



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 04:20 PM GMT

PDB ID : 3CCM  
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2611U  
Authors : Blaha, G.; Gurel, G.  
Deposited on : 2008-02-26  
Resolution : 2.55 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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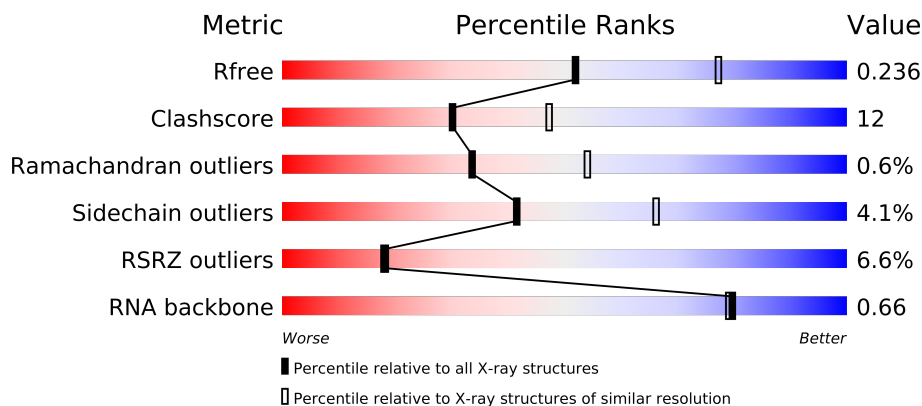
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.55 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	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)
RNA backbone	1838	1058 (3.10-1.98)

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	8004	-	X
32	MG	0	8006	-	X
32	MG	0	8007	-	X
32	MG	0	8008	-	X
32	MG	0	8009	-	X
32	MG	0	8012	-	X
32	MG	0	8014	-	X
32	MG	0	8015	-	X
32	MG	0	8017	-	X
32	MG	0	8018	-	X
32	MG	0	8019	-	X
32	MG	0	8028	-	X
32	MG	0	8030	-	X
32	MG	0	8032	-	X
32	MG	0	8037	-	X
32	MG	0	8038	-	X
32	MG	0	8039	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8040	-	X
32	MG	0	8041	-	X
32	MG	0	8044	-	X
32	MG	0	8045	-	X
32	MG	0	8047	-	X
32	MG	0	8048	-	X
32	MG	0	8049	-	X
32	MG	0	8050	-	X
32	MG	0	8055	-	X
32	MG	0	8056	-	X
32	MG	0	8061	-	X
32	MG	0	8062	-	X
32	MG	0	8063	-	X
32	MG	0	8065	-	X
32	MG	0	8066	-	X
32	MG	0	8068	-	X
32	MG	0	8071	-	X
32	MG	0	8073	-	X
32	MG	0	8076	-	X
32	MG	0	8078	-	X
32	MG	0	8079	-	X
32	MG	0	8081	-	X
32	MG	0	8085	-	X
32	MG	0	8092	-	X
32	MG	0	8093	-	X
32	MG	9	8074	-	X
32	MG	A	8051	-	X
32	MG	B	8042	-	X
34	NA	0	8502	-	X
34	NA	0	8504	-	X
34	NA	0	8505	-	X
34	NA	0	8507	-	X
34	NA	0	8508	-	X
34	NA	0	8509	-	X
34	NA	0	8511	-	X
34	NA	0	8516	-	X
34	NA	0	8517	-	X
34	NA	0	8518	-	X
34	NA	0	8520	-	X
34	NA	0	8521	-	X
34	NA	0	8524	-	X
34	NA	0	8525	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	NA	0	8528	-	X
34	NA	0	8530	-	X
34	NA	0	8535	-	X
34	NA	0	8536	-	X
34	NA	0	8542	-	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	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
34	NA	0	8561	-	X
34	NA	0	8562	-	X
34	NA	0	8563	-	X
34	NA	0	8564	-	X
34	NA	0	8566	-	X
34	NA	0	8567	-	X
34	NA	0	8569	-	X
34	NA	0	8571	-	X
34	NA	0	8573	-	X
34	NA	0	8574	-	X
34	NA	0	8575	-	X
35	CL	B	8819	-	X
36	SR	0	8902	-	X
36	SR	0	8903	-	X
36	SR	0	8905	-	X
36	SR	0	8907	-	X
36	SR	0	8910	-	X
36	SR	0	8918	-	X
36	SR	0	8922	-	X
36	SR	0	8926	-	X
36	SR	0	8927	-	X
36	SR	0	8938	-	X
36	SR	0	8949	-	X
36	SR	0	8955	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	SR	0	8957	-	X
36	SR	0	8962	-	X
36	SR	0	8971	-	X
36	SR	0	8974	-	X
36	SR	0	8976	-	X
36	SR	0	8979	-	X
36	SR	0	8983	-	X
36	SR	0	8987	-	X
36	SR	0	8989	-	X
36	SR	0	8991	-	X
36	SR	0	8994	-	X
36	SR	0	8996	-	X
36	SR	0	8997	-	X
36	SR	0	9000	-	X
36	SR	0	9002	-	X
36	SR	0	9007	-	X
36	SR	9	8968	-	X
36	SR	9	8980	-	X

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99119 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
			59017	26348	10870	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	87	Total	Mg	0	0
			87	87		
32	Y	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	9	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	T	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	L	1	Total 1	Cl 1	0	0
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	94	Total 94	Sr 94	0	0
36	1	2	Total 2	Sr 2	0	0
36	B	1	Total 1	Sr 1	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	3	Total 3	Sr 3	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	5938	Total O 5938 5938	0	0
38	9	145	Total O 145 145	0	0
38	A	117	Total O 117 117	0	0
38	B	139	Total O 139 139	0	0
38	C	165	Total O 165 165	0	0
38	D	48	Total O 48 48	0	0
38	E	49	Total O 49 49	0	0
38	F	25	Total O 25 25	0	0
38	G	18	Total O 18 18	0	0
38	H	71	Total O 71 71	0	0
38	I	8	Total O 8 8	0	0
38	J	55	Total O 55 55	0	0
38	K	55	Total O 55 55	0	0
38	L	79	Total O 79 79	0	0
38	M	138	Total O 138 138	0	0
38	N	58	Total O 58 58	0	0
38	O	40	Total O 40 40	0	0
38	P	61	Total O 61 61	0	0
38	Q	49	Total O 49 49	0	0
38	R	78	Total O 78 78	0	0
38	S	32	Total O 32 32	0	0

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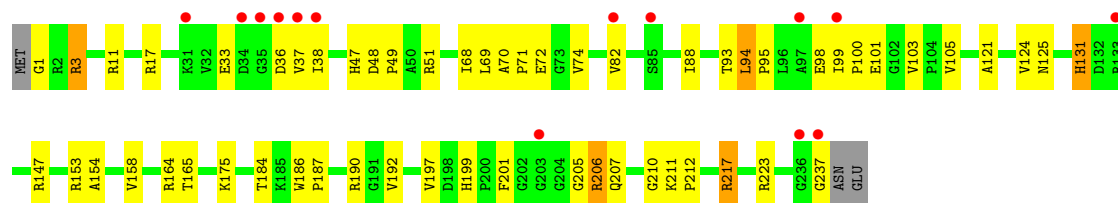
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	T	36	Total 36	O 36	0	0
38	U	28	Total 28	O 28	0	0
38	V	13	Total 13	O 13	0	0
38	W	68	Total 68	O 68	0	0
38	X	24	Total 24	O 24	0	0
38	Y	97	Total 97	O 97	0	0
38	Z	29	Total 29	O 29	0	0
38	1	51	Total 51	O 51	0	0
38	2	37	Total 37	O 37	0	0
38	3	72	Total 72	O 72	0	0

### 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.

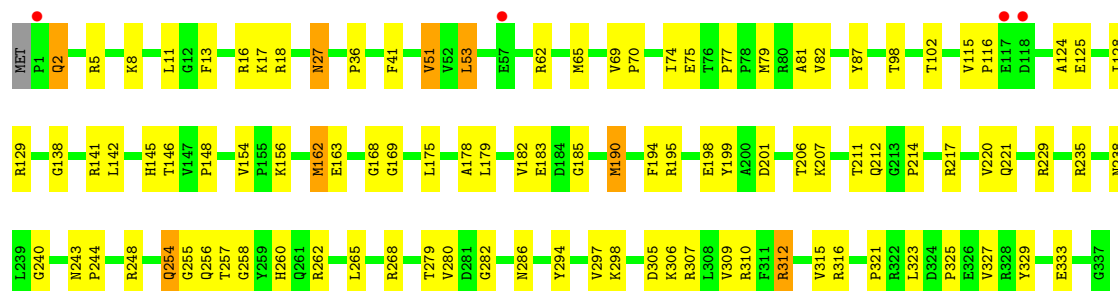
- Molecule 1: 50S ribosomal protein L2P

Chain A: 



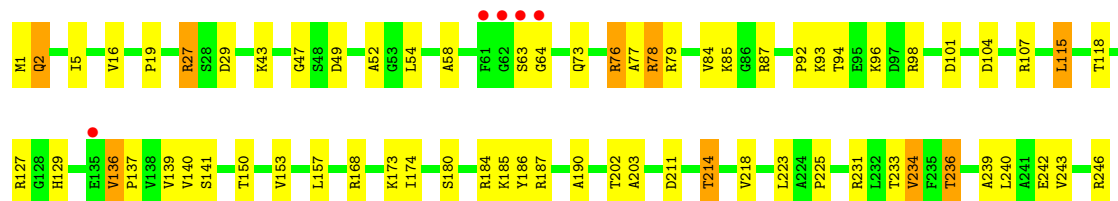
- Molecule 2: 50S ribosomal protein L3P

Chain B: 



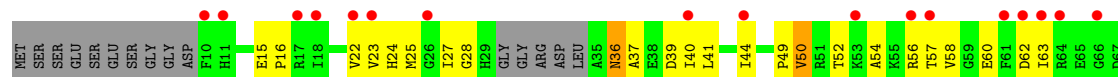
- Molecule 3: 50S ribosomal protein L4P

Chain C: 

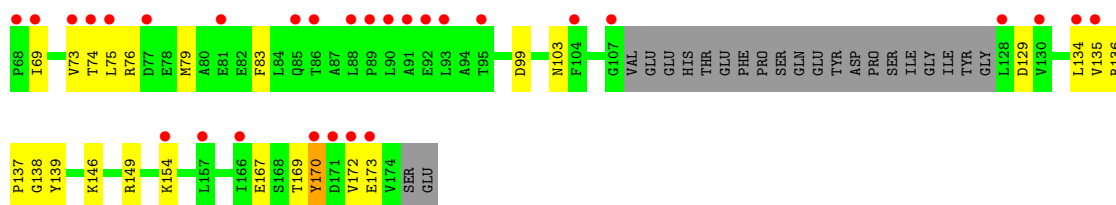


- Molecule 4: 50S ribosomal protein L5P

Chain D: 

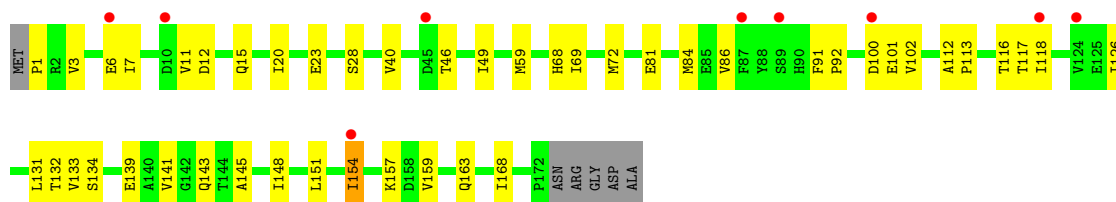






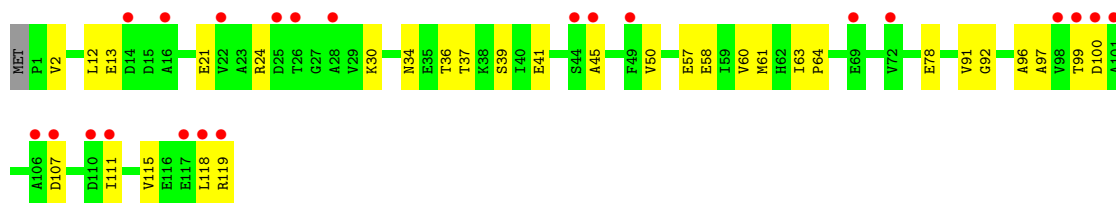
• Molecule 5: 50S ribosomal protein L6P

Chain E:



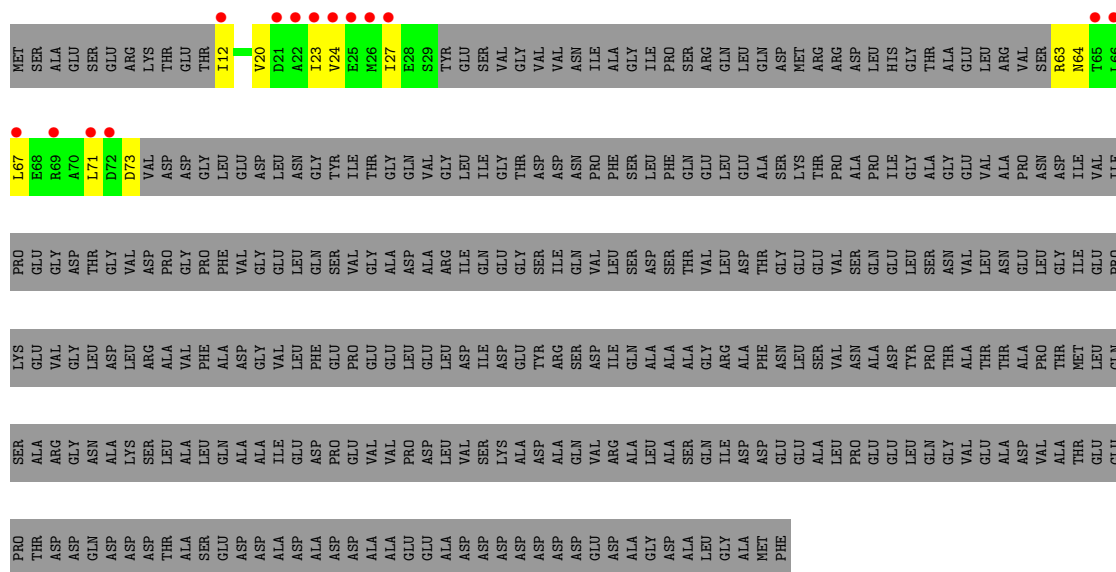
• Molecule 6: 50S ribosomal protein L7Ae

Chain F:



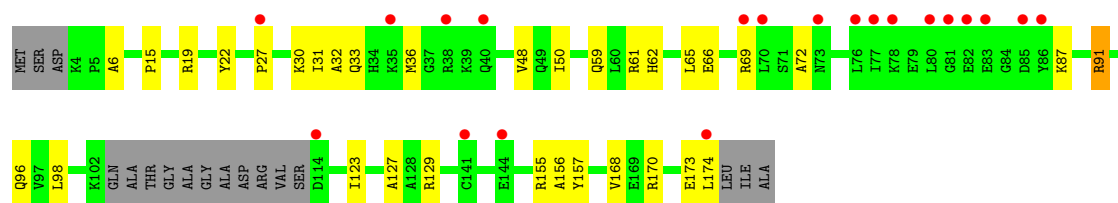
• Molecule 7: 50S ribosomal protein L10E

Chain G:



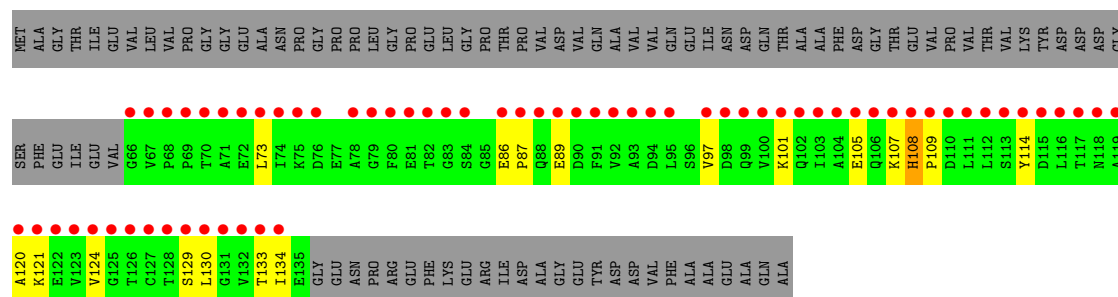
• Molecule 8: 50S ribosomal protein L10e

Chain H:



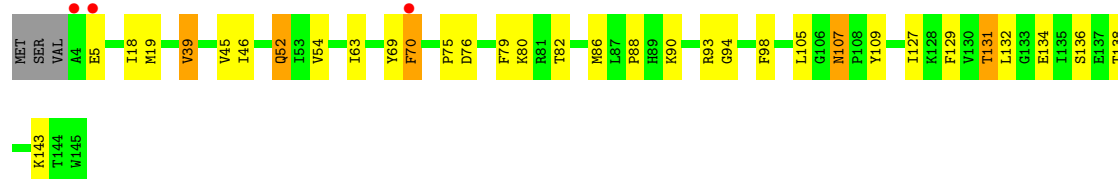
• Molecule 9: 50S ribosomal protein L11P

Chain I:



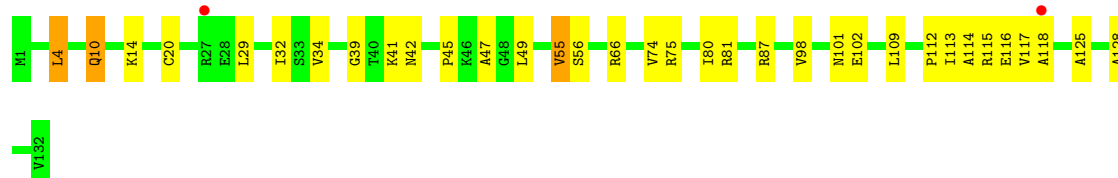
• Molecule 10: 50S ribosomal protein L13P

Chain J:



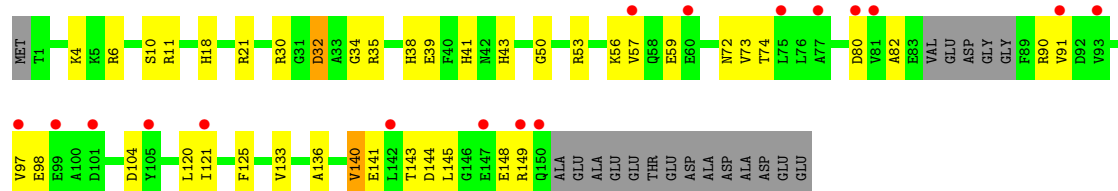
• Molecule 11: 50S ribosomal protein L14P

Chain K:



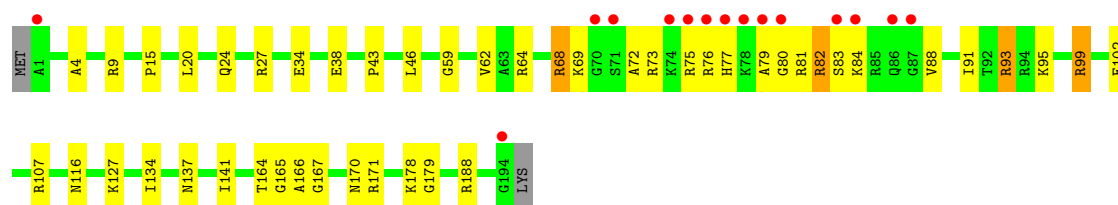
• Molecule 12: 50S ribosomal protein L15P

Chain L:



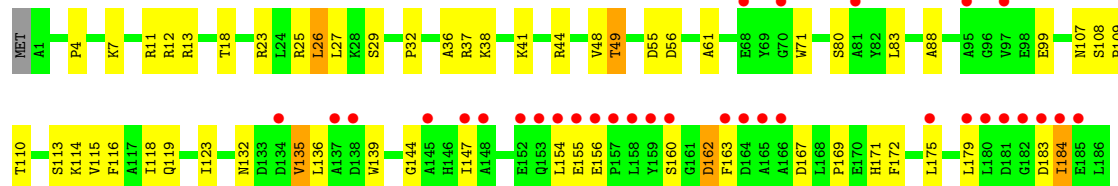
• Molecule 13: 50S ribosomal protein L15e

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:



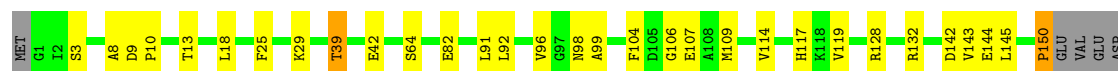
- Molecule 17: 50S ribosomal protein L21e

Chain Q:



- Molecule 18: 50S ribosomal protein L22P

Chain R:



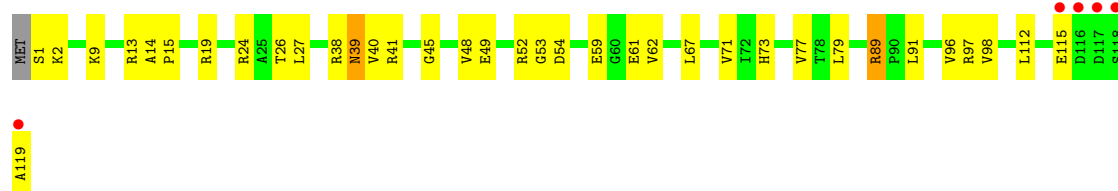
- Molecule 19: 50S ribosomal protein L23P

Chain S:



- Molecule 20: 50S ribosomal protein L24P

Chain T:



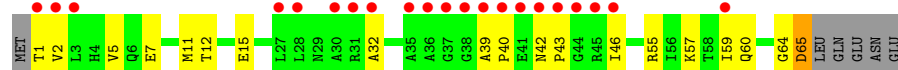
- Molecule 21: 50S ribosomal protein L24e

Chain U:



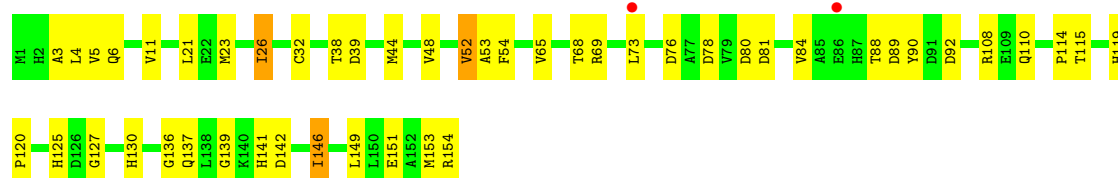
- Molecule 22: 50S ribosomal protein L29P

Chain V:



- Molecule 23: 50S ribosomal protein L30P

Chain W:



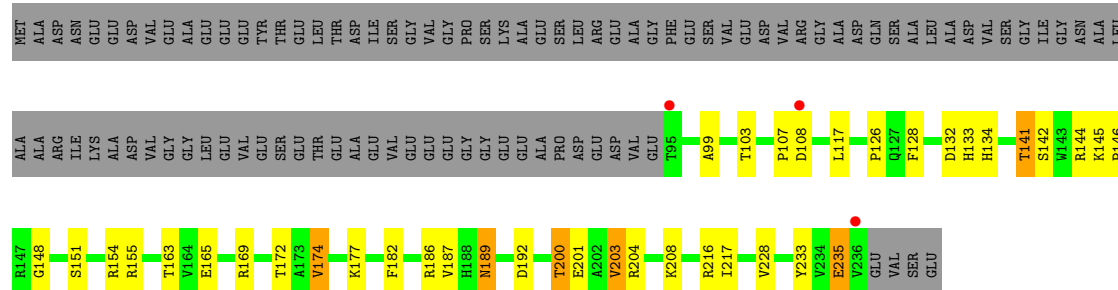
- Molecule 24: 50S ribosomal protein L31e

Chain X:



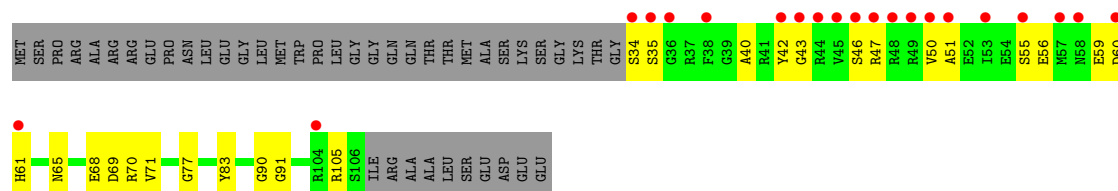
- Molecule 25: 50S ribosomal protein L32e

Chain Y:



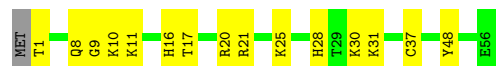
- Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



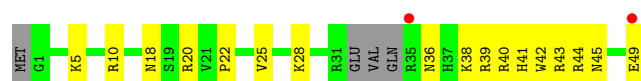
- Molecule 27: 50S ribosomal protein L37e

Chain 1:



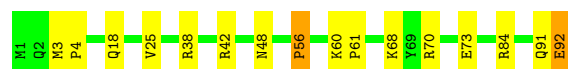
- Molecule 28: 50S ribosomal protein L39e

Chain 2:



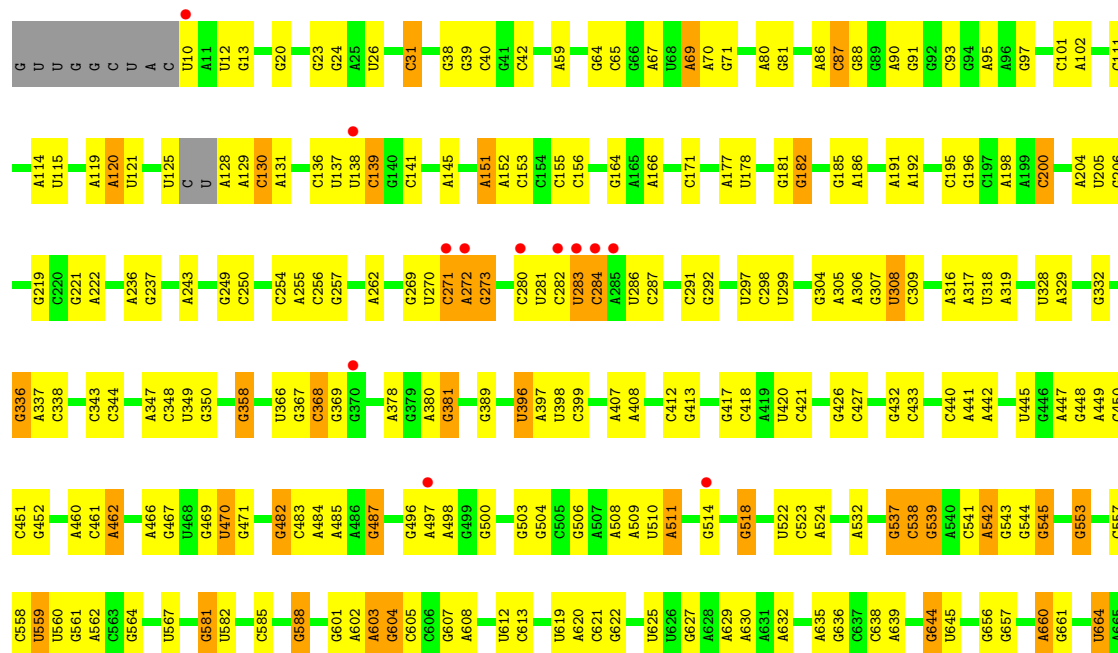
- Molecule 29: 50S ribosomal protein L44E

Chain 3:

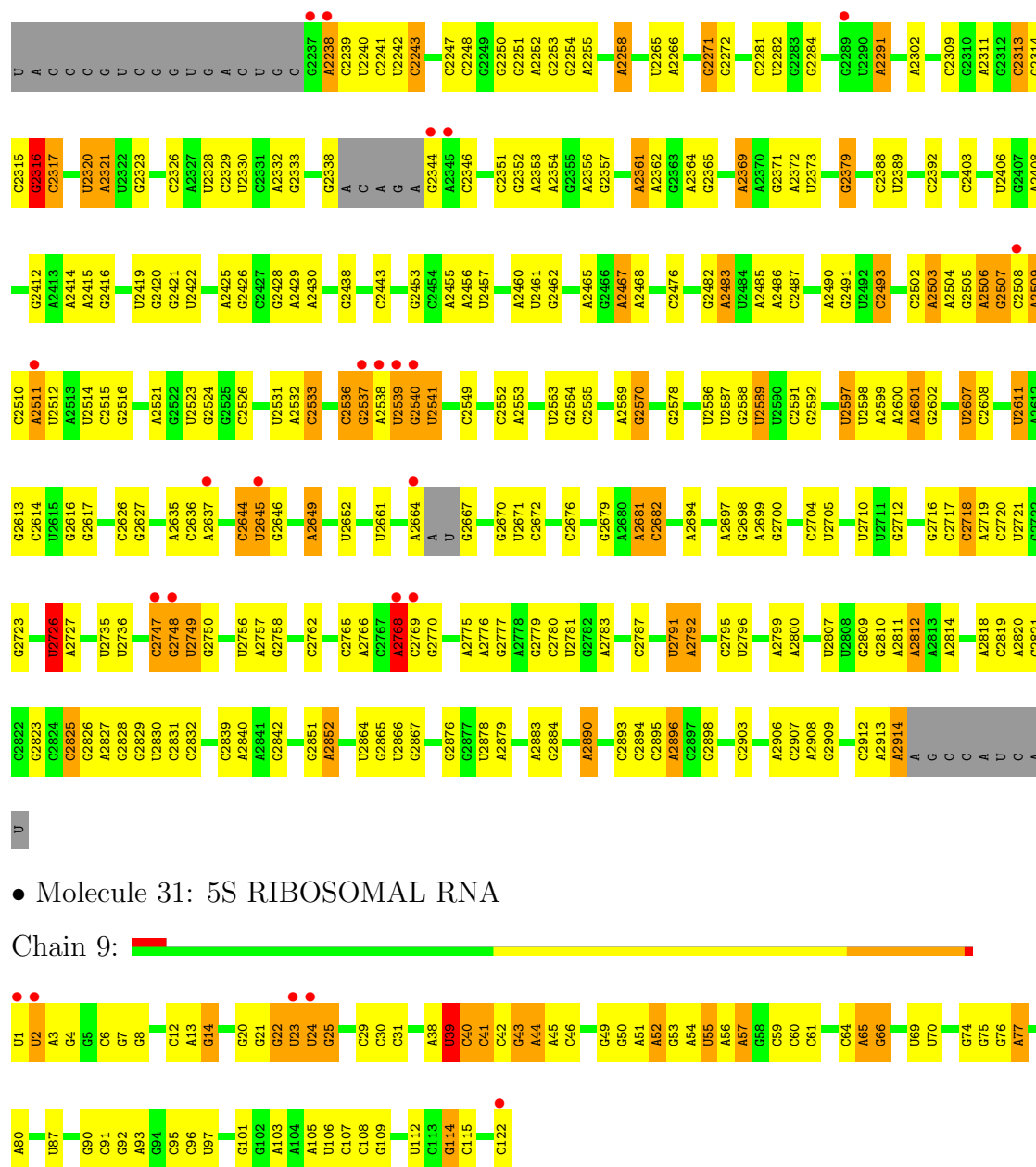


- Molecule 30: 23S RIBOSOMAL RNA

Chain 0:







• Molecule 31: 5S RIBOSOMAL RNA

Chain 9:

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.53Å 298.18Å 573.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.55 85.30 – 2.39	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.70-2.55) 90.6 (85.30-2.39)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.201 , 0.240 0.203 , 0.236	Depositor DCC
$R_{free}$ test set	5933 reflections (0.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.9	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	0 of 691614 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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	0.33	0/1786	0.65	0/2408
2	B	0.33	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.65	0/2552
4	D	0.30	0/1111	0.56	1/1498 (0.1%)
5	E	0.31	0/1382	0.56	0/1880
6	F	0.33	0/901	0.56	0/1224
7	G	0.29	0/241	0.45	0/324
8	H	0.33	0/1302	0.64	0/1743
9	I	0.29	0/526	0.47	0/716
10	J	0.36	0/1136	0.58	0/1530
11	K	0.32	0/1004	0.66	0/1351
12	L	0.33	0/1130	0.63	0/1509
13	M	0.35	0/1582	0.62	0/2116
14	N	0.29	0/1474	0.63	0/1999
15	O	0.32	0/874	0.60	0/1181
16	P	0.33	0/1147	0.53	0/1528
17	Q	0.35	0/749	0.69	0/1005
18	R	1.26	7/1172 (0.6%)	1.11	6/1578 (0.4%)
19	S	0.33	0/648	0.56	0/875
20	T	0.32	0/958	0.64	0/1289
21	U	0.34	0/417	0.55	0/562
22	V	0.30	0/502	0.51	0/675
23	W	0.33	0/1219	0.60	0/1655
24	X	0.32	0/664	0.57	0/895
25	Y	0.36	0/1146	0.63	0/1536
26	Z	0.36	0/584	0.60	0/781
27	1	0.39	0/438	0.65	0/578
28	2	0.35	0/401	0.56	0/529
29	3	0.38	0/771	0.57	0/1024
30	0	0.35	0/65953	0.69	25/102860 (0.0%)
31	9	0.30	0/2904	0.70	1/4526 (0.0%)
All	All	0.37	7/98697 (0.0%)	0.68	33/147579 (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	46
31	9	0	3
All	All	1	49

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	26.57	2.82	1.50
18	R	150	PRO	CA-C	-19.00	1.14	1.52
18	R	150	PRO	CG-CD	14.11	1.97	1.50
18	R	150	PRO	C-O	11.94	1.47	1.23
18	R	150	PRO	N-CA	11.60	1.67	1.47
18	R	150	PRO	N-CD	10.77	1.62	1.47
18	R	150	PRO	CA-CB	7.91	1.69	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.33	56.17	112.00
18	R	150	PRO	N-CA-C	-19.61	61.12	112.10
18	R	150	PRO	CA-N-CD	12.19	128.76	111.70
18	R	150	PRO	N-CA-CB	10.92	116.40	103.30
30	0	1942	A	C5'-C4'-C3'	8.23	129.17	116.00
18	R	150	PRO	CA-C-O	-8.07	100.83	120.20
30	0	871	G	C5'-C4'-O4'	-7.66	99.91	109.10
30	0	1942	A	C5'-C4'-O4'	6.92	117.41	109.10
30	0	1592	G	N9-C1'-C2'	6.74	122.76	114.00
30	0	1504	A	C1'-O4'-C4'	-6.26	104.89	109.90
30	0	1819	G	C5'-C4'-C3'	6.22	125.96	116.00
31	9	39	U	N1-C1'-C2'	6.17	122.03	114.00
30	0	777	U	O4'-C1'-N1	5.90	112.92	108.20
30	0	921	G	N9-C1'-C2'	5.80	121.54	114.00
30	0	1942	A	C1'-O4'-C4'	-5.80	105.26	109.90
18	R	150	PRO	CA-CB-CG	-5.79	93.00	104.00
30	0	2316	G	C5'-C4'-C3'	-5.76	106.78	116.00
30	0	1737	A	C5'-C4'-C3'	-5.68	106.91	116.00
30	0	1819	G	C1'-O4'-C4'	-5.67	105.37	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1819	G	C4'-C3'-C2'	-5.63	96.97	102.60
30	0	1452	G	C5'-C4'-C3'	-5.53	107.15	116.00
30	0	1942	A	C4'-C3'-C2'	-5.52	97.08	102.60
30	0	2467	A	C1'-O4'-C4'	-5.52	105.48	109.90
30	0	206	G	C5'-C4'-C3'	-5.41	107.34	116.00
30	0	2536	C	N1-C1'-C2'	5.37	120.98	114.00
4	D	170	TYR	N-CA-C	5.32	125.35	111.00
30	0	1504	A	N9-C1'-C2'	5.28	120.87	114.00
30	0	1878	G	N9-C1'-C2'	-5.20	106.28	112.00
30	0	1615	A	C5'-C4'-C3'	5.12	124.19	116.00
30	0	1342	C	N1-C1'-C2'	-5.10	106.39	112.00
30	0	2726	U	N1-C1'-C2'	5.08	120.61	114.00
30	0	2313	C	C5'-C4'-O4'	5.07	115.18	109.10
30	0	841	A	C1'-O4'-C4'	-5.03	105.87	109.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1122	U	Sidechain
30	0	1237	U	Sidechain
30	0	1340	G	Sidechain
30	0	1342	C	Sidechain
30	0	1417	G	Sidechain
30	0	1488	U	Sidechain
30	0	1714	C	Sidechain
30	0	1744	G	Sidechain
30	0	1777	G	Sidechain
30	0	1819	G	Sidechain
30	0	182	G	Sidechain
30	0	1829	A	Sidechain
30	0	1863	G	Sidechain
30	0	1867	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1979	G	Sidechain
30	0	2036	C	Sidechain
30	0	2316	G	Sidechain

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Mol	Chain	Res	Type	Group
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2552	C	Sidechain
30	0	2597	U	Sidechain
30	0	2599	A	Sidechain
30	0	26	U	Sidechain
30	0	2607	U	Sidechain
30	0	270	U	Sidechain
30	0	2768	A	Sidechain
30	0	2842	G	Sidechain
30	0	332	G	Sidechain
30	0	396	U	Sidechain
30	0	460	A	Sidechain
30	0	462	A	Sidechain
30	0	469	G	Sidechain
30	0	470	U	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	664	U	Sidechain
30	0	795	G	Sidechain
30	0	817	G	Sidechain
30	0	867	A	Sidechain
30	0	868	G	Sidechain
31	9	39	U	Sidechain
31	9	87	U	Sidechain
31	9	90	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	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2625	0	2533	86	0
3	C	1860	0	1813	57	0
4	D	1094	0	1085	37	0
5	E	1357	0	1266	35	0
6	F	890	0	843	25	0
7	G	240	0	231	6	0
8	H	1282	0	1292	31	0
9	I	519	0	500	19	0
10	J	1120	0	1098	37	0
11	K	994	0	1027	36	0
12	L	1118	0	1076	35	0
13	M	1558	0	1572	48	0
14	N	1445	0	1401	50	0
15	O	865	0	873	24	0
16	P	1136	0	1123	23	0
17	Q	735	0	729	16	0
18	R	1149	0	1122	32	0
19	S	641	0	605	9	0
20	T	950	0	924	25	0
21	U	410	0	364	15	0
22	V	499	0	511	15	0
23	W	1196	0	1137	52	0
24	X	654	0	653	15	0
25	Y	1130	0	1133	36	0
26	Z	573	0	531	15	0
27	1	431	0	426	22	0
28	2	396	0	413	19	0
29	3	755	0	728	13	0
30	0	59017	0	29811	1046	0
31	9	2599	0	1325	78	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	T	1	0	0	0	0
35	0	10	0	0	1	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	2	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	94	0	0	0	0
36	1	2	0	0	0	0
36	3	2	0	0	0	0
36	9	3	0	0	0	0
36	A	3	0	0	0	0
36	B	1	0	0	0	0
36	F	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	5938	0	0	160	0
38	1	51	0	0	1	0
38	2	37	0	0	1	0
38	3	72	0	0	4	0
38	9	145	0	0	9	0
38	A	117	0	0	8	0
38	B	139	0	0	16	0
38	C	165	0	0	10	0
38	D	48	0	0	5	0
38	E	49	0	0	1	0
38	F	25	0	0	1	0
38	G	18	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H	71	0	0	5	0
38	I	8	0	0	0	0
38	J	55	0	0	1	0
38	K	55	0	0	2	0
38	L	79	0	0	8	0
38	M	138	0	0	3	0
38	N	58	0	0	6	0
38	O	40	0	0	0	0
38	P	61	0	0	1	0
38	Q	49	0	0	2	0
38	R	78	0	0	2	0
38	S	32	0	0	3	0
38	T	36	0	0	3	0
38	U	28	0	0	2	0
38	V	13	0	0	2	0
38	W	68	0	0	5	0
38	X	24	0	0	3	0
38	Y	97	0	0	8	0
38	Z	29	0	0	3	0
All	All	99119	0	59911	1801	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 12.

All (1801) 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	1.97	1.41
30:0:2537:G:H5''	30:0:2538:A:H5''	1.17	1.14
30:0:871:G:C8	30:0:871:G:H5'	1.83	1.14
30:0:1205:U:H2'	30:0:1206:U:H5''	1.27	1.12
30:0:1160:G:H5'	30:0:1161:A:H5'	1.13	1.11
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.30	1.11
15:O:3:THR:HG22	30:0:656:G:H5'	1.26	1.10
14:N:37:ARG:NH1	31:9:6:C:H5''	1.67	1.09
30:0:2102:G:H21	30:0:2103:A:H2'	0.97	1.09
30:0:1160:G:C5'	30:0:1161:A:H5'	1.84	1.07
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.07
30:0:871:G:H8	30:0:871:G:H5'	1.12	1.07
30:0:1165:G:H1'	30:0:1174:A:H1'	1.34	1.07
30:0:1189:A:H3'	38:0:7701:HOH:O	1.56	1.04
9:I:130:LEU:HD21	30:0:1167:G:H4'	1.40	1.04
10:J:82:THR:HG23	30:0:1242:A:H5'	1.37	1.02

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:542:A:H5'	30:0:542:A:H8	1.24	1.02
31:9:56:A:H2'	31:9:57:A:H5''	1.42	1.01
30:0:1166:A:H61	30:0:1180:U:H3	1.04	1.01
30:0:1160:G:H5'	30:0:1161:A:C5'	1.91	1.01
3:C:236:THR:HG22	3:C:239:ALA:H	1.22	1.01
30:0:2748:G:OP1	30:0:2749:U:H5''	1.58	1.00
31:9:76:G:H3'	31:9:77:A:H5''	1.41	1.00
13:M:171:ARG:HD3	30:0:156:C:H5''	1.39	0.98
30:0:2100:A:H5'	38:0:7413:HOH:O	1.63	0.98
30:0:870:G:H2'	30:0:871:G:H5''	1.42	0.98
22:V:1:THR:HB	30:0:93:C:H5''	1.43	0.97
30:0:282:C:O2'	30:0:283:U:H5'	1.64	0.96
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.11	0.96
30:0:1372:A:H3'	38:0:7215:HOH:O	1.65	0.95
30:0:1625:U:H4'	38:0:4678:HOH:O	1.67	0.95
30:0:2102:G:H1'	30:0:2103:A:C8	2.02	0.95
30:0:2541:U:H5'	30:0:2541:U:C6	2.00	0.95
30:0:2102:G:N2	30:0:2103:A:H2'	1.82	0.95
30:0:2588:OMG:H5''	38:0:7509:HOH:O	1.64	0.94
16:P:115:SER:H	16:P:118:GLN:HE21	1.09	0.94
30:0:2717:C:C2'	30:0:2718:C:H5''	1.98	0.94
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.48	0.93
30:0:2710:U:H1'	38:0:7642:HOH:O	1.66	0.93
11:K:10:GLN:H	11:K:10:GLN:HE21	1.05	0.93
30:0:2491:G:H1'	38:0:6895:HOH:O	1.68	0.93
38:B:9058:HOH:O	30:0:2672:C:H1'	1.67	0.92
30:0:1116:U:H3	30:0:1246:A:H62	1.16	0.92
30:0:1205:U:C2'	30:0:1206:U:H5''	1.99	0.92
30:0:2896:A:H5''	38:0:6127:HOH:O	1.70	0.92
30:0:2103:A:H62	30:0:2538:A:H8	1.16	0.91
30:0:2851:G:C2'	30:0:2852:A:H5'	2.01	0.91
30:0:1878:G:H1'	38:0:6149:HOH:O	1.71	0.91
30:0:1290:G:H3'	38:0:5188:HOH:O	1.70	0.90
30:0:1701:A:H4'	30:0:1702:U:H5''	1.54	0.90
30:0:2748:G:H5'	38:0:7565:HOH:O	1.71	0.90
30:0:2406:U:H1'	38:0:6728:HOH:O	1.71	0.90
30:0:2506:A:O2'	30:0:2507:G:H8	1.55	0.90
30:0:2851:G:H2'	30:0:2852:A:H5'	1.54	0.89
30:0:1118:A:H3'	30:0:1118:A:H8	1.36	0.88
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.55	0.88
30:0:1184:C:H1'	38:0:7491:HOH:O	1.73	0.88
30:0:2812:A:H2	30:0:2814:A:H62	1.06	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1835:U:H5	30:0:1840:A:N7	1.72	0.88
30:0:2541:U:H5'	30:0:2541:U:H6	1.34	0.88
30:0:2717:C:H2'	30:0:2718:C:H5''	1.54	0.88
30:0:1300:G:H1'	38:0:4694:HOH:O	1.72	0.88
30:0:2637:A:H5'	38:0:9280:HOH:O	1.73	0.87
30:0:871:G:H8	30:0:871:G:C5'	1.88	0.87
28:2:41:HIS:H	28:2:45:ASN:HD22	1.22	0.87
1:A:211:LYS:HG2	1:A:212:PRO:HD2	1.55	0.87
30:0:1118:A:H3'	30:0:1118:A:C8	2.09	0.86
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.40	0.86
30:0:2537:G:C5'	30:0:2538:A:H5''	2.03	0.86
2:B:238:ASN:HD22	2:B:240:GLY:H	1.19	0.85
30:0:256:C:H5''	38:0:5505:HOH:O	1.77	0.85
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.19	0.85
30:0:506:G:H22	30:0:509:A:C5'	1.89	0.85
30:0:1119:G:N2	30:0:1246:A:C2	2.43	0.85
30:0:545:G:H8	30:0:545:G:H5'	1.41	0.85
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.41	0.85
30:0:2004:U:H2'	30:0:2004:U:O2	1.76	0.85
30:0:1426:C:H2'	38:0:9601:HOH:O	1.76	0.84
30:0:1183:C:N4	30:0:1184:C:H41	1.75	0.84
30:0:2586:U:H3	30:0:2592:G:H22	1.24	0.84
8:H:30:LYS:H	8:H:62:HIS:HD2	1.26	0.84
15:O:3:THR:CG2	30:0:656:G:H5'	2.08	0.84
31:9:23:U:O2'	31:9:24:U:H4'	1.78	0.84
15:O:57:THR:HB	15:O:111:VAL:HG23	1.60	0.83
30:0:1632:A:H2'	30:0:1633:C:H5'	1.60	0.83
30:0:1750:C:H4'	38:0:7509:HOH:O	1.76	0.83
30:0:559:U:H5'	30:0:559:U:H6	1.42	0.83
30:0:2505:G:O2'	30:0:2506:A:H5'	1.79	0.83
30:0:1165:G:O3'	30:0:1174:A:H4'	1.78	0.82
30:0:2783:A:H3'	38:0:5253:HOH:O	1.78	0.82
30:0:1666:C:O2'	30:0:1667:A:H5''	1.78	0.82
30:0:960:G:H3'	30:0:960:G:N3	1.94	0.82
30:0:1615:A:H5'	38:0:4198:HOH:O	1.76	0.82
11:K:39:GLY:HA2	38:0:5242:HOH:O	1.79	0.82
14:N:113:SER:HB2	38:N:8854:HOH:O	1.78	0.82
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.15	0.82
30:0:1116:U:HO2'	30:0:1118:A:H2	0.82	0.82
30:0:544:G:H2'	30:0:545:G:H5''	1.62	0.81
30:0:2506:A:HO2'	30:0:2507:G:H8	0.82	0.81
22:V:1:THR:HG23	22:V:2:VAL:H	1.43	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:558:C:C2'	30:0:559:U:H5''	2.10	0.81
30:0:558:C:O2'	30:0:559:U:H5''	1.81	0.81
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.28	0.81
30:0:1667:A:H8	30:0:1667:A:H5'	1.45	0.81
30:0:1183:C:H2'	38:0:6274:HOH:O	1.79	0.81
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.95	0.81
30:0:2005:G:H3'	30:0:2005:G:OP2	1.81	0.81
30:0:1632:A:C2'	30:0:1633:C:H5'	2.10	0.81
30:0:69:A:H5'	30:0:69:A:C8	2.16	0.81
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.16	0.80
30:0:870:G:C2'	30:0:871:G:H5''	2.09	0.80
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.62	0.80
4:D:172:VAL:HG12	4:D:173:GLU:H	1.47	0.80
31:9:56:A:C2'	31:9:57:A:H5''	2.12	0.80
30:0:282:C:H1'	30:0:368:C:N4	1.97	0.80
30:0:272:A:H3'	38:0:7553:HOH:O	1.81	0.80
30:0:1474:C:H6	30:0:1474:C:H5'	1.47	0.79
30:0:1189:A:H1'	30:0:1209:C:O4'	1.82	0.79
27:1:25:LYS:HD2	28:2:49:GLU:H	1.48	0.79
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.64	0.79
30:0:558:C:H2'	30:0:559:U:C5'	2.13	0.79
30:0:1973:A:H5'	30:0:1973:A:H8	1.46	0.79
30:0:2100:A:H1'	38:0:5670:HOH:O	1.83	0.79
2:B:206:THR:HG21	30:0:2716:G:H5''	1.65	0.79
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.64	0.79
1:A:199:HIS:HD2	1:A:201:PHE:H	1.28	0.79
31:9:29:C:H2'	31:9:30:C:H5'	1.65	0.78
30:0:1634:G:H3'	38:0:3910:HOH:O	1.82	0.78
30:0:1118:A:H62	30:0:1244:U:H3	1.31	0.78
2:B:211:THR:HG23	30:0:2840:A:OP1	1.82	0.78
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.12	0.78
30:0:381:G:H5''	38:0:4335:HOH:O	1.82	0.78
31:9:39:U:H1'	31:9:44:A:H61	1.46	0.78
30:0:2524:G:N2	30:0:2526:C:H41	1.82	0.78
30:0:1279:U:O2	30:0:1279:U:H2'	1.83	0.78
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.14	0.78
30:0:1377:C:H6	30:0:1377:C:H5'	1.48	0.77
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.67	0.77
30:0:69:A:H5'	30:0:69:A:H8	1.48	0.77
3:C:63:SER:OG	30:0:2101:A:H2'	1.85	0.77
23:W:21:LEU:HD22	23:W:26:ILE:HD13	1.67	0.77
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.66	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.67	0.77
30:0:2852:A:H5"	38:0:5255:HOH:O	1.85	0.77
30:0:877:G:H5'	30:0:878:G:OP1	1.84	0.77
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.50	0.76
28:2:20:ARG:HG3	28:2:39:ARG:HH21	1.49	0.76
30:0:1175:G:H1'	30:0:1193:A:H2'	1.65	0.76
30:0:2765:C:H4'	38:0:5545:HOH:O	1.85	0.76
30:0:1730:G:H5"	30:0:1731:C:H6	1.51	0.76
30:0:2769:C:O2'	30:0:2770:G:H5'	1.86	0.76
30:0:1700:C:H5"	30:0:1701:A:OP2	1.86	0.76
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.51	0.76
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.67	0.76
30:0:2537:G:H5"	30:0:2538:A:C5'	2.10	0.75
30:0:2769:C:C2'	30:0:2770:G:H5'	2.17	0.75
30:0:1603:A:H5'	30:0:1605:G:O4'	1.86	0.75
31:9:39:U:H1'	31:9:44:A:N6	2.01	0.75
30:0:1165:G:H21	30:0:1173:A:H5"	1.52	0.75
30:0:2502:C:C2'	30:0:2503:A:H5'	2.17	0.75
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.69	0.75
30:0:506:G:H22	30:0:509:A:H5"	1.50	0.75
6:F:91:VAL:HG12	6:F:92:GLY:H	1.51	0.75
30:0:1116:U:O2'	30:0:1118:A:H2	1.66	0.75
21:U:14:GLU:O	21:U:17:THR:HB	1.87	0.75
1:A:48:ASP:HB3	38:A:9069:HOH:O	1.87	0.74
30:0:2524:G:H21	30:0:2526:C:H41	1.31	0.74
30:0:1206:U:H6	30:0:1206:U:H5'	1.52	0.74
31:9:2:U:H4'	38:9:9099:HOH:O	1.88	0.74
23:W:88:THR:HB	38:W:6679:HOH:O	1.88	0.74
14:N:144:GLY:O	14:N:147:ILE:HG22	1.87	0.74
4:D:154:LYS:HD2	4:D:154:LYS:H	1.53	0.74
30:0:1666:C:H2'	30:0:1667:A:H5'	1.69	0.74
30:0:1552:G:N2	30:0:1634:G:H1'	2.03	0.74
18:R:128:ARG:NH2	30:0:2054:A:N3	2.36	0.74
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.68	0.74
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.68	0.74
30:0:541:C:C2'	30:0:542:A:H5"	2.17	0.74
30:0:1701:A:H4'	30:0:1702:U:C5'	2.17	0.74
30:0:541:C:H2'	30:0:542:A:C5'	2.18	0.74
30:0:871:G:C8	30:0:871:G:C5'	2.64	0.73
30:0:396:U:H1'	38:0:7649:HOH:O	1.87	0.73
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.69	0.73
18:R:39:THR:HG22	18:R:42:GLU:H	1.53	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1209:C:H2'	30:0:1210:G:H8	1.53	0.73
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.69	0.73
30:0:2438:G:H5'	38:0:6199:HOH:O	1.87	0.73
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.71	0.73
4:D:58:VAL:HB	4:D:62:ASP:HB3	1.69	0.73
13:M:171:ARG:CD	30:0:156:C:H5''	2.17	0.73
30:0:558:C:H2'	30:0:559:U:H5'	1.71	0.73
31:9:14:G:H5'	31:9:14:G:H8	1.53	0.73
30:0:1201:C:H5''	38:0:6263:HOH:O	1.87	0.73
30:0:542:A:H5'	30:0:542:A:C8	2.15	0.73
30:0:1165:G:C1'	30:0:1174:A:H1'	2.17	0.73
29:3:48:ASN:HD21	30:0:2468:A:H61	1.37	0.73
30:0:1166:A:N6	30:0:1180:U:H3	1.85	0.72
30:0:2502:C:H2'	30:0:2503:A:H5'	1.71	0.72
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.71	0.72
30:0:2769:C:H2'	30:0:2770:G:O4'	1.88	0.72
30:0:2812:A:C2	30:0:2814:A:N6	2.54	0.72
30:0:1476:A:O2'	30:0:1477:C:H5'	1.89	0.72
30:0:119:A:H2'	30:0:120:A:H5''	1.71	0.72
30:0:1165:G:H1'	30:0:1174:A:C1'	2.15	0.72
30:0:1119:G:H22	30:0:1246:A:H2	1.37	0.72
30:0:1730:G:H5''	30:0:1731:C:C6	2.23	0.72
30:0:2718:C:H6	30:0:2718:C:H5'	1.54	0.72
30:0:544:G:C2'	30:0:545:G:H5''	2.19	0.72
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.37	0.72
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.02	0.71
30:0:138:U:H5''	30:0:139:C:OP2	1.90	0.71
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.72	0.71
30:0:2908:A:H2'	30:0:2909:G:O4'	1.90	0.71
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.71	0.71
30:0:2635:A:O2'	30:0:2636:C:H5'	1.91	0.71
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.70	0.71
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.73	0.71
3:C:139:VAL:HG13	38:C:8641:HOH:O	1.89	0.71
30:0:506:G:H22	30:0:509:A:H5'	1.55	0.71
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.21	0.71
30:0:848:C:H5'	38:0:7298:HOH:O	1.91	0.71
30:0:2747:C:O3'	30:0:2748:G:H4'	1.90	0.71
18:R:25:PHE:CE2	18:R:29:LYS:HE2	2.26	0.71
30:0:1878:G:O2'	30:0:1879:U:C6	2.44	0.71
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.90	0.70
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	1.72	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2106:C:H5'	30:0:2284:G:H21	1.55	0.70
30:0:2507:G:H2'	30:0:2510:C:H42	1.57	0.70
30:0:2487:C:H5	38:0:4903:HOH:O	1.74	0.70
30:0:272:A:H5'	30:0:273:G:OP2	1.91	0.70
30:0:2578:G:H5'	30:0:2578:G:H8	1.56	0.70
30:0:282:C:C2'	30:0:283:U:H5'	2.21	0.70
30:0:1730:G:H5'	30:0:1731:C:C5	2.27	0.70
18:R:29:LYS:HD3	30:0:524:A:H5''	1.73	0.70
30:0:1058:A:H2'	30:0:1060:C:H5''	1.73	0.70
30:0:1724:U:H5''	38:0:3745:HOH:O	1.92	0.70
30:0:462:A:H2'	38:0:4898:HOH:O	1.91	0.70
30:0:1278:A:O2'	30:0:1279:U:H3'	1.92	0.69
31:9:49:G:H5''	38:9:9086:HOH:O	1.91	0.69
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.74	0.69
30:0:1165:G:H21	30:0:1173:A:C5'	2.04	0.69
30:0:280:C:H2'	30:0:281:U:O4'	1.90	0.69
30:0:1380:U:O4	30:0:2748:G:H1'	1.92	0.69
30:0:1299:G:H5'	38:0:4092:HOH:O	1.92	0.69
30:0:281:U:H2'	30:0:282:C:O4'	1.91	0.69
30:0:1666:C:C2'	30:0:1667:A:H5''	2.22	0.69
30:0:2748:G:C8	30:0:2748:G:H5'	2.28	0.69
30:0:1666:C:H2'	30:0:1667:A:C5'	2.22	0.69
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.41	0.69
18:R:39:THR:HG23	18:R:107:GLU:O	1.92	0.69
30:0:2541:U:H3'	38:0:9415:HOH:O	1.93	0.69
30:0:2717:C:O2'	30:0:2718:C:H5''	1.91	0.69
30:0:2064:U:H5'	30:0:2652:U:H4'	1.75	0.69
30:0:2421:G:H4'	38:0:4795:HOH:O	1.92	0.69
30:0:681:G:N3	30:0:681:G:H5'	2.08	0.69
30:0:282:C:H1'	30:0:368:C:H42	1.58	0.69
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.74	0.69
9:I:108:HIS:H	9:I:109:PRO:HD2	1.56	0.69
30:0:292:G:H2'	30:0:358:G:N2	2.08	0.69
2:B:238:ASN:HD22	2:B:240:GLY:N	1.91	0.69
1:A:199:HIS:CD2	1:A:201:PHE:H	2.09	0.69
30:0:2533:C:H6	30:0:2533:C:H5'	1.57	0.69
30:0:1505:U:H1'	38:0:7611:HOH:O	1.92	0.68
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.07	0.68
30:0:2524:G:H21	30:0:2526:C:N4	1.90	0.68
31:9:13:A:O2'	31:9:14:G:H5''	1.92	0.68
3:C:1:MET:HG2	3:C:2:GLN:H	1.59	0.68
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.90	0.68
23:W:84:VAL:HG12	38:W:6679:HOH:O	1.94	0.68
30:0:2102:G:H2'	38:0:7788:HOH:O	1.93	0.68
30:0:558:C:C2'	30:0:559:U:C5'	2.72	0.68
8:H:168:VAL:HG13	38:H:214:HOH:O	1.93	0.68
30:0:2896:A:N3	30:0:2896:A:H2'	2.08	0.68
28:2:28:LYS:O	30:0:87:C:H2'	1.93	0.68
14:N:7:LYS:HE3	17:Q:21:ARG:O	1.92	0.68
30:0:1118:A:C8	30:0:1118:A:C3'	2.73	0.67
30:0:2420:G:O2'	30:0:2421:G:H5'	1.94	0.67
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.76	0.67
30:0:2291:A:C8	30:0:2309:C:H5'	2.29	0.67
23:W:108:ARG:HH21	23:W:114:PRO:HG2	1.59	0.67
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.75	0.67
1:A:51:ARG:HB2	38:A:9069:HOH:O	1.94	0.67
14:N:160:SER:HB3	31:9:51:A:H5'	1.77	0.67
25:Y:235:GLU:H	25:Y:235:GLU:CD	1.96	0.67
6:F:96:ALA:HA	38:F:3111:HOH:O	1.94	0.67
3:C:27:ARG:NH2	30:0:657:G:OP1	2.27	0.67
30:0:2661:U:H3	30:0:2812:A:H62	1.42	0.67
30:0:1377:C:H5'	30:0:1377:C:C6	2.29	0.67
30:0:2505:G:C2'	30:0:2506:A:H5'	2.25	0.67
30:0:2878:U:H2'	30:0:2879:A:O4'	1.94	0.67
30:0:1641:A:H2'	30:0:1642:A:H5'	1.77	0.67
28:2:49:GLU:HB2	38:2:131:HOH:O	1.93	0.67
14:N:160:SER:CB	31:9:51:A:H5'	2.25	0.67
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.29	0.67
12:L:18:HIS:HD2	30:0:902:G:N7	1.93	0.67
12:L:136:ALA:HB3	38:L:8867:HOH:O	1.95	0.67
10:J:131:THR:HG22	10:J:134:GLU:H	1.61	0.66
18:R:150:PRO:O	18:R:150:PRO:CG	2.42	0.66
14:N:37:ARG:NH1	31:9:6:C:C5'	2.53	0.66
25:Y:200:THR:HG22	25:Y:201:GLU:HG3	1.77	0.66
30:0:182:G:H5'	38:0:5177:HOH:O	1.96	0.66
30:0:2004:U:O2	30:0:2004:U:C2'	2.43	0.66
30:0:1603:A:H5''	30:0:1605:G:H5'	1.77	0.66
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.77	0.66
30:0:541:C:H2'	30:0:542:A:H5''	1.78	0.66
27:1:16:HIS:HD2	30:0:470:U:O2'	1.78	0.66
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.78	0.66
10:J:127:ILE:HG22	35:J:8801:CL:CL	2.33	0.66
30:0:1730:G:C5'	30:0:1731:C:C6	2.79	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:26:ILE:HB	38:W:5420:HOH:O	1.96	0.65
30:0:2426:G:H1'	38:0:6120:HOH:O	1.95	0.65
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.77	0.65
30:0:256:C:H2'	30:0:257:G:O4'	1.96	0.65
30:0:1187:U:H5''	38:0:6214:HOH:O	1.96	0.65
30:0:1119:G:N2	30:0:1246:A:H2	1.94	0.65
30:0:545:G:C8	30:0:545:G:H5'	2.30	0.65
2:B:211:THR:HG21	38:0:7480:HOH:O	1.96	0.65
30:0:2032:U:H2'	30:0:2033:G:C5'	2.26	0.65
30:0:567:U:H5''	38:0:6432:HOH:O	1.96	0.65
30:0:299:U:H5'	38:0:7361:HOH:O	1.96	0.65
30:0:1878:G:HO2'	30:0:1879:U:H6	1.41	0.65
30:0:2524:G:H21	30:0:2526:C:H5	1.44	0.65
24:X:61:ARG:HH11	24:X:65:ASN:HB3	1.62	0.65
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.89	0.65
15:O:32:ARG:HH21	15:O:35:LYS:NZ	1.94	0.65
2:B:51:VAL:CG1	2:B:53:LEU:HD13	2.26	0.65
12:L:140:VAL:HB	38:L:8851:HOH:O	1.96	0.65
31:9:24:U:H3'	31:9:25:G:H5'	1.79	0.64
30:0:125:U:H2'	38:0:3780:HOH:O	1.97	0.64
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.80	0.64
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.78	0.64
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.97	0.64
30:0:1166:A:H1'	30:0:1192:A:N3	2.13	0.64
30:0:1187:U:H1'	30:0:1189:A:H2	1.62	0.64
30:0:1166:A:H1'	30:0:1192:A:C2	2.31	0.64
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.79	0.64
17:Q:25:PRO:HB2	38:9:9078:HOH:O	1.98	0.64
3:C:174:ILE:CD1	30:0:338:C:H4'	2.28	0.64
30:0:271:C:H41	30:0:378:A:H2	1.46	0.64
30:0:1451:C:H5'	30:0:1505:U:C5	2.33	0.64
30:0:196:G:H2'	38:0:6681:HOH:O	1.98	0.64
30:0:1187:U:HO2'	30:0:1188:A:H8	1.44	0.64
30:0:2539:U:H3'	38:0:9174:HOH:O	1.96	0.64
10:J:76:ASP:HA	38:J:5907:HOH:O	1.97	0.64
20:T:9:LYS:HD3	38:0:3770:HOH:O	1.97	0.64
24:X:61:ARG:NH1	24:X:65:ASN:HB3	2.12	0.64
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.78	0.64
27:1:10:LYS:HG3	38:1:2979:HOH:O	1.98	0.64
30:0:541:C:H2'	30:0:542:A:H5'	1.78	0.64
8:H:59:GLN:HE22	8:H:96:GLN:HG2	1.62	0.64
30:0:380:A:H2'	38:0:7253:HOH:O	1.97	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:80:ASP:O	23:W:84:VAL:HG23	1.97	0.63
3:C:2:GLN:HB3	38:C:8580:HOH:O	1.97	0.63
31:9:54:A:H2	38:9:9062:HOH:O	1.80	0.63
18:R:98:ASN:HD21	30:0:500:G:H21	1.46	0.63
6:F:91:VAL:HG12	6:F:92:GLY:N	2.13	0.63
30:0:1187:U:O2'	30:0:1188:A:H8	1.80	0.63
30:0:1666:C:C2'	30:0:1667:A:C5'	2.77	0.63
27:1:20:ARG:HG2	30:0:111:C:O2'	1.98	0.63
2:B:179:LEU:O	2:B:183:GLU:HG2	1.99	0.63
30:0:283:U:H5	30:0:284:C:N3	1.97	0.63
30:0:1919:A:H4'	38:0:4866:HOH:O	1.98	0.63
30:0:1207:A:OP2	30:0:1207:A:H8	1.81	0.63
30:0:1878:G:O2'	30:0:1879:U:H6	1.82	0.63
24:X:25:ARG:HD2	38:X:5356:HOH:O	1.98	0.63
18:R:117:HIS:HD2	30:0:20:G:H21	1.46	0.63
16:P:115:SER:H	16:P:118:GLN:NE2	1.90	0.63
10:J:18:ILE:HD13	30:0:1244:U:OP1	1.99	0.63
30:0:2908:A:C2'	30:0:2909:G:H5'	2.29	0.63
30:0:2670:G:O2'	30:0:2671:U:H5'	1.99	0.63
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.81	0.62
30:0:441:A:H1'	30:0:442:A:N7	2.13	0.62
30:0:1835:U:C5	30:0:1840:A:N7	2.62	0.62
31:9:1:U:H5''	31:9:3:A:OP1	1.99	0.62
30:0:1681:G:H5''	30:0:1682:A:H5'	1.80	0.62
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.81	0.62
30:0:2537:G:H3'	38:0:3125:HOH:O	1.98	0.62
1:A:211:LYS:O	30:0:1943:C:H4'	1.99	0.62
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.29	0.62
25:Y:169:ARG:HD2	30:0:1328:A:OP1	2.00	0.62
30:0:1359:U:C6	30:0:2537:G:N2	2.67	0.62
7:G:12:ILE:HG23	38:0:5483:HOH:O	1.98	0.62
30:0:2112:A:H2'	30:0:2113:G:C8	2.33	0.62
30:0:42:C:H1'	38:0:4687:HOH:O	1.98	0.62
11:K:10:GLN:N	11:K:10:GLN:HE21	1.88	0.62
2:B:214:PRO:HD2	38:B:8953:HOH:O	2.00	0.62
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.82	0.62
22:V:5:VAL:HG23	38:V:2271:HOH:O	1.99	0.62
15:O:3:THR:HG22	30:0:656:G:C5'	2.16	0.62
4:D:57:THR:HG23	4:D:63:ILE:HA	1.80	0.62
30:0:1205:U:H2'	30:0:1206:U:C5'	2.18	0.62
23:W:65:VAL:HA	23:W:68:THR:HG22	1.81	0.62
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.30	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:125:ASN:HB3	1:A:158:VAL:HG12	1.81	0.62
23:W:125:HIS:HD2	23:W:127:GLY:H	1.48	0.62
30:0:1167:G:H2'	30:0:1168:C:O4'	1.99	0.61
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.81	0.61
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.40	0.61
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.82	0.61
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.82	0.61
30:0:1183:C:H5	30:0:1192:A:OP1	1.83	0.61
3:C:236:THR:HG22	3:C:239:ALA:N	2.05	0.61
31:9:92:G:H2'	31:9:93:A:C8	2.35	0.61
30:0:2607:U:H4'	38:0:9446:HOH:O	1.99	0.61
4:D:103:ASN:ND2	4:D:134:LEU:H	1.98	0.61
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.98	0.61
30:0:2748:G:H8	38:0:7565:HOH:O	1.84	0.61
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.31	0.61
30:0:1200:A:H3'	38:0:5785:HOH:O	2.00	0.61
30:0:1973:A:H5'	30:0:1973:A:C8	2.33	0.61
12:L:6:ARG:HD3	30:0:1299:G:O6	2.00	0.61
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.65	0.61
31:9:29:C:C2'	31:9:30:C:H5'	2.30	0.61
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.81	0.61
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.81	0.61
5:E:68:HIS:O	5:E:72:MET:HG3	2.00	0.61
30:0:1187:U:O2'	30:0:1188:A:C8	2.54	0.60
3:C:140:VAL:HB	38:C:8644:HOH:O	2.00	0.60
30:0:558:C:H2'	30:0:559:U:H5''	1.77	0.60
22:V:42:ASN:HB3	38:V:7247:HOH:O	2.00	0.60
17:Q:95:GLU:HA	30:0:949:U:H4'	1.82	0.60
1:A:3:ARG:HD3	30:0:870:G:OP2	2.01	0.60
31:9:14:G:H5'	31:9:14:G:C8	2.35	0.60
30:0:204:A:C2'	30:0:205:U:H5'	2.31	0.60
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.37	0.60
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.15	0.60
31:9:54:A:O2'	31:9:55:U:H5'	2.01	0.60
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.83	0.60
14:N:80:SER:HB2	38:N:8834:HOH:O	2.01	0.60
2:B:254:GLN:HG2	2:B:255:GLY:N	2.16	0.60
30:0:1189:A:H1'	30:0:1209:C:C1'	2.31	0.60
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.83	0.60
30:0:1679:C:H5'	38:0:9330:HOH:O	2.02	0.60
13:M:164:THR:HG22	13:M:166:ALA:H	1.66	0.60
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:38:LYS:HE2	14:N:107:ASN:HD21	1.67	0.60
23:W:21:LEU:CD2	23:W:48:VAL:HG11	2.29	0.60
13:M:83:SER:HB3	38:O:4395:HOH:O	2.01	0.60
25:Y:141:THR:HG23	38:Y:8888:HOH:O	2.00	0.60
4:D:25:MET:SD	4:D:40:ILE:HD11	2.42	0.60
30:O:1342:C:C2'	30:O:1343:C:H5'	2.32	0.60
13:M:82:ARG:HD2	38:O:9124:HOH:O	2.01	0.60
30:O:254:C:O2	30:O:254:C:H2'	2.01	0.60
30:O:1189:A:O2'	30:O:1208:C:H2'	2.02	0.60
12:L:104:ASP:HB2	38:L:8857:HOH:O	2.00	0.60
30:O:1667:A:C8	30:O:1667:A:H5'	2.33	0.60
30:O:1476:A:N7	38:O:5190:HOH:O	2.32	0.60
30:O:1766:U:O2	30:O:1778:A:H5'	2.02	0.60
2:B:145:HIS:HD2	2:B:146:THR:O	1.85	0.60
30:O:1528:A:H2'	30:O:1529:G:O4'	2.02	0.60
15:O:32:ARG:HD3	15:O:32:ARG:O	2.02	0.59
30:O:2769:C:H2'	30:O:2770:G:C5'	2.32	0.59
23:W:125:HIS:CD2	23:W:127:GLY:H	2.20	0.59
30:O:1632:A:C3'	30:O:1633:C:H5'	2.33	0.59
2:B:41:PHE:CD2	2:B:190:MET:HE3	2.37	0.59
14:N:179:LEU:HA	14:N:184:ILE:HD12	1.84	0.59
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.84	0.59
30:O:2825:C:H4'	30:O:2826:G:O5'	2.02	0.59
14:N:11:ARG:HD3	31:9:114:G:O6	2.02	0.59
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.84	0.59
30:O:1116:U:O2'	30:O:1118:A:C2	2.47	0.59
30:O:2073:G:OP2	30:O:2490:A:H5'	2.03	0.59
30:O:1342:C:O2'	30:O:1343:C:H5'	2.01	0.59
12:L:30:ARG:HD3	30:O:164:G:H4'	1.85	0.59
38:Z:8718:HOH:O	30:O:819:A:H5''	2.01	0.59
30:O:2626:C:H2'	30:O:2627:G:C8	2.38	0.59
16:P:81:LYS:HG2	38:O:9547:HOH:O	2.02	0.59
20:T:112:LEU:HD23	20:T:119:ALA:HB3	1.84	0.59
30:O:2239:C:H2'	30:O:2240:U:H6	1.67	0.59
28:2:10:ARG:NH2	30:O:121:U:OP2	2.32	0.59
11:K:32:ILE:HD11	11:K:56:SER:HB2	1.84	0.59
17:Q:45:PRO:O	30:O:2365:G:H4'	2.03	0.59
30:O:1278:A:H4'	30:O:1279:U:C4	2.37	0.59
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.85	0.59
4:D:57:THR:HA	38:D:5728:HOH:O	2.01	0.59
3:C:214:THR:HB	38:O:9688:HOH:O	2.02	0.59
30:O:407:A:H3'	38:O:4474:HOH:O	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.84	0.59
30:0:960:G:C3'	30:0:960:G:N3	2.66	0.59
30:0:291:C:H2'	30:0:292:G:O4'	2.03	0.59
30:0:1862:C:H1'	38:0:7245:HOH:O	2.01	0.59
20:T:26:THR:HA	20:T:39:ASN:HB3	1.85	0.59
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.85	0.59
3:C:174:ILE:HD11	30:0:338:C:H4'	1.85	0.59
30:0:2239:C:H2'	30:0:2240:U:C6	2.38	0.59
30:0:834:G:H4'	30:0:835:U:OP2	2.03	0.59
30:0:1182:C:H1'	30:0:1192:A:C8	2.38	0.59
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.68	0.59
30:0:603:A:H4'	30:0:604:G:O5'	2.03	0.59
30:0:2372:A:H2'	30:0:2373:U:C6	2.38	0.59
30:0:1819:G:H2'	30:0:1820:G:H4'	1.85	0.59
10:J:93:ARG:HH11	10:J:93:ARG:HB3	1.68	0.59
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.84	0.58
30:0:2102:G:H21	30:0:2103:A:C2'	1.91	0.58
30:0:2894:C:O2'	30:0:2895:C:H5'	2.02	0.58
30:0:1218:U:H2'	30:0:1219:U:C6	2.38	0.58
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.84	0.58
30:0:1118:A:H8	30:0:1119:G:H5''	1.68	0.58
30:0:396:U:O2'	30:0:418:C:H4'	2.03	0.58
30:0:2089:A:O2'	30:0:2090:G:H5'	2.03	0.58
30:0:1165:G:N2	30:0:1173:A:C5'	2.67	0.58
30:0:200:C:H2'	38:0:3459:HOH:O	2.03	0.58
30:0:2453:G:H5''	38:0:4736:HOH:O	2.04	0.58
2:B:16:ARG:NH1	38:B:9042:HOH:O	2.35	0.58
3:C:202:THR:HG22	30:0:328:U:O4'	2.04	0.58
16:P:55:LYS:HG2	16:P:56:GLY:N	2.19	0.58
2:B:162:MET:CE	2:B:310:ARG:HD3	2.33	0.58
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.85	0.58
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.01	0.58
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.19	0.58
12:L:39:GLU:OE2	30:0:926:A:H5'	2.02	0.58
14:N:162:ASP:HA	38:N:8831:HOH:O	2.03	0.58
20:T:1:SER:HB2	30:0:447:A:P	2.44	0.58
30:0:541:C:C2'	30:0:542:A:C5'	2.80	0.58
30:0:999:C:C2'	30:0:1000:C:H5'	2.34	0.58
30:0:2541:U:C6	30:0:2541:U:C5'	2.82	0.58
2:B:298:LYS:HG2	38:0:5545:HOH:O	2.04	0.58
30:0:1595:G:O2'	30:0:1596:U:H5'	2.04	0.58
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.19	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1730:G:C5'	30:0:1731:C:C5	2.86	0.57
30:0:12:U:H2'	30:0:13:G:H5'	1.86	0.57
2:B:17:LYS:O	2:B:260:HIS:HD2	1.87	0.57
30:0:2102:G:H1'	30:0:2103:A:H8	1.65	0.57
4:D:103:ASN:HD22	4:D:134:LEU:H	1.50	0.57
22:V:55:ARG:O	22:V:59:ILE:HG12	2.05	0.57
23:W:44:MET:CE	30:0:944:G:H21	2.16	0.57
30:0:130:C:H5'	38:0:5234:HOH:O	2.02	0.57
30:0:1667:A:H2'	30:0:1668:U:H6	1.70	0.57
28:2:36:ASN:HB3	28:2:39:ARG:HG3	1.86	0.57
30:0:2032:U:H2'	30:0:2033:G:H5'	1.86	0.57
20:T:1:SER:HB2	30:0:447:A:OP2	2.05	0.57
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.39	0.57
30:0:951:A:C2'	30:0:952:G:H5'	2.34	0.57
30:0:2320:U:H4'	30:0:2321:A:O4'	2.05	0.57
19:S:57:THR:HG22	19:S:58:MET:N	2.20	0.57
22:V:1:THR:CB	30:0:93:C:H5''	2.28	0.57
15:O:32:ARG:NE	15:O:35:LYS:HD2	2.16	0.57
31:9:2:U:OP2	31:9:3:A:H5'	2.05	0.57
30:0:1044:C:H3'	30:0:1045:G:H5''	1.86	0.57
30:0:1355:A:H2'	38:0:4139:HOH:O	2.05	0.57
30:0:2717:C:H2'	30:0:2718:C:C5'	2.30	0.57
11:K:29:LEU:HB3	11:K:55:VAL:HG21	1.85	0.57
30:0:59:A:H5'	38:0:4347:HOH:O	2.05	0.57
30:0:1878:G:H4'	38:0:4133:HOH:O	2.05	0.57
16:P:10:ALA:HA	16:P:13:VAL:HG12	1.87	0.57
10:J:45:VAL:HG21	10:J:129:PHE:CD1	2.39	0.57
30:0:1201:C:H2'	30:0:1202:A:H5'	1.86	0.57
30:0:2541:U:H6	30:0:2541:U:C5'	2.11	0.57
31:9:24:U:H3'	31:9:25:G:C5'	2.35	0.57
4:D:58:VAL:HG12	4:D:60:GLU:HG2	1.87	0.57
10:J:63:ILE:HD11	30:0:1236:A:C8	2.40	0.57
30:0:2827:A:H2'	30:0:2828:G:O4'	2.05	0.57
30:0:1174:A:C5	30:0:1201:C:H4'	2.39	0.56
3:C:236:THR:HG21	38:C:8570:HOH:O	2.04	0.56
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.40	0.56
6:F:58:GLU:HG3	6:F:61:MET:HE1	1.87	0.56
26:Z:34:SER:HB3	30:0:797:A:H4'	1.86	0.56
30:0:1165:G:N2	30:0:1173:A:H5''	2.17	0.56
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.41	0.56
24:X:30:MET:HG2	30:0:1384:C:H5'	1.85	0.56
10:J:19:MET:CE	10:J:132:LEU:HD11	2.35	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2316:G:H4'	38:0:6120:HOH:O	2.05	0.56
30:0:2912:C:H3'	38:0:6403:HOH:O	2.03	0.56
5:E:15:GLN:HG3	5:E:20:ILE:HG12	1.88	0.56
30:0:2361:A:H2'	30:0:2362:A:C8	2.40	0.56
30:0:2866:U:H4'	30:0:2867:G:H5'	1.87	0.56
21:U:49:LEU:HG	38:U:3805:HOH:O	2.05	0.56
30:0:1474:C:C6	30:0:1474:C:H5'	2.34	0.56
30:0:1838:U:O2'	30:0:2644:C:H5'	2.05	0.56
29:3:61:PRO:HG2	38:0:7581:HOH:O	2.04	0.56
29:3:73:GLU:HB3	38:3:9055:HOH:O	2.04	0.56
30:0:2851:G:O2'	30:0:2852:A:H5'	2.04	0.56
18:R:9:ASP:O	18:R:13:THR:HG22	2.06	0.56
30:0:2697:A:H2'	30:0:2698:G:O4'	2.06	0.56
38:Z:8706:HOH:O	30:0:1886:A:H4'	2.05	0.56
30:0:432:G:O2'	30:0:433:C:H5'	2.06	0.56
29:3:70:ARG:HG2	38:3:9067:HOH:O	2.05	0.56
30:0:2712:G:H5'	38:0:5242:HOH:O	2.03	0.56
8:H:155:ARG:NH1	30:0:2503:A:H5''	2.21	0.56
31:9:1:U:O3'	31:9:3:A:H5''	2.05	0.56
30:0:2032:U:O2'	30:0:2033:G:H5''	2.05	0.56
30:0:1921:A:C6	30:0:1922:A:C2	2.93	0.56
30:0:1667:A:H2'	30:0:1668:U:C6	2.41	0.56
30:0:1527:A:H1'	30:0:1528:A:C8	2.41	0.56
30:0:349:U:O2'	30:0:350:G:H5'	2.06	0.56
30:0:2524:G:N2	30:0:2526:C:H5	2.04	0.56
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.87	0.56
30:0:1819:G:H5'	38:0:4724:HOH:O	2.04	0.56
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.70	0.56
14:N:4:PRO:HG3	31:9:69:U:OP1	2.06	0.56
30:0:1166:A:P	30:0:1174:A:H4'	2.46	0.56
10:J:82:THR:HG23	30:0:1242:A:C5'	2.25	0.56
5:E:3:VAL:CG2	5:E:49:ILE:HB	2.35	0.56
30:0:204:A:H2'	30:0:205:U:H5'	1.86	0.56
24:X:22:ASN:ND2	30:0:2726:U:O2'	2.39	0.56
18:R:150:PRO:CG	18:R:150:PRO:CB	2.82	0.56
18:R:99:ALA:HB1	18:R:109:MET:CE	2.34	0.56
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.88	0.56
3:C:115:LEU:O	3:C:118:THR:HB	2.06	0.56
30:0:602:A:O2'	30:0:605:C:H4'	2.05	0.56
30:0:2100:A:C8	30:0:2538:A:C2	2.94	0.55
3:C:214:THR:HG23	38:C:8628:HOH:O	2.05	0.55
31:9:76:G:C3'	31:9:77:A:H5''	2.27	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:211:LYS:CG	1:A:212:PRO:HD2	2.32	0.55
30:0:2645:U:O2'	30:0:2646:G:P	2.65	0.55
30:0:2101:A:O4'	30:0:2537:G:H1'	2.05	0.55
30:0:1477:C:H5'	30:0:1868:G:H5'	1.87	0.55
9:I:87:PRO:HD2	30:0:1180:U:O2'	2.06	0.55
30:0:1279:U:O2	30:0:1279:U:C2'	2.53	0.55
30:0:1477:C:H5'	30:0:1868:G:C5'	2.36	0.55
13:M:69:LYS:O	13:M:73:ARG:NH2	2.39	0.55
30:0:1044:C:H5	38:0:6631:HOH:O	1.90	0.55
31:9:52:A:O2'	31:9:53:G:H5'	2.06	0.55
31:9:7:G:H5'	38:9:9096:HOH:O	2.06	0.55
5:E:143:GLN:NE2	30:0:2779:G:H21	2.05	0.55
13:M:76:ARG:HG3	13:M:88:VAL:HG21	1.89	0.55
14:N:110:THR:HB	14:N:113:SER:OG	2.07	0.55
30:0:271:C:C2	30:0:273:G:O4'	2.60	0.55
30:0:1972:U:H2'	30:0:1973:A:C5'	2.36	0.55
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.87	0.55
12:L:143:THR:HG22	12:L:144:ASP:N	2.22	0.55
30:0:2415:A:H2'	30:0:2416:G:H5'	1.87	0.55
6:F:118:LEU:O	6:F:119:ARG:HB3	2.07	0.55
26:Z:51:ALA:HA	38:Z:8715:HOH:O	2.05	0.55
30:0:1191:A:H2	30:0:1206:U:H3	1.55	0.55
31:9:3:A:H2'	38:9:9042:HOH:O	2.05	0.55
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.71	0.55
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.89	0.55
2:B:162:MET:HE2	2:B:310:ARG:HD3	1.87	0.55
9:I:101:LYS:O	9:I:105:GLU:HG3	2.07	0.55
30:0:1406:A:H4'	30:0:1407:A:H5''	1.87	0.55
9:I:129:SER:HB3	30:0:1192:A:H61	1.72	0.55
14:N:37:ARG:NH1	31:9:6:C:OP1	2.37	0.55
10:J:70:PHE:HD1	30:0:2676:C:H4'	1.71	0.55
13:M:9:ARG:HD2	30:0:380:A:OP2	2.07	0.55
30:0:999:C:O2'	30:0:1000:C:H5'	2.07	0.55
30:0:1946:C:H2'	30:0:1971:G:C8	2.41	0.55
3:C:79:ARG:O	3:C:87:ARG:HG2	2.06	0.55
30:0:2718:C:H5'	30:0:2718:C:C6	2.40	0.55
30:0:2908:A:H2'	30:0:2909:G:C4'	2.37	0.55
8:H:61:ARG:HG3	8:H:61:ARG:HH11	1.71	0.55
3:C:184:ARG:NH2	30:0:450:C:OP1	2.34	0.55
27:1:16:HIS:HE1	30:0:775:G:OP1	1.90	0.54
26:Z:40:ALA:HA	30:0:1773:G:C8	2.41	0.54
25:Y:133:HIS:HD2	38:Y:8882:HOH:O	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.70	0.54
30:0:271:C:H4'	30:0:272:A:OP1	2.08	0.54
31:9:42:C:H5'	31:9:43:G:OP2	2.07	0.54
30:0:2323:G:H5''	38:0:4795:HOH:O	2.05	0.54
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.35	0.54
11:K:81:ARG:HD3	11:K:87:ARG:CZ	2.37	0.54
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.90	0.54
15:O:37:ARG:HD2	30:0:656:G:OP2	2.08	0.54
30:0:1118:A:C8	30:0:1119:G:H5''	2.42	0.54
30:0:1730:G:H5'	30:0:1731:C:H5	1.70	0.54
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.36	0.54
2:B:297:VAL:HB	38:B:9030:HOH:O	2.08	0.54
30:0:2769:C:H2'	30:0:2770:G:H5'	1.89	0.54
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.88	0.54
30:0:541:C:O2'	30:0:542:A:H5''	2.07	0.54
30:0:952:G:N3	30:0:2302:A:H2'	2.22	0.54
22:V:64:GLY:O	22:V:65:ASP:HB2	2.06	0.54
30:0:482:G:H4'	30:0:508:A:N1	2.22	0.54
30:0:249:G:O2'	30:0:250:C:H5'	2.08	0.54
30:0:1183:C:H42	30:0:1184:C:H41	1.51	0.54
31:9:52:A:H2'	31:9:53:G:O4'	2.06	0.54
30:0:2681:A:H4'	30:0:2682:C:H5'	1.90	0.54
30:0:1350:U:H4'	38:0:5141:HOH:O	2.06	0.54
23:W:21:LEU:O	23:W:26:ILE:HG23	2.08	0.54
30:0:2032:U:C2'	30:0:2033:G:H5''	2.38	0.54
30:0:1175:G:H1'	30:0:1193:A:C2'	2.34	0.54
23:W:48:VAL:HG12	23:W:48:VAL:O	2.07	0.54
14:N:37:ARG:NE	38:N:8832:HOH:O	2.36	0.54
15:O:24:ALA:HB3	30:0:710:G:OP1	2.07	0.54
20:T:49:GLU:HB3	20:T:59:GLU:HG2	1.90	0.54
30:0:1206:U:H2'	30:0:1207:A:O4'	2.06	0.54
13:M:80:GLY:O	13:M:81:ARG:HD2	2.08	0.54
23:W:130:HIS:O	23:W:136:GLY:HA3	2.08	0.54
3:C:43:LYS:HG2	30:0:449:A:N7	2.23	0.54
30:0:1878:G:C1'	38:0:6149:HOH:O	2.40	0.54
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.38	0.54
8:H:30:LYS:N	8:H:62:HIS:HD2	2.02	0.53
27:1:17:THR:HG21	30:0:120:A:C6	2.43	0.53
13:M:59:GLY:HA3	13:M:141:ILE:HD12	1.89	0.53
4:D:135:VAL:HG22	4:D:136:ARG:H	1.73	0.53
23:W:38:THR:HB	38:W:5390:HOH:O	2.08	0.53
1:A:17:ARG:HD2	38:A:9013:HOH:O	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.89	0.53
30:0:2102:G:N3	30:0:2103:A:C8	2.75	0.53
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.08	0.53
15:O:39:THR:O	15:O:115:ARG:NH2	2.41	0.53
25:Y:186:ARG:HG2	25:Y:186:ARG:HH11	1.72	0.53
30:0:2506:A:O2'	30:0:2507:G:C8	2.42	0.53
30:0:2506:A:N6	30:0:2511:A:O2'	2.40	0.53
2:B:125:GLU:O	2:B:129:ARG:HG3	2.08	0.53
27:1:9:GLY:HA2	30:0:1687:C:O2	2.09	0.53
30:0:2104:C:O2	30:0:2485:A:N1	2.41	0.53
4:D:169:THR:HG22	4:D:170:TYR:HD1	1.72	0.53
30:0:368:C:H2'	30:0:369:G:H5'	1.91	0.53
10:J:19:MET:HE2	10:J:132:LEU:HD11	1.90	0.53
30:0:2766:A:H5'	38:0:9572:HOH:O	2.06	0.53
31:9:39:U:C2'	31:9:40:C:OP1	2.56	0.53
3:C:64:GLY:O	30:0:2100:A:H4'	2.08	0.53
38:B:9058:HOH:O	30:0:2818:A:H2	1.92	0.53
14:N:29:SER:HB3	30:0:2415:A:O2'	2.08	0.53
30:0:307:G:H3'	38:0:6710:HOH:O	2.06	0.53
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.90	0.53
23:W:38:THR:HG22	23:W:39:ASP:N	2.23	0.53
30:0:1741:U:O2'	30:0:2723:G:H4'	2.09	0.53
20:T:19:ARG:HD3	20:T:67:LEU:O	2.09	0.53
8:H:66:GLU:HA	38:H:234:HOH:O	2.09	0.53
30:0:821:U:H2'	30:0:822:C:H6	1.73	0.53
30:0:2591:C:H2'	30:0:2592:G:O4'	2.09	0.53
30:0:2795:C:O2'	30:0:2796:U:H5'	2.09	0.53
13:M:178:LYS:HB2	38:0:6901:HOH:O	2.08	0.53
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.91	0.53
24:X:23:HIS:CD2	24:X:24:LYS:HG3	2.44	0.53
23:W:5:VAL:HG11	23:W:153:MET:HE3	1.91	0.53
1:A:210:GLY:N	38:A:9052:HOH:O	2.40	0.53
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.23	0.53
30:0:2505:G:H2'	30:0:2506:A:H5'	1.91	0.53
30:0:2112:A:H2'	30:0:2113:G:H8	1.72	0.53
30:0:407:A:H5'	38:0:6054:HOH:O	2.09	0.53
30:0:151:A:H2'	30:0:152:A:O4'	2.09	0.53
30:0:2735:U:H2'	30:0:2736:U:C6	2.44	0.53
30:0:347:A:H2'	30:0:348:C:O4'	2.08	0.53
30:0:2505:G:HO2'	30:0:2506:A:H5'	1.73	0.52
30:0:1972:U:H2'	30:0:1973:A:H5'	1.91	0.52
28:2:20:ARG:HG3	28:2:39:ARG:NH2	2.23	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:41:HIS:HD2	30:0:926:A:O2'	1.91	0.52
30:0:2379:G:N7	30:0:2408:A:N1	2.57	0.52
30:0:644:G:N3	30:0:644:G:H5'	2.24	0.52
12:L:133:VAL:HA	38:L:8867:HOH:O	2.10	0.52
30:0:2515:C:C2'	30:0:2516:G:H5'	2.39	0.52
23:W:119:HIS:HE1	38:0:9563:HOH:O	1.91	0.52
30:0:2563:U:H2'	30:0:2565:C:O5'	2.09	0.52
25:Y:204:ARG:HH22	30:0:553:G:P	2.32	0.52
30:0:559:U:H6	30:0:559:U:C5'	2.19	0.52
13:M:164:THR:HG22	13:M:165:GLY:N	2.24	0.52
11:K:41:LYS:HE3	38:0:6239:HOH:O	2.08	0.52
13:M:15:PRO:HA	13:M:20:LEU:HD23	1.91	0.52
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.08	0.52
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.91	0.52
30:0:136:C:H2'	30:0:137:U:O4'	2.10	0.52
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.07	0.52
30:0:485:A:N3	30:0:487:G:H5''	2.24	0.52
30:0:920:C:H4'	30:0:921:G:C2	2.45	0.52
4:D:50:VAL:HG13	31:9:41:C:O4'	2.10	0.52
1:A:192:VAL:HB	38:0:5683:HOH:O	2.09	0.52
2:B:53:LEU:HD11	2:B:327:VAL:HG22	1.92	0.52
14:N:4:PRO:HD2	38:0:6797:HOH:O	2.09	0.52
30:0:958:G:O2'	30:0:959:C:H5'	2.10	0.52
30:0:2346:C:H6	30:0:2346:C:O5'	1.92	0.52
7:G:64:ASN:N	7:G:64:ASN:HD22	2.08	0.52
10:J:52:GLN:NE2	30:0:1119:G:H8	2.07	0.52
30:0:137:U:H2'	30:0:139:C:C5	2.44	0.52
31:9:92:G:H2'	31:9:93:A:H8	1.74	0.52
12:L:41:HIS:CD2	30:0:926:A:O2'	2.63	0.52
11:K:29:LEU:HB3	11:K:55:VAL:CG2	2.40	0.52
14:N:132:ASN:O	14:N:135:VAL:HG12	2.10	0.52
2:B:229:ARG:HD2	38:0:9115:HOH:O	2.09	0.52
30:0:2820:A:H2'	30:0:2821:C:C6	2.44	0.52
30:0:1878:G:O2'	30:0:1879:U:P	2.68	0.52
13:M:82:ARG:HB3	38:0:7854:HOH:O	2.09	0.52
14:N:11:ARG:NH1	31:9:8:G:O6	2.42	0.52
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.24	0.52
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.39	0.52
20:T:38:ARG:HH21	30:0:306:A:P	2.33	0.52
30:0:1160:G:H5'	30:0:1161:A:C4'	2.40	0.52
30:0:2070:G:H2'	30:0:2072:G:OP1	2.10	0.52
2:B:53:LEU:HD12	2:B:327:VAL:HA	1.90	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.92	0.52
30:0:95:A:H5''	30:0:97:G:O4'	2.10	0.52
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.90	0.52
2:B:268:ARG:NH2	2:B:325:PRO:HG3	2.23	0.52
30:0:1724:U:H4'	38:0:4582:HOH:O	2.09	0.52
30:0:2072:G:C6	30:0:2533:C:H1'	2.45	0.52
30:0:1778:A:H2'	30:0:1779:A:H5'	1.92	0.52
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.73	0.52
29:3:84:ARG:NE	38:3:9045:HOH:O	2.43	0.52
30:0:255:A:H2'	30:0:256:C:C6	2.45	0.52
30:0:544:G:H2'	30:0:545:G:C5'	2.37	0.52
2:B:27:ASN:HD21	30:0:2807:U:P	2.32	0.52
30:0:2531:U:O2'	30:0:2532:A:H5'	2.10	0.52
30:0:790:A:H1'	30:0:1710:A:H2'	1.92	0.52
2:B:178:ALA:O	2:B:182:VAL:HG23	2.10	0.52
26:Z:42:TYR:HA	30:0:1829:A:N6	2.25	0.52
30:0:1164:U:O2	30:0:1166:A:H4'	2.09	0.51
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.55	0.51
30:0:2252:A:C5	30:0:2253:G:H1'	2.43	0.51
23:W:151:GLU:O	23:W:154:ARG:HB2	2.10	0.51
27:1:25:LYS:HD2	28:2:49:GLU:N	2.21	0.51
13:M:69:LYS:HG3	13:M:127:LYS:HG3	1.91	0.51
25:Y:144:ARG:NE	38:Y:8913:HOH:O	2.43	0.51
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.46	0.51
30:0:343:C:O2'	30:0:344:C:H5'	2.09	0.51
30:0:389:G:H5''	38:0:6487:HOH:O	2.10	0.51
29:3:91:GLN:O	29:3:92:GLU:HB2	2.10	0.51
30:0:1209:C:H2'	30:0:1210:G:C8	2.41	0.51
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.74	0.51
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.92	0.51
31:9:20:G:O2'	31:9:21:G:H5'	2.10	0.51
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.76	0.51
30:0:2883:A:H2'	30:0:2884:G:O4'	2.10	0.51
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.10	0.51
30:0:564:G:H1'	38:0:6341:HOH:O	2.10	0.51
4:D:49:PRO:HB3	4:D:73:VAL:HG22	1.93	0.51
21:U:37:GLU:HB3	38:U:408:HOH:O	2.09	0.51
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.45	0.51
30:0:542:A:H2'	30:0:543:G:O4'	2.11	0.51
30:0:661:G:C5	30:0:686:A:C2	2.99	0.51
9:I:114:TYR:CE1	30:0:1186:C:H5''	2.45	0.51
2:B:307:ARG:NH1	2:B:307:ARG:HG3	2.17	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:87:ARG:NH2	30:0:894:A:N1	2.58	0.51
30:0:856:G:C8	38:0:5452:HOH:O	2.54	0.51
24:X:43:VAL:HG12	24:X:44:ASP:N	2.25	0.51
25:Y:174:VAL:HG22	25:Y:177:LYS:HD2	1.92	0.51
30:0:1909:A:N1	30:0:2128:G:H1'	2.25	0.51
30:0:1506:U:H5'	30:0:1506:U:H6	1.75	0.51
1:A:206:ARG:HD3	1:A:206:ARG:H	1.75	0.51
6:F:58:GLU:HA	6:F:61:MET:HE2	1.93	0.51
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.58	0.51
30:0:2251:G:H2'	30:0:2252:A:C8	2.46	0.51
12:L:90:ARG:NH2	12:L:121:ILE:HD11	2.25	0.51
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.73	0.51
30:0:2510:C:H5'	30:0:2511:A:OP2	2.11	0.51
30:0:2908:A:H2'	30:0:2909:G:H5'	1.92	0.51
2:B:190:MET:HE2	2:B:194:PHE:HD1	1.76	0.51
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.92	0.51
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.08	0.51
30:0:1067:A:H5'	38:0:4364:HOH:O	2.10	0.51
30:0:282:C:O2'	30:0:283:U:C5'	2.48	0.51
30:0:2414:A:H2'	30:0:2415:A:C8	2.46	0.51
30:0:1947:G:N2	30:0:1966:U:C2	2.79	0.51
23:W:139:GLY:O	23:W:141:HIS:HD2	1.93	0.51
28:2:18:ASN:ND2	28:2:40:ARG:H	2.08	0.51
26:Z:35:SER:CB	26:Z:47:ARG:HB2	2.39	0.51
30:0:1218:U:H2'	30:0:1219:U:H6	1.75	0.51
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.11	0.51
2:B:294:TYR:HE2	38:B:9074:HOH:O	1.94	0.51
30:0:1182:C:H4'	30:0:1192:A:N7	2.26	0.51
8:H:31:ILE:HG23	38:H:234:HOH:O	2.11	0.51
16:P:1:THR:O	30:0:1396:C:H1'	2.10	0.51
22:V:39:ALA:N	22:V:40:PRO:HD2	2.26	0.51
31:9:108:C:H2'	31:9:109:G:C8	2.46	0.51
3:C:153:VAL:O	3:C:157:LEU:HG	2.11	0.51
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.46	0.51
30:0:101:C:H2'	30:0:102:A:C8	2.46	0.51
30:0:440:C:H2'	30:0:441:A:C8	2.46	0.50
30:0:1739:G:H1'	30:0:2726:U:O4	2.11	0.50
1:A:223:ARG:NH1	38:A:8987:HOH:O	2.44	0.50
10:J:39:VAL:HG21	10:J:107:ASN:ND2	2.25	0.50
30:0:1196:C:H2'	30:0:1197:G:H5'	1.93	0.50
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.76	0.50
30:0:1745:G:H22	30:0:2033:G:H5'	1.76	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2515:C:H2'	30:0:2516:G:H5'	1.93	0.50
3:C:93:LYS:O	3:C:98:ARG:NH2	2.44	0.50
11:K:10:GLN:H	11:K:10:GLN:NE2	1.90	0.50
31:9:51:A:H8	31:9:51:A:OP2	1.94	0.50
30:0:2908:A:H2'	30:0:2909:G:C5'	2.40	0.50
30:0:441:A:H8	30:0:441:A:O5'	1.94	0.50
30:0:407:A:H2'	30:0:408:A:C8	2.47	0.50
30:0:1948:G:H2'	30:0:1949:G:O4'	2.11	0.50
16:P:59:ARG:NH2	16:P:66:GLN:HE22	1.98	0.50
30:0:2769:C:C2'	30:0:2770:G:C5'	2.87	0.50
30:0:1060:C:H6	30:0:1060:C:H5'	1.76	0.50
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.12	0.50
10:J:86:MET:HE2	30:0:1241:G:H2'	1.93	0.50
30:0:522:U:O2'	30:0:1366:C:H5'	2.12	0.50
5:E:145:ALA:HB1	5:E:168:ILE:CD1	2.41	0.50
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.12	0.50
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.69	0.50
31:9:49:G:H2'	31:9:50:G:O4'	2.12	0.50
14:N:160:SER:HB2	31:9:51:A:H5'	1.92	0.50
30:0:2032:U:H2'	30:0:2033:G:H5''	1.91	0.50
23:W:119:HIS:HD2	23:W:120:PRO:O	1.95	0.50
30:0:2265:U:H2'	30:0:2266:A:C8	2.47	0.50
30:0:1149:U:H5''	30:0:1151:G:O4'	2.11	0.50
30:0:532:A:H3'	38:0:9472:HOH:O	2.11	0.50
30:0:2756:U:O2	30:0:2896:A:H2	1.95	0.50
8:H:48:VAL:HA	8:H:170:ARG:O	2.12	0.50
30:0:830:G:O2'	30:0:831:U:H5'	2.12	0.50
30:0:1314:U:H5''	30:0:1316:G:O4'	2.11	0.50
16:P:73:HIS:HE1	30:0:1789:G:O6	1.95	0.50
30:0:612:U:H2'	30:0:613:C:C6	2.47	0.50
31:9:49:G:O2'	31:9:50:G:H5'	2.12	0.50
30:0:920:C:H5''	30:0:921:G:O5'	2.11	0.50
30:0:2252:A:H2'	30:0:2253:G:O4'	2.12	0.50
25:Y:144:ARG:NH1	38:Y:8875:HOH:O	2.44	0.50
30:0:585:C:H5''	38:0:4886:HOH:O	2.10	0.50
30:0:497:A:H5''	38:0:3610:HOH:O	2.11	0.50
24:X:78:GLU:HB3	38:X:5564:HOH:O	2.12	0.50
30:0:2587:OMU:HM23	30:0:2589:U:C6	2.47	0.50
20:T:61:GLU:HG2	38:T:3851:HOH:O	2.10	0.50
30:0:1193:A:C2	30:0:1194:A:N6	2.80	0.50
5:E:20:ILE:HD11	5:E:40:VAL:CG1	2.41	0.50
27:1:1:THR:HA	38:0:9363:HOH:O	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1131:G:C6	30:0:1230:A:C4	2.99	0.50
12:L:145:LEU:O	12:L:148:GLU:HG3	2.12	0.50
30:0:2649:A:H5'	30:0:2649:A:C8	2.47	0.50
30:0:2649:A:H5'	30:0:2649:A:H8	1.77	0.50
2:B:321:PRO:HA	38:B:9081:HOH:O	2.11	0.50
30:0:282:C:C2'	30:0:283:U:C5'	2.89	0.50
8:H:48:VAL:HG13	38:H:214:HOH:O	2.11	0.50
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.47	0.50
5:E:81:GLU:HG2	5:E:134:SER:CB	2.42	0.50
30:0:861:A:H4'	30:0:1697:G:H4'	1.94	0.50
13:M:188:ARG:HD3	30:0:155:C:OP2	2.11	0.50
30:0:69:A:H8	30:0:69:A:C5'	2.23	0.49
30:0:834:G:H3'	30:0:835:U:H4'	1.94	0.49
13:M:75:ARG:HH11	30:0:1864:C:H5	1.58	0.49
30:0:1422:U:H2'	30:0:1423:C:C6	2.47	0.49
30:0:2032:U:C2'	30:0:2033:G:C5'	2.89	0.49
12:L:143:THR:HG22	12:L:144:ASP:H	1.75	0.49
30:0:1168:C:H5	38:0:7521:HOH:O	1.94	0.49
18:R:29:LYS:NZ	38:R:8943:HOH:O	2.46	0.49
30:0:603:A:H5''	30:0:604:G:OP1	2.11	0.49
25:Y:165:GLU:HB3	38:0:6729:HOH:O	2.12	0.49
9:I:120:ALA:O	9:I:124:VAL:HG23	2.11	0.49
31:9:64:C:C2'	31:9:65:A:H5'	2.42	0.49
1:A:121:ALA:O	1:A:124:VAL:HG22	2.11	0.49
30:0:1159:G:H1	30:0:1208:C:H42	1.58	0.49
30:0:1207:A:C8	30:0:1208:C:C5	3.00	0.49
30:0:1044:C:H5''	38:0:9029:HOH:O	2.12	0.49
31:9:105:A:H2'	31:9:106:U:H5'	1.94	0.49
30:0:1834:C:H2'	30:0:1840:A:N6	2.27	0.49
2:B:280:VAL:HG13	2:B:333:GLU:O	2.12	0.49
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.45	0.49
12:L:41:HIS:HE1	38:0:9778:HOH:O	1.95	0.49
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.94	0.49
28:2:42:TRP:HB3	30:0:1418:U:OP1	2.12	0.49
30:0:912:A:C4	30:0:1294:A:C2	3.01	0.49
11:K:66:ARG:HH22	30:0:1994:A:P	2.35	0.49
30:0:1163:G:N2	30:0:1184:C:C4	2.81	0.49
28:2:41:HIS:HD2	28:2:44:ARG:H	1.60	0.49
3:C:1:MET:HG2	3:C:2:GLN:N	2.25	0.49
27:1:28:HIS:HE1	30:0:776:A:OP1	1.95	0.49
25:Y:146:PRO:O	25:Y:154:ARG:HG3	2.13	0.49
2:B:36:PRO:HG3	2:B:169:GLY:H	1.76	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.43	0.49
6:F:58:GLU:HA	6:F:61:MET:CE	2.42	0.49
13:M:59:GLY:HA3	13:M:141:ILE:CD1	2.42	0.49
30:0:1865:A:C2	38:0:3075:HOH:O	2.55	0.49
3:C:77:ALA:O	3:C:78:ARG:HD3	2.12	0.49
20:T:53:GLY:HA3	38:T:6384:HOH:O	2.12	0.49
12:L:125:PHE:CE1	12:L:140:VAL:HG13	2.48	0.49
30:0:1909:A:H2'	30:0:1910:A:C8	2.47	0.49
1:A:175:LYS:HG3	30:0:1847:A:OP1	2.13	0.49
30:0:1761:U:H2'	30:0:1762:C:C6	2.47	0.49
30:0:1562:C:N4	38:0:5891:HOH:O	2.45	0.49
5:E:101:GLU:HB3	5:E:117:THR:HA	1.94	0.49
14:N:41:LYS:HD3	38:9:9059:HOH:O	2.12	0.49
15:O:59:VAL:HG23	15:O:111:VAL:HG22	1.94	0.49
30:0:304:G:H1'	30:0:347:A:N6	2.27	0.49
30:0:2587:OMU:H6	30:0:2587:OMU:O5'	2.12	0.49
2:B:87:TYR:HD1	38:B:9004:HOH:O	1.95	0.49
30:0:1414:A:H2'	30:0:1415:G:O4'	2.12	0.49
30:0:426:G:H2'	30:0:427:C:O4'	2.12	0.49
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.94	0.49
27:1:20:ARG:HH21	30:0:120:A:H5'	1.77	0.49
18:R:117:HIS:CD2	30:0:20:G:H21	2.30	0.49
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.42	0.49
29:3:60:LYS:HE2	30:0:2428:G:N7	2.27	0.49
2:B:256:GLN:HG2	38:B:9080:HOH:O	2.11	0.49
30:0:1196:C:C2'	30:0:1197:G:H5'	2.42	0.49
11:K:66:ARG:HD2	30:0:1992:U:OP2	2.13	0.49
30:0:1755:A:H2'	30:0:1756:G:O4'	2.13	0.49
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.95	0.49
30:0:1166:A:C6	30:0:1181:A:C2	3.01	0.48
2:B:221:GLN:HE22	11:K:42:ASN:ND2	2.04	0.48
23:W:4:LEU:O	23:W:32:CYS:HA	2.13	0.48
12:L:6:ARG:NH2	38:L:8843:HOH:O	2.45	0.48
2:B:41:PHE:HB3	2:B:190:MET:CE	2.43	0.48
27:1:28:HIS:CD2	27:1:31:LYS:H	2.31	0.48
20:T:54:ASP:OD2	30:0:316:A:H5'	2.13	0.48
30:0:1321:A:H2'	30:0:1322:G:C8	2.48	0.48
14:N:169:PRO:O	14:N:172:PHE:HB3	2.13	0.48
30:0:696:C:O2'	30:0:697:G:H5'	2.13	0.48
30:0:2637:A:C5'	38:0:4944:HOH:O	2.61	0.48
2:B:258:GLY:H	2:B:260:HIS:CE1	2.30	0.48
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:105:VAL:HG11	1:A:154:ALA:HB1	1.95	0.48
2:B:8:LYS:HG3	2:B:220:VAL:HG12	1.95	0.48
30:0:2512:U:H4'	30:0:2514:U:O4	2.13	0.48
2:B:248:ARG:NH2	30:0:2549:C:H1'	2.28	0.48
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.13	0.48
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.45	0.48
30:0:820:G:O2'	30:0:856:G:H4'	2.13	0.48
3:C:173:LYS:HE3	30:0:1311:G:O6	2.13	0.48
30:0:221:G:H5''	38:0:5772:HOH:O	2.13	0.48
10:J:88:PRO:O	10:J:94:GLY:HA3	2.13	0.48
11:K:49:LEU:CD2	11:K:80:ILE:HD13	2.43	0.48
13:M:107:ARG:NH2	30:0:181:G:H4'	2.27	0.48
30:0:635:A:H2'	30:0:636:G:H5''	1.95	0.48
30:0:1185:U:H2'	30:0:1186:C:C6	2.48	0.48
14:N:147:ILE:HD12	38:9:9086:HOH:O	2.13	0.48
30:0:120:A:H2'	30:0:120:A:N3	2.28	0.48
30:0:625:U:H5''	30:0:1044:C:N4	2.28	0.48
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.94	0.48
26:Z:55:SER:O	26:Z:59:GLU:HG3	2.14	0.48
10:J:52:GLN:HE22	30:0:1119:G:H8	1.62	0.48
10:J:75:PRO:HD3	10:J:136:SER:OG	2.12	0.48
30:0:1205:U:C3'	30:0:1206:U:H5''	2.43	0.48
30:0:1205:U:H5	38:0:4455:HOH:O	1.97	0.48
30:0:2506:A:H1'	38:0:3761:HOH:O	2.13	0.48
6:F:91:VAL:HG11	30:0:262:A:OP2	2.14	0.48
30:0:856:G:H2'	38:0:5452:HOH:O	2.13	0.48
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.43	0.48
30:0:1353:C:H6	30:0:1353:C:H5'	1.78	0.48
30:0:2134:G:C6	30:0:2258:A:C8	3.02	0.48
30:0:1972:U:C2'	30:0:1973:A:H5''	2.44	0.48
30:0:1298:U:H2'	30:0:1299:G:C8	2.48	0.48
2:B:254:GLN:HG3	38:B:8960:HOH:O	2.13	0.48
30:0:447:A:O2'	30:0:448:G:H5'	2.14	0.48
30:0:316:A:N3	30:0:336:G:O2'	2.42	0.48
2:B:305:ASP:O	2:B:306:LYS:HB2	2.14	0.48
30:0:1790:C:H2'	30:0:1791:U:C6	2.49	0.48
30:0:627:G:H2'	30:0:2071:C:C4	2.48	0.48
30:0:2101:A:H1'	30:0:2537:G:O4'	2.14	0.48
30:0:1117:A:C2	30:0:1244:U:C2	3.01	0.48
30:0:1632:A:H2'	30:0:1633:C:C5'	2.38	0.48
30:0:1838:U:H1'	30:0:2644:C:H5'	1.96	0.48
30:0:152:A:O2'	30:0:153:C:H5'	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:10:U:H6	30:0:10:U:H3'	1.79	0.48
30:0:1559:A:H4'	38:0:5891:HOH:O	2.13	0.48
3:C:233:THR:HG22	3:C:234:VAL:N	2.28	0.48
1:A:36:ASP:O	1:A:38:ILE:N	2.38	0.48
30:0:1902:G:H2'	30:0:1903:U:O4'	2.14	0.48
11:K:87:ARG:NH2	30:0:2720:C:O2	2.47	0.48
30:0:697:G:H4'	30:0:730:G:O3'	2.14	0.48
25:Y:145:LYS:HE2	38:Y:8907:HOH:O	2.14	0.48
30:0:1081:A:H5''	38:0:3162:HOH:O	2.14	0.48
6:F:111:ILE:O	6:F:115:VAL:HG23	2.14	0.48
30:0:1194:A:C2	30:0:1206:U:H1'	2.48	0.48
30:0:2809:G:H2'	30:0:2810:G:O4'	2.14	0.48
30:0:1535:G:H2'	30:0:1536:C:C6	2.49	0.48
30:0:1555:G:H4'	30:0:1630:A:H2	1.79	0.48
30:0:1181:A:N1	30:0:1192:A:O2'	2.41	0.47
30:0:960:G:N3	30:0:960:G:C2'	2.76	0.47
12:L:30:ARG:HD2	38:0:9024:HOH:O	2.14	0.47
30:0:2238:A:C2	30:0:2239:C:C6	3.02	0.47
30:0:821:U:H2'	30:0:822:C:C6	2.49	0.47
2:B:102:THR:HG21	2:B:182:VAL:O	2.14	0.47
23:W:154:ARG:NH1	30:0:588:G:O6	2.47	0.47
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.43	0.47
28:2:5:LYS:HD2	30:0:1675:C:H5''	1.96	0.47
3:C:246:ARG:NE	38:C:8616:HOH:O	2.38	0.47
30:0:1333:U:H2'	30:0:1334:C:C6	2.49	0.47
12:L:53:ARG:NH2	12:L:57:VAL:HG12	2.28	0.47
30:0:1524:U:HO2'	30:0:1525:G:P	2.37	0.47
13:M:64:ARG:HD2	38:M:8887:HOH:O	2.15	0.47
14:N:155:GLU:O	14:N:156:GLU:HG3	2.14	0.47
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.14	0.47
30:0:23:G:C6	30:0:24:G:N1	2.83	0.47
12:L:73:VAL:HG23	12:L:74:THR:H	1.79	0.47
19:S:76:GLU:HB3	38:S:7263:HOH:O	2.13	0.47
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.30	0.47
1:A:237:GLY:HA3	30:0:1939:U:H5''	1.95	0.47
14:N:114:LYS:O	14:N:118:ILE:HG13	2.14	0.47
30:0:999:C:H2'	30:0:1000:C:H5'	1.95	0.47
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.96	0.47
30:0:2102:G:H3'	38:0:3643:HOH:O	2.14	0.47
30:0:1182:C:C1'	30:0:1192:A:C8	2.97	0.47
31:9:50:G:H2'	31:9:51:A:C8	2.48	0.47
15:O:25:VAL:HG13	30:0:710:G:H5'	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:1:28:HIS:HD2	27:1:30:LYS:H	1.61	0.47
25:Y:155:ARG:NH1	38:Y:8857:HOH:O	2.47	0.47
30:0:1132:A:N6	30:0:1229:C:H2'	2.30	0.47
30:0:1656:A:H2'	30:0:1657:A:O4'	2.15	0.47
3:C:242:GLU:HB2	38:C:8578:HOH:O	2.14	0.47
30:0:2001:G:O2'	30:0:2002:C:H5'	2.14	0.47
25:Y:216:ARG:HD2	38:Y:8869:HOH:O	2.12	0.47
30:0:1406:A:H4'	30:0:1407:A:C5'	2.45	0.47
25:Y:144:ARG:NH1	30:0:905:C:OP1	2.48	0.47
7:G:23:ILE:O	7:G:27:ILE:HG13	2.14	0.47
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.96	0.47
17:Q:75:ILE:HD13	17:Q:84:ILE:HD11	1.95	0.47
30:0:1165:G:N2	30:0:1173:A:H5'	2.30	0.47
30:0:1178:G:C6	30:0:1179:C:N4	2.83	0.47
3:C:127:ARG:HD3	3:C:129:HIS:CE1	2.50	0.47
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.97	0.47
30:0:2502:C:H2'	30:0:2503:A:C5'	2.42	0.47
30:0:1477:C:H2'	30:0:1478:U:C6	2.50	0.47
30:0:538:C:H5''	30:0:539:G:C8	2.48	0.47
23:W:5:VAL:HG11	23:W:153:MET:CE	2.44	0.47
4:D:52:THR:HG21	30:0:2346:C:O2'	2.14	0.47
31:9:65:A:N6	31:9:112:U:C6	2.82	0.47
20:T:79:LEU:HG	20:T:89:ARG:HB2	1.96	0.47
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.80	0.47
26:Z:46:SER:O	26:Z:50:VAL:HG23	2.14	0.47
30:0:2616:G:N3	30:0:2616:G:H2'	2.28	0.47
30:0:1925:G:O2'	30:0:1926:G:H5'	2.15	0.47
17:Q:32:GLU:HA	17:Q:71:TYR:OH	2.15	0.47
23:W:11:VAL:HG11	30:0:1086:A:C6	2.49	0.47
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.45	0.47
30:0:1181:A:H2'	30:0:1182:C:H5'	1.95	0.47
30:0:1193:A:H2	30:0:1194:A:N6	2.13	0.47
30:0:2541:U:H5''	38:0:5423:HOH:O	2.14	0.47
30:0:999:C:H2'	30:0:1000:C:C5'	2.45	0.47
6:F:50:VAL:CG1	6:F:60:VAL:HG11	2.45	0.47
10:J:39:VAL:HG22	10:J:107:ASN:HA	1.95	0.47
30:0:10:U:O4	30:0:532:A:OP2	2.32	0.47
25:Y:148:GLY:HA3	30:0:622:G:P	2.55	0.47
28:2:38:LYS:HE3	38:0:4243:HOH:O	2.15	0.47
30:0:561:G:O2'	30:0:562:A:H5'	2.15	0.47
30:0:2456:A:H2'	30:0:2457:U:C6	2.50	0.47
12:L:91:VAL:HG13	12:L:120:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:280:C:O2'	30:0:281:U:H5'	2.15	0.47
30:0:1985:U:C2	30:0:1996:U:O4'	2.68	0.47
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.40	0.47
10:J:107:ASN:HD22	10:J:109:TYR:H	1.63	0.47
30:0:1014:A:H5''	31:9:101:G:O2'	2.15	0.47
30:0:1252:A:H2'	30:0:1253:C:O4'	2.15	0.47
9:I:114:TYR:HE1	30:0:1186:C:H5''	1.78	0.47
10:J:52:GLN:NE2	30:0:1119:G:H2'	2.30	0.47
30:0:2828:G:O2'	30:0:2829:G:H5'	2.14	0.47
30:0:1496:A:H2'	30:0:1497:G:O4'	2.15	0.47
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.15	0.47
31:9:95:C:O2'	31:9:96:C:H5'	2.15	0.47
30:0:1163:G:N1	30:0:1184:C:N4	2.63	0.46
27:1:25:LYS:CD	28:2:49:GLU:H	2.24	0.46
20:T:49:GLU:CB	20:T:59:GLU:HG2	2.46	0.46
30:0:64:G:H2'	30:0:65:C:O4'	2.15	0.46
7:G:20:VAL:O	7:G:24:VAL:HG23	2.15	0.46
30:0:1160:G:H5''	30:0:1161:A:H5'	1.87	0.46
14:N:37:ARG:HH11	31:9:6:C:P	2.37	0.46
8:H:30:LYS:H	8:H:62:HIS:CD2	2.17	0.46
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.28	0.46
2:B:258:GLY:HA2	38:0:4025:HOH:O	2.15	0.46
10:J:45:VAL:CG2	10:J:129:PHE:HD1	2.29	0.46
30:0:2247:C:H2'	30:0:2248:C:H6	1.81	0.46
30:0:1120:U:H5''	30:0:1120:U:C6	2.51	0.46
31:9:60:C:O2'	31:9:61:C:H5'	2.15	0.46
16:P:16:VAL:HG12	16:P:17:GLY:N	2.30	0.46
30:0:1735:C:O2'	30:0:1736:A:H5'	2.14	0.46
10:J:45:VAL:CG2	10:J:129:PHE:CD1	2.98	0.46
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.96	0.46
13:M:77:HIS:HD2	13:M:79:ALA:O	1.98	0.46
30:0:1592:G:O2'	30:0:1593:C:O5'	2.34	0.46
5:E:126:ILE:HB	5:E:131:LEU:HD23	1.97	0.46
2:B:282:GLY:O	30:0:2898:G:H1'	2.15	0.46
30:0:1164:U:C2	30:0:1166:A:H4'	2.50	0.46
30:0:1192:A:H3'	30:0:1193:A:H5'	1.98	0.46
30:0:2372:A:H2'	30:0:2373:U:H6	1.80	0.46
16:P:40:VAL:O	16:P:44:VAL:HG23	2.16	0.46
13:M:68:ARG:NH2	13:M:73:ARG:HD3	2.30	0.46
30:0:2515:C:H2'	30:0:2516:G:C5'	2.46	0.46
30:0:1120:U:H5'	30:0:1121:G:OP2	2.16	0.46
30:0:1942:A:H3'	38:0:7372:HOH:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2241:C:O2'	30:0:2242:U:H5'	2.15	0.46
30:0:690:G:H4'	30:0:741:C:O2	2.16	0.46
30:0:1518:A:H2'	30:0:1519:U:C6	2.50	0.46
1:A:211:LYS:HB3	38:0:7455:HOH:O	2.15	0.46
30:0:255:A:C5	30:0:256:C:C4	3.03	0.46
2:B:307:ARG:HD2	38:B:9077:HOH:O	2.15	0.46
30:0:2004:U:H5''	30:0:2005:G:C8	2.50	0.46
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.97	0.46
27:1:48:TYR:HE2	38:0:9317:HOH:O	1.99	0.46
1:A:71:PRO:HD2	1:A:74:VAL:HG21	1.98	0.46
6:F:37:THR:O	6:F:41:GLU:HG3	2.15	0.46
30:0:703:G:O2'	30:0:704:C:H5'	2.16	0.46
30:0:2103:A:N6	30:0:2538:A:H8	1.97	0.46
30:0:2507:G:H2'	30:0:2510:C:N4	2.27	0.46
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.45	0.46
30:0:1203:G:O2'	30:0:1204:C:H5'	2.16	0.46
30:0:2356:A:H5'	38:0:5662:HOH:O	2.15	0.46
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.97	0.46
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.84	0.46
6:F:107:ASP:O	6:F:111:ILE:HG13	2.16	0.46
2:B:148:PRO:HD2	38:B:9005:HOH:O	2.15	0.46
1:A:11:ARG:HD3	38:0:9224:HOH:O	2.15	0.46
30:0:816:G:C6	30:0:817:G:N1	2.84	0.46
38:Q:2875:HOH:O	30:0:2392:C:H4'	2.15	0.46
30:0:1211:G:H2'	30:0:1212:C:H6	1.81	0.46
30:0:2072:G:H3'	30:0:2073:G:C5'	2.46	0.46
18:R:3:SER:HB2	30:0:20:G:O3'	2.16	0.46
30:0:1819:G:H2'	30:0:1820:G:C4'	2.45	0.46
21:U:33:SER:O	21:U:37:GLU:HG3	2.15	0.46
30:0:2587:OMU:CM2	30:0:2589:U:C6	2.99	0.46
8:H:27:PRO:HD3	8:H:123:ILE:HG22	1.98	0.46
12:L:32:ASP:HB3	30:0:222:A:H5''	1.97	0.46
30:0:2351:C:H2'	30:0:2352:G:O4'	2.16	0.46
10:J:80:LYS:HE2	10:J:98:PHE:CE1	2.51	0.46
30:0:1641:A:C2'	30:0:1642:A:H5'	2.45	0.46
30:0:1996:U:O2'	30:0:1997:A:H5'	2.16	0.46
31:9:22:G:H5'	31:9:23:U:OP1	2.16	0.46
30:0:1615:A:H4'	38:0:5912:HOH:O	2.16	0.46
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.98	0.46
1:A:105:VAL:HG11	1:A:154:ALA:CB	2.46	0.46
13:M:75:ARG:NH1	30:0:1864:C:H5	2.14	0.46
30:0:1524:U:OP1	30:0:1524:U:H4'	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1014:A:H2'	30:0:1015:C:H5'	1.97	0.46
30:0:1484:G:H3'	38:0:7841:HOH:O	2.16	0.46
30:0:1851:G:O2'	30:0:1852:A:H5'	2.16	0.46
17:Q:67:GLN:NE2	30:0:2403:C:O2	2.47	0.46
30:0:2839:C:H2'	30:0:2840:A:H5''	1.98	0.46
13:M:82:ARG:HA	38:M:8836:HOH:O	2.16	0.46
30:0:407:A:H8	38:0:4474:HOH:O	1.99	0.46
13:M:79:ALA:HB3	13:M:81:ARG:NH1	2.31	0.46
23:W:149:LEU:HG	23:W:153:MET:HE2	1.98	0.46
30:0:830:G:H2'	30:0:831:U:C6	2.51	0.46
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.78	0.46
12:L:97:VAL:HG12	12:L:98:GLU:O	2.16	0.46
30:0:1175:G:H8	30:0:1193:A:HO2'	1.64	0.45
4:D:76:ARG:CZ	31:9:44:A:H1'	2.46	0.45
30:0:2421:G:H2'	38:0:4096:HOH:O	2.16	0.45
30:0:2282:U:H4'	30:0:2309:C:C5	2.51	0.45
30:0:666:A:H2'	30:0:667:C:O4'	2.16	0.45
4:D:36:ASN:HB3	38:D:7502:HOH:O	2.15	0.45
2:B:316:ARG:HB2	30:0:2768:A:C8	2.51	0.45
3:C:180:SER:HB2	38:C:8638:HOH:O	2.15	0.45
30:0:2748:G:C5'	30:0:2748:G:C8	2.98	0.45
30:0:2506:A:H2'	30:0:2506:A:O5'	2.16	0.45
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.98	0.45
30:0:664:U:O4	30:0:681:G:H5''	2.16	0.45
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.98	0.45
2:B:13:PHE:HB2	2:B:16:ARG:NH1	2.31	0.45
15:O:96:VAL:HG13	15:O:100:GLN:HB2	1.98	0.45
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.16	0.45
30:0:1185:U:H5'	38:0:7491:HOH:O	2.15	0.45
15:O:32:ARG:HH21	15:O:35:LYS:HZ3	1.62	0.45
29:3:42:ARG:NH1	30:0:396:U:H5'	2.31	0.45
4:D:37:ALA:HA	38:D:5583:HOH:O	2.16	0.45
30:0:1008:C:H2'	30:0:1009:U:C6	2.51	0.45
30:0:1948:G:H2'	30:0:1949:G:H8	1.80	0.45
30:0:560:U:C2	30:0:561:G:C8	3.04	0.45
5:E:126:ILE:HB	5:E:131:LEU:CD2	2.46	0.45
5:E:1:PRO:HG2	5:E:59:MET:SD	2.57	0.45
30:0:2906:A:H5'	30:0:2907:C:O4'	2.17	0.45
11:K:114:ALA:HB3	11:K:117:VAL:HG23	1.97	0.45
19:S:67:ARG:HD3	38:S:3430:HOH:O	2.17	0.45
30:0:2314:G:C2'	30:0:2315:C:H5'	2.47	0.45
9:I:129:SER:HB3	30:0:1192:A:N6	2.31	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.15	0.45
30:0:1739:G:O2'	30:0:1740:U:H5'	2.16	0.45
24:X:22:ASN:O	24:X:64:ALA:HA	2.17	0.45
30:0:2679:G:H2'	30:0:2681:A:OP2	2.17	0.45
27:1:28:HIS:HD2	27:1:31:LYS:H	1.64	0.45
27:1:28:HIS:CD2	27:1:30:LYS:HB2	2.51	0.45
30:0:1335:C:H2'	30:0:1336:U:C6	2.51	0.45
30:0:24:G:N2	30:0:518:G:H1'	2.31	0.45
31:9:59:C:H2'	31:9:60:C:C6	2.52	0.45
30:0:1021:G:O2'	30:0:1022:A:H5'	2.17	0.45
3:C:150:THR:HA	3:C:203:ALA:O	2.17	0.45
30:0:1163:G:H2'	30:0:1164:U:C5	2.51	0.45
31:9:76:G:H3'	31:9:77:A:C5'	2.30	0.45
30:0:1119:G:C5	30:0:1243:C:C4	3.04	0.45
31:9:29:C:H2'	31:9:30:C:C5'	2.43	0.45
1:A:125:ASN:CB	1:A:158:VAL:HG12	2.44	0.45
30:0:1236:A:H2'	30:0:1237:U:O4'	2.16	0.45
30:0:806:A:H2'	30:0:807:A:O4'	2.16	0.45
30:0:2502:C:O2'	30:0:2503:A:H5'	2.17	0.45
2:B:212:GLN:HA	30:0:1733:A:H4'	1.98	0.45
30:0:2831:C:H2'	30:0:2832:C:H5'	1.99	0.45
11:K:113:ILE:HD12	11:K:128:ALA:HB2	1.98	0.45
30:0:1182:C:H1'	30:0:1192:A:H8	1.82	0.45
9:I:121:LYS:HB3	30:0:1184:C:H4'	1.98	0.45
30:0:2508:C:H2'	30:0:2509:A:O5'	2.17	0.45
23:W:3:ALA:O	23:W:54:PHE:HA	2.16	0.45
30:0:2238:A:O2'	30:0:2239:C:H5'	2.17	0.45
30:0:407:A:O2'	30:0:408:A:H5'	2.17	0.45
30:0:969:G:H1	30:0:999:C:N4	2.15	0.45
30:0:95:A:O5'	30:0:97:G:H5'	2.17	0.45
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.52	0.45
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.52	0.45
1:A:186:TRP:CG	1:A:187:PRO:HA	2.52	0.45
20:T:52:ARG:O	30:0:317:A:OP1	2.33	0.45
14:N:108:SER:HA	14:N:109:PRO:HD3	1.76	0.45
30:0:2493:C:H2'	30:0:2493:C:O2	2.16	0.45
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.97	0.45
9:I:108:HIS:N	9:I:109:PRO:HD2	2.29	0.45
13:M:164:THR:CG2	13:M:165:GLY:N	2.80	0.45
30:0:1391:G:H2'	30:0:1392:A:H5'	1.99	0.45
30:0:1419:U:H2'	30:0:1685:A:C2	2.51	0.45
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.37	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:U:52:THR:HG22	21:U:55:ALA:H	1.81	0.45
3:C:236:THR:HA	38:C:8644:HOH:O	2.16	0.45
3:C:218:VAL:N	38:C:8616:HOH:O	2.48	0.45
21:U:52:THR:CG2	21:U:54:THR:HB	2.47	0.45
30:0:2429:A:H2'	30:0:2430:A:C8	2.52	0.45
5:E:6:GLU:HA	5:E:46:THR:HG22	1.99	0.45
1:A:165:THR:HG22	38:A:9083:HOH:O	2.17	0.45
30:0:1714:C:O2'	30:0:1715:C:H5'	2.17	0.45
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.52	0.45
30:0:2102:G:H1'	30:0:2103:A:N7	2.29	0.45
30:0:2509:A:OP2	30:0:2510:C:H5	2.00	0.45
30:0:2096:A:N7	30:0:2539:U:C4	2.84	0.45
17:Q:49:ASN:HB2	38:Q:5227:HOH:O	2.17	0.45
4:D:23:VAL:HG11	4:D:83:PHE:CZ	2.52	0.45
38:K:7438:HOH:O	21:U:20:MET:HE1	2.16	0.45
30:0:1759:A:N3	30:0:1818:C:H2'	2.32	0.45
30:0:195:C:H5''	38:0:5427:HOH:O	2.17	0.45
30:0:368:C:C2'	30:0:369:G:H5'	2.46	0.44
30:0:1588:G:C5	30:0:1589:G:C6	3.05	0.44
30:0:1198:U:C6	30:0:1200:A:OP2	2.70	0.44
2:B:235:ARG:HD3	30:0:2091:G:O3'	2.16	0.44
16:P:68:LYS:HE2	30:0:1787:C:OP1	2.17	0.44
30:0:2775:A:C6	30:0:2799:A:C8	3.04	0.44
18:R:119:VAL:HG21	18:R:142:ASP:CG	2.37	0.44
14:N:37:ARG:HD2	31:9:6:C:OP1	2.16	0.44
4:D:173:GLU:HA	38:D:6326:HOH:O	2.17	0.44
30:0:2072:G:P	38:0:3107:HOH:O	2.76	0.44
30:0:2425:A:H5'	30:0:2426:G:OP2	2.18	0.44
3:C:118:THR:HG22	3:C:137:PRO:HB3	1.99	0.44
8:H:33:GLN:H	8:H:69:ARG:NH1	2.15	0.44
30:0:2819:C:H2'	30:0:2820:A:C8	2.53	0.44
31:9:105:A:C2'	31:9:106:U:H5'	2.46	0.44
30:0:2038:A:O2'	30:0:2039:A:H5'	2.16	0.44
30:0:638:C:H2'	30:0:639:A:C8	2.52	0.44
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.17	0.44
30:0:2506:A:O2'	30:0:2507:G:P	2.75	0.44
30:0:2064:U:H5'	30:0:2652:U:O3'	2.17	0.44
30:0:1334:C:O2'	30:0:1335:C:H5'	2.17	0.44
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.99	0.44
30:0:1592:G:O2'	30:0:1593:C:O4'	2.27	0.44
30:0:699:C:H2'	30:0:744:G:O4'	2.16	0.44
2:B:154:VAL:HG12	2:B:156:LYS:HG2	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:286:U:H2'	30:0:287:C:C6	2.52	0.44
30:0:2896:A:C2'	30:0:2896:A:N3	2.78	0.44
30:0:319:A:H4'	30:0:338:C:C4	2.53	0.44
11:K:20:CYS:HB2	11:K:29:LEU:HG	2.00	0.44
20:T:52:ARG:HD2	30:0:317:A:H5''	1.98	0.44
30:0:750:A:H2'	30:0:751:U:C6	2.53	0.44
30:0:557:C:C2	30:0:601:G:N2	2.85	0.44
25:Y:142:SER:OG	30:0:1331:G:OP2	2.31	0.44
14:N:171:HIS:CE1	38:N:8860:HOH:O	2.70	0.44
30:0:876:A:N3	30:0:876:A:H2'	2.33	0.44
23:W:115:THR:HG23	38:W:5420:HOH:O	2.16	0.44
30:0:2090:G:H2'	30:0:2091:G:C8	2.53	0.44
25:Y:144:ARG:NH2	38:Y:8913:HOH:O	2.51	0.44
12:L:56:LYS:HE3	30:0:2443:C:O3'	2.16	0.44
20:T:77:VAL:HG11	20:T:91:LEU:HD11	1.98	0.44
31:9:74:G:C6	31:9:75:G:N7	2.85	0.44
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.17	0.44
30:0:1182:C:O2'	30:0:1192:A:H8	1.99	0.44
30:0:2505:G:H2'	30:0:2506:A:C5'	2.48	0.44
30:0:1588:G:C6	30:0:1589:G:N1	2.86	0.44
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.17	0.44
30:0:1819:G:H2'	30:0:1820:G:C5'	2.48	0.44
20:T:2:LYS:HG2	30:0:447:A:OP1	2.17	0.44
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.17	0.44
31:9:65:A:C2'	31:9:66:G:OP2	2.65	0.44
30:0:1790:C:H2'	30:0:1791:U:H6	1.83	0.44
16:P:16:VAL:CG1	16:P:20:ARG:HB2	2.47	0.44
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.33	0.44
30:0:1183:C:H41	30:0:1192:A:P	2.41	0.44
23:W:88:THR:HG22	23:W:89:ASP:N	2.32	0.44
4:D:135:VAL:HG22	4:D:136:ARG:N	2.32	0.44
14:N:71:TRP:HB2	38:N:8837:HOH:O	2.17	0.44
30:0:1471:A:H5'	38:0:3202:HOH:O	2.17	0.44
30:0:366:U:H2'	30:0:367:G:O4'	2.17	0.44
35:0:8813:CL:CL	38:0:4694:HOH:O	2.58	0.44
30:0:1603:A:C5'	30:0:1605:G:O4'	2.59	0.44
31:9:1:U:O3'	31:9:3:A:C5'	2.66	0.44
23:W:52:VAL:HG13	23:W:53:ALA:N	2.32	0.44
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.17	0.44
25:Y:151:SER:HB3	25:Y:154:ARG:HB2	1.99	0.44
30:0:1121:G:H4'	38:0:5565:HOH:O	2.17	0.44
14:N:119:GLN:O	14:N:123:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:496:G:H3'	38:0:7689:HOH:O	2.18	0.44
30:0:1367:A:H2'	30:0:1368:U:O4'	2.18	0.44
22:V:12:THR:HG22	22:V:15:GLU:CG	2.48	0.44
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.01	0.44
30:0:1996:U:H6	30:0:2586:U:O2	2.00	0.44
27:1:17:THR:HG21	30:0:120:A:C5	2.52	0.44
30:0:101:C:H2'	30:0:102:A:H8	1.83	0.44
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.99	0.44
30:0:816:G:H5'	30:0:1598:A:H4'	2.00	0.44
2:B:75:GLU:C	2:B:77:PRO:HD3	2.38	0.44
30:0:1304:U:H2'	30:0:1305:C:C6	2.53	0.44
30:0:2611:U:O2'	30:0:2614:C:OP2	2.32	0.44
30:0:1883:U:H5'	30:0:2012:U:OP2	2.18	0.44
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.76	0.44
30:0:1210:G:O2'	30:0:1211:G:H5'	2.17	0.43
30:0:1211:G:O2'	30:0:1212:C:H5'	2.18	0.43
13:M:95:LYS:HG2	13:M:99:ARG:HB3	2.00	0.43
30:0:2105:C:H2'	30:0:2106:C:C6	2.53	0.43
11:K:75:ARG:HD3	11:K:112:PRO:O	2.18	0.43
30:0:59:A:C5'	38:0:4347:HOH:O	2.64	0.43
20:T:97:ARG:NH2	30:0:308:U:H5'	2.32	0.43
19:S:8:PRO:HD2	22:V:32:ALA:HA	2.00	0.43
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.99	0.43
3:C:49:ASP:HB3	3:C:52:ALA:HB2	1.99	0.43
14:N:116:PHE:HB3	14:N:136:LEU:HD23	2.00	0.43
30:0:2617:G:H2'	30:0:2617:G:N3	2.32	0.43
30:0:2756:U:N3	30:0:2896:A:C2	2.76	0.43
30:0:523:C:H2'	30:0:524:A:C8	2.53	0.43
30:0:445:U:H1'	38:0:7361:HOH:O	2.18	0.43
12:L:50:GLY:C	30:0:2453:G:H4'	2.38	0.43
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.83	0.43
14:N:36:ALA:HB1	14:N:118:ILE:HD12	2.01	0.43
12:L:21:ARG:N	38:L:8826:HOH:O	2.51	0.43
30:0:2369:A:C8	30:0:2371:G:C6	3.06	0.43
30:0:1257:C:H2'	30:0:1258:G:O4'	2.19	0.43
30:0:177:A:H2'	30:0:178:U:O4'	2.18	0.43
31:9:39:U:HO2'	31:9:42:C:H5	1.59	0.43
8:H:59:GLN:NE2	8:H:96:GLN:HG2	2.30	0.43
10:J:132:LEU:HA	10:J:132:LEU:HD23	1.80	0.43
30:0:951:A:H2'	30:0:952:G:H5'	1.99	0.43
30:0:776:A:H1'	30:0:779:U:O4	2.19	0.43
20:T:62:VAL:N	38:T:3851:HOH:O	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1736:A:H1'	38:0:7607:HOH:O	2.18	0.43
30:0:2099:A:N6	30:0:2100:A:N6	2.66	0.43
30:0:542:A:C5'	30:0:542:A:C8	2.96	0.43
11:K:74:VAL:HG13	11:K:113:ILE:HG23	2.00	0.43
3:C:118:THR:CG2	3:C:137:PRO:HB3	2.48	0.43
30:0:1849:G:H1'	30:0:2011:A:N1	2.34	0.43
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.83	0.43
25:Y:208:LYS:O	30:0:1313:A:H5'	2.18	0.43
30:0:305:A:C5	30:0:329:A:C2	3.06	0.43
2:B:82:VAL:HG12	2:B:82:VAL:O	2.18	0.43
2:B:62:ARG:HA	2:B:65:MET:CE	2.48	0.43
5:E:159:VAL:O	5:E:163:GLN:HG2	2.18	0.43
30:0:2004:U:H2'	30:0:2005:G:OP1	2.18	0.43
30:0:960:G:C2'	30:0:961:A:OP2	2.66	0.43
23:W:108:ARG:NH2	23:W:114:PRO:HG2	2.31	0.43
30:0:38:G:N2	38:0:7361:HOH:O	2.50	0.43
8:H:6:ALA:CA	8:H:61:ARG:HH12	2.31	0.43
30:0:1787:C:H4'	30:0:2883:A:O4'	2.19	0.43
30:0:1015:C:H2'	30:0:1016:U:H6	1.84	0.43
31:9:96:C:H2'	31:9:97:U:C6	2.54	0.43
30:0:1940:C:H4'	38:0:7372:HOH:O	2.17	0.43
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.48	0.43
30:0:887:G:H2'	30:0:888:U:C6	2.53	0.43
29:3:3:MET:CG	29:3:4:PRO:HD2	2.49	0.43
30:0:1098:A:H2'	30:0:1099:G:O4'	2.19	0.43
30:0:1183:C:H42	30:0:1184:C:N4	2.16	0.43
30:0:1972:U:C2'	30:0:1973:A:C5'	2.97	0.43
30:0:1377:C:H6	30:0:1377:C:C5'	2.24	0.43
30:0:39:G:H2'	30:0:40:C:O4'	2.19	0.43
30:0:708:A:H2'	30:0:709:G:O4'	2.18	0.43
21:U:20:MET:CG	21:U:28:THR:HG23	2.48	0.43
3:C:104:ASP:HA	3:C:107:ARG:HH12	1.83	0.43
3:C:104:ASP:HA	3:C:107:ARG:NH1	2.34	0.43
30:0:2329:C:O2'	30:0:2330:U:H5'	2.17	0.43
30:0:1871:U:O4'	30:0:1873:G:C8	2.72	0.43
30:0:1179:C:H2'	30:0:1180:U:H6	1.83	0.43
30:0:2004:U:H4'	38:0:5331:HOH:O	2.19	0.43
30:0:1682:A:H2'	38:0:9811:HOH:O	2.19	0.43
24:X:80:GLU:HB3	38:X:5564:HOH:O	2.18	0.43
2:B:286:ASN:O	2:B:306:LYS:HE3	2.18	0.43
31:9:12:C:H5'	31:9:70:U:O4'	2.18	0.43
22:V:43:PRO:O	22:V:46:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:82:VAL:HG13	1:A:93:THR:HB	2.00	0.43
30:0:2460:A:C2	30:0:2461:U:C2	3.06	0.43
30:0:31:C:H4'	38:0:7452:HOH:O	2.19	0.43
30:0:1280:A:H3'	30:0:1280:A:P	2.58	0.43
30:0:1588:G:C6	30:0:1589:G:C6	3.06	0.43
30:0:2321:A:C5	30:0:2323:G:C8	3.06	0.43
12:L:59:GLU:HB3	38:L:8857:HOH:O	2.17	0.43
14:N:26:LEU:HD13	30:0:2415:A:N3	2.33	0.43
3:C:54:LEU:HD23	3:C:79:ARG:HG3	2.01	0.43
30:0:2252:A:H2'	30:0:2253:G:H5'	1.99	0.43
30:0:767:A:H2	30:0:2110:G:N3	2.16	0.43
1:A:164:ARG:NE	38:A:9053:HOH:O	2.47	0.43
6:F:34:ASN:HA	13:M:4:ALA:HB2	2.01	0.43
30:0:2569:A:H2'	30:0:2570:G:O4'	2.19	0.43
12:L:72:ASN:HB2	38:L:8876:HOH:O	2.19	0.43
1:A:33:GLU:CD	1:A:33:GLU:H	2.22	0.43
9:I:86:GLU:CG	30:0:1180:U:H4'	2.43	0.43
3:C:140:VAL:HG12	3:C:141:SER:N	2.33	0.43
31:9:114:G:H2'	31:9:115:C:C6	2.54	0.43
15:O:25:VAL:HG12	30:0:709:G:O2'	2.19	0.43
2:B:199:TYR:CE2	2:B:268:ARG:HB2	2.54	0.43
15:O:96:VAL:CG1	15:O:100:GLN:HB2	2.49	0.43
30:0:2791:U:H1'	30:0:2792:A:H5''	2.00	0.43
30:0:2704:C:H2'	30:0:2705:U:O4'	2.19	0.43
31:9:45:A:C5	31:9:46:C:C4	3.06	0.43
30:0:883:U:H3'	30:0:883:U:O2	2.19	0.43
5:E:11:VAL:HG12	5:E:12:ASP:N	2.33	0.43
30:0:2523:U:O2'	30:0:2524:G:H5'	2.19	0.43
2:B:333:GLU:HB2	21:U:14:GLU:OE2	2.18	0.43
4:D:25:MET:HE1	4:D:37:ALA:O	2.19	0.43
12:L:121:ILE:HG12	12:L:141:GLU:HB2	2.01	0.43
30:0:2456:A:H2'	30:0:2457:U:H6	1.84	0.43
30:0:2787:C:H5	38:0:4644:HOH:O	2.02	0.43
30:0:1482:A:O2'	30:0:1483:C:H5'	2.19	0.43
30:0:398:U:H2'	30:0:399:C:C6	2.54	0.43
17:Q:9:GLY:HA2	38:0:7028:HOH:O	2.19	0.43
30:0:1188:A:H62	30:0:1189:A:N6	2.17	0.42
30:0:2505:G:C2'	30:0:2506:A:C5'	2.94	0.42
18:R:96:VAL:HG13	18:R:106:GLY:HA3	2.00	0.42
30:0:523:C:H2'	30:0:524:A:H8	1.83	0.42
13:M:24:GLN:HA	13:M:24:GLN:NE2	2.34	0.42
11:K:115:ARG:HG3	11:K:116:GLU:N	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2893:C:O2'	30:0:2894:C:H5'	2.19	0.42
23:W:38:THR:HG22	23:W:39:ASP:H	1.83	0.42
2:B:102:THR:CG2	2:B:182:VAL:HG12	2.48	0.42
2:B:198:GLU:HA	38:B:9081:HOH:O	2.18	0.42
18:R:18:LEU:HB2	18:R:143:VAL:HG13	2.01	0.42
9:I:133:THR:HG22	9:I:134:ILE:N	2.34	0.42
30:0:1503:U:H2'	30:0:1504:A:O4'	2.19	0.42
8:H:91:ARG:HG2	8:H:91:ARG:H	1.69	0.42
30:0:2344:G:N3	30:0:2344:G:H2'	2.34	0.42
30:0:2588:OMG:HM23	30:0:2617:G:C2	2.54	0.42
28:2:40:ARG:HG3	28:2:45:ASN:HB2	2.00	0.42
30:0:69:A:C8	30:0:69:A:C5'	2.96	0.42
30:0:1279:U:C5'	30:0:1280:A:OP2	2.68	0.42
30:0:2316:G:OP1	30:0:2317:C:H1'	2.19	0.42
2:B:16:ARG:NH2	38:B:8982:HOH:O	2.49	0.42
30:0:951:A:O2'	30:0:952:G:H5'	2.20	0.42
30:0:1659:A:H2'	30:0:1660:G:O4'	2.18	0.42
30:0:1213:C:O2'	30:0:1214:G:H5'	2.19	0.42
30:0:1249:U:H2'	30:0:1250:C:C6	2.54	0.42
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.84	0.42
30:0:1934:A:C8	30:0:1935:C:C5	3.07	0.42
30:0:2536:C:HO2'	30:0:2537:G:P	2.42	0.42
30:0:1163:G:H2'	30:0:1164:U:H5	1.84	0.42
14:N:37:ARG:HH11	31:9:6:C:H5''	1.71	0.42
22:V:1:THR:HG23	22:V:2:VAL:N	2.24	0.42
4:D:172:VAL:HG12	4:D:173:GLU:N	2.23	0.42
30:0:2486:A:H3'	38:0:4903:HOH:O	2.18	0.42
2:B:102:THR:HG23	2:B:182:VAL:HG12	2.01	0.42
30:0:660:A:H4'	30:0:661:G:O5'	2.20	0.42
30:0:1522:A:H2'	30:0:1523:G:H5'	2.01	0.42
14:N:115:VAL:HG13	38:9:9105:HOH:O	2.19	0.42
4:D:99:ASP:HB3	4:D:103:ASN:H	1.84	0.42
23:W:44:MET:HE2	30:0:944:G:H21	1.83	0.42
16:P:13:VAL:HG11	16:P:40:VAL:HG12	2.00	0.42
30:0:2829:G:O2'	30:0:2830:U:H5'	2.20	0.42
30:0:2540:G:N2	38:0:9380:HOH:O	2.52	0.42
5:E:145:ALA:HB1	5:E:168:ILE:HD11	2.02	0.42
13:M:179:GLY:O	30:0:399:C:H5'	2.19	0.42
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.54	0.42
30:0:2254:G:O2'	30:0:2255:A:H5'	2.19	0.42
30:0:128:A:H3'	30:0:128:A:C8	2.55	0.42
30:0:1183:C:C6	30:0:1192:A:N7	2.87	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:236:THR:H	3:C:239:ALA:HB3	1.85	0.42
16:P:115:SER:OG	16:P:118:GLN:HG3	2.20	0.42
30:0:1701:A:H4'	30:0:1702:U:O5'	2.20	0.42
30:0:2637:A:H5''	38:0:4944:HOH:O	2.18	0.42
30:0:1552:G:N2	30:0:1634:G:C1'	2.80	0.42
23:W:88:THR:HG22	23:W:90:TYR:CD1	2.51	0.42
25:Y:169:ARG:HB2	30:0:1268:C:O2'	2.20	0.42
5:E:101:GLU:HA	5:E:118:ILE:HG13	2.01	0.42
30:0:1099:G:H2'	30:0:1100:G:O4'	2.20	0.42
15:O:44:ASN:OD1	15:O:67:SER:HB2	2.20	0.42
2:B:124:ALA:O	2:B:128:ILE:HG13	2.19	0.42
30:0:867:A:H2	30:0:880:C:O2	2.03	0.42
30:0:1972:U:H2'	30:0:1973:A:H5''	1.99	0.42
6:F:58:GLU:OE1	13:M:27:ARG:NH2	2.45	0.42
30:0:1342:C:H2'	30:0:1343:C:H5'	2.02	0.42
30:0:2645:U:OP2	30:0:2645:U:C6	2.72	0.42
26:Z:56:GLU:O	26:Z:61:HIS:HE1	2.03	0.42
30:0:807:A:N1	30:0:808:A:C2	2.88	0.42
30:0:1842:A:C4	30:0:1979:G:C6	3.06	0.42
2:B:244:PRO:HB3	30:0:1234:U:N3	2.35	0.42
3:C:168:ARG:NH2	3:C:190:ALA:O	2.53	0.42
30:0:1380:U:C4	30:0:2748:G:H1'	2.54	0.42
18:R:106:GLY:HA2	18:R:109:MET:HE3	2.02	0.42
30:0:138:U:OP2	30:0:139:C:H5	2.02	0.42
3:C:87:ARG:NH2	30:0:894:A:C2	2.88	0.42
5:E:84:MET:HE1	5:E:148:ILE:HD12	2.02	0.42
17:Q:11:ARG:HB2	38:0:7028:HOH:O	2.20	0.42
18:R:92:LEU:HD23	18:R:145:LEU:HD21	2.02	0.42
30:0:1042:U:O2'	30:0:1043:C:H5'	2.19	0.42
19:S:33:SER:O	19:S:37:VAL:HG23	2.19	0.42
30:0:1520:G:H2'	30:0:1521:C:C6	2.54	0.42
30:0:812:A:H2'	30:0:813:C:C6	2.54	0.42
7:G:63:ARG:N	38:G:2569:HOH:O	2.52	0.42
30:0:1167:G:N2	30:0:1180:U:C2	2.88	0.42
30:0:1201:C:C2'	30:0:1202:A:H5'	2.49	0.42
30:0:2504:A:H2'	30:0:2505:G:O4'	2.20	0.42
6:F:91:VAL:CG1	6:F:92:GLY:N	2.83	0.42
30:0:2419:U:H5''	30:0:2420:G:H5'	2.02	0.42
8:H:61:ARG:HG3	8:H:61:ARG:NH1	2.34	0.42
30:0:1066:U:H2'	30:0:1067:A:C8	2.54	0.42
31:9:108:C:H2'	31:9:109:G:H8	1.82	0.42
18:R:18:LEU:HD12	18:R:143:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:2356:A:H2'	30:0:2357:G:O4'	2.19	0.42
30:0:1367:A:H2'	30:0:1368:U:H5'	2.02	0.42
25:Y:107:PRO:HD3	25:Y:182:PHE:CE1	2.55	0.42
38:A:9042:HOH:O	30:0:2271:G:H5'	2.20	0.42
13:M:84:LYS:HG3	30:0:171:C:OP2	2.20	0.42
30:0:451:C:O2'	30:0:452:G:H5'	2.19	0.42
31:9:38:A:H2	31:9:43:G:H5''	1.84	0.42
13:M:68:ARG:HD3	13:M:68:ARG:O	2.19	0.42
30:0:1335:C:H2'	30:0:1336:U:H6	1.85	0.42
30:0:1926:G:H2'	30:0:1927:A:C8	2.54	0.42
30:0:2699:A:H2'	30:0:2700:G:O4'	2.19	0.42
12:L:10:SER:O	12:L:11:ARG:HB3	2.19	0.42
30:0:90:A:H2'	30:0:91:G:O4'	2.19	0.42
31:9:80:A:C2	31:9:103:A:C4	3.08	0.42
19:S:43:GLU:HB3	38:S:7106:HOH:O	2.18	0.42
25:Y:203:VAL:HG12	25:Y:228:VAL:HG22	2.02	0.42
30:0:1626:A:H2'	30:0:1627:G:O4'	2.20	0.42
30:0:629:A:H2'	30:0:630:A:O4'	2.20	0.42
30:0:1181:A:C2'	30:0:1182:C:H5'	2.49	0.42
30:0:1189:A:H1'	30:0:1209:C:H1'	2.02	0.42
15:O:32:ARG:HH21	15:O:35:LYS:HZ2	1.68	0.42
27:1:16:HIS:CD2	30:0:470:U:O2'	2.67	0.42
8:H:36:MET:SD	8:H:69:ARG:HD2	2.60	0.42
31:9:107:C:O2'	31:9:108:C:H5'	2.20	0.42
30:0:1103:C:C2	30:0:1241:G:N2	2.88	0.42
30:0:2326:C:H4'	30:0:2412:G:C4'	2.50	0.42
16:P:37:ARG:HD2	30:0:1501:A:OP2	2.20	0.42
15:O:87:THR:O	15:O:91:GLN:HG3	2.19	0.42
30:0:1055:G:N7	38:0:4091:HOH:O	2.51	0.42
30:0:2757:A:H2'	30:0:2758:G:O4'	2.20	0.42
30:0:734:U:O2'	30:0:737:A:N6	2.53	0.42
1:A:217:ARG:HH11	1:A:217:ARG:CG	2.31	0.42
14:N:13:ARG:HA	14:N:13:ARG:HD2	1.89	0.42
30:0:2099:A:N6	30:0:2100:A:H61	2.17	0.41
30:0:1183:C:N3	30:0:1184:C:C5	2.88	0.41
9:I:86:GLU:HA	9:I:87:PRO:HD2	1.94	0.41
30:0:506:G:N2	30:0:509:A:H5''	2.27	0.41
31:9:49:G:C2'	31:9:50:G:H5'	2.50	0.41
30:0:1298:U:H2'	30:0:1299:G:H8	1.85	0.41
30:0:2281:C:C2'	30:0:2282:U:H5'	2.49	0.41
5:E:84:MET:HG2	5:E:168:ILE:HD13	2.02	0.41
30:0:2776:A:H2'	30:0:2777:G:O4'	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1309:U:O2'	30:0:1310:U:H5'	2.20	0.41
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.55	0.41
30:0:1183:C:C5	30:0:1192:A:C8	3.08	0.41
30:0:1641:A:C8	30:0:1702:U:O4	2.73	0.41
31:9:40:C:H2'	31:9:41:C:OP1	2.20	0.41
11:K:101:ASN:O	11:K:102:GLU:HB2	2.20	0.41
10:J:88:PRO:HD3	30:0:1104:C:H4'	2.01	0.41
16:P:16:VAL:CG1	16:P:17:GLY:N	2.83	0.41
30:0:1367:A:C2'	30:0:1368:U:H5'	2.51	0.41
30:0:2011:A:H4'	30:0:2012:U:O5'	2.20	0.41
30:0:1006:A:N1	30:0:2311:A:H1'	2.35	0.41
3:C:76:ARG:HH22	30:0:1363:G:P	2.42	0.41
30:0:607:G:H2'	30:0:608:A:O4'	2.21	0.41
30:0:1878:G:O2'	30:0:1879:U:OP2	2.38	0.41
21:U:17:THR:CG2	21:U:18:GLY:N	2.83	0.41
31:9:31:C:C2	31:9:50:G:N2	2.89	0.41
30:0:537:G:O4'	30:0:538:C:C5	2.73	0.41
30:0:2089:A:C2'	30:0:2090:G:H5'	2.50	0.41
11:K:81:ARG:HB2	11:K:87:ARG:HH11	1.84	0.41
12:L:56:LYS:HE3	30:0:2443:C:H1'	2.02	0.41
30:0:876:A:N3	30:0:876:A:C2'	2.83	0.41
2:B:243:ASN:HA	2:B:244:PRO:C	2.39	0.41
30:0:1980:U:O2'	30:0:1981:A:H5'	2.20	0.41
30:0:1116:U:H3	30:0:1246:A:N6	1.98	0.41
30:0:1552:G:C6	30:0:1553:C:C4	3.08	0.41
30:0:254:C:C2'	30:0:254:C:O2	2.64	0.41
29:3:73:GLU:HB2	38:3:9023:HOH:O	2.20	0.41
25:Y:117:LEU:HB2	25:Y:174:VAL:HG21	2.01	0.41
25:Y:174:VAL:CG2	25:Y:177:LYS:HD2	2.50	0.41
30:0:696:C:C2'	30:0:697:G:H5'	2.51	0.41
30:0:1657:A:H2'	30:0:1658:A:C8	2.55	0.41
30:0:581:G:O2'	30:0:582:U:H5'	2.21	0.41
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.55	0.41
6:F:99:THR:HG23	6:F:99:THR:O	2.20	0.41
5:E:143:GLN:OE1	30:0:2796:U:H1'	2.21	0.41
30:0:969:G:H1	30:0:999:C:H42	1.67	0.41
30:0:1406:A:H5'	30:0:1407:A:C8	2.56	0.41
30:0:1971:G:H5'	38:0:7098:HOH:O	2.20	0.41
30:0:1948:G:H2'	30:0:1949:G:C8	2.55	0.41
31:9:64:C:H2'	31:9:65:A:H5'	2.01	0.41
22:V:7:GLU:O	22:V:11:MET:HG3	2.20	0.41
30:0:80:A:H4'	30:0:81:G:O5'	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:174:LEU:HD21	30:0:1220:U:H4'	2.03	0.41
14:N:44:ARG:NH1	31:9:4:G:H21	2.18	0.41
30:0:2667:G:H1'	30:0:2914:A:N3	2.36	0.41
3:C:19:PRO:HD2	3:C:240:LEU:HD11	2.03	0.41
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.55	0.41
30:0:236:A:H8	30:0:236:A:OP1	2.03	0.41
30:0:1211:G:H2'	30:0:1212:C:C6	2.56	0.41
23:W:146:ILE:HA	23:W:146:ILE:HD13	1.83	0.41
30:0:1116:U:C2	30:0:1246:A:N6	2.88	0.41
30:0:484:A:N1	30:0:506:G:H4'	2.35	0.41
30:0:559:U:H5'	30:0:559:U:C6	2.34	0.41
30:0:204:A:O2'	30:0:205:U:H5'	2.20	0.41
2:B:254:GLN:NE2	38:B:9014:HOH:O	2.52	0.41
30:0:2823:G:H4'	30:0:2827:A:O4'	2.20	0.41
13:M:79:ALA:HB1	30:0:770:C:OP1	2.21	0.41
30:0:612:U:H2'	30:0:613:C:H6	1.86	0.41
30:0:2094:G:O6	30:0:2649:A:H2	2.04	0.41
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.87	0.41
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.20	0.41
30:0:2864:U:O2'	30:0:2865:G:H5'	2.20	0.41
3:C:5:ILE:HD11	3:C:16:VAL:HG13	2.03	0.41
20:T:40:VAL:HG22	20:T:41:ARG:N	2.35	0.41
21:U:6:CYS:HB2	21:U:32:CYS:HB3	2.03	0.41
17:Q:30:VAL:O	17:Q:30:VAL:HG12	2.20	0.41
30:0:2506:A:C2'	30:0:2506:A:O5'	2.68	0.41
1:A:211:LYS:CB	38:0:7455:HOH:O	2.69	0.41
30:0:69:A:C8	30:0:69:A:C3'	3.04	0.41
30:0:2644:C:O2'	30:0:2645:U:O5'	2.37	0.41
13:M:68:ARG:HG3	13:M:73:ARG:HE	1.84	0.41
30:0:1131:G:H4'	31:9:91:C:O4'	2.20	0.41
30:0:1523:G:C6	30:0:1524:U:O4	2.74	0.41
17:Q:75:ILE:CD1	17:Q:84:ILE:HD11	2.51	0.41
13:M:137:ASN:ND2	30:0:145:A:H4'	2.36	0.41
30:0:2600:A:H2'	30:0:2601:A:O4'	2.21	0.41
30:0:503:G:H2'	30:0:504:G:H8	1.84	0.41
20:T:27:LEU:HD23	20:T:98:VAL:HB	2.02	0.41
4:D:138:GLY:N	38:D:7597:HOH:O	2.53	0.41
18:R:114:VAL:HA	18:R:144:GLU:O	2.21	0.41
14:N:32:PRO:HD2	14:N:99:GLU:O	2.21	0.41
30:0:466:A:H2'	30:0:467:G:O4'	2.20	0.41
30:0:2826:G:C5	30:0:2913:A:C6	3.08	0.41
16:P:55:LYS:CG	16:P:56:GLY:N	2.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:107:ASN:HD22	10:J:107:ASN:C	2.24	0.41
30:0:2597:U:H2'	30:0:2598:U:H5'	2.02	0.41
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.89	0.41
12:L:4:LYS:HE2	30:0:645:U:OP2	2.20	0.41
30:0:2388:C:H2'	30:0:2389:U:O4'	2.21	0.41
30:0:1046:G:N3	30:0:1082:A:H2	2.19	0.41
5:E:133:VAL:HG12	5:E:141:VAL:HG13	2.02	0.41
30:0:1206:U:C5'	30:0:1206:U:H6	2.28	0.41
30:0:1165:G:H3'	30:0:1166:A:C5'	2.50	0.41
30:0:2526:C:H5''	38:0:7627:HOH:O	2.20	0.41
4:D:154:LYS:HD2	4:D:154:LYS:N	2.30	0.41
13:M:102:GLU:OE1	13:M:164:THR:HG21	2.20	0.41
30:0:2453:G:H5'	38:0:4702:HOH:O	2.21	0.41
30:0:2644:C:HO2'	30:0:2645:U:P	2.44	0.41
3:C:118:THR:O	3:C:136:VAL:HG13	2.20	0.41
2:B:87:TYR:O	2:B:138:GLY:N	2.47	0.41
30:0:2455:A:H2'	30:0:2456:A:O4'	2.20	0.41
30:0:1592:G:H2'	30:0:1593:C:C6	2.56	0.41
8:H:98:LEU:HD11	8:H:127:ALA:HB2	2.02	0.41
30:0:2061:C:C2'	30:0:2062:A:H5'	2.51	0.41
2:B:81:ALA:HB1	2:B:142:LEU:HD13	2.03	0.41
14:N:23:ARG:O	14:N:27:LEU:HG	2.21	0.41
30:0:1076:G:C2	30:0:1084:C:C2	3.09	0.41
18:R:64:SER:OG	30:0:1369:A:H4'	2.21	0.41
30:0:757:C:H2'	30:0:758:A:C8	2.56	0.41
13:M:91:ILE:HG23	38:M:8953:HOH:O	2.20	0.41
6:F:21:GLU:O	6:F:24:ARG:HG2	2.21	0.41
30:0:1441:G:O2'	30:0:1442:A:H5'	2.21	0.41
30:0:243:A:H61	30:0:269:G:H1'	1.86	0.41
8:H:50:ILE:HG21	38:H:231:HOH:O	2.21	0.41
22:V:1:THR:CG2	22:V:2:VAL:H	2.21	0.41
30:0:2588:OMG:HM23	30:0:2617:G:N2	2.36	0.41
19:S:57:THR:HG22	19:S:58:MET:H	1.84	0.41
30:0:2645:U:H2'	30:0:2645:U:H6	1.62	0.41
15:O:25:VAL:HG13	30:0:709:G:O3'	2.20	0.41
4:D:167:GLU:C	4:D:169:THR:H	2.24	0.41
30:0:1484:G:H2'	38:0:9110:HOH:O	2.20	0.41
30:0:1768:C:H2'	30:0:1769:C:O4'	2.21	0.41
30:0:1816:C:H2'	30:0:1817:U:O4'	2.21	0.41
7:G:67:LEU:O	7:G:71:LEU:HG	2.21	0.41
30:0:2748:G:P	30:0:2749:U:H5''	2.59	0.40
5:E:143:GLN:HE22	30:0:2779:G:H21	1.67	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:9:ASP:HA	18:R:10:PRO:HD2	1.94	0.40
30:0:2831:C:C2'	30:0:2832:C:H5'	2.51	0.40
4:D:40:ILE:HG13	4:D:41:LEU:N	2.36	0.40
30:0:12:U:C2'	30:0:13:G:H5'	2.49	0.40
30:0:304:G:H1'	30:0:347:A:H61	1.86	0.40
30:0:553:G:O4'	30:0:1325:G:H5'	2.21	0.40
30:0:336:G:H5''	38:0:3737:HOH:O	2.21	0.40
30:0:1400:C:H1'	38:0:4150:HOH:O	2.20	0.40
11:K:118:ALA:HA	11:K:125:ALA:HB2	2.03	0.40
18:R:132:ARG:NH2	38:R:8983:HOH:O	2.54	0.40
3:C:185:LYS:HD3	3:C:186:TYR:CE1	2.56	0.40
15:O:53:GLN:HG2	15:O:56:GLU:OE1	2.21	0.40
30:0:2102:G:C2	30:0:2103:A:C4	3.10	0.40
9:I:87:PRO:C	9:I:89:GLU:H	2.23	0.40
1:A:212:PRO:HA	30:0:1943:C:O4'	2.21	0.40
29:3:38:ARG:HB3	29:3:42:ARG:HH12	1.85	0.40
12:L:6:ARG:NH1	30:0:1299:G:N7	2.69	0.40
20:T:2:LYS:HE2	38:0:7433:HOH:O	2.21	0.40
1:A:36:ASP:C	1:A:38:ILE:H	2.21	0.40
15:O:77:ALA:HA	15:O:96:VAL:O	2.20	0.40
30:0:1573:A:H2'	30:0:1574:C:O4'	2.21	0.40
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.89	0.40
30:0:669:G:O2'	30:0:670:G:H5'	2.21	0.40
30:0:2332:A:H5'	30:0:2333:G:OP2	2.20	0.40
30:0:787:G:O2'	30:0:788:A:H5'	2.20	0.40
30:0:1624:A:H4'	30:0:1625:U:H5'	2.03	0.40
30:0:2712:G:P	38:0:5242:HOH:O	2.80	0.40
2:B:16:ARG:NE	38:B:8982:HOH:O	2.46	0.40
25:Y:186:ARG:HG2	25:Y:186:ARG:NH1	2.35	0.40
30:0:2819:C:H2'	30:0:2820:A:H8	1.87	0.40
30:0:2250:G:H2'	30:0:2251:G:O4'	2.20	0.40
30:0:2328:U:C4	30:0:2329:C:C5	3.09	0.40
30:0:1339:G:C6	30:0:1340:G:N1	2.89	0.40
6:F:30:LYS:HD3	6:F:30:LYS:HA	1.88	0.40
16:P:115:SER:HB2	38:P:4299:HOH:O	2.21	0.40
30:0:1476:A:H1'	30:0:1867:G:O2'	2.21	0.40
30:0:2578:G:C8	30:0:2578:G:H5'	2.44	0.40
6:F:57:GLU:O	6:F:61:MET:HG3	2.21	0.40
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.92	0.40
30:0:907:A:H4'	30:0:1328:A:C2	2.57	0.40
30:0:482:G:O4'	30:0:511:A:C2	2.74	0.40
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:1524:U:H3'	38:0:5355:HOH:O	2.21	0.40
30:0:1398:G:H2'	30:0:1399:A:C8	2.56	0.40
23:W:23:MET:O	30:0:1025:C:H5'	2.21	0.40
3:C:84:VAL:O	3:C:85:LYS:HB2	2.22	0.40
30:0:412:C:H2'	30:0:413:G:O4'	2.21	0.40
10:J:90:LYS:HB2	35:J:8802:CL:CL	2.57	0.40
30:0:297:U:H2'	30:0:298:C:C6	2.55	0.40
30:0:2482:G:H4'	30:0:2483:A:C5'	2.52	0.40
30:0:2135:A:O4'	30:0:2243:C:N4	2.55	0.40
30:0:2102:G:HO2'	30:0:2103:A:P	2.44	0.40
30:0:483:C:C4	30:0:484:A:C6	3.10	0.40
18:R:104:PHE:HB3	18:R:109:MET:HE1	2.04	0.40
30:0:1589:G:N2	30:0:1605:G:H1'	2.35	0.40
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.88	0.40
30:0:968:G:C2	30:0:1001:U:O2	2.75	0.40
16:P:83:LYS:HG2	30:0:793:A:H5''	2.03	0.40
30:0:1511:U:O2'	30:0:1512:G:H5'	2.21	0.40
30:0:420:U:H2'	30:0:421:C:C6	2.57	0.40
30:0:1345:A:H2'	30:0:1346:U:C6	2.55	0.40
1:A:1:GLY:HA2	1:A:197:VAL:HG23	2.04	0.40
23:W:73:LEU:HA	23:W:73:LEU:HD12	1.87	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%)	209 (89%)	24 (10%)	2 (1%)	25	41
2	B	335/338 (99%)	315 (94%)	18 (5%)	2 (1%)	33	54
3	C	244/246 (99%)	233 (96%)	11 (4%)	0	100	100
4	D	134/177 (76%)	111 (83%)	20 (15%)	3 (2%)	10	15
5	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
6	F	117/120 (98%)	105 (90%)	11 (9%)	1 (1%)	25	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	149 (96%)	7 (4%)	0	100	100
9	I	68/162 (42%)	55 (81%)	12 (18%)	1 (2%)	15	25
10	J	140/145 (97%)	133 (95%)	5 (4%)	2 (1%)	16	27
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
12	L	141/165 (86%)	124 (88%)	14 (10%)	3 (2%)	11	16
13	M	192/196 (98%)	183 (95%)	9 (5%)	0	100	100
14	N	184/187 (98%)	171 (93%)	8 (4%)	5 (3%)	8	10
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
19	S	79/85 (93%)	77 (98%)	2 (2%)	0	100	100
20	T	117/120 (98%)	113 (97%)	3 (3%)	1 (1%)	25	41
21	U	51/67 (76%)	49 (96%)	2 (4%)	0	100	100
22	V	63/71 (89%)	60 (95%)	3 (5%)	0	100	100
23	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
24	X	80/92 (87%)	76 (95%)	2 (2%)	2 (2%)	9	11
25	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
26	Z	71/116 (61%)	63 (89%)	7 (10%)	1 (1%)	16	27
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	21	34
All	All	3705/4472 (83%)	3486 (94%)	195 (5%)	24 (1%)	33	54

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
10	J	5	GLU
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
1	A	205	GLY

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Mol	Chain	Res	Type
12	L	149	ARG
14	N	167	ASP
12	L	80	ASP
26	Z	105	ARG
2	B	2	GLN
2	B	185	GLY
4	D	56	ARG
20	T	45	GLY
24	X	87	ALA
4	D	137	PRO
10	J	143	LYS
12	L	82	ALA
14	N	162	ASP
4	D	27	ILE
6	F	100	ASP
24	X	70	ILE
29	3	56	PRO
9	I	108	HIS

### 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%)	170 (95%)	9 (5%)	34	56
2	B	282/283 (100%)	268 (95%)	14 (5%)	34	56
3	C	193/193 (100%)	178 (92%)	15 (8%)	18	31
4	D	117/148 (79%)	112 (96%)	5 (4%)	40	64
5	E	152/156 (97%)	147 (97%)	5 (3%)	50	75
6	F	93/94 (99%)	92 (99%)	1 (1%)	84	96
7	G	27/282 (10%)	26 (96%)	1 (4%)	45	71
8	H	134/145 (92%)	129 (96%)	5 (4%)	45	71
9	I	58/130 (45%)	58 (100%)	0	100	100
10	J	118/121 (98%)	111 (94%)	7 (6%)	28	46
11	K	106/106 (100%)	103 (97%)	3 (3%)	56	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	113/127 (89%)	109 (96%)	4 (4%)	48	73
13	M	158/160 (99%)	152 (96%)	6 (4%)	44	70
14	N	149/150 (99%)	145 (97%)	4 (3%)	57	82
15	O	93/94 (99%)	88 (95%)	5 (5%)	31	51
16	P	113/117 (97%)	110 (97%)	3 (3%)	57	82
17	Q	79/80 (99%)	76 (96%)	3 (4%)	44	70
18	R	117/122 (96%)	115 (98%)	2 (2%)	73	92
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	98 (93%)	7 (7%)	23	39
21	U	44/53 (83%)	43 (98%)	1 (2%)	63	86
22	V	51/57 (90%)	50 (98%)	1 (2%)	68	89
23	W	130/130 (100%)	124 (95%)	6 (5%)	37	60
24	X	66/74 (89%)	61 (92%)	5 (8%)	19	33
25	Y	120/196 (61%)	110 (92%)	10 (8%)	16	28
26	Z	60/94 (64%)	58 (97%)	2 (3%)	50	75
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	42 (100%)	0	100	100
29	3	79/79 (100%)	76 (96%)	3 (4%)	44	70
All	All	3095/3646 (85%)	2968 (96%)	127 (4%)	41	66

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	68	ILE
1	A	69	LEU
1	A	94	LEU
1	A	131	HIS
1	A	147	ARG
1	A	184	THR
1	A	206	ARG
1	A	217	ARG
2	B	2	GLN
2	B	5	ARG
2	B	11	LEU
2	B	27	ASN

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Mol	Chain	Res	Type
2	B	51	VAL
2	B	53	LEU
2	B	98	THR
2	B	162	MET
2	B	175	LEU
2	B	190	MET
2	B	254	GLN
2	B	265	LEU
2	B	279	THR
2	B	312	ARG
3	C	2	GLN
3	C	27	ARG
3	C	76	ARG
3	C	78	ARG
3	C	94	THR
3	C	101	ASP
3	C	115	LEU
3	C	136	VAL
3	C	187	ARG
3	C	211	ASP
3	C	214	THR
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	243	VAL
4	D	24	HIS
4	D	36	ASN
4	D	39	ASP
4	D	50	VAL
4	D	149	ARG
5	E	7	ILE
5	E	86	VAL
5	E	102	VAL
5	E	132	THR
5	E	154	ILE
6	F	12	LEU
7	G	73	ASP
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
8	H	173	GLU

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Mol	Chain	Res	Type
10	J	39	VAL
10	J	46	ILE
10	J	52	GLN
10	J	70	PHE
10	J	79	PHE
10	J	107	ASN
10	J	131	THR
11	K	4	LEU
11	K	10	GLN
11	K	55	VAL
12	L	32	ASP
12	L	35	ARG
12	L	43	HIS
12	L	140	VAL
13	M	46	LEU
13	M	68	ARG
13	M	82	ARG
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
14	N	26	LEU
14	N	49	THR
14	N	135	VAL
14	N	163	PHE
15	O	3	THR
15	O	25	VAL
15	O	38	ARG
15	O	43	VAL
15	O	111	VAL
16	P	21	VAL
16	P	91	LYS
16	P	98	ILE
17	Q	11	ARG
17	Q	16	ASN
17	Q	95	GLU
18	R	39	THR
18	R	82	GLU
20	T	39	ASN
20	T	48	VAL
20	T	71	VAL
20	T	73	HIS
20	T	89	ARG

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Mol	Chain	Res	Type
20	T	96	VAL
20	T	115	GLU
21	U	17	THR
22	V	65	ASP
23	W	26	ILE
23	W	52	VAL
23	W	76	ASP
23	W	78	ASP
23	W	142	ASP
23	W	146	ILE
24	X	27	ASP
24	X	72	VAL
24	X	79	GLU
24	X	80	GLU
24	X	82	GLU
25	Y	103	THR
25	Y	108	ASP
25	Y	141	THR
25	Y	163	THR
25	Y	172	THR
25	Y	174	VAL
25	Y	189	ASN
25	Y	200	THR
25	Y	203	VAL
25	Y	235	GLU
26	Z	65	ASN
26	Z	68	GLU
29	3	18	GLN
29	3	56	PRO
29	3	92	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) 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	260	HIS
2	B	320	GLN

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Mol	Chain	Res	Type
2	B	332	ASN
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
3	C	163	HIS
4	D	103	ASN
4	D	133	ASN
5	E	106	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	25	GLN
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	44	HIS
12	L	18	HIS
12	L	41	HIS
12	L	116	HIS
13	M	24	GLN
13	M	58	GLN
13	M	77	HIS
13	M	137	ASN
13	M	170	ASN
14	N	21	HIS
14	N	107	ASN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	16	ASN
17	Q	40	HIS
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
19	S	44	GLN

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Mol	Chain	Res	Type
19	S	51	GLN
19	S	53	ASN
20	T	37	GLN
20	T	39	ASN
21	U	39	ASN
21	U	48	ASN
22	V	60	GLN
23	W	87	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	22	ASN
24	X	23	HIS
25	Y	133	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	15	ASN
29	3	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	242 (8%)	28 (1%)
31	9	121/122 (99%)	17 (14%)	3 (2%)
All	All	2866/3045 (94%)	259 (9%)	31 (1%)

All (259) 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	131	A
30	0	139	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	185	G
30	0	186	A
30	0	191	A
30	0	192	A
30	0	198	A
30	0	200	C
30	0	219	G
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	368	C
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

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Mol	Chain	Res	Type
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	581	G
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	701	U
30	0	702	G
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	868	G
30	0	869	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	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	1087	G
30	0	1088	A
30	0	1100	G
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
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	1207	A
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	1280	A
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1357	A
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1474	C
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A

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Mol	Chain	Res	Type
30	0	1562	C
30	0	1592	G
30	0	1603	A
30	0	1625	U
30	0	1626	A
30	0	1633	C
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	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	1943	C
30	0	1971	G
30	0	1973	A
30	0	1979	G
30	0	1996	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U

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Mol	Chain	Res	Type
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2100	A
30	0	2101	A
30	0	2102	G
30	0	2103	A
30	0	2110	G
30	0	2238	A
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	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	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2533	C
30	0	2537	G
30	0	2539	U
30	0	2540	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C

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Mol	Chain	Res	Type
30	0	2611	U
30	0	2613	G
30	0	2644	C
30	0	2645	U
30	0	2649	A
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2719	A
30	0	2726	U
30	0	2727	A
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	2852	A
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	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	39	U
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G

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Mol	Chain	Res	Type
31	9	77	A
31	9	114	G
31	9	122	C

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	603	A
30	0	644	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1232	A
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1506	U
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1856	C
30	0	1942	A
30	0	1979	G
30	0	2313	C
30	0	2467	A
30	0	2541	U
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2748	G
30	0	2791	U
31	9	43	G
31	9	55	U
31	9	65	A

## 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	0.83	1 (5%)	24,31,34	0.75	0
30	OMG	0	2588	30	24,26,27	0.89	1 (4%)	32,38,41	4.86	3 (9%)
30	UR3	0	2619	30	20,22,23	0.73	0	23,32,35	0.88	0
30	PSU	0	2621	30	19,21,22	1.16	1 (5%)	23,30,33	1.09	2 (8%)
30	1MA	0	628	30,34	23,25,26	0.81	0	32,37,40	0.92	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	0/1/3/3
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	0/1/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	3.00	1.43	1.37
30	0	2587	OMU	P-OP1	2.78	1.49	1.46
30	0	2588	OMG	P-OP1	2.42	1.49	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-C5-N7	-26.91	130.52	134.14
30	0	2588	OMG	C6-N1-C2	3.22	125.15	119.51
30	0	628	1MA	C2-N3-C4	-3.18	110.79	116.23
30	0	2621	PSU	C5-C1'-C2'	-2.32	111.52	115.61
30	0	2588	OMG	C2-N3-C4	-2.18	112.03	115.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	C5-C4-N3	-2.17	114.90	118.86

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%)	0.28	14 (5%) 22 23	20, 40, 77, 100	0
2	B	337/338 (99%)	0.12	4 (1%) 75 78	21, 44, 73, 83	0
3	C	246/246 (100%)	0.10	5 (2%) 62 65	17, 36, 60, 73	0
4	D	140/177 (79%)	1.82	46 (32%) 1 1	48, 89, 116, 126	0
5	E	172/178 (96%)	0.57	9 (5%) 26 27	34, 59, 79, 85	0
6	F	119/120 (99%)	1.01	22 (18%) 2 2	34, 61, 91, 105	0
7	G	29/348 (8%)	2.08	14 (48%) 1 0	70, 87, 96, 98	0
8	H	160/177 (90%)	0.77	20 (12%) 5 4	32, 50, 85, 91	0
9	I	70/162 (43%)	5.34	66 (94%) 0 0	124, 138, 156, 156	0
10	J	142/145 (97%)	0.08	3 (2%) 60 64	27, 41, 63, 89	0
11	K	132/132 (100%)	-0.09	2 (1%) 70 73	23, 39, 63, 72	0
12	L	145/165 (87%)	0.73	17 (11%) 5 5	18, 55, 103, 118	0
13	M	194/196 (98%)	0.21	15 (7%) 13 13	23, 34, 54, 59	0
14	N	186/187 (99%)	0.87	32 (17%) 2 2	34, 52, 104, 112	0
15	O	115/116 (99%)	0.24	2 (1%) 67 70	31, 45, 61, 69	0
16	P	143/149 (95%)	0.00	1 (0%) 84 87	28, 43, 56, 68	0
17	Q	95/96 (98%)	0.01	0 100 100	29, 37, 55, 66	0
18	R	150/155 (96%)	-0.05	0 100 100	23, 36, 57, 71	0
19	S	81/85 (95%)	0.53	9 (11%) 6 6	33, 48, 70, 81	0
20	T	119/120 (99%)	0.34	5 (4%) 35 37	29, 46, 74, 101	0
21	U	53/67 (79%)	0.48	1 (1%) 64 67	33, 46, 65, 74	0
22	V	65/71 (91%)	2.07	21 (32%) 1 1	41, 63, 106, 113	0
23	W	154/154 (100%)	0.14	2 (1%) 74 77	26, 42, 59, 71	0
24	X	82/92 (89%)	0.46	5 (6%) 21 21	34, 49, 77, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/241 (58%)	-0.09	3 (2%) 60 64	19, 34, 58, 80	0
26	Z	73/116 (62%)	1.35	21 (28%) 1 1	36, 55, 72, 89	0
27	1	56/57 (98%)	-0.14	0 100 100	18, 24, 34, 41	0
28	2	46/50 (92%)	0.37	2 (4%) 34 36	25, 49, 74, 86	0
29	3	92/92 (100%)	0.23	0 100 100	27, 45, 60, 74	0
30	0	2754/2923 (94%)	-0.07	98 (3%) 41 43	14, 35, 77, 154	0
31	9	122/122 (100%)	-0.00	5 (4%) 35 38	29, 54, 76, 138	0
All	All	6651/7517 (88%)	0.26	444 (6%) 18 17	14, 41, 89, 156	0

All (444) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	39	ALA	15.3
22	V	1	THR	15.0
4	D	63	ILE	14.3
22	V	40	PRO	12.9
30	0	2101	A	12.0
9	I	74	ILE	11.8
9	I	70	THR	10.8
9	I	97	VAL	10.4
9	I	104	ALA	10.0
30	0	2537	G	9.8
4	D	57	THR	9.6
9	I	128	THR	9.6
14	N	166	ALA	9.5
9	I	127	CYS	9.3
30	0	2102	G	9.3
9	I	103	ILE	9.1
9	I	66	GLY	9.0
30	0	2103	A	8.8
9	I	132	VAL	8.8
9	I	72	GLU	8.7
9	I	80	PHE	8.6
9	I	113	SER	8.5
9	I	111	LEU	8.3
9	I	91	PHE	8.1
26	Z	35	SER	7.9
9	I	120	ALA	7.9
26	Z	46	SER	7.8
9	I	108	HIS	7.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	I	73	LEU	7.5
9	I	116	LEU	7.5
9	I	100	VAL	7.5
9	I	69	PRO	7.3
30	0	1951	G	7.2
9	I	82	THR	7.1
9	I	98	ASP	7.1
9	I	121	LYS	7.1
1	A	37	VAL	6.9
30	0	1199	A	6.9
30	0	1172	G	6.7
7	G	23	ILE	6.6
4	D	90	LEU	6.6
19	S	81	ILE	6.6
30	0	2100	A	6.5
13	M	71	SER	6.5
30	0	2540	G	6.4
9	I	112	LEU	6.4
9	I	133	THR	6.4
30	0	2538	A	6.3
26	Z	45	VAL	6.3
22	V	38	GLY	6.3
9	I	117	THR	6.1
4	D	10	PHE	6.1
4	D	61	PHE	6.0
9	I	71	ALA	6.0
9	I	102	GLN	6.0
9	I	106	GLN	6.0
20	T	119	ALA	6.0
26	Z	49	ARG	5.9
9	I	114	TYR	5.6
30	0	1163	G	5.6
28	2	49	GLU	5.4
30	0	1177	A	5.4
26	Z	34	SER	5.4
30	0	2769	C	5.3
30	0	1948	G	5.3
30	0	1173	A	5.2
30	0	1192	A	5.2
9	I	83	GLY	5.2
30	0	1198	U	5.2
9	I	76	ASP	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	35	GLY	5.2
9	I	123	VAL	5.1
9	I	109	PRO	5.1
30	0	1202	A	5.0
8	H	81	GLY	5.0
30	0	1965	C	5.0
5	E	100	ASP	5.0
30	0	514	G	5.0
9	I	129	SER	4.9
9	I	99	GLN	4.9
9	I	101	LYS	4.9
31	9	1	U	4.8
9	I	118	ASN	4.8
24	X	88	GLU	4.8
7	G	26	MET	4.7
14	N	155	GLU	4.7
30	0	1200	A	4.7
30	0	2539	U	4.7
13	M	70	GLY	4.6
26	Z	58	ASN	4.6
20	T	116	ASP	4.6
1	A	31	LYS	4.6
5	E	45	ASP	4.6
5	E	6	GLU	4.6
4	D	64	ARG	4.6
30	0	2637	A	4.6
26	Z	60	ASP	4.5
9	I	81	GLU	4.5
22	V	32	ALA	4.5
8	H	174	LEU	4.5
30	0	1950	G	4.5
9	I	94	ASP	4.5
20	T	117	ASP	4.5
9	I	92	VAL	4.5
30	0	999	C	4.5
7	G	24	VAL	4.4
30	0	1164	U	4.4
30	0	2645	U	4.4
10	J	70	PHE	4.3
4	D	62	ASP	4.3
7	G	69	ARG	4.2
14	N	147	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
9	I	130	LEU	4.2
30	0	282	C	4.1
22	V	41	GLU	4.1
14	N	165	ALA	4.1
9	I	122	GLU	4.1
26	Z	55	SER	4.1
24	X	80	GLU	4.0
9	I	119	ALA	4.0
30	0	1181	A	4.0
13	M	75	ARG	4.0
4	D	93	LEU	4.0
12	L	75	LEU	4.0
6	F	100	ASP	3.9
30	0	1203	G	3.9
9	I	105	GLU	3.9
30	0	1169	U	3.9
9	I	86	GLU	3.9
30	0	960	G	3.9
30	0	2237	G	3.9
13	M	79	ALA	3.9
30	0	1162	G	3.9
8	H	77	ILE	3.9
8	H	86	TYR	3.9
22	V	46	ILE	3.9
1	A	237	GLY	3.9
30	0	1171	A	3.8
31	9	2	U	3.8
26	Z	38	PHE	3.8
12	L	150	GLN	3.8
4	D	40	ILE	3.8
4	D	170	TYR	3.8
30	0	272	A	3.8
31	9	24	U	3.8
7	G	27	ILE	3.8
9	I	124	VAL	3.7
4	D	166	ILE	3.7
4	D	134	LEU	3.7
4	D	172	VAL	3.7
30	0	1189	A	3.7
30	0	1190	G	3.7
4	D	11	HIS	3.7
14	N	160	SER	3.7

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Mol	Chain	Res	Type	RSRZ
9	I	88	GLN	3.7
30	0	1966	U	3.6
30	0	1197	G	3.6
4	D	92	GLU	3.6
30	0	1170	U	3.6
30	0	2004	U	3.6
12	L	80	ASP	3.6
30	0	970	U	3.6
8	H	76	LEU	3.6
12	L	91	VAL	3.6
9	I	78	ALA	3.5
4	D	56	ARG	3.5
1	A	38	ILE	3.5
6	F	117	GLU	3.5
30	0	497	A	3.5
8	H	40	GLN	3.5
4	D	91	ALA	3.5
4	D	69	ILE	3.5
13	M	80	GLY	3.5
26	Z	36	GLY	3.5
4	D	73	VAL	3.5
22	V	45	ARG	3.5
22	V	2	VAL	3.5
22	V	27	LEU	3.5
14	N	158	LEU	3.4
30	0	1161	A	3.4
30	0	1165	G	3.4
19	S	2	TRP	3.4
4	D	18	ILE	3.4
30	0	1182	C	3.4
30	0	1183	C	3.4
22	V	37	GLY	3.4
26	Z	48	ARG	3.4
12	L	81	VAL	3.4
26	Z	42	TYR	3.4
9	I	125	GLY	3.3
6	F	25	ASP	3.3
30	0	1178	G	3.3
19	S	77	VAL	3.3
4	D	23	VAL	3.3
6	F	110	ASP	3.3
13	M	74	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
30	0	1180	U	3.2
6	F	28	ALA	3.2
26	Z	43	GLY	3.2
9	I	95	LEU	3.2
1	A	85	SER	3.2
19	S	20	PHE	3.2
4	D	66	GLY	3.2
30	0	1186	C	3.2
30	0	1525	G	3.2
9	I	110	ASP	3.2
30	0	1168	C	3.2
30	0	1196	C	3.2
3	C	64	GLY	3.2
7	G	71	LEU	3.2
30	0	2748	G	3.2
21	U	47	ARG	3.2
14	N	175	LEU	3.2
6	F	45	ALA	3.1
22	V	43	PRO	3.1
12	L	97	VAL	3.1
22	V	42	ASN	3.1
4	D	135	VAL	3.1
14	N	81	ALA	3.1
5	E	87	PHE	3.1
6	F	99	THR	3.1
9	I	115	ASP	3.1
30	0	969	G	3.1
30	0	1179	C	3.1
4	D	154	LYS	3.1
14	N	179	LEU	3.1
31	9	23	U	3.1
14	N	159	TYR	3.1
22	V	36	ALA	3.1
14	N	184	ILE	3.0
15	O	23	GLY	3.0
2	B	1	PRO	3.0
30	0	10	U	3.0
4	D	157	LEU	3.0
14	N	180	LEU	3.0
30	0	138	U	3.0
30	0	1947	G	3.0
4	D	171	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
4	D	130	VAL	3.0
26	Z	104	ARG	3.0
9	I	126	THR	3.0
8	H	38	ARG	3.0
5	E	10	ASP	2.9
30	0	1201	C	2.9
14	N	163	PHE	2.9
19	S	78	ALA	2.9
30	0	1166	A	2.9
30	0	1188	A	2.9
8	H	85	ASP	2.9
12	L	101	ASP	2.9
30	0	280	C	2.9
30	0	1176	C	2.9
13	M	87	GLY	2.9
11	K	118	ALA	2.9
14	N	164	ASP	2.9
14	N	183	ASP	2.9
26	Z	44	ARG	2.9
30	0	1625	U	2.9
30	0	1195	G	2.9
12	L	60	GLU	2.9
30	0	1175	G	2.9
14	N	97	VAL	2.9
13	M	86	GLN	2.8
22	V	31	ARG	2.8
1	A	236	GLY	2.8
12	L	147	GLU	2.8
12	L	93	VAL	2.8
9	I	67	VAL	2.8
5	E	118	ILE	2.8
19	S	1	SER	2.8
13	M	194	GLY	2.7
30	0	1967	U	2.7
30	0	1174	A	2.7
16	P	143	ALA	2.7
13	M	78	LYS	2.7
14	N	185	GLU	2.7
4	D	88	LEU	2.7
20	T	118	SER	2.7
6	F	49	PHE	2.7
23	W	86	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
13	M	76	ARG	2.7
4	D	89	PRO	2.7
8	H	141	CYS	2.7
1	A	36	ASP	2.7
9	I	90	ASP	2.7
7	G	25	GLU	2.6
6	F	72	VAL	2.6
4	D	74	THR	2.6
30	O	1929	G	2.6
26	Z	47	ARG	2.6
14	N	182	GLY	2.6
22	V	35	ALA	2.6
30	O	1279	U	2.6
4	D	26	GLY	2.6
3	C	61	PHE	2.6
30	O	2238	A	2.6
15	O	60	VAL	2.6
9	I	93	ALA	2.6
19	S	76	GLU	2.6
1	A	99	ILE	2.6
8	H	35	LYS	2.6
1	A	82	VAL	2.6
7	G	72	ASP	2.6
1	A	97	ALA	2.6
12	L	99	GLU	2.6
30	O	1157	C	2.6
14	N	156	GLU	2.6
24	X	85	VAL	2.6
7	G	66	LEU	2.5
26	Z	50	VAL	2.5
4	D	107	GLY	2.5
26	Z	61	HIS	2.5
19	S	21	GLN	2.5
4	D	44	ILE	2.5
14	N	181	ASP	2.5
14	N	154	LEU	2.5
30	O	1184	C	2.5
6	F	106	ALA	2.5
13	M	1	ALA	2.5
14	N	137	ALA	2.5
12	L	105	TYR	2.5
22	V	3	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
13	M	84	LYS	2.5
25	Y	108	ASP	2.5
30	0	1000	C	2.5
8	H	82	GLU	2.5
9	I	107	LYS	2.5
4	D	85	GLN	2.5
13	M	77	HIS	2.5
30	0	2344	G	2.5
30	0	2345	A	2.5
12	L	77	ALA	2.5
4	D	68	PRO	2.5
30	0	271	C	2.5
22	V	44	GLY	2.5
4	D	17	ARG	2.4
4	D	173	GLU	2.4
6	F	16	ALA	2.4
3	C	62	GLY	2.4
1	A	34	ASP	2.4
28	2	35	ARG	2.4
30	0	2508	C	2.4
2	B	57	GLU	2.4
8	H	144	GLU	2.4
7	G	65	THR	2.4
30	0	284	C	2.4
7	G	12	ILE	2.4
3	C	63	SER	2.4
14	N	153	GLN	2.4
6	F	107	ASP	2.4
25	Y	95	THR	2.4
30	0	1185	U	2.4
8	H	114	ASP	2.4
6	F	22	VAL	2.4
4	D	86	THR	2.4
31	9	122	C	2.4
8	H	73	ASN	2.3
30	0	1167	G	2.3
8	H	80	LEU	2.3
4	D	77	ASP	2.3
10	J	5	GLU	2.3
10	J	4	ALA	2.3
6	F	111	ILE	2.3
30	0	1964	U	2.3

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Mol	Chain	Res	Type	RSRZ
26	Z	51	ALA	2.3
9	I	89	GLU	2.3
20	T	115	GLU	2.3
30	0	1187	U	2.3
14	N	95	ALA	2.3
22	V	30	ALA	2.3
4	D	95	THR	2.3
6	F	26	THR	2.3
30	0	370	G	2.3
30	0	2768	A	2.3
14	N	145	ALA	2.3
2	B	117	GLU	2.3
8	H	70	LEU	2.3
12	L	142	LEU	2.3
30	0	1949	G	2.3
9	I	131	GLY	2.3
22	V	59	ILE	2.3
6	F	98	VAL	2.3
6	F	44	SER	2.3
9	I	84	SER	2.3
14	N	152	GLU	2.3
7	G	22	ALA	2.2
8	H	83	GLU	2.2
14	N	68	GLU	2.2
6	F	119	ARG	2.2
26	Z	57	MET	2.2
30	0	1208	C	2.2
30	0	283	U	2.2
30	0	1970	G	2.2
5	E	124	VAL	2.2
4	D	53	LYS	2.2
9	I	79	GLY	2.2
4	D	128	LEU	2.2
1	A	203	GLY	2.2
6	F	101	ALA	2.2
4	D	104	PHE	2.2
30	0	2511	A	2.2
30	0	2664	A	2.2
25	Y	236	VAL	2.2
5	E	154	ILE	2.2
9	I	68	PRO	2.2
9	I	87	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
6	F	69	GLU	2.2
5	E	89	SER	2.2
19	S	80	ARG	2.2
24	X	77	PHE	2.2
4	D	81	GLU	2.2
26	Z	53	ILE	2.2
8	H	69	ARG	2.1
4	D	75	LEU	2.1
23	W	73	LEU	2.1
2	B	118	ASP	2.1
30	0	1206	U	2.1
9	I	134	ILE	2.1
6	F	118	LEU	2.1
30	0	2289	G	2.1
30	0	285	A	2.1
11	K	27	ARG	2.1
8	H	27	PRO	2.1
14	N	70	GLY	2.1
13	M	83	SER	2.1
6	F	14	ASP	2.1
7	G	21	ASP	2.1
12	L	57	VAL	2.1
14	N	138	ASP	2.1
14	N	157	PRO	2.1
30	0	2747	C	2.1
7	G	67	LEU	2.1
22	V	28	LEU	2.1
9	I	75	LYS	2.0
12	L	121	ILE	2.0
1	A	133	ARG	2.0
12	L	149	ARG	2.0
14	N	134	ASP	2.0
24	X	7	GLU	2.0
4	D	22	VAL	2.0
14	N	148	ALA	2.0
3	C	135	GLU	2.0
8	H	78	LYS	2.0
30	0	735	C	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	1MA	0	628	23/24	0.15	-0.03	20,23,25,25	0
30	UR3	0	2619	21/22	0.14	-0.53	43,48,52,56	0
30	OMU	0	2587	21/22	0.11	-0.57	23,27,29,29	0
30	PSU	0	2621	20/21	0.13	-0.97	29,31,42,42	0
30	OMG	0	2588	24/25	0.11	-2.12	23,29,30,31	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	9007	1/1	1.30	163.44	178,178,178,178	0
36	SR	0	8962	1/1	1.13	128.50	165,165,165,165	0
32	MG	0	8065	1/1	0.85	63.20	68,68,68,68	0
34	NA	0	8555	1/1	0.67	60.02	59,59,59,59	0
36	SR	0	8955	1/1	0.20	56.57	140,140,140,140	0
34	NA	0	8521	1/1	0.57	53.37	70,70,70,70	0
36	SR	0	8949	1/1	0.49	48.62	184,184,184,184	0
32	MG	0	8073	1/1	0.29	47.26	72,72,72,72	0
32	MG	0	8049	1/1	0.48	46.20	78,78,78,78	0
34	NA	0	8567	1/1	0.38	37.36	59,59,59,59	0
34	NA	0	8548	1/1	0.27	34.70	41,41,41,41	0
32	MG	0	8040	1/1	0.36	33.47	81,81,81,81	0
36	SR	0	8902	1/1	0.55	32.32	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
34	NA	0	8562	1/1	0.39	30.34	61,61,61,61	0
34	NA	0	8554	1/1	0.30	29.56	55,55,55,55	0
36	SR	0	8987	1/1	0.70	29.48	199,199,199,199	0
34	NA	0	8561	1/1	0.28	27.28	67,67,67,67	0
36	SR	0	8983	1/1	0.24	27.02	151,151,151,151	0
32	MG	0	8018	1/1	0.23	26.45	13,13,13,13	0
32	MG	0	8030	1/1	0.26	25.72	51,51,51,51	0
34	NA	0	8505	1/1	0.36	25.25	37,37,37,37	0
32	MG	0	8092	1/1	0.18	25.02	53,53,53,53	0
32	MG	0	8038	1/1	0.38	22.30	80,80,80,80	0
32	MG	0	8017	1/1	0.53	21.98	67,67,67,67	0
34	NA	0	8509	1/1	0.15	21.92	60,60,60,60	0
36	SR	0	8994	1/1	0.45	21.92	173,173,173,173	0
34	NA	0	8569	1/1	0.32	21.12	61,61,61,61	0
34	NA	0	8549	1/1	0.37	20.95	73,73,73,73	0
36	SR	0	8991	1/1	0.27	19.94	171,171,171,171	0
32	MG	0	8085	1/1	0.26	18.72	90,90,90,90	0
32	MG	0	8037	1/1	0.29	18.23	77,77,77,77	0
34	NA	0	8552	1/1	0.32	18.16	51,51,51,51	0
34	NA	0	8502	1/1	0.20	18.15	52,52,52,52	0
32	MG	0	8006	1/1	0.27	17.16	1,1,1,1	0
32	MG	0	8044	1/1	0.23	16.25	62,62,62,62	0
34	NA	0	8518	1/1	0.47	15.40	81,81,81,81	0
32	MG	0	8039	1/1	0.28	14.53	42,42,42,42	0
34	NA	0	8575	1/1	0.45	13.65	78,78,78,78	0
34	NA	0	8553	1/1	0.24	13.26	61,61,61,61	0
34	NA	0	8547	1/1	0.24	12.89	49,49,49,49	0
34	NA	0	8530	1/1	0.26	12.14	41,41,41,41	0
36	SR	0	8997	1/1	0.19	12.13	115,115,115,115	0
32	MG	0	8050	1/1	0.51	12.01	63,63,63,63	0
34	NA	0	8558	1/1	0.22	11.73	39,39,39,39	0
32	MG	0	8063	1/1	0.29	11.57	74,74,74,74	0
34	NA	0	8535	1/1	0.23	11.13	55,55,55,55	0
34	NA	0	8563	1/1	0.36	11.11	64,64,64,64	0
36	SR	0	8976	1/1	0.27	10.99	122,122,122,122	0
36	SR	0	8922	1/1	0.51	10.69	164,164,164,164	0
32	MG	0	8032	1/1	0.16	10.68	42,42,42,42	0
32	MG	0	8047	1/1	0.34	10.07	66,66,66,66	0
32	MG	0	8009	1/1	0.27	10.02	1,1,1,1	0
32	MG	0	8028	1/1	0.24	9.85	1,1,1,1	0
36	SR	0	8910	1/1	0.21	9.62	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8996	1/1	0.26	9.36	173,173,173,173	0
36	SR	9	8980	1/1	0.18	9.34	144,144,144,144	0
36	SR	0	8905	1/1	0.22	9.26	43,43,43,43	0
32	MG	0	8041	1/1	0.22	9.23	52,52,52,52	0
34	NA	0	8542	1/1	0.26	8.83	44,44,44,44	0
34	NA	0	8536	1/1	0.12	8.44	62,62,62,62	0
32	MG	0	8076	1/1	0.18	8.43	52,52,52,52	0
32	MG	0	8008	1/1	0.21	8.37	27,27,27,27	0
32	MG	0	8019	1/1	0.20	8.31	18,18,18,18	0
34	NA	0	8559	1/1	0.18	8.24	67,67,67,67	0
34	NA	0	8511	1/1	0.18	7.81	61,61,61,61	0
36	SR	0	8971	1/1	0.15	7.80	153,153,153,153	0
32	MG	0	8071	1/1	0.24	7.75	73,73,73,73	0
36	SR	0	8918	1/1	0.19	7.70	45,45,45,45	0
32	MG	0	8012	1/1	0.19	7.42	4,4,4,4	0
32	MG	9	8074	1/1	0.26	7.36	42,42,42,42	0
36	SR	0	8989	1/1	0.24	7.14	149,149,149,149	0
34	NA	0	8524	1/1	0.19	6.92	27,27,27,27	0
32	MG	0	8079	1/1	0.23	6.86	52,52,52,52	0
32	MG	0	8045	1/1	0.23	6.72	40,40,40,40	0
34	NA	0	8516	1/1	0.24	6.71	50,50,50,50	0
32	MG	0	8048	1/1	0.22	6.68	55,55,55,55	0
32	MG	0	8081	1/1	0.18	6.62	65,65,65,65	0
36	SR	0	8957	1/1	0.28	6.60	149,149,149,149	0
32	MG	0	8062	1/1	0.26	6.55	46,46,46,46	0
34	NA	0	8571	1/1	0.21	6.51	83,83,83,83	0
32	MG	0	8055	1/1	0.21	6.46	12,12,12,12	0
36	SR	0	8974	1/1	0.26	6.11	119,119,119,119	0
36	SR	0	8903	1/1	0.15	5.89	36,36,36,36	0
32	MG	0	8014	1/1	0.19	5.56	23,23,23,23	0
32	MG	0	8066	1/1	0.23	5.51	67,67,67,67	0
32	MG	0	8068	1/1	0.15	5.33	50,50,50,50	0
34	NA	0	8564	1/1	0.17	5.27	49,49,49,49	0
32	MG	0	8004	1/1	0.17	5.24	13,13,13,13	0
34	NA	0	8574	1/1	0.23	5.22	47,47,47,47	0
32	MG	0	8007	1/1	0.20	5.19	53,53,53,53	0
32	MG	0	8078	1/1	0.20	5.18	52,52,52,52	0
36	SR	0	9002	1/1	0.21	4.71	141,141,141,141	0
34	NA	0	8508	1/1	0.17	4.62	36,36,36,36	0
32	MG	0	8093	1/1	0.15	4.55	29,29,29,29	0
32	MG	0	8061	1/1	0.21	4.38	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
36	SR	0	8938	1/1	0.19	4.31	102,102,102,102	0
34	NA	0	8566	1/1	0.20	3.95	37,37,37,37	0
34	NA	0	8520	1/1	0.23	3.94	49,49,49,49	0
32	MG	A	8051	1/1	0.30	3.92	51,51,51,51	0
36	SR	0	8907	1/1	0.18	3.79	50,50,50,50	0
36	SR	9	8968	1/1	0.13	3.73	96,96,96,96	0
34	NA	0	8517	1/1	0.31	3.69	68,68,68,68	0
32	MG	0	8015	1/1	0.16	3.61	50,50,50,50	0
34	NA	0	8528	1/1	0.18	3.56	67,67,67,67	0
34	NA	0	8560	1/1	0.28	3.46	67,67,67,67	0
34	NA	0	8504	1/1	0.17	3.37	34,34,34,34	0
35	CL	B	8819	1/1	0.20	3.35	57,57,57,57	0
36	SR	0	8926	1/1	0.15	3.25	69,69,69,69	0
34	NA	0	8525	1/1	0.15	3.11	57,57,57,57	0
36	SR	0	8979	1/1	0.19	3.00	193,193,193,193	0
34	NA	0	8546	1/1	0.28	2.83	51,51,51,51	0
36	SR	0	9000	1/1	0.15	2.57	125,125,125,125	0
34	NA	0	8507	1/1	0.15	2.52	19,19,19,19	0
34	NA	0	8545	1/1	0.17	2.49	40,40,40,40	0
32	MG	0	8056	1/1	0.14	2.37	66,66,66,66	0
34	NA	0	8573	1/1	0.16	2.27	69,69,69,69	0
34	NA	0	8556	1/1	0.33	2.23	38,38,38,38	0
32	MG	B	8042	1/1	0.17	2.14	75,75,75,75	0
36	SR	0	8927	1/1	0.14	2.05	58,58,58,58	0
32	MG	0	8080	1/1	0.14	1.90	54,54,54,54	0
34	NA	0	8512	1/1	0.41	1.85	63,63,63,63	0
32	MG	0	8064	1/1	0.14	1.69	54,54,54,54	0
32	MG	0	8067	1/1	0.45	1.64	55,55,55,55	0
34	NA	0	8523	1/1	0.15	1.61	48,48,48,48	0
34	NA	0	8533	1/1	0.18	1.43	57,57,57,57	0
34	NA	0	8514	1/1	0.19	1.40	34,34,34,34	0
36	SR	0	8919	1/1	0.15	1.12	167,167,167,167	0
32	MG	0	8035	1/1	0.12	1.07	63,63,63,63	0
37	CD	Z	8703	1/1	0.20	1.05	67,67,67,67	0
36	SR	0	8914	1/1	0.17	0.91	67,67,67,67	0
33	K	0	8401	1/1	0.35	0.90	97,97,97,97	0
32	MG	0	8025	1/1	0.14	0.86	40,40,40,40	0
35	CL	0	8816	1/1	0.16	0.77	49,49,49,49	0
36	SR	0	8969	1/1	0.15	0.73	115,115,115,115	0
32	MG	0	8011	1/1	0.18	0.70	26,26,26,26	0
34	NA	0	8541	1/1	0.16	0.70	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8901	1/1	0.14	0.66	35,35,35,35	0
36	SR	0	8985	1/1	0.17	0.63	98,98,98,98	0
36	SR	0	8921	1/1	0.12	0.61	46,46,46,46	0
32	MG	0	8003	1/1	0.14	0.58	24,24,24,24	0
34	NA	9	8572	1/1	0.15	0.57	66,66,66,66	0
32	MG	0	8020	1/1	0.14	0.57	22,22,22,22	0
37	CD	U	8701	1/1	0.17	0.47	62,62,62,62	0
34	NA	0	8522	1/1	0.14	0.44	52,52,52,52	0
36	SR	0	9004	1/1	0.47	0.44	182,182,182,182	0
33	K	0	8402	1/1	0.19	0.34	77,77,77,77	0
36	SR	0	8906	1/1	0.17	0.31	50,50,50,50	0
36	SR	0	8982	1/1	0.12	0.30	116,116,116,116	0
36	SR	0	8947	1/1	0.16	0.29	73,73,73,73	0
34	NA	0	8570	1/1	0.13	0.29	35,35,35,35	0
37	CD	1	8702	1/1	0.13	0.22	54,54,54,54	0
32	MG	0	8082	1/1	0.28	0.18	63,63,63,63	0
32	MG	0	8084	1/1	0.14	0.03	59,59,59,59	0
34	NA	0	8534	1/1	0.23	0.02	56,56,56,56	0
36	SR	0	8908	1/1	0.12	0.00	46,46,46,46	0
36	SR	0	8986	1/1	0.17	-0.00	136,136,136,136	0
36	SR	0	8965	1/1	0.12	0.00	80,80,80,80	0
36	SR	0	8981	1/1	0.14	-0.02	115,115,115,115	0
34	NA	C	8503	1/1	0.15	-0.08	19,19,19,19	0
32	MG	0	8036	1/1	0.12	-0.10	37,37,37,37	0
32	MG	0	8001	1/1	0.16	-0.10	9,9,9,9	0
36	SR	0	8972	1/1	0.16	-0.25	121,121,121,121	0
32	MG	0	8016	1/1	0.24	-0.25	75,75,75,75	0
36	SR	0	8944	1/1	0.14	-0.26	117,117,117,117	0
36	SR	0	8925	1/1	0.11	-0.27	55,55,55,55	0
34	NA	0	8550	1/1	0.16	-0.28	37,37,37,37	0
36	SR	0	8995	1/1	0.15	-0.35	94,94,94,94	0
36	SR	0	8992	1/1	0.12	-0.40	108,108,108,108	0
35	CL	J	8821	1/1	0.15	-0.41	52,52,52,52	0
32	MG	0	8058	1/1	0.14	-0.43	3,3,3,3	0
35	CL	0	8803	1/1	0.12	-0.48	38,38,38,38	0
32	MG	0	8022	1/1	0.12	-0.53	7,7,7,7	0
34	NA	0	8515	1/1	0.14	-0.56	28,28,28,28	0
37	CD	3	8704	1/1	0.14	-0.56	63,63,63,63	0
34	NA	J	8538	1/1	0.13	-0.57	47,47,47,47	0
32	MG	0	8005	1/1	0.15	-0.57	29,29,29,29	0
36	SR	A	8977	1/1	0.14	-0.59	88,88,88,88	0
36	SR	0	8956	1/1	0.12	-0.59	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8568	1/1	0.15	-0.61	33,33,33,33	0
35	CL	0	8822	1/1	0.13	-0.68	46,46,46,46	0
34	NA	0	8551	1/1	0.12	-0.73	40,40,40,40	0
36	SR	0	8909	1/1	0.11	-0.82	44,44,44,44	0
32	MG	0	8053	1/1	0.13	-0.83	45,45,45,45	0
34	NA	0	8513	1/1	0.14	-0.84	32,32,32,32	0
34	NA	R	8532	1/1	0.13	-0.89	32,32,32,32	0
36	SR	0	8954	1/1	0.10	-0.91	60,60,60,60	0
32	MG	T	8057	1/1	0.17	-0.92	32,32,32,32	0
34	NA	M	8539	1/1	0.11	-0.96	34,34,34,34	0
36	SR	0	8993	1/1	0.07	-1.01	154,154,154,154	0
32	MG	0	8026	1/1	0.11	-1.05	44,44,44,44	0
36	SR	A	8930	1/1	0.10	-1.08	57,57,57,57	0
32	MG	0	8002	1/1	0.15	-1.09	33,33,33,33	0
32	MG	0	8010	1/1	0.27	-1.10	69,69,69,69	0
36	SR	0	8960	1/1	0.09	-1.11	100,100,100,100	0
36	SR	R	8912	1/1	0.12	-1.13	55,55,55,55	0
36	SR	0	8998	1/1	0.13	-1.14	99,99,99,99	0
32	MG	0	8069	1/1	0.18	-1.24	75,75,75,75	0
32	MG	0	8070	1/1	0.11	-1.28	50,50,50,50	0
36	SR	0	8963	1/1	0.13	-1.33	135,135,135,135	0
36	SR	F	9005	1/1	0.11	-1.34	77,77,77,77	0
36	SR	0	8942	1/1	0.09	-1.46	55,55,55,55	0
35	CL	O	8808	1/1	0.09	-1.49	52,52,52,52	0
36	SR	0	8924	1/1	0.09	-1.50	50,50,50,50	0
36	SR	0	8911	1/1	0.10	-1.51	48,48,48,48	0
36	SR	0	9001	1/1	0.09	-1.57	142,142,142,142	0
34	NA	9	8543	1/1	0.15	-1.60	60,60,60,60	0
34	NA	Q	8540	1/1	0.08	-1.65	39,39,39,39	0
34	NA	0	8506	1/1	0.10	-1.68	44,44,44,44	0
32	MG	0	8043	1/1	0.10	-1.71	51,51,51,51	0
35	CL	J	8801	1/1	0.08	-1.72	42,42,42,42	0
35	CL	0	8812	1/1	0.09	-1.72	43,43,43,43	0
32	MG	0	8023	1/1	0.10	-1.73	30,30,30,30	0
36	SR	A	8929	1/1	0.08	-1.75	78,78,78,78	0
34	NA	0	8544	1/1	0.10	-1.80	53,53,53,53	0
35	CL	L	8810	1/1	0.13	-1.81	43,43,43,43	0
32	MG	0	8013	1/1	0.10	-1.83	41,41,41,41	0
32	MG	0	8060	1/1	0.08	-1.88	41,41,41,41	0
32	MG	0	8075	1/1	0.10	-1.92	37,37,37,37	0
35	CL	0	8811	1/1	0.11	-1.93	54,54,54,54	0
34	NA	0	8557	1/1	0.10	-2.01	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	1	8913	1/1	0.10	-2.02	32,32,32,32	0
36	SR	0	8946	1/1	0.13	-2.04	75,75,75,75	0
36	SR	0	8940	1/1	0.09	-2.08	62,62,62,62	0
35	CL	N	8807	1/1	0.10	-2.14	43,43,43,43	0
34	NA	0	8529	1/1	0.06	-2.15	29,29,29,29	0
32	MG	Y	8086	1/1	0.10	-2.16	30,30,30,30	0
34	NA	0	8565	1/1	0.09	-2.17	39,39,39,39	0
36	SR	0	8959	1/1	0.08	-2.28	129,129,129,129	0
32	MG	0	8090	1/1	0.10	-2.29	51,51,51,51	0
36	SR	S	8961	1/1	0.09	-2.39	98,98,98,98	0
35	CL	A	8809	1/1	0.12	-2.41	51,51,51,51	0
36	SR	3	8999	1/1	0.10	-2.45	63,63,63,63	0
36	SR	B	8950	1/1	0.10	-2.62	83,83,83,83	0
35	CL	J	8802	1/1	0.07	-2.63	49,49,49,49	0
36	SR	0	8915	1/1	0.09	-2.67	58,58,58,58	0
32	MG	0	8052	1/1	0.09	-2.72	29,29,29,29	0
36	SR	0	8917	1/1	0.12	-2.76	46,46,46,46	0
36	SR	0	8975	1/1	0.06	-2.79	114,114,114,114	0
36	SR	1	8952	1/1	0.11	-2.80	47,47,47,47	0
34	NA	T	8537	1/1	0.08	-2.83	26,26,26,26	0
36	SR	0	8966	1/1	0.09	-2.92	68,68,68,68	0
34	NA	0	8526	1/1	0.08	-2.99	43,43,43,43	0
36	SR	0	8943	1/1	0.06	-3.01	49,49,49,49	0
32	MG	0	8077	1/1	0.07	-3.04	34,34,34,34	0
32	MG	0	8031	1/1	0.08	-3.05	39,39,39,39	0
32	MG	0	8087	1/1	0.09	-3.06	33,33,33,33	0
32	MG	0	8072	1/1	0.10	-3.16	36,36,36,36	0
34	NA	S	8510	1/1	0.06	-3.20	32,32,32,32	0
32	MG	K	8054	1/1	0.09	-3.24	20,20,20,20	0
32	MG	0	8021	1/1	0.09	-3.42	24,24,24,24	0
36	SR	0	8964	1/1	0.07	-3.48	76,76,76,76	0
36	SR	0	8967	1/1	0.09	-3.56	86,86,86,86	0
35	CL	Y	8820	1/1	0.04	-3.61	27,27,27,27	0
32	MG	0	8083	1/1	0.05	-3.63	35,35,35,35	0
36	SR	0	8945	1/1	0.08	-3.67	71,71,71,71	0
35	CL	0	8817	1/1	0.09	-3.75	33,33,33,33	0
36	SR	0	9008	1/1	0.09	-3.85	59,59,59,59	0
35	CL	M	8818	1/1	0.08	-4.01	22,22,22,22	0
36	SR	0	8951	1/1	0.07	-4.06	99,99,99,99	0
36	SR	0	8973	1/1	0.09	-4.12	79,79,79,79	0
36	SR	0	8935	1/1	0.07	-4.17	54,54,54,54	0
36	SR	0	8953	1/1	0.06	-4.21	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8916	1/1	0.08	-4.24	45,45,45,45	0
36	SR	9	9003	1/1	0.06	-4.42	122,122,122,122	0
36	SR	3	8932	1/1	0.07	-4.52	65,65,65,65	0
34	NA	0	8527	1/1	0.11	-4.67	35,35,35,35	0
36	SR	0	8939	1/1	0.09	-4.68	62,62,62,62	0
35	CL	3	8804	1/1	0.05	-4.75	48,48,48,48	0
32	MG	0	8034	1/1	0.07	-4.92	25,25,25,25	0
36	SR	0	8941	1/1	0.10	-5.01	60,60,60,60	0
35	CL	0	8805	1/1	0.06	-5.16	39,39,39,39	0
36	SR	0	8970	1/1	0.09	-5.31	73,73,73,73	0
36	SR	0	8948	1/1	0.09	-5.33	57,57,57,57	0
32	MG	0	8027	1/1	0.06	-5.47	36,36,36,36	0
32	MG	0	8091	1/1	0.11	-5.50	50,50,50,50	0
32	MG	0	8046	1/1	0.10	-5.54	1,1,1,1	0
36	SR	0	8936	1/1	0.09	-5.72	44,44,44,44	0
36	SR	0	8937	1/1	0.11	-6.02	53,53,53,53	0
36	SR	0	8931	1/1	0.08	-6.24	61,61,61,61	0
35	CL	0	8815	1/1	0.07	-6.35	38,38,38,38	0
32	MG	0	8029	1/1	0.09	-6.46	35,35,35,35	0
36	SR	0	8934	1/1	0.07	-6.68	52,52,52,52	0
36	SR	0	8958	1/1	0.08	-6.88	57,57,57,57	0
35	CL	0	8814	1/1	0.06	-7.01	35,35,35,35	0
36	SR	0	8984	1/1	0.07	-7.51	75,75,75,75	0
35	CL	R	8806	1/1	0.08	-7.71	28,28,28,28	0
32	MG	0	8088	1/1	0.06	-7.75	25,25,25,25	0
36	SR	0	8978	1/1	0.08	-7.77	47,47,47,47	0
34	NA	0	8501	1/1	0.07	-7.91	30,30,30,30	0
32	MG	0	8059	1/1	0.09	-7.94	31,31,31,31	0
36	SR	0	8988	1/1	0.11	-8.25	110,110,110,110	0
37	CD	O	8705	1/1	0.04	-8.42	88,88,88,88	0
32	MG	0	8033	1/1	0.07	-8.55	45,45,45,45	0
34	NA	0	8519	1/1	0.07	-8.73	29,29,29,29	0
36	SR	0	8904	1/1	0.05	-8.78	20,20,20,20	0
36	SR	0	8928	1/1	0.07	-9.18	67,67,67,67	0
35	CL	0	8813	1/1	0.06	-9.26	34,34,34,34	0
32	MG	0	8024	1/1	0.13	-9.72	45,45,45,45	0
36	SR	0	8920	1/1	0.06	-9.89	63,63,63,63	0
36	SR	0	8923	1/1	0.08	-10.89	54,54,54,54	0
36	SR	0	8933	1/1	0.05	-12.30	54,54,54,54	0
34	NA	0	8531	1/1	0.06	-12.79	17,17,17,17	0
36	SR	0	8990	1/1	0.12	-12.83	132,132,132,132	0
32	MG	0	8089	1/1	0.12	-59.00	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	9006	1/1	0.43	-	199,199,199,199	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.