149 (95%)	0.38	4 (2%) 50 56	37, 53, 67, 76	0
17	Q	95/96 (98%)	0.00	1 (1%) 77 82	33, 43, 59, 76	0
18	R	150/155 (96%)	-0.12	0 100 100	30, 43, 62, 77	0
19	S	81/85 (95%)	0.76	6 (7%) 14 15	38, 57, 78, 89	0
20	T	119/120 (99%)	0.58	10 (8%) 11 12	37, 54, 86, 111	0
21	U	53/67 (79%)	0.35	1 (1%) 64 70	40, 54, 72, 80	0
22	V	65/71 (91%)	1.92	24 (36%) 1 1	51, 71, 116, 122	0
23	W	154/154 (100%)	-0.07	0 100 100	32, 48, 64, 77	0
24	X	82/92 (89%)	0.20	1 (1%) 75 81	39, 58, 83, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/241 (58%)	0.13	4 (2%) 50 56	23, 43, 66, 86	0
26	Z	73/116 (62%)	0.89	15 (20%) 1 2	49, 67, 83, 95	0
27	1	56/57 (98%)	-0.24	0 100 100	25, 31, 39, 47	0
28	2	46/50 (92%)	0.30	2 (4%) 34 38	31, 59, 88, 100	0
29	3	92/92 (100%)	0.56	6 (6%) 18 21	33, 55, 68, 83	0
30	0	2754/2923 (94%)	-0.00	77 (2%) 50 56	19, 42, 87, 162	0
31	9	122/122 (100%)	0.17	6 (4%) 28 31	35, 61, 85, 146	0
All	All	6651/7517 (88%)	0.30	467 (7%) 17 17	19, 49, 98, 163	0

All (467) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	63	ILE	14.7
22	V	1	THR	13.4
9	I	66	GLY	11.5
9	I	74	ILE	11.2
9	I	112	LEU	10.3
4	D	57	THR	9.1
9	I	128	THR	9.1
31	9	1	U	8.6
22	V	40	PRO	8.5
22	V	39	ALA	8.4
9	I	108	HIS	8.4
4	D	64	ARG	8.4
9	I	72	GLU	8.4
9	I	104	ALA	8.3
9	I	111	LEU	8.3
9	I	132	VAL	8.2
9	I	70	THR	8.1
9	I	71	ALA	8.1
22	V	43	PRO	7.7
9	I	97	VAL	7.4
4	D	69	ILE	7.3
9	I	67	VAL	7.2
9	I	109	PRO	6.8
9	I	106	GLN	6.8
19	S	81	ILE	6.8
4	D	18	ILE	6.6
14	N	166	ALA	6.6
30	0	1172	G	6.6

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Mol	Chain	Res	Type	RSRZ
4	D	26	GLY	6.5
12	L	80	ASP	6.5
9	I	69	PRO	6.3
4	D	61	PHE	6.3
7	G	27	ILE	6.3
6	F	106	ALA	6.2
20	T	119	ALA	6.0
4	D	27	ILE	6.0
9	I	73	LEU	6.0
12	L	91	VAL	6.0
9	I	100	VAL	5.9
30	0	735	C	5.8
30	0	282	C	5.8
30	0	1199	A	5.7
9	I	79	GLY	5.6
9	I	113	SER	5.6
30	0	1163	G	5.6
30	0	1173	A	5.6
30	0	1190	G	5.5
14	N	147	ILE	5.5
4	D	10	PHE	5.5
12	L	81	VAL	5.4
20	T	116	ASP	5.3
4	D	70	GLY	5.2
4	D	128	LEU	5.2
9	I	92	VAL	5.1
9	I	91	PHE	5.1
4	D	23	VAL	5.1
30	0	1177	A	5.1
9	I	110	ASP	5.0
9	I	93	ALA	5.0
4	D	17	ARG	5.0
9	I	105	GLU	5.0
9	I	68	PRO	5.0
9	I	80	PHE	5.0
9	I	127	CYS	5.0
30	0	1165	G	4.9
30	0	1181	A	4.9
12	L	120	LEU	4.8
9	I	102	GLN	4.8
9	I	83	GLY	4.8
30	0	1951	G	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
30	0	1171	A	4.8
9	I	82	THR	4.7
4	D	66	GLY	4.6
12	L	105	TYR	4.6
30	0	2237	G	4.6
9	I	103	ILE	4.6
12	L	106	VAL	4.5
30	0	1192	A	4.5
12	L	89	PHE	4.5
4	D	56	ARG	4.5
30	0	1162	G	4.5
26	Z	44	ARG	4.4
9	I	99	GLN	4.4
26	Z	46	SER	4.4
9	I	86	GLU	4.3
30	0	1200	A	4.2
9	I	123	VAL	4.2
4	D	58	VAL	4.2
30	0	2769	C	4.2
30	0	2004	U	4.2
12	L	75	LEU	4.1
4	D	44	ILE	4.1
12	L	99	GLU	4.1
9	I	114	TYR	4.1
4	D	75	LEU	4.1
16	P	67	LYS	4.1
4	D	11	HIS	4.1
31	9	24	U	4.0
30	0	1186	C	4.0
25	Y	235	GLU	4.0
31	9	2	U	4.0
30	0	1168	C	3.9
22	V	44	GLY	3.9
12	L	73	VAL	3.9
30	0	1166	A	3.9
9	I	130	LEU	3.9
30	0	1174	A	3.8
14	N	75	THR	3.8
12	L	60	GLU	3.8
12	L	145	LEU	3.8
14	N	183	ASP	3.8
30	0	1161	A	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	237	GLY	3.8
26	Z	45	VAL	3.8
12	L	90	ARG	3.7
26	Z	49	ARG	3.7
4	D	134	LEU	3.7
9	I	126	THR	3.7
30	0	1164	U	3.7
30	0	1167	G	3.7
30	0	1198	U	3.7
29	3	1	MET	3.7
12	L	77	ALA	3.7
30	0	1178	G	3.7
8	H	174	LEU	3.7
9	I	88	GLN	3.7
9	I	76	ASP	3.6
6	F	47	LEU	3.6
30	0	284	C	3.6
30	0	1170	U	3.6
4	D	73	VAL	3.6
30	0	138	U	3.6
4	D	139	TYR	3.6
9	I	129	SER	3.6
22	V	41	GLU	3.6
14	N	179	LEU	3.6
4	D	25	MET	3.6
30	0	1279	U	3.6
22	V	45	ARG	3.6
30	0	1176	C	3.5
5	E	154	ILE	3.5
4	D	65	GLU	3.5
4	D	93	LEU	3.5
4	D	130	VAL	3.5
7	G	23	ILE	3.5
4	D	74	THR	3.5
6	F	28	ALA	3.4
12	L	123	ASP	3.4
4	D	106	PHE	3.4
4	D	62	ASP	3.4
22	V	2	VAL	3.4
4	D	68	PRO	3.4
11	K	118	ALA	3.4
9	I	81	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
4	D	135	VAL	3.4
4	D	141	VAL	3.4
25	Y	108	ASP	3.4
9	I	122	GLU	3.4
6	F	16	ALA	3.3
7	G	71	LEU	3.3
9	I	116	LEU	3.3
22	V	38	GLY	3.3
30	0	1191	A	3.3
9	I	119	ALA	3.3
30	0	1202	A	3.3
4	D	47	GLN	3.3
6	F	119	ARG	3.3
4	D	143	LYS	3.3
5	E	10	ASP	3.3
4	D	22	VAL	3.3
9	I	125	GLY	3.3
28	2	49	GLU	3.3
30	0	2238	A	3.3
4	D	90	LEU	3.3
12	L	149	ARG	3.2
30	0	1175	G	3.2
4	D	19	GLU	3.2
16	P	71	TYR	3.2
1	A	37	VAL	3.2
30	0	272	A	3.2
30	0	999	C	3.2
7	G	72	ASP	3.2
12	L	147	GLU	3.2
2	B	119	HIS	3.2
4	D	28	GLY	3.2
29	3	41	GLU	3.2
30	0	2345	A	3.2
4	D	88	LEU	3.2
7	G	26	MET	3.2
30	0	1169	U	3.2
5	E	100	ASP	3.1
12	L	76	LEU	3.1
30	0	736	A	3.1
5	E	118	ILE	3.1
30	0	285	A	3.1
1	A	99	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
6	F	49	PHE	3.1
1	A	103	VAL	3.1
4	D	13	MET	3.1
4	D	85	GLN	3.1
5	E	122	THR	3.1
31	9	23	U	3.1
5	E	45	ASP	3.1
1	A	82	VAL	3.1
6	F	17	LEU	3.1
7	G	70	ALA	3.1
14	N	42	HIS	3.1
4	D	71	ALA	3.1
4	D	48	MET	3.1
30	0	1950	G	3.1
3	C	246	ARG	3.0
4	D	40	ILE	3.0
30	0	2664	A	3.0
4	D	43	GLU	3.0
20	T	118	SER	3.0
15	O	69	VAL	3.0
22	V	49	LEU	3.0
20	T	117	ASP	3.0
30	0	10	U	3.0
7	G	69	ARG	3.0
22	V	37	GLY	3.0
1	A	58	VAL	3.0
5	E	123	ASP	3.0
14	N	155	GLU	3.0
30	0	1189	A	3.0
10	J	70	PHE	2.9
12	L	121	ILE	2.9
12	L	82	ALA	2.9
9	I	118	ASN	2.9
30	0	970	U	2.9
30	0	960	G	2.9
30	0	1947	G	2.9
5	E	87	PHE	2.9
20	T	112	LEU	2.9
1	A	36	ASP	2.9
6	F	27	GLY	2.9
1	A	88	ILE	2.9
30	0	2344	G	2.9

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Mol	Chain	Res	Type	RSRZ
26	Z	104	ARG	2.9
8	H	35	LYS	2.9
22	V	8	ILE	2.9
1	A	35	GLY	2.9
9	I	120	ALA	2.9
30	0	1207	A	2.9
9	I	133	THR	2.8
6	F	117	GLU	2.8
14	N	149	GLU	2.8
22	V	36	ALA	2.8
9	I	95	LEU	2.8
3	C	135	GLU	2.8
5	E	6	GLU	2.8
12	L	96	VAL	2.8
9	I	75	LYS	2.8
9	I	107	LYS	2.8
8	H	40	GLN	2.8
24	X	85	VAL	2.8
30	0	1184	C	2.8
26	Z	35	SER	2.8
20	T	115	GLU	2.8
14	N	138	ASP	2.8
26	Z	60	ASP	2.8
19	S	20	PHE	2.8
4	D	29	HIS	2.8
7	G	25	GLU	2.8
9	I	78	ALA	2.8
30	0	1193	A	2.8
30	0	1626	A	2.8
9	I	124	VAL	2.7
12	L	119	THR	2.7
25	Y	234	VAL	2.7
9	I	131	GLY	2.7
26	Z	50	VAL	2.7
12	L	118	LEU	2.7
1	A	38	ILE	2.7
26	Z	34	SER	2.7
4	D	165	PHE	2.7
4	D	51	ARG	2.7
4	D	166	ILE	2.7
6	F	75	ILE	2.7
30	0	497	A	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	104	PHE	2.6
30	0	1179	C	2.6
4	D	50	VAL	2.6
30	0	283	U	2.6
4	D	41	LEU	2.6
7	G	24	VAL	2.6
14	N	145	ALA	2.6
9	I	84	SER	2.6
26	Z	43	GLY	2.6
2	B	91	PRO	2.6
4	D	24	HIS	2.6
14	N	62	HIS	2.6
30	0	280	C	2.6
12	L	150	GLN	2.6
26	Z	58	ASN	2.6
8	H	86	TYR	2.6
9	I	134	ILE	2.6
14	N	152	GLU	2.6
4	D	107	GLY	2.6
1	A	60	PHE	2.6
12	L	141	GLU	2.6
4	D	137	PRO	2.5
6	F	99	THR	2.5
4	D	72	LYS	2.5
1	A	94	LEU	2.5
5	E	5	LEU	2.5
30	0	1948	G	2.5
14	N	67	ALA	2.5
6	F	14	ASP	2.5
5	E	119	HIS	2.5
22	V	51	LYS	2.5
4	D	170	TYR	2.5
30	0	1000	C	2.5
30	0	2239	C	2.5
1	A	65	ARG	2.5
22	V	31	ARG	2.5
13	M	194	GLY	2.5
6	F	105	ASP	2.5
13	M	1	ALA	2.5
11	K	49	LEU	2.5
9	I	98	ASP	2.5
12	L	122	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
4	D	157	LEU	2.5
14	N	158	LEU	2.5
1	A	30	ARG	2.5
1	A	236	GLY	2.5
9	I	121	LYS	2.5
6	F	103	GLU	2.5
20	T	109	GLU	2.5
5	E	11	VAL	2.5
22	V	5	VAL	2.5
22	V	48	GLU	2.5
30	0	2241	C	2.5
12	L	114	VAL	2.5
7	G	15	TRP	2.4
7	G	28	GLU	2.4
4	D	45	THR	2.4
6	F	91	VAL	2.4
30	0	1180	U	2.4
30	0	1195	G	2.4
30	0	1197	G	2.4
14	N	43	VAL	2.4
25	Y	98	GLN	2.4
11	K	132	VAL	2.4
14	N	148	ALA	2.4
22	V	32	ALA	2.4
26	Z	53	ILE	2.4
14	N	95	ALA	2.4
30	0	1188	A	2.4
29	3	3	MET	2.4
12	L	104	ASP	2.4
26	Z	54	GLU	2.4
4	D	80	ALA	2.4
31	9	122	C	2.4
6	F	107	ASP	2.4
12	L	144	ASP	2.4
12	L	62	ALA	2.4
4	D	98	PHE	2.4
8	H	82	GLU	2.4
16	P	108	LEU	2.4
6	F	108	VAL	2.3
12	L	97	VAL	2.3
1	A	64	ASP	2.3
12	L	124	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
14	N	63	SER	2.3
1	A	68	ILE	2.3
22	V	7	GLU	2.3
7	G	73	ASP	2.3
31	9	3	A	2.3
4	D	133	ASN	2.3
12	L	130	ARG	2.3
12	L	139	SER	2.3
4	D	92	GLU	2.3
17	Q	95	GLU	2.3
7	G	65	THR	2.3
20	T	42	VAL	2.3
30	0	1203	G	2.3
30	0	368	C	2.3
2	B	57	GLU	2.3
19	S	76	GLU	2.3
30	0	1625	U	2.3
1	A	59	GLU	2.3
12	L	125	PHE	2.3
30	0	130	C	2.3
12	L	108	VAL	2.3
29	3	83	TRP	2.3
12	L	140	VAL	2.3
21	U	48	ASN	2.3
4	D	142	ALA	2.2
22	V	46	ILE	2.2
30	0	1185	U	2.2
4	D	16	PRO	2.2
9	I	87	PRO	2.2
30	0	1182	C	2.2
1	A	145	MET	2.2
14	N	115	VAL	2.2
26	Z	38	PHE	2.2
2	B	92	TYR	2.2
20	T	35	TYR	2.2
30	0	1525	G	2.2
19	S	77	VAL	2.2
22	V	52	ALA	2.2
29	3	22	VAL	2.2
4	D	76	ARG	2.2
14	N	66	LEU	2.2
6	F	26	THR	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	87	ALA	2.2
7	G	63	ARG	2.2
5	E	78	GLU	2.2
14	N	64	SER	2.2
1	A	154	ALA	2.2
4	D	81	GLU	2.2
14	N	184	ILE	2.2
4	D	84	LEU	2.2
7	G	21	ASP	2.2
5	E	29	VAL	2.2
30	0	1194	A	2.2
12	L	79	ASP	2.2
28	2	27	LEU	2.2
29	3	8	ASN	2.2
4	D	132	VAL	2.2
22	V	3	LEU	2.2
14	N	69	TYR	2.1
4	D	67	ASP	2.1
4	D	129	ASP	2.1
20	T	103	LEU	2.1
26	Z	36	GLY	2.1
22	V	33	VAL	2.1
4	D	171	ASP	2.1
4	D	154	LYS	2.1
2	B	118	ASP	2.1
6	F	100	ASP	2.1
4	D	59	GLY	2.1
30	0	1150	A	2.1
14	N	159	TYR	2.1
14	N	81	ALA	2.1
19	S	47	VAL	2.1
30	0	1981	A	2.1
5	E	121	ASP	2.1
6	F	18	GLU	2.1
6	F	98	VAL	2.1
14	N	185	GLU	2.1
4	D	162	ALA	2.1
4	D	144	ARG	2.1
8	H	74	ARG	2.1
4	D	53	LYS	2.0
12	L	100	ALA	2.0
16	P	62	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
7	G	68	GLU	2.0
14	N	76	GLY	2.0
8	H	76	LEU	2.0
30	O	370	G	2.0
1	A	133	ARG	2.0
6	F	110	ASP	2.0
9	I	94	ASP	2.0
12	L	95	ASP	2.0
4	D	55	LYS	2.0
5	E	20	ILE	2.0
14	N	41	LYS	2.0
15	O	48	ILE	2.0
4	D	101	THR	2.0
6	F	90	GLU	2.0
22	V	35	ALA	2.0
19	S	45	TYR	2.0
3	C	245	GLU	2.0
1	A	85	SER	2.0
3	C	139	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
30	UR3	0	2619	21/22	0.16	1.69	34,37,39,43	0
30	1MA	0	628	23/24	0.17	0.99	22,25,28,28	0
30	OMU	0	2587	21/22	0.13	-0.30	29,32,34,36	0
30	PSU	0	2621	20/21	0.14	-1.27	24,26,33,33	0
30	OMG	0	2588	24/25	0.14	-1.62	28,32,34,36	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
36	SR	0	9006	1/1	1.03	179.20	200,200,200,200	0
34	NA	0	8554	1/1	0.63	165.77	63,63,63,63	0
36	SR	0	8997	1/1	0.58	143.85	190,190,190,190	0
34	NA	0	8505	1/1	0.77	89.24	45,45,45,45	0
34	NA	0	8561	1/1	0.39	78.83	68,68,68,68	0
36	SR	0	8982	1/1	0.73	69.38	189,189,189,189	0
32	MG	0	8030	1/1	0.34	54.94	60,60,60,60	0
36	SR	J	8986	1/1	1.95	49.94	200,200,200,200	0
32	MG	0	8040	1/1	0.50	45.02	84,84,84,84	0
32	MG	0	8031	1/1	0.37	41.45	55,55,55,55	0
34	NA	0	8574	1/1	0.50	41.44	61,61,61,61	0
36	SR	0	9007	1/1	0.54	34.44	200,200,200,200	0
34	NA	0	8565	1/1	0.35	29.65	57,57,57,57	0
32	MG	0	8037	1/1	0.32	25.44	89,89,89,89	0
34	NA	0	8555	1/1	0.50	24.45	61,61,61,61	0
34	NA	0	8547	1/1	0.49	23.75	51,51,51,51	0
36	SR	0	8994	1/1	0.47	23.65	198,198,198,198	0
34	NA	0	8562	1/1	0.35	23.47	62,62,62,62	0
36	SR	0	8955	1/1	0.25	20.21	189,189,189,189	0
32	MG	0	8081	1/1	0.22	20.01	64,64,64,64	0
34	NA	0	8525	1/1	0.28	19.77	79,79,79,79	0
34	NA	0	8542	1/1	0.31	18.93	42,42,42,42	0
34	NA	0	8558	1/1	0.39	18.74	44,44,44,44	0
34	NA	0	8566	1/1	0.32	18.63	58,58,58,58	0
36	SR	0	8996	1/1	0.44	17.70	200,200,200,200	0
34	NA	0	8549	1/1	0.32	17.35	58,58,58,58	0
32	MG	0	8071	1/1	0.21	17.28	53,53,53,53	0
36	SR	B	8987	1/1	0.48	17.00	200,200,200,200	0
36	SR	0	8934	1/1	0.22	16.70	108,108,108,108	0
32	MG	0	8047	1/1	0.33	15.01	44,44,44,44	0
36	SR	0	8919	1/1	0.19	14.53	173,173,173,173	0
34	NA	0	8513	1/1	0.31	13.72	45,45,45,45	0
34	NA	0	8546	1/1	0.63	12.96	77,77,77,77	0
34	NA	0	8511	1/1	0.26	12.67	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8571	1/1	0.33	12.23	73,73,73,73	0
36	SR	0	8962	1/1	0.29	11.97	164,164,164,164	0
32	MG	0	8049	1/1	0.31	11.52	65,65,65,65	0
36	SR	0	8976	1/1	0.36	11.28	194,194,194,194	0
34	NA	0	8524	1/1	0.34	10.87	41,41,41,41	0
34	NA	0	8567	1/1	0.35	10.68	65,65,65,65	0
34	NA	9	8572	1/1	0.42	10.64	64,64,64,64	0
34	NA	0	8548	1/1	0.25	10.57	59,59,59,59	0
34	NA	0	8553	1/1	0.22	10.35	67,67,67,67	0
36	SR	0	8998	1/1	0.29	10.27	171,171,171,171	0
36	SR	0	8989	1/1	0.23	10.09	168,168,168,168	0
34	NA	0	8559	1/1	0.19	10.06	71,71,71,71	0
32	MG	0	8024	1/1	0.23	9.70	61,61,61,61	0
36	SR	0	8914	1/1	0.24	9.55	107,107,107,107	0
34	NA	0	8506	1/1	0.26	9.24	66,66,66,66	0
34	NA	0	8545	1/1	0.18	9.18	38,38,38,38	0
34	NA	0	8527	1/1	0.27	8.99	43,43,43,43	0
33	K	0	8401	1/1	0.19	8.84	88,88,88,88	0
34	NA	0	8535	1/1	0.22	8.68	46,46,46,46	0
36	SR	0	8992	1/1	0.23	8.52	125,125,125,125	0
35	CL	0	8822	1/1	0.30	8.31	74,74,74,74	0
34	NA	0	8544	1/1	0.20	8.23	64,64,64,64	0
36	SR	0	8922	1/1	0.29	8.17	160,160,160,160	0
32	MG	0	8069	1/1	0.39	7.48	65,65,65,65	0
32	MG	A	8051	1/1	0.27	7.48	72,72,72,72	0
34	NA	0	8502	1/1	0.22	7.23	55,55,55,55	0
34	NA	0	8560	1/1	0.33	7.23	92,92,92,92	0
36	SR	0	9004	1/1	0.41	7.20	200,200,200,200	0
34	NA	0	8552	1/1	0.29	7.09	59,59,59,59	0
34	NA	0	8568	1/1	0.24	6.84	53,53,53,53	0
34	NA	0	8569	1/1	0.28	6.37	53,53,53,53	0
34	NA	0	8551	1/1	0.21	5.99	47,47,47,47	0
32	MG	0	8062	1/1	0.26	5.98	47,47,47,47	0
32	MG	0	8079	1/1	0.20	5.71	50,50,50,50	0
34	NA	0	8564	1/1	0.28	5.66	63,63,63,63	0
34	NA	0	8521	1/1	0.20	5.57	54,54,54,54	0
32	MG	0	8083	1/1	0.31	5.40	55,55,55,55	0
34	NA	R	8575	1/1	0.29	5.30	82,82,82,82	0
34	NA	0	8517	1/1	0.20	5.20	31,31,31,31	0
34	NA	0	8522	1/1	0.33	5.16	58,58,58,58	0
32	MG	0	8063	1/1	0.17	5.14	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8905	1/1	0.25	4.71	54,54,54,54	0
34	NA	0	8526	1/1	0.31	4.55	46,46,46,46	0
36	SR	0	8947	1/1	0.27	4.53	178,178,178,178	0
36	SR	0	8991	1/1	0.23	4.52	188,188,188,188	0
32	MG	0	8018	1/1	0.18	4.45	36,36,36,36	0
34	NA	0	8519	1/1	0.20	4.26	36,36,36,36	0
32	MG	0	8041	1/1	0.19	4.13	19,19,19,19	0
34	NA	0	8541	1/1	0.22	4.08	50,50,50,50	0
32	MG	0	8009	1/1	0.21	3.94	19,19,19,19	0
34	NA	0	8556	1/1	0.45	3.93	41,41,41,41	0
36	SR	9	8980	1/1	0.14	3.89	177,177,177,177	0
36	SR	0	8974	1/1	0.24	3.83	166,166,166,166	0
32	MG	0	8017	1/1	0.23	3.79	23,23,23,23	0
32	MG	0	8001	1/1	0.18	3.61	29,29,29,29	0
36	SR	0	8907	1/1	0.21	3.58	53,53,53,53	0
32	MG	0	8090	1/1	0.20	3.57	55,55,55,55	0
34	NA	0	8512	1/1	0.19	3.47	38,38,38,38	0
34	NA	0	8550	1/1	0.21	3.29	55,55,55,55	0
36	SR	0	8979	1/1	0.21	3.04	199,199,199,199	0
34	NA	0	8514	1/1	0.19	2.83	41,41,41,41	0
36	SR	0	8906	1/1	0.20	2.69	52,52,52,52	0
34	NA	0	8563	1/1	0.21	2.52	65,65,65,65	0
32	MG	0	8061	1/1	0.18	2.46	29,29,29,29	0
36	SR	0	8959	1/1	0.23	2.35	159,159,159,159	0
32	MG	0	8078	1/1	0.19	2.32	43,43,43,43	0
36	SR	0	8985	1/1	0.17	2.16	118,118,118,118	0
32	MG	0	8039	1/1	0.18	2.01	64,64,64,64	0
34	NA	0	8509	1/1	0.14	1.96	50,50,50,50	0
36	SR	0	8957	1/1	0.17	1.79	188,188,188,188	0
36	SR	0	8904	1/1	0.17	1.51	49,49,49,49	0
34	NA	0	8518	1/1	0.26	1.42	65,65,65,65	0
36	SR	0	8903	1/1	0.16	1.41	45,45,45,45	0
34	NA	0	8570	1/1	0.15	1.37	44,44,44,44	0
32	MG	0	8068	1/1	0.16	1.17	64,64,64,64	0
32	MG	0	8005	1/1	0.19	1.03	29,29,29,29	0
32	MG	0	8012	1/1	0.18	0.99	22,22,22,22	0
32	MG	0	8048	1/1	0.17	0.93	27,27,27,27	0
32	MG	0	8011	1/1	0.19	0.83	24,24,24,24	0
32	MG	0	8019	1/1	0.16	0.74	20,20,20,20	0
32	MG	0	8029	1/1	0.14	0.66	52,52,52,52	0
34	NA	R	8532	1/1	0.18	0.61	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8082	1/1	0.19	0.51	56,56,56,56	0
35	CL	0	8816	1/1	0.17	0.46	54,54,54,54	0
33	K	0	8402	1/1	0.17	0.38	62,62,62,62	0
34	NA	0	8530	1/1	0.16	0.20	47,47,47,47	0
32	MG	0	8015	1/1	0.13	0.00	27,27,27,27	0
36	SR	0	8990	1/1	0.16	-0.04	113,113,113,113	0
32	MG	0	8085	1/1	0.15	-0.11	73,73,73,73	0
34	NA	0	8504	1/1	0.15	-0.12	33,33,33,33	0
35	CL	J	8801	1/1	0.15	-0.13	54,54,54,54	0
32	MG	0	8004	1/1	0.15	-0.18	21,21,21,21	0
36	SR	R	8912	1/1	0.15	-0.33	73,73,73,73	0
32	MG	0	8006	1/1	0.14	-0.36	23,23,23,23	0
36	SR	0	8981	1/1	0.15	-0.40	153,153,153,153	0
34	NA	0	8528	1/1	0.13	-0.41	40,40,40,40	0
36	SR	0	8972	1/1	0.15	-0.49	112,112,112,112	0
36	SR	0	8944	1/1	0.14	-0.51	161,161,161,161	0
35	CL	J	8821	1/1	0.15	-0.54	59,59,59,59	0
32	MG	0	8080	1/1	0.12	-0.60	66,66,66,66	0
34	NA	0	8520	1/1	0.12	-0.61	54,54,54,54	0
36	SR	0	8927	1/1	0.13	-0.65	150,150,150,150	0
34	NA	0	8573	1/1	0.14	-0.67	69,69,69,69	0
35	CL	N	8807	1/1	0.20	-0.73	68,68,68,68	0
32	MG	0	8084	1/1	0.11	-0.76	27,27,27,27	0
36	SR	0	8983	1/1	0.14	-0.78	177,177,177,177	0
36	SR	0	8963	1/1	0.14	-0.82	105,105,105,105	0
35	CL	O	8808	1/1	0.14	-0.83	62,62,62,62	0
32	MG	0	8076	1/1	0.13	-0.85	32,32,32,32	0
36	SR	0	9002	1/1	0.13	-0.87	175,175,175,175	0
36	SR	0	8956	1/1	0.09	-0.88	128,128,128,128	0
36	SR	F	9005	1/1	0.09	-0.95	122,122,122,122	0
34	NA	0	8501	1/1	0.13	-1.01	24,24,24,24	0
34	NA	0	8523	1/1	0.14	-1.05	29,29,29,29	0
34	NA	0	8557	1/1	0.10	-1.11	68,68,68,68	0
32	MG	0	8003	1/1	0.14	-1.13	26,26,26,26	0
32	MG	0	8010	1/1	0.15	-1.15	23,23,23,23	0
35	CL	0	8815	1/1	0.11	-1.17	58,58,58,58	0
34	NA	0	8515	1/1	0.13	-1.17	35,35,35,35	0
34	NA	C	8503	1/1	0.13	-1.23	31,31,31,31	0
37	CD	Z	8703	1/1	0.09	-1.26	71,71,71,71	0
34	NA	J	8538	1/1	0.10	-1.27	57,57,57,57	0
34	NA	9	8543	1/1	0.12	-1.29	47,47,47,47	0
36	SR	0	8993	1/1	0.09	-1.34	165,165,165,165	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8921	1/1	0.12	-1.43	84,84,84,84	0
36	SR	A	8977	1/1	0.08	-1.50	158,158,158,158	0
36	SR	0	8943	1/1	0.11	-1.52	104,104,104,104	0
36	SR	0	8909	1/1	0.12	-1.54	75,75,75,75	0
37	CD	U	8701	1/1	0.07	-1.68	51,51,51,51	0
35	CL	L	8810	1/1	0.11	-1.71	50,50,50,50	0
36	SR	0	8953	1/1	0.15	-1.72	143,143,143,143	0
32	MG	0	8008	1/1	0.11	-1.73	23,23,23,23	0
32	MG	0	8053	1/1	0.09	-1.75	53,53,53,53	0
36	SR	0	8917	1/1	0.12	-1.76	95,95,95,95	0
36	SR	0	8937	1/1	0.15	-1.78	103,103,103,103	0
34	NA	0	8537	1/1	0.10	-1.79	32,32,32,32	0
37	CD	3	8704	1/1	0.07	-1.81	64,64,64,64	0
35	CL	A	8809	1/1	0.15	-1.82	60,60,60,60	0
36	SR	0	8935	1/1	0.11	-1.82	68,68,68,68	0
32	MG	0	8064	1/1	0.14	-1.85	43,43,43,43	0
32	MG	0	8046	1/1	0.13	-1.85	28,28,28,28	0
32	MG	B	8043	1/1	0.07	-1.91	48,48,48,48	0
34	NA	0	8533	1/1	0.10	-1.91	55,55,55,55	0
32	MG	0	8055	1/1	0.14	-1.97	30,30,30,30	0
32	MG	0	8025	1/1	0.12	-1.99	31,31,31,31	0
36	SR	3	8932	1/1	0.10	-2.00	67,67,67,67	0
35	CL	J	8802	1/1	0.06	-2.07	56,56,56,56	0
35	CL	0	8811	1/1	0.10	-2.08	58,58,58,58	0
34	NA	0	8508	1/1	0.11	-2.10	39,39,39,39	0
37	CD	O	8705	1/1	0.07	-2.11	83,83,83,83	0
32	MG	0	8092	1/1	0.11	-2.11	51,51,51,51	0
36	SR	0	8925	1/1	0.11	-2.14	84,84,84,84	0
32	MG	B	8042	1/1	0.07	-2.14	47,47,47,47	0
36	SR	0	8918	1/1	0.12	-2.15	76,76,76,76	0
32	MG	Y	8086	1/1	0.10	-2.16	33,33,33,33	0
32	MG	0	8045	1/1	0.11	-2.29	39,39,39,39	0
36	SR	3	8999	1/1	0.06	-2.30	93,93,93,93	0
32	MG	0	8073	1/1	0.11	-2.43	79,79,79,79	0
32	MG	0	8007	1/1	0.13	-2.67	27,27,27,27	0
36	SR	0	8939	1/1	0.09	-2.71	146,146,146,146	0
36	SR	A	8929	1/1	0.10	-2.77	113,113,113,113	0
36	SR	0	9000	1/1	0.11	-2.83	157,157,157,157	0
36	SR	9	9003	1/1	0.16	-2.84	169,169,169,169	0
35	CL	0	8812	1/1	0.06	-2.85	40,40,40,40	0
34	NA	0	8507	1/1	0.13	-2.85	40,40,40,40	0
34	NA	0	8516	1/1	0.12	-2.98	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	CL	0	8805	1/1	0.10	-2.99	58,58,58,58	0
32	MG	0	8060	1/1	0.11	-3.00	54,54,54,54	0
32	MG	0	8016	1/1	0.14	-3.01	43,43,43,43	0
35	CL	R	8806	1/1	0.11	-3.03	42,42,42,42	0
37	CD	1	8702	1/1	0.07	-3.13	53,53,53,53	0
32	MG	T	8057	1/1	0.10	-3.15	58,58,58,58	0
36	SR	0	8940	1/1	0.09	-3.18	70,70,70,70	0
32	MG	0	8075	1/1	0.10	-3.18	49,49,49,49	0
36	SR	0	8954	1/1	0.08	-3.24	94,94,94,94	0
36	SR	0	8965	1/1	0.08	-3.26	117,117,117,117	0
32	MG	9	8074	1/1	0.11	-3.29	74,74,74,74	0
34	NA	M	8539	1/1	0.08	-3.29	33,33,33,33	0
36	SR	0	8975	1/1	0.07	-3.39	120,120,120,120	0
36	SR	0	8933	1/1	0.11	-3.43	127,127,127,127	0
36	SR	0	8911	1/1	0.06	-3.49	74,74,74,74	0
36	SR	0	8968	1/1	0.08	-3.49	146,146,146,146	0
32	MG	0	8028	1/1	0.11	-3.53	18,18,18,18	0
35	CL	0	8814	1/1	0.11	-3.54	48,48,48,48	0
32	MG	0	8020	1/1	0.09	-3.63	38,38,38,38	0
36	SR	0	8969	1/1	0.11	-3.64	134,134,134,134	0
32	MG	A	8050	1/1	0.08	-3.65	24,24,24,24	0
32	MG	0	8066	1/1	0.12	-3.66	57,57,57,57	0
32	MG	0	8058	1/1	0.06	-3.69	25,25,25,25	0
32	MG	0	8093	1/1	0.10	-3.76	29,29,29,29	0
36	SR	0	8960	1/1	0.07	-3.77	141,141,141,141	0
36	SR	0	8931	1/1	0.07	-3.81	94,94,94,94	0
36	SR	0	8941	1/1	0.11	-3.86	113,113,113,113	0
32	MG	0	8021	1/1	0.07	-3.90	31,31,31,31	0
35	CL	B	8819	1/1	0.10	-3.92	50,50,50,50	0
36	SR	0	8946	1/1	0.13	-3.99	102,102,102,102	0
32	MG	0	8070	1/1	0.10	-4.02	40,40,40,40	0
35	CL	M	8818	1/1	0.07	-4.10	33,33,33,33	0
32	MG	0	8035	1/1	0.10	-4.11	62,62,62,62	0
35	CL	3	8804	1/1	0.09	-4.13	53,53,53,53	0
32	MG	0	8014	1/1	0.12	-4.15	19,19,19,19	0
36	SR	0	9008	1/1	0.13	-4.18	85,85,85,85	0
36	SR	0	8978	1/1	0.05	-4.29	108,108,108,108	0
36	SR	0	8973	1/1	0.09	-4.30	121,121,121,121	0
36	SR	0	8967	1/1	0.06	-4.39	116,116,116,116	0
36	SR	0	8964	1/1	0.06	-4.50	110,110,110,110	0
36	SR	0	8926	1/1	0.09	-4.51	107,107,107,107	0
36	SR	0	8966	1/1	0.08	-4.51	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8529	1/1	0.04	-4.54	38,38,38,38	0
34	NA	Q	8540	1/1	0.07	-4.59	41,41,41,41	0
36	SR	1	8913	1/1	0.07	-4.61	78,78,78,78	0
36	SR	0	9001	1/1	0.09	-4.64	171,171,171,171	0
32	MG	0	8067	1/1	0.11	-4.65	26,26,26,26	0
35	CL	0	8803	1/1	0.08	-4.67	50,50,50,50	0
32	MG	0	8038	1/1	0.10	-4.74	68,68,68,68	0
36	SR	0	8928	1/1	0.07	-4.85	125,125,125,125	0
32	MG	0	8023	1/1	0.08	-4.86	18,18,18,18	0
36	SR	A	8930	1/1	0.05	-4.87	100,100,100,100	0
36	SR	0	8902	1/1	0.13	-4.95	58,58,58,58	0
36	SR	0	8908	1/1	0.08	-5.07	80,80,80,80	0
36	SR	0	8923	1/1	0.08	-5.14	85,85,85,85	0
36	SR	0	8958	1/1	0.08	-5.21	86,86,86,86	0
32	MG	0	8022	1/1	0.10	-5.22	32,32,32,32	0
36	SR	0	8970	1/1	0.06	-5.25	115,115,115,115	0
36	SR	0	8949	1/1	0.09	-5.30	90,90,90,90	0
32	MG	0	8087	1/1	0.13	-5.31	31,31,31,31	0
34	NA	0	8534	1/1	0.11	-5.35	25,25,25,25	0
36	SR	0	8951	1/1	0.04	-5.38	132,132,132,132	0
32	MG	0	8072	1/1	0.11	-5.66	53,53,53,53	0
36	SR	0	8920	1/1	0.05	-5.72	113,113,113,113	0
36	SR	0	8936	1/1	0.08	-5.74	84,84,84,84	0
32	MG	0	8065	1/1	0.09	-5.90	47,47,47,47	0
32	MG	0	8077	1/1	0.07	-5.97	35,35,35,35	0
35	CL	0	8817	1/1	0.09	-6.19	50,50,50,50	0
34	NA	0	8531	1/1	0.07	-6.26	41,41,41,41	0
32	MG	0	8013	1/1	0.07	-6.48	24,24,24,24	0
32	MG	0	8056	1/1	0.12	-6.52	41,41,41,41	0
36	SR	0	8988	1/1	0.11	-6.53	158,158,158,158	0
32	MG	0	8036	1/1	0.07	-6.59	49,49,49,49	0
34	NA	0	8536	1/1	0.08	-6.60	44,44,44,44	0
32	MG	0	8002	1/1	0.09	-6.69	21,21,21,21	0
35	CL	0	8813	1/1	0.07	-6.75	44,44,44,44	0
36	SR	0	8945	1/1	0.06	-6.82	105,105,105,105	0
36	SR	0	8984	1/1	0.07	-6.99	105,105,105,105	0
32	MG	0	8088	1/1	0.09	-7.00	34,34,34,34	0
36	SR	0	8910	1/1	0.06	-7.03	84,84,84,84	0
32	MG	0	8044	1/1	0.06	-7.06	46,46,46,46	0
36	SR	0	8924	1/1	0.09	-7.17	134,134,134,134	0
32	MG	0	8027	1/1	0.09	-7.63	39,39,39,39	0
32	MG	0	8052	1/1	0.06	-7.66	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8026	1/1	0.08	-7.74	27,27,27,27	0
32	MG	0	8033	1/1	0.04	-7.78	51,51,51,51	0
36	SR	0	8995	1/1	0.08	-8.11	117,117,117,117	0
36	SR	B	8950	1/1	0.08	-8.16	101,101,101,101	0
36	SR	0	8971	1/1	0.10	-8.40	165,165,165,165	0
36	SR	0	8942	1/1	0.07	-8.66	115,115,115,115	0
36	SR	0	8901	1/1	0.08	-8.76	73,73,73,73	0
36	SR	0	8915	1/1	0.06	-9.38	115,115,115,115	0
36	SR	0	8948	1/1	0.08	-10.12	77,77,77,77	0
32	MG	0	8034	1/1	0.08	-10.28	36,36,36,36	0
36	SR	1	8952	1/1	0.07	-11.75	74,74,74,74	0
35	CL	Y	8820	1/1	0.09	-12.30	38,38,38,38	0
32	MG	K	8054	1/1	0.07	-15.61	37,37,37,37	0
34	NA	S	8510	1/1	0.11	-16.06	34,34,34,34	0
32	MG	0	8032	1/1	0.05	-16.12	36,36,36,36	0
36	SR	0	8938	1/1	0.05	-17.34	139,139,139,139	0
32	MG	0	8059	1/1	0.07	-17.67	35,35,35,35	0
32	MG	0	8089	1/1	0.13	-24.33	40,40,40,40	0
36	SR	0	8916	1/1	0.06	-24.72	98,98,98,98	0
32	MG	0	8091	1/1	0.11	-51.00	54,54,54,54	0
36	SR	S	8961	1/1	0.06	-	113,113,113,113	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.