



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:42 PM GMT

PDB ID : 1VQO  
Title : The structure of CCPMN bound to the large ribosomal subunit haloarcula marismortui  
Authors : Schmeing, T.M.; Steitz, T.A.  
Deposited on : 2004-12-16  
Resolution : 2.20 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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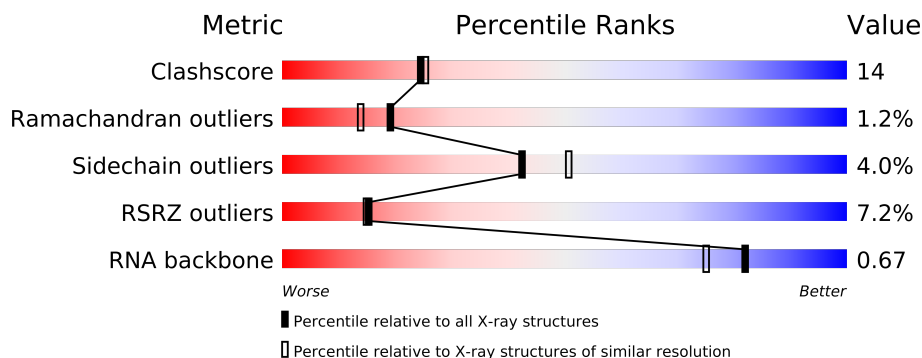
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)
RNA backbone	1838	1120 (3.00-1.40)

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	0	2922	
2	9	122	
3	4	3	
4	A	240	
5	B	338	
6	C	246	
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	

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Mol	Chain	Length	Quality of chain
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	
31	3	92	
32	I	162	

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

Mol	Type	Chain	Res	Geometry	Electron density
33	MG	0	8001	-	X
33	MG	0	8002	-	X
33	MG	0	8008	-	X
33	MG	0	8012	-	X
33	MG	0	8013	-	X
33	MG	0	8014	-	X
33	MG	0	8017	-	X
33	MG	0	8021	-	X
33	MG	0	8022	-	X
33	MG	0	8024	-	X
33	MG	0	8025	-	X
33	MG	0	8026	-	X
33	MG	0	8027	-	X
33	MG	0	8029	-	X
33	MG	0	8038	-	X
33	MG	0	8040	-	X
33	MG	0	8041	-	X
33	MG	0	8045	-	X
33	MG	0	8047	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
33	MG	0	8051	-	X
33	MG	0	8052	-	X
33	MG	0	8056	-	X
33	MG	0	8057	-	X
33	MG	0	8058	-	X
33	MG	0	8059	-	X
33	MG	0	8060	-	X
33	MG	0	8061	-	X
33	MG	0	8065	-	X
33	MG	0	8072	-	X
33	MG	0	8082	-	X
33	MG	0	8084	-	X
33	MG	0	8085	-	X
33	MG	0	8089	-	X
33	MG	0	8090	-	X
33	MG	0	8092	-	X
33	MG	0	8094	-	X
33	MG	0	8101	-	X
33	MG	0	8103	-	X
33	MG	0	8107	-	X
33	MG	0	8108	-	X
33	MG	0	8114	-	X
33	MG	0	8118	-	X
33	MG	9	8095	-	X
33	MG	A	8066	-	X
33	MG	B	8055	-	X
33	MG	K	8069	-	X
34	K	0	9001	-	X
35	NA	0	9101	-	X
35	NA	0	9102	-	X
35	NA	0	9106	-	X
35	NA	0	9107	-	X
35	NA	0	9111	-	X
35	NA	0	9116	-	X
35	NA	0	9118	-	X
35	NA	0	9120	-	X
35	NA	0	9122	-	X
35	NA	0	9125	-	X
35	NA	0	9129	-	X
35	NA	0	9132	-	X
35	NA	0	9141	-	X
35	NA	0	9149	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	NA	0	9152	-	X
35	NA	0	9154	-	X
35	NA	0	9155	-	X
35	NA	0	9156	-	X
35	NA	0	9157	-	X
35	NA	0	9158	-	X
35	NA	0	9163	-	X
35	NA	0	9164	-	X
35	NA	0	9165	-	X
35	NA	0	9169	-	X
35	NA	0	9170	-	X
35	NA	0	9171	-	X
35	NA	0	9172	-	X
35	NA	0	9173	-	X
35	NA	0	9175	-	X
35	NA	0	9177	-	X
35	NA	0	9178	-	X
35	NA	0	9179	-	X
35	NA	0	9182	-	X
35	NA	0	9184	-	X
35	NA	0	9185	-	X
35	NA	9	9183	-	X
35	NA	B	9161	-	X
35	NA	R	9186	-	X
36	CL	0	9316	-	X
36	CL	0	9322	-	X
37	SR	0	9405	-	X
37	SR	0	9406	-	X
37	SR	0	9408	-	X
37	SR	0	9432	-	X
37	SR	0	9452	-	X
37	SR	0	9474	-	X
37	SR	0	9482	-	X
37	SR	0	9500	-	X
37	SR	0	9501	-	X
37	SR	0	9539	-	X
37	SR	0	9547	-	X
37	SR	0	9601	-	X
37	SR	0	9626	-	X
37	SR	B	9521	-	X

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99040 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 RNA chain called 23S ribosomal rna.

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

There are 5 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	88	Total	Mg	0	0
			88	88		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	64	Total Na 64 64	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	D	1	Total Na 1 1	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	9	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	3	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	98	Total 98	Sr 98	0	0
37	1	2	Total 2	Sr 2	0	0
37	H	1	Total 1	Sr 1	0	0
37	B	2	Total 2	Sr 2	0	0
37	3	1	Total 1	Sr 1	0	0
37	A	3	Total 3	Sr 3	0	0
37	R	1	Total 1	Sr 1	0	0
37	9	3	Total 3	Sr 3	0	0
37	L	1	Total 1	Sr 1	0	0
37	S	1	Total 1	Sr 1	0	0
37	F	1	Total 1	Sr 1	0	0

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5780	Total	O	0	0
			5780	5780		
39	9	136	Total	O	0	0
			136	136		
39	4	4	Total	O	0	0
			4	4		
39	A	124	Total	O	0	0
			124	124		
39	B	141	Total	O	0	0
			141	141		
39	C	177	Total	O	0	0
			177	177		
39	D	46	Total	O	0	0
			46	46		
39	E	43	Total	O	0	0
			43	43		
39	F	25	Total	O	0	0
			25	25		
39	G	16	Total	O	0	0
			16	16		
39	H	71	Total	O	0	0
			71	71		
39	J	58	Total	O	0	0
			58	58		
39	K	60	Total	O	0	0
			60	60		
39	L	82	Total	O	0	0
			82	82		
39	M	125	Total	O	0	0
			125	125		
39	N	62	Total	O	0	0
			62	62		
39	O	40	Total	O	0	0
			40	40		
39	P	60	Total	O	0	0
			60	60		

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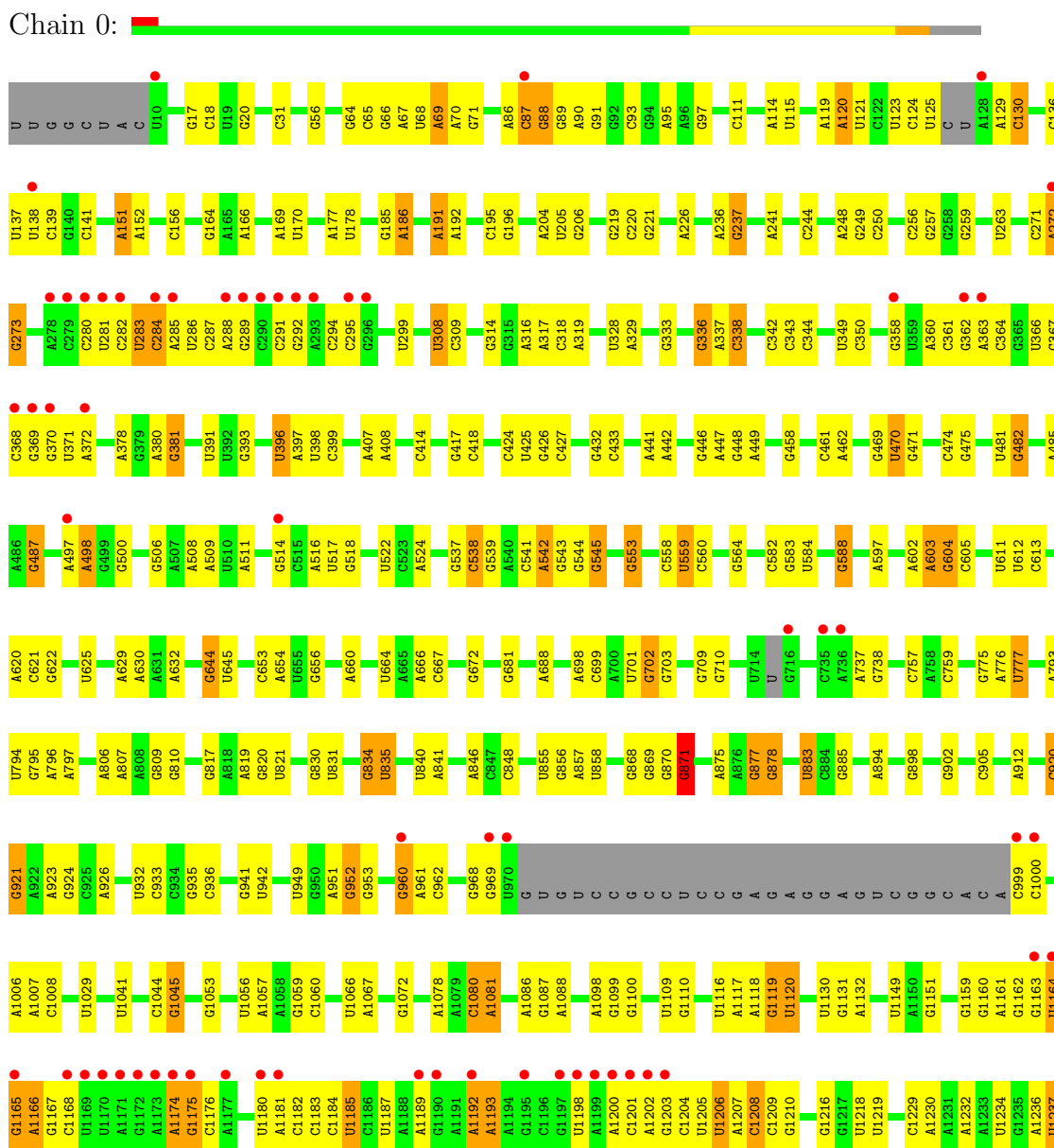
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	Q	49	Total 49	O 49	0	0
39	R	83	Total 83	O 83	0	0
39	S	30	Total 30	O 30	0	0
39	T	36	Total 36	O 36	0	0
39	U	28	Total 28	O 28	0	0
39	V	12	Total 12	O 12	0	0
39	W	68	Total 68	O 68	0	0
39	X	26	Total 26	O 26	0	0
39	Y	93	Total 93	O 93	0	0
39	Z	29	Total 29	O 29	0	0
39	1	52	Total 52	O 52	0	0
39	2	40	Total 40	O 40	0	0
39	3	66	Total 66	O 66	0	0
39	I	8	Total 8	O 8	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.

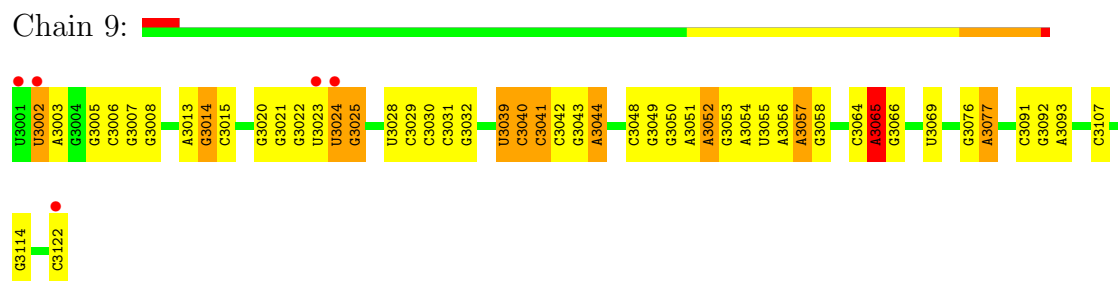
- Molecule 1: 23S ribosomal rna





C2857	U2858	C2761	C2762	C2765	U2531	C2644	U2645	A2649	U2652	C2536	U2661	G2662	U2663	A2664	A	U	C2549	G2462	A2465	U2466	A2467	A2468	U2469	C2472	C2476	A2568	U2569	G2578	A2481	G2482	U2483	U2484	A2485	A2490	U2491	U2492	C2493	C2399	A2600	U2601	G2602	G2715	G2716	C2717	C2824	C2825	G2826	U2827	G2828	C2831	C2832	U2837	C2839	A2840	C2841	G2842	G2851	A2852	U2853																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
C2426	C2427	C2428	U2435	C2443	C2534	U2535	C2536	U2537	A2538	G2539	U2540	U2541	C2549	A2456	U2457	G2462	C2552	A2465	U2466	A2467	A2468	U2469	C2472	C2476	A2568	U2569	G2578	A2481	G2482	U2483	U2484	A2485	A2490	U2491	U2492	C2493	C2374	A2600	U2601	G2602	G2715	G2716	C2717	C2824	C2825	G2826	U2827	G2828	C2831	C2832	U2837	C2839	A2840	C2841	G2842	G2851	A2852	U2853																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
U2320	A2321	G2324	C2329	U2330	G2337	U2338	A	C	A	G	A	A	C2549	A2456	U2457	G2462	C2552	A2465	U2466	A2467	A2468	U2469	C2472	C2476	A2568	U2569	G2578	A2481	G2482	U2483	U2484	A2485	A2490	U2491	U2492	C2493	C2374	A2600	U2601	G2602	G2715	G2716	C2717	C2824	C2825	G2826	U2827	G2828	C2831	C2832	U2837	C2839	A2840	C2841	G2842	G2851	A2852	U2853																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
U	A	C	U	A	C	U	C	U	C	U	C	U	C	A	C	A	C	A2353	A2354	G2355	A2356	G2357	A2361	A2362	G2363	A2364	G2365	A2369	U2370	U2371	U2372	U2373	U2374	U2375	U2376	U2377	U2378	U2379	U2380	U2381	U2382	U2383	U2384	U2385	U2386	U2387	U2388	U2389	U2390	U2391	U2392	U2393	U2394	U2395	U2396	U2397	U2398	U2399	U2400	U2401	U2402	U2403	U2404	U2405	U2406	U2407	U2408	U2409	U2410	U2411	U2412	U2413	U2414	U2415	U2416	U2417	U2418	U2419	U2420	U2421	U2422																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
C	A	U	A	C	G	A	C	A	C	U	C	U	C	A	C	A	C	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A

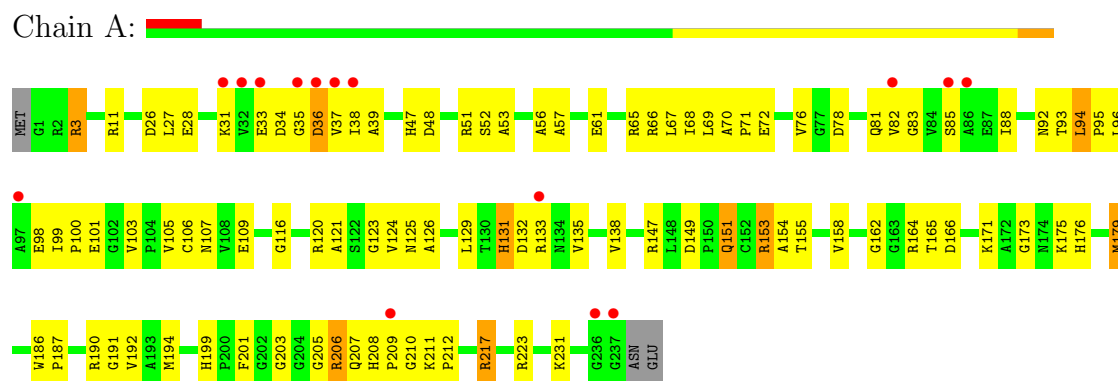
- Molecule 2: 5S ribosomal RNA



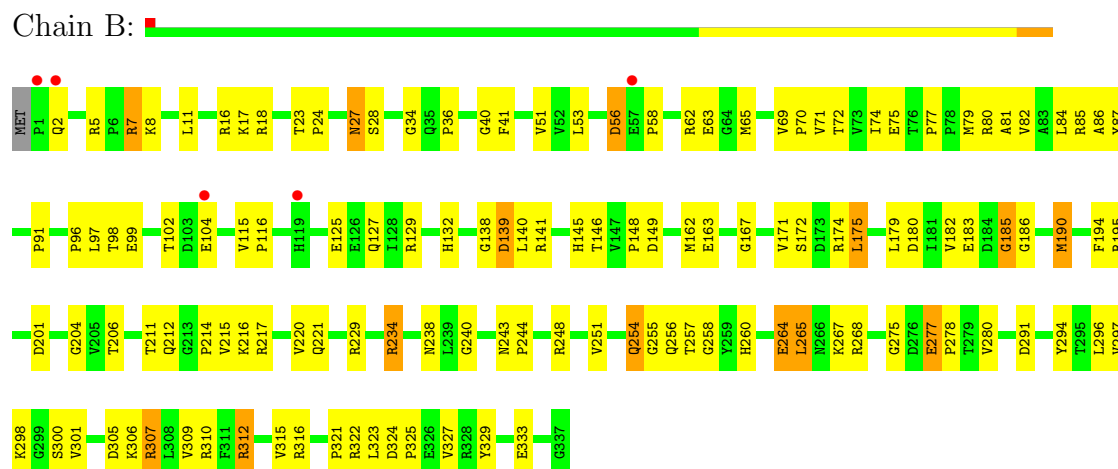
- Molecule 3: 5'-R(\*CP\*CP\*(PPU))-3'



- Molecule 4: 50S ribosomal protein L2P

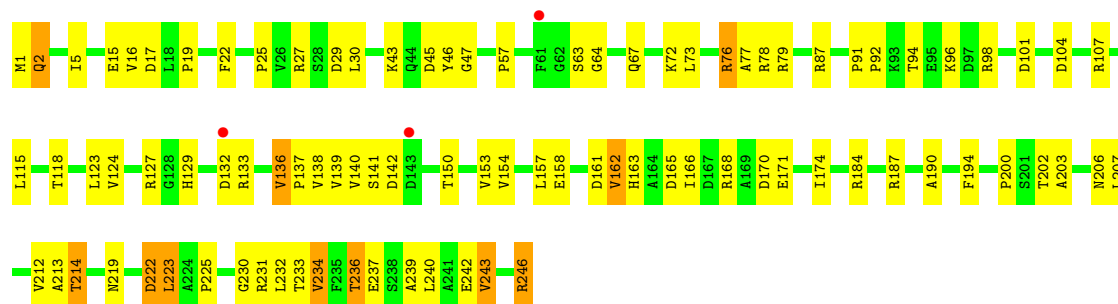


- Molecule 5: 50S ribosomal protein L3P



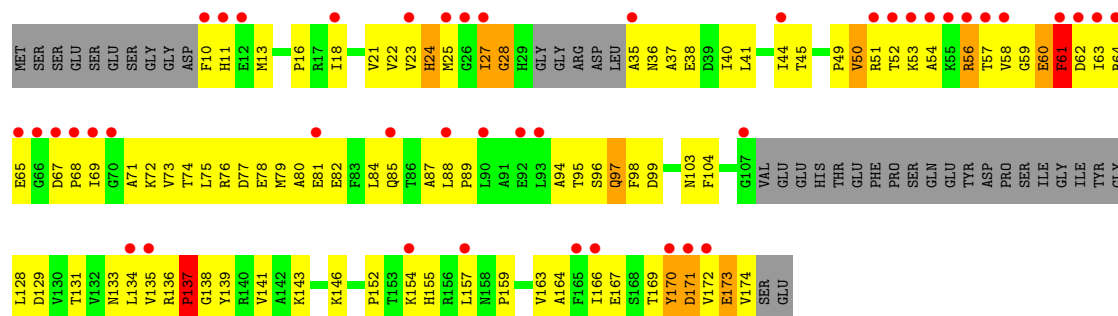
- Molecule 6: 50S ribosomal protein L4E





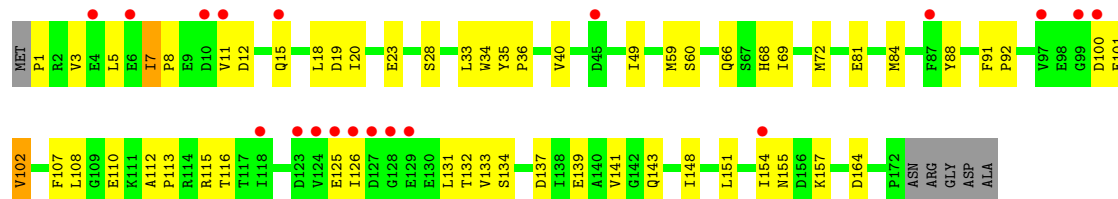
• Molecule 7: 50S ribosomal protein L5P

Chain D:



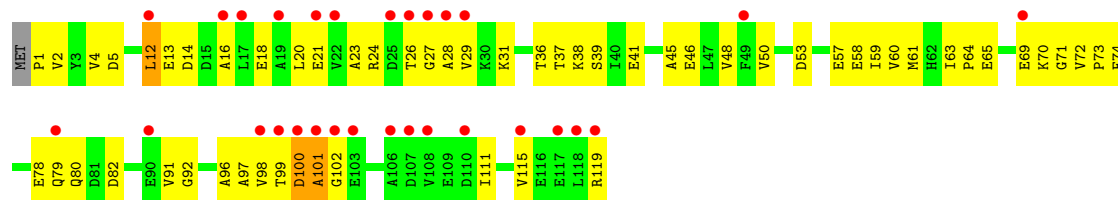
• Molecule 8: 50S ribosomal protein L6P

Chain E:



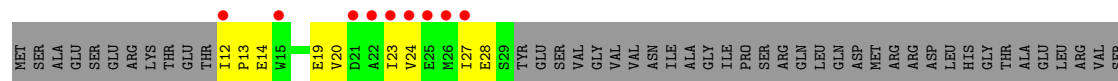
• Molecule 9: 50S ribosomal protein L7AE

Chain F:

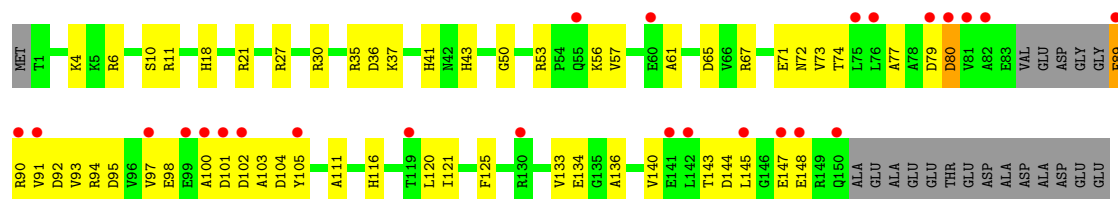


• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

Chain G:

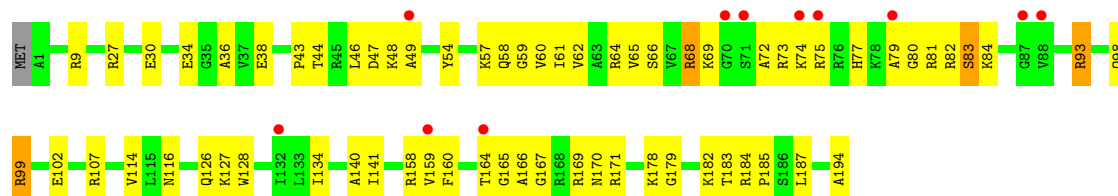






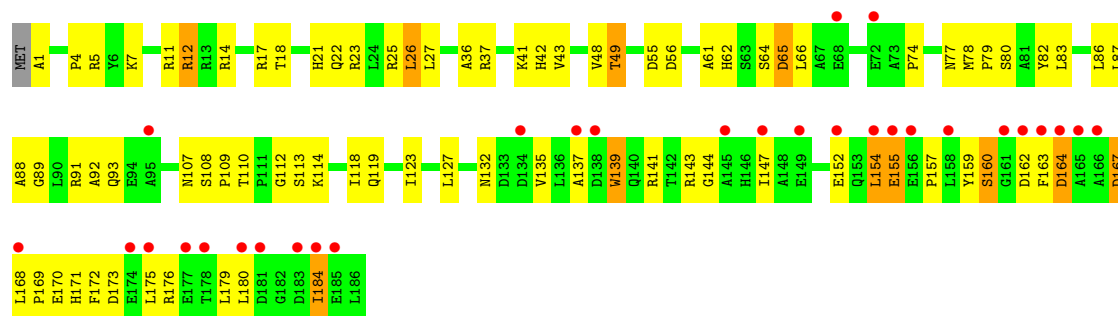
• Molecule 15: 50S Ribosomal Protein L15E

Chain M:



• Molecule 16: 50S ribosomal protein L18P

Chain N:



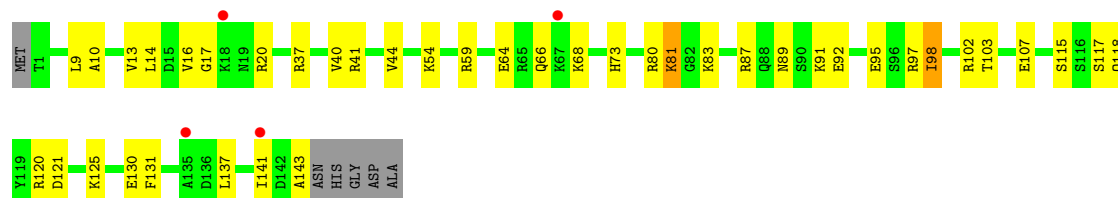
• Molecule 17: 50S ribosomal protein L18e

Chain O:



• Molecule 18: 50S ribosomal protein L19E

Chain P:



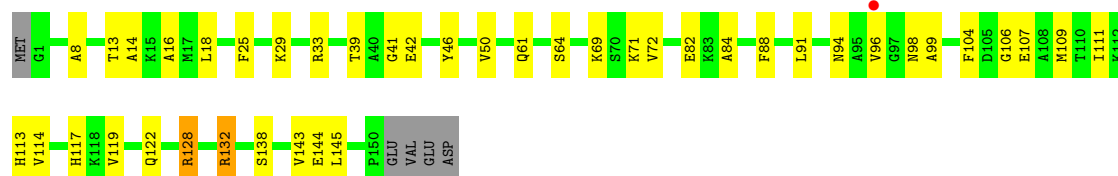
• Molecule 19: 50S ribosomal protein L21e

Chain Q:



- Molecule 20: 50S ribosomal protein L22P

Chain R:



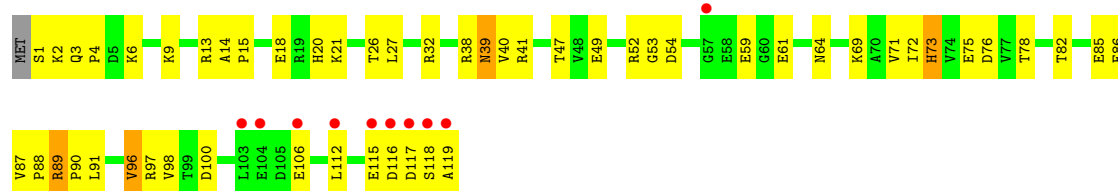
- Molecule 21: 50S ribosomal protein L23P

Chain S:



- Molecule 22: 50S ribosomal protein L24P

Chain T:



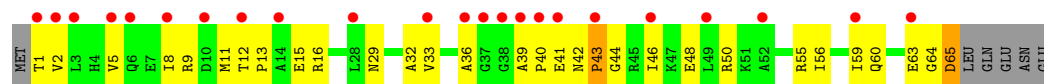
- Molecule 23: 50S ribosomal protein L24E

Chain U:



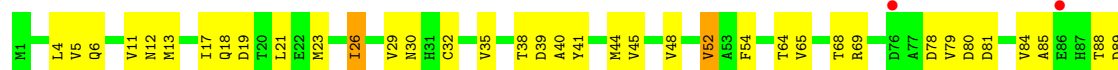
- Molecule 24: 50S ribosomal protein L29P

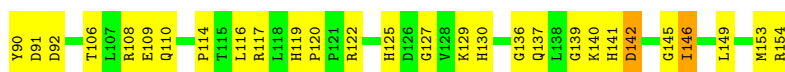
Chain V:



- Molecule 25: 50S ribosomal protein L30P

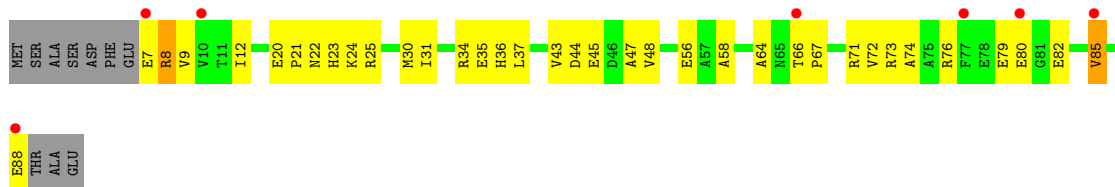
Chain W:





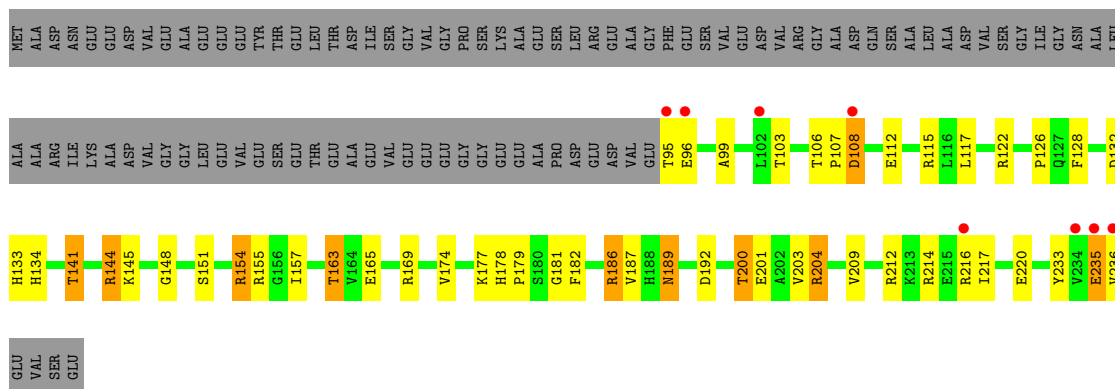
- Molecule 26: 50S ribosomal protein L31e

Chain X:



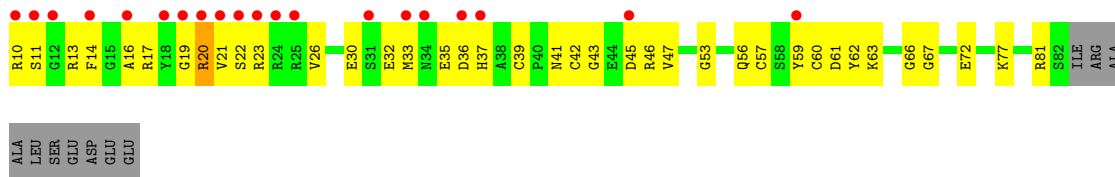
- Molecule 27: 50S ribosomal protein L32E

Chain Y:



- Molecule 28: 50S ribosomal protein L37Ae

Chain Z:



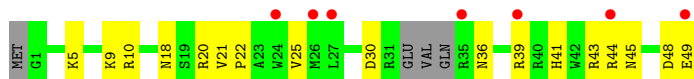
- Molecule 29: 50S ribosomal protein L37e

Chain 1:

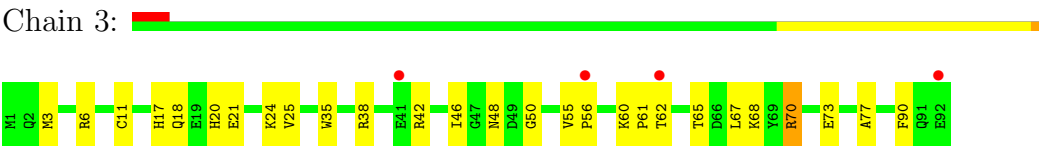


- Molecule 30: 50S ribosomal protein L39e

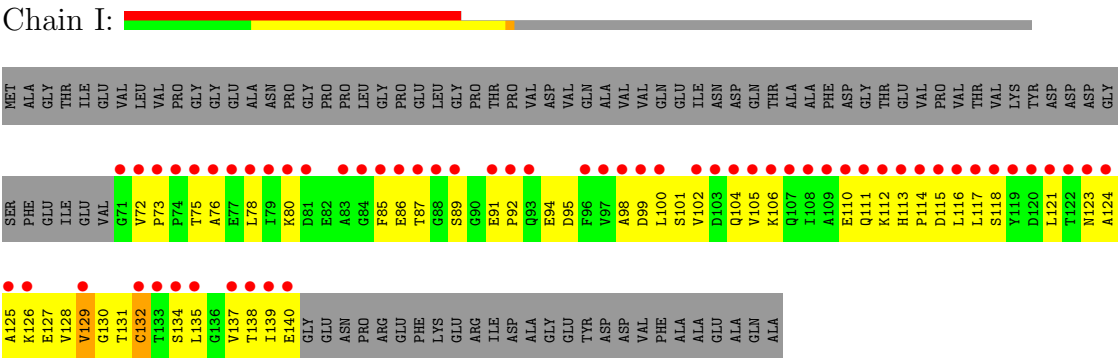
Chain 2:



- Molecule 31: 50S ribosomal protein L44E



● Molecule 32: 50S RIBOSOMAL PROTEIN L11P





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.04Å 299.41Å 575.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 49.39 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.20) 88.8 (49.39-2.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.215 , 0.246 0.214 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 892831 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	99040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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, PPU, 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	0	0.37	0/65959	0.70	24/102870 (0.0%)
2	9	0.33	0/2905	0.71	1/4528 (0.0%)
3	4	0.43	0/40	0.63	0/60
4	A	0.32	0/1786	0.64	0/2408
5	B	0.35	0/2690	0.67	0/3652
6	C	0.37	0/1884	0.65	0/2551
7	D	0.29	0/1111	0.53	0/1498
8	E	0.32	0/1382	0.57	0/1880
9	F	0.32	0/901	0.53	0/1224
10	G	0.26	0/241	0.46	0/324
11	H	0.33	0/1287	0.64	0/1725
12	J	0.35	0/1136	0.61	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.32	0/1130	0.66	0/1509
15	M	0.34	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.59	0/1999
17	O	0.32	0/874	0.58	1/1181 (0.1%)
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.34	0/749	0.69	1/1005 (0.1%)
20	R	0.35	0/1172	0.67	1/1578 (0.1%)
21	S	0.31	0/648	0.56	0/875
22	T	0.29	0/958	0.62	0/1289
23	U	0.34	0/417	0.56	0/562
24	V	0.25	0/502	0.51	0/675
25	W	0.34	0/1219	0.61	0/1655
26	X	0.32	0/664	0.59	0/895
27	Y	0.35	0/1146	0.66	0/1536
28	Z	0.32	0/589	0.59	0/787
29	1	0.44	0/438	0.66	0/578
30	2	0.34	0/401	0.58	0/529
31	3	0.35	0/771	0.58	0/1024
32	I	0.28	0/526	0.49	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.36	0/98732	0.68	28/147637 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	40
2	9	0	1
All	All	1	41

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.80	131.06	109.50
1	0	871	G	C5'-C4'-O4'	-8.85	98.48	109.10
1	0	1942	A	C5'-C4'-C3'	8.20	129.12	116.00
1	0	777	U	O4'-C1'-N1	6.82	113.66	108.20
1	0	1819	G	C5'-C4'-C3'	6.76	126.81	116.00
1	0	1979	G	C2'-C3'-O3'	6.69	124.41	113.70
1	0	1819	G	C1'-O4'-C4'	-6.50	104.70	109.90
1	0	1592	G	N9-C1'-C2'	6.20	122.06	114.00
1	0	1504	A	C1'-O4'-C4'	-5.86	105.22	109.90
1	0	883	U	N1-C1'-C2'	5.84	121.59	114.00
1	0	2467	A	C1'-O4'-C4'	-5.83	105.24	109.90
2	9	3039	U	N1-C1'-C2'	5.69	121.39	114.00
1	0	1819	G	C4'-C3'-C2'	-5.58	97.02	102.60
1	0	206	G	C5'-C4'-C3'	-5.57	107.09	116.00
1	0	1120	U	C5'-C4'-C3'	-5.51	107.19	116.00
1	0	1504	A	N9-C1'-C2'	5.48	121.12	114.00
1	0	1829	A	N9-C1'-C2'	-5.46	105.99	112.00
1	0	1615	A	C5'-C4'-C3'	5.31	124.50	116.00
1	0	2313	C	C5'-C4'-O4'	5.30	115.46	109.10
1	0	1942	A	C4'-C3'-C2'	-5.20	97.40	102.60
19	Q	17	LYS	N-CA-C	-5.19	96.99	111.00
20	R	128	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	0	1942	A	C1'-O4'-C4'	-5.15	105.78	109.90
1	0	841	A	C1'-O4'-C4'	-5.14	105.78	109.90
1	0	1878	G	O4'-C1'-N9	5.12	112.30	108.20
1	0	2291	A	N9-C1'-C2'	5.06	120.58	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1352	A	OP1-P-O3'	5.04	116.28	105.20
17	O	66	GLY	N-CA-C	5.01	125.62	113.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1327	G	Sidechain
1	0	1340	G	Sidechain
1	0	1376	G	Sidechain
1	0	1430	G	Sidechain
1	0	1458	A	Sidechain
1	0	1592	G	Sidechain
1	0	1647	G	Sidechain
1	0	1726	G	Sidechain
1	0	1744	G	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	191	A	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2599	A	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2679	G	Sidechain
1	0	2681	A	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain

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Mol	Chain	Res	Type	Group
1	0	458	G	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	952	G	Sidechain
2	9	3065	A	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	0	59021	0	29812	718	0
2	9	2600	0	1326	56	0
3	4	74	0	51	2	0
4	A	1753	0	1766	117	0
5	B	2625	0	2532	131	0
6	C	1859	0	1816	111	0
7	D	1094	0	1085	101	0
8	E	1357	0	1266	53	0
9	F	890	0	843	52	0
10	G	240	0	231	15	0
11	H	1266	0	1268	68	0
12	J	1120	0	1098	68	0
13	K	992	0	1031	49	0
14	L	1118	0	1076	59	0
15	M	1560	0	1568	67	0
16	N	1445	0	1401	89	0
17	O	865	0	873	38	0
18	P	1136	0	1123	40	0
19	Q	735	0	728	18	0
20	R	1149	0	1122	46	0
21	S	641	0	605	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	T	950	0	924	53	0
23	U	410	0	364	26	0
24	V	499	0	511	37	0
25	W	1196	0	1137	76	0
26	X	654	0	653	42	0
27	Y	1130	0	1133	55	0
28	Z	578	0	539	33	0
29	1	431	0	426	24	0
30	2	396	0	413	23	0
31	3	755	0	728	23	0
32	I	519	0	500	54	0
33	0	88	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	64	0	0	0	0
35	9	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	9	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	98	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	1	2	0	0	0	0
37	3	1	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5780	0	0	111	0
39	1	52	0	0	3	0
39	2	40	0	0	2	0
39	3	66	0	0	4	0
39	4	4	0	0	0	0
39	9	136	0	0	10	0
39	A	124	0	0	12	0
39	B	141	0	0	19	0
39	C	177	0	0	16	0
39	D	46	0	0	10	0
39	E	43	0	0	1	0
39	F	25	0	0	4	0
39	G	16	0	0	3	0
39	H	71	0	0	8	0
39	I	8	0	0	0	0
39	J	58	0	0	3	0
39	K	60	0	0	8	0
39	L	82	0	0	12	0
39	M	125	0	0	6	0
39	N	62	0	0	7	0
39	O	40	0	0	4	0
39	P	60	0	0	4	0
39	Q	49	0	0	3	0
39	R	83	0	0	5	0
39	S	30	0	0	0	0
39	T	36	0	0	4	0
39	U	28	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	V	12	0	0	1	0
39	W	68	0	0	4	0
39	X	26	0	0	6	0
39	Y	93	0	0	11	0
39	Z	29	0	0	2	0
All	All	99040	0	59949	2117	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 14.

All (2117) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.32	1.10
6:C:236:THR:HG22	6:C:239:ALA:H	1.10	1.10
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.34	1.10
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.32	1.08
2:9:3006:C:H5''	16:N:37:ARG:NH1	1.68	1.07
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.27	1.07
9:F:91:VAL:HG12	9:F:92:GLY:H	1.24	1.02
1:0:871:G:C8	1:0:871:G:H5'	1.95	1.01
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.40	1.00
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.24	0.99
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.23	0.99
1:0:156:C:H5''	15:M:171:ARG:HD3	1.40	0.99
5:B:86:ALA:HA	39:B:9580:HOH:O	1.64	0.96
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.44	0.96
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.13	0.95
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.48	0.95
2:9:3076:G:H3'	2:9:3077:A:H5''	1.49	0.95
1:0:2506:A:HO2'	1:0:2507:G:H8	0.97	0.94
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.11	0.94
7:D:25:MET:HE2	7:D:41:LEU:HG	1.50	0.94
1:0:871:G:H8	1:0:871:G:H5'	1.32	0.93
6:C:78:ARG:HG3	6:C:78:ARG:HH11	1.32	0.93
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.82	0.93
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.50	0.93
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.50	0.93
30:2:41:HIS:H	30:2:45:ASN:HD22	1.18	0.93
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.48	0.92
2:9:3006:C:H5''	16:N:37:ARG:HH12	1.29	0.92
29:1:25:LYS:HD2	30:2:49:GLU:H	1.31	0.92
4:A:211:LYS:HG2	4:A:212:PRO:HD2	1.52	0.92

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1372:A:H3'	39:0:7690:HOH:O	1.70	0.92
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.52	0.92
13:K:10:GLN:H	13:K:10:GLN:NE2	1.66	0.91
16:N:144:GLY:O	16:N:147:ILE:HG22	1.71	0.91
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.50	0.91
13:K:39:GLY:HA2	39:K:4183:HOH:O	1.70	0.90
18:P:115:SER:H	18:P:118:GLN:HE21	1.19	0.90
1:0:1242:A:H5'	12:J:82:THR:HG23	1.52	0.90
5:B:140:LEU:HA	39:B:9580:HOH:O	1.71	0.90
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.33	0.90
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.49	0.90
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.52	0.89
5:B:162:MET:SD	5:B:310:ARG:HD3	2.11	0.89
2:9:3056:A:H2'	2:9:3057:A:H5''	1.52	0.89
1:0:289:G:H22	1:0:363:A:H2	1.19	0.89
7:D:136:ARG:HH12	7:D:157:LEU:HA	1.36	0.89
13:K:10:GLN:H	13:K:10:GLN:HE21	0.89	0.89
26:X:25:ARG:HG2	39:X:5356:HOH:O	1.73	0.89
25:W:125:HIS:HD2	25:W:127:GLY:H	1.19	0.89
1:0:2524:G:H21	1:0:2526:C:H41	1.21	0.88
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.14	0.88
13:K:10:GLN:N	13:K:10:GLN:HE21	1.71	0.88
7:D:58:VAL:HB	7:D:62:ASP:HB3	1.54	0.88
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.39	0.88
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.39	0.87
7:D:57:THR:HG23	7:D:63:ILE:HA	1.56	0.87
5:B:238:ASN:HD22	5:B:240:GLY:H	1.22	0.87
1:0:288:A:H61	1:0:364:C:H42	1.20	0.87
6:C:1:MET:HG2	6:C:2:GLN:H	1.36	0.87
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.55	0.87
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.54	0.87
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.57	0.87
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.55	0.86
1:0:542:A:H5'	1:0:542:A:H8	1.38	0.86
6:C:236:THR:HG22	6:C:239:ALA:N	1.89	0.86
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.57	0.86
1:0:1603:A:H5'	1:0:1605:G:O4'	1.76	0.86
1:0:870:G:H2'	1:0:871:G:H5''	1.57	0.86
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.56	0.85
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.57	0.85
1:0:2812:A:H2	1:0:2814:A:H62	1.21	0.85
1:0:1116:U:HO2'	1:0:1118:A:H2	0.86	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:P:115:SER:OG	18:P:118:GLN:HG3	1.77	0.84
1:0:2717:C:C2'	1:0:2718:C:H5''	2.07	0.84
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.59	0.84
5:B:51:VAL:HG23	5:B:329:TYR:O	1.78	0.84
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.79	0.84
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.60	0.84
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.60	0.83
16:N:113:SER:HB2	39:N:9356:HOH:O	1.77	0.83
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.92	0.83
1:0:1593:C:OP1	18:P:117:SER:HB3	1.77	0.83
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.44	0.83
1:0:1474:C:H5'	1:0:1474:C:H6	1.44	0.83
1:0:1041:U:H5'	39:L:9490:HOH:O	1.78	0.83
1:0:506:G:H22	1:0:509:A:H5''	1.42	0.83
25:W:88:THR:HB	39:W:6679:HOH:O	1.78	0.83
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.60	0.83
25:W:88:THR:HG23	25:W:110:GLN:NE2	1.94	0.82
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.79	0.82
4:A:192:VAL:HB	39:A:9582:HOH:O	1.78	0.82
4:A:192:VAL:HG22	39:A:9621:HOH:O	1.78	0.82
1:0:560:C:H42	1:0:597:A:H61	1.23	0.82
1:0:1701:A:H4'	1:0:1702:U:H5''	1.61	0.82
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.61	0.82
39:O:5410:HOH:O	12:J:47:THR:HB	1.80	0.82
1:0:2717:C:H2'	1:0:2718:C:H5''	1.62	0.82
1:0:1835:U:H5	1:0:1840:A:N7	1.77	0.82
12:J:93:ARG:NH1	12:J:93:ARG:HB3	1.94	0.81
21:S:57:THR:HG22	21:S:59:ASP:H	1.45	0.81
24:V:1:THR:HG23	24:V:2:VAL:H	1.44	0.81
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.46	0.81
1:0:544:G:H2'	1:0:545:G:H5''	1.62	0.80
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.61	0.80
27:Y:154:ARG:HH12	27:Y:155:ARG:HG2	1.46	0.80
11:H:27:LYS:H	11:H:59:HIS:HD2	1.29	0.80
5:B:179:LEU:O	5:B:183:GLU:HG2	1.82	0.80
1:0:1205:U:H2'	1:0:1206:U:H5''	1.62	0.80
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.62	0.80
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.62	0.80
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.63	0.80
25:W:13:MET:HE1	25:W:18:GLN:HA	1.62	0.79
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.00	0.79
4:A:199:HIS:HD2	4:A:201:PHE:H	1.27	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:559:U:H5'	1:0:559:U:H6	1.47	0.79
6:C:107:ARG:NH1	6:C:107:ARG:HB3	1.98	0.79
4:A:191:GLY:HA2	4:A:194:MET:CE	2.12	0.79
2:9:3039:U:H1'	2:9:3044:A:H61	1.48	0.79
39:0:6083:HOH:O	5:B:298:LYS:HG2	1.82	0.78
1:0:962:C:H1'	16:N:5:ARG:NH1	1.99	0.78
5:B:141:ARG:HD2	5:B:163:GLU:OE2	1.84	0.78
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.14	0.78
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.13	0.78
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.65	0.78
1:0:645:U:OP2	14:L:4:LYS:HE2	1.84	0.78
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.63	0.77
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.64	0.77
1:0:506:G:H22	1:0:509:A:C5'	1.97	0.77
6:C:246:ARG:NH1	6:C:246:ARG:HB3	1.99	0.77
1:0:871:G:H8	1:0:871:G:C5'	1.97	0.77
1:0:1667:A:H8	1:0:1667:A:H5'	1.50	0.77
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.19	0.77
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.84	0.77
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.14	0.77
1:0:2054:A:N3	20:R:128:ARG:NH2	2.33	0.77
1:0:2635:A:O2'	1:0:2636:C:H5'	1.85	0.77
1:0:1160:G:C5'	1:0:1161:A:H5'	2.13	0.77
5:B:56:ASP:HB3	5:B:322:ARG:HE	1.50	0.76
1:0:2748:G:H2'	39:0:8086:HOH:O	1.86	0.76
4:A:35:GLY:O	4:A:36:ASP:HB3	1.86	0.76
1:0:656:G:H5'	17:O:3:THR:HG22	1.67	0.76
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.67	0.75
1:0:553:G:P	27:Y:204:ARG:HH22	2.09	0.75
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.02	0.75
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.68	0.75
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.16	0.75
12:J:45:VAL:HG11	12:J:121:LEU:HD22	1.68	0.75
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.86	0.75
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.69	0.75
22:T:9:LYS:HE2	22:T:13:ARG:NH1	2.02	0.75
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.17	0.75
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.22	0.75
1:0:2840:A:OP1	5:B:211:THR:HG23	1.85	0.75
16:N:80:SER:HB2	39:N:9335:HOH:O	1.87	0.75
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.69	0.75
1:0:871:G:C8	1:0:871:G:C5'	2.70	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2506:A:O2'	1:0:2507:G:H8	1.68	0.75
16:N:164:ASP:CG	16:N:167:ASP:HA	2.07	0.75
1:0:1160:G:H5'	1:0:1161:A:C5'	2.16	0.74
1:0:236:A:H4'	1:0:237:G:H5'	1.69	0.74
2:9:3014:G:H8	2:9:3014:G:H5'	1.52	0.74
1:0:1973:A:H5'	1:0:1973:A:H8	1.52	0.74
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.68	0.74
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.52	0.74
1:0:1116:U:O2'	1:0:1118:A:H2	1.68	0.74
1:0:545:G:H8	1:0:545:G:H5'	1.51	0.74
39:0:7941:HOH:O	5:B:211:THR:HG21	1.85	0.74
6:C:236:THR:CG2	6:C:239:ALA:H	1.96	0.74
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.01	0.73
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.71	0.73
6:C:115:LEU:HD21	6:C:243:VAL:HG13	1.68	0.73
1:0:2716:G:H5''	5:B:206:THR:HG21	1.70	0.73
6:C:132:ASP:HB3	39:C:9166:HOH:O	1.87	0.73
9:F:58:GLU:HA	9:F:61:MET:HE2	1.70	0.73
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.70	0.73
1:0:2491:G:H1'	39:0:7383:HOH:O	1.88	0.73
8:E:15:GLN:HG2	8:E:19:ASP:O	1.89	0.73
1:0:1377:C:H6	1:0:1377:C:H5'	1.52	0.73
5:B:195:ARG:HG2	5:B:323:LEU:HD22	1.68	0.73
20:R:99:ALA:HB1	20:R:109:MET:CE	2.19	0.73
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.54	0.73
1:0:2005:G:H3'	1:0:2005:G:OP2	1.89	0.73
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.70	0.73
39:0:4356:HOH:O	22:T:9:LYS:HD2	1.89	0.72
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.71	0.72
5:B:16:ARG:NH1	39:B:9614:HOH:O	2.20	0.72
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.69	0.72
26:X:71:ARG:HD3	39:X:2171:HOH:O	1.88	0.72
6:C:246:ARG:HH11	6:C:246:ARG:HB3	1.52	0.72
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.72	0.72
1:0:481:U:H5''	39:0:6210:HOH:O	1.90	0.72
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.70	0.72
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.90	0.72
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.90	0.72
1:0:1183:C:N4	1:0:1184:C:H41	1.88	0.72
1:0:1206:U:H6	1:0:1206:U:H5'	1.54	0.72
1:0:281:U:H2'	1:0:282:C:O4'	1.89	0.71
1:0:870:G:C2'	1:0:871:G:H5''	2.20	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1118:A:H62	1:0:1244:U:H3	1.38	0.71
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.18	0.71
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.39	0.71
25:W:88:THR:HG22	25:W:89:ASP:N	2.05	0.71
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.56	0.71
1:0:796:A:HO2'	28:Z:10:ARG:N	1.87	0.71
11:H:170:ASN:N	11:H:170:ASN:HD22	1.86	0.71
1:0:2765:C:H4'	39:0:6083:HOH:O	1.91	0.71
14:L:73:VAL:HG23	14:L:74:THR:H	1.55	0.71
1:0:1299:G:O6	14:L:6:ARG:HD3	1.90	0.71
1:0:1166:A:H1'	1:0:1192:A:C2	2.26	0.70
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.73	0.70
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.18	0.70
12:J:74:ARG:O	12:J:78:ILE:HG12	1.92	0.70
31:3:70:ARG:HG3	31:3:77:ALA:HB2	1.74	0.70
2:9:3029:C:H2'	2:9:3030:C:H5'	1.73	0.70
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.03	0.70
18:P:115:SER:H	18:P:118:GLN:NE2	1.88	0.70
1:0:56:G:H5''	24:V:50:ARG:NH1	2.06	0.70
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.22	0.70
23:U:17:THR:HG22	23:U:18:GLY:N	2.07	0.70
1:0:1166:A:H61	1:0:1180:U:H3	1.37	0.70
15:M:99:ARG:NH2	15:M:170:ASN:HD22	1.89	0.70
1:0:542:A:H5'	1:0:542:A:C8	2.25	0.70
1:0:1751:G:H2'	1:0:1752:G:H5''	1.74	0.70
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.21	0.70
1:0:1165:G:H4'	1:0:1174:A:O2'	1.91	0.70
24:V:12:THR:HG22	24:V:15:GLU:CG	2.20	0.70
25:W:125:HIS:CD2	25:W:127:GLY:H	2.07	0.70
31:3:70:ARG:HG2	39:3:9501:HOH:O	1.91	0.70
1:0:2524:G:N2	1:0:2526:C:H41	1.90	0.70
24:V:39:ALA:N	24:V:40:PRO:HD2	2.07	0.70
1:0:1205:U:H2'	1:0:1206:U:C5'	2.21	0.69
1:0:2586:U:H3	1:0:2592:G:H22	1.37	0.69
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.22	0.69
1:0:1159:G:H21	1:0:1189:A:H8	1.40	0.69
6:C:162:VAL:HG22	6:C:232:LEU:HD21	1.74	0.69
9:F:13:GLU:OE2	9:F:78:GLU:HG2	1.92	0.69
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.06	0.69
1:0:2749:U:H5'	39:0:8486:HOH:O	1.92	0.69
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.56	0.69
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.75	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:280:C:H2'	1:0:281:U:O4'	1.92	0.69
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.22	0.69
1:0:902:G:N7	14:L:18:HIS:HD2	1.90	0.69
1:0:2851:G:C2'	1:0:2852:A:H5'	2.23	0.69
15:M:164:THR:HG22	15:M:166:ALA:H	1.58	0.69
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.73	0.69
1:0:1118:A:H3'	1:0:1118:A:H8	1.58	0.69
26:X:71:ARG:HB3	26:X:88:GLU:OE1	1.93	0.69
9:F:96:ALA:HA	39:F:3111:HOH:O	1.92	0.69
1:0:1641:A:H2'	1:0:1642:A:H5'	1.73	0.69
1:0:2524:G:H21	1:0:2526:C:N4	1.90	0.69
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.75	0.69
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.74	0.69
25:W:88:THR:HG22	25:W:89:ASP:H	1.56	0.69
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.38	0.69
14:L:67:ARG:O	14:L:71:GLU:HG3	1.93	0.69
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.22	0.68
2:9:3006:C:C5'	16:N:37:ARG:NH1	2.54	0.68
9:F:91:VAL:HG12	9:F:92:GLY:N	2.03	0.68
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.91	0.68
27:Y:115:ARG:HH11	27:Y:115:ARG:HB3	1.59	0.68
1:0:2676:C:H4'	12:J:70:PHE:CD1	2.27	0.68
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.75	0.68
1:0:1118:A:H3'	1:0:1118:A:C8	2.28	0.68
4:A:199:HIS:CD2	4:A:201:PHE:H	2.10	0.68
1:0:282:C:O2'	1:0:283:U:H5'	1.92	0.68
1:0:2533:C:H5'	1:0:2533:C:H6	1.58	0.68
2:9:3014:G:C8	2:9:3014:G:H5'	2.28	0.68
1:0:2534:C:H1'	39:O:4100:HOH:O	1.93	0.68
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.75	0.68
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.57	0.68
6:C:140:VAL:HB	39:C:9254:HOH:O	1.93	0.68
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.93	0.68
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.76	0.68
1:0:1119:G:N2	1:0:1246:A:C2	2.56	0.68
1:0:2820:A:OP1	5:B:98:THR:HG22	1.93	0.68
22:T:26:THR:HA	22:T:39:ASN:HB3	1.76	0.68
1:0:544:G:C2'	1:0:545:G:H5''	2.22	0.68
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.24	0.68
16:N:169:PRO:O	16:N:172:PHE:HB3	1.94	0.68
18:P:91:LYS:O	18:P:95:GLU:HG3	1.93	0.68
15:M:164:THR:HG22	15:M:166:ALA:N	2.09	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.07	0.67
1:0:1201:C:H2'	1:0:1202:A:H5'	1.74	0.67
14:L:143:THR:HG22	14:L:144:ASP:H	1.57	0.67
5:B:102:THR:HG21	5:B:182:VAL:O	1.94	0.67
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.94	0.67
1:0:1116:U:O2'	1:0:1118:A:C2	2.46	0.67
1:0:1838:U:O2'	1:0:2644:C:H5'	1.94	0.67
1:0:1206:U:H2'	1:0:1207:A:O4'	1.94	0.67
27:Y:144:ARG:HG3	27:Y:144:ARG:HH11	1.57	0.67
9:F:37:THR:O	9:F:41:GLU:HG3	1.94	0.67
1:0:1189:A:H3'	39:0:8245:HOH:O	1.94	0.67
1:0:1979:G:H2'	39:0:3902:HOH:O	1.93	0.67
1:0:1119:G:H2'	12:J:52:GLN:NE2	2.09	0.67
16:N:23:ARG:NH1	16:N:27:LEU:HD11	2.09	0.67
29:1:25:LYS:HD2	30:2:49:GLU:N	2.07	0.67
9:F:58:GLU:HG3	9:F:61:MET:HE1	1.75	0.67
32:I:75:THR:HA	32:I:112:LYS:HZ3	1.59	0.67
1:0:1878:G:H1'	39:0:6661:HOH:O	1.94	0.67
4:A:51:ARG:HB2	39:A:9594:HOH:O	1.94	0.67
22:T:71:VAL:HG12	22:T:72:ILE:N	2.10	0.67
5:B:53:LEU:HD11	5:B:327:VAL:HG22	1.76	0.67
17:O:32:ARG:HD3	17:O:32:ARG:O	1.94	0.67
1:0:797:A:H5'	28:Z:10:ARG:N	2.09	0.67
14:L:143:THR:HG22	14:L:144:ASP:N	2.10	0.67
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.75	0.67
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.60	0.67
1:0:1205:U:C2'	1:0:1206:U:H5''	2.25	0.67
15:M:80:GLY:O	15:M:81:ARG:HD2	1.93	0.67
2:9:3056:A:C2'	2:9:3057:A:H5''	2.23	0.66
2:9:3039:U:H1'	2:9:3044:A:N6	2.09	0.66
1:0:1666:C:H2'	1:0:1667:A:H5'	1.77	0.66
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.77	0.66
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.77	0.66
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.31	0.66
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.30	0.66
10:G:12:ILE:N	10:G:13:PRO:HD3	2.11	0.66
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.10	0.66
4:A:48:ASP:HB3	39:A:9594:HOH:O	1.95	0.66
2:9:3051:A:H5'	16:N:160:SER:HB3	1.77	0.66
1:0:1474:C:H5'	1:0:1474:C:C6	2.31	0.66
25:W:48:VAL:HG12	25:W:48:VAL:O	1.95	0.66
1:0:797:A:C4'	28:Z:10:ARG:N	2.59	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:9:3013:A:O2'	2:9:3014:G:H5''	1.95	0.66
1:0:396:U:O2'	1:0:418:C:H4'	1.96	0.66
1:0:2420:G:O2'	1:0:2421:G:H5'	1.96	0.66
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.60	0.66
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.16	0.66
29:1:25:LYS:HE2	39:2:7213:HOH:O	1.95	0.66
27:Y:151:SER:O	27:Y:155:ARG:HG3	1.96	0.66
17:O:45:LEU:CD1	17:O:88:LYS:HD2	2.26	0.66
32:I:106:LYS:O	32:I:110:GLU:HG3	1.96	0.66
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.95	0.66
14:L:80:ASP:HB2	14:L:90:ARG:O	1.95	0.66
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.76	0.65
26:X:9:VAL:HG22	26:X:88:GLU:OE2	1.97	0.65
1:0:1701:A:H4'	1:0:1702:U:C5'	2.26	0.65
25:W:13:MET:CE	25:W:17:ILE:HG22	2.26	0.65
2:9:3014:G:O2'	16:N:1:ALA:HB2	1.97	0.65
5:B:102:THR:HG23	5:B:182:VAL:HG12	1.77	0.65
1:0:2291:A:C8	1:0:2309:C:H5'	2.31	0.65
14:L:133:VAL:HA	39:L:9471:HOH:O	1.97	0.65
6:C:1:MET:HG2	6:C:2:GLN:N	2.11	0.65
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.27	0.65
5:B:62:ARG:HA	5:B:65:MET:HE3	1.78	0.65
1:0:558:C:C2'	1:0:559:U:H5''	2.27	0.65
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.12	0.65
17:O:42:GLU:HB2	39:O:2176:HOH:O	1.96	0.65
21:S:57:THR:HG22	21:S:59:ASP:N	2.12	0.65
11:H:166:SER:CB	11:H:167:PRO:CD	2.75	0.65
32:I:99:ASP:OD1	32:I:138:THR:HB	1.96	0.65
13:K:55:VAL:HG12	13:K:56:SER:N	2.11	0.65
11:H:30:GLN:H	11:H:66:ARG:NH1	1.95	0.65
5:B:238:ASN:HD22	5:B:240:GLY:N	1.95	0.65
5:B:125:GLU:O	5:B:129:ARG:HG3	1.97	0.65
1:0:2578:G:H5'	1:0:2578:G:H8	1.61	0.65
8:E:7:ILE:HD11	8:E:12:ASP:HA	1.79	0.65
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.78	0.64
5:B:307:ARG:NH1	5:B:307:ARG:HG3	2.06	0.64
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.11	0.64
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.79	0.64
1:0:2505:G:O2'	1:0:2506:A:H5'	1.98	0.64
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.79	0.64
32:I:102:VAL:O	32:I:106:LYS:HG3	1.97	0.64
24:V:56:ILE:O	24:V:60:GLN:HG3	1.96	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:Y:154:ARG:HH11	27:Y:154:ARG:HB3	1.61	0.64
1:0:470:U:O2'	29:1:16:HIS:HD2	1.81	0.64
1:0:541:C:H2'	1:0:542:A:C5'	2.27	0.64
14:L:36:ASP:HB2	39:L:9431:HOH:O	1.98	0.64
5:B:254:GLN:HG2	5:B:255:GLY:N	2.10	0.64
1:0:282:C:H1'	1:0:368:C:N4	2.12	0.64
2:9:3051:A:H5'	16:N:160:SER:CB	2.27	0.64
32:I:110:GLU:HA	32:I:113:HIS:CE1	2.33	0.64
27:Y:165:GLU:HB3	39:Y:9391:HOH:O	1.96	0.64
6:C:163:HIS:HD2	39:C:9241:HOH:O	1.80	0.64
2:9:3006:C:OP1	16:N:37:ARG:NH1	2.31	0.64
5:B:62:ARG:HA	5:B:65:MET:CE	2.28	0.64
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.96	0.64
15:M:69:LYS:O	15:M:73:ARG:NH2	2.31	0.64
21:S:51:GLN:HE21	21:S:53:ASN:ND2	1.93	0.64
12:J:19:MET:CE	12:J:132:LEU:HD11	2.27	0.63
27:Y:144:ARG:CZ	39:Y:9409:HOH:O	2.45	0.63
6:C:45:ASP:OD2	6:C:98:ARG:HD2	1.98	0.63
6:C:236:THR:HG21	39:C:9178:HOH:O	1.98	0.63
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.28	0.63
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.79	0.63
1:0:949:U:H4'	19:Q:95:GLU:HA	1.78	0.63
4:A:179:MET:HG2	4:A:186:TRP:CB	2.28	0.63
1:0:962:C:H1'	16:N:5:ARG:HH12	1.63	0.63
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.61	0.63
1:0:541:C:C2'	1:0:542:A:H5''	2.28	0.63
1:0:2346:C:O2'	7:D:52:THR:HG21	1.98	0.63
16:N:154:LEU:O	16:N:155:GLU:HB3	1.98	0.63
1:0:2481:G:H5''	39:0:5130:HOH:O	1.97	0.63
26:X:25:ARG:HD3	26:X:64:ALA:O	1.98	0.63
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.29	0.63
1:0:681:G:N3	1:0:681:G:H5'	2.14	0.63
7:D:65:GLU:HA	39:D:6752:HOH:O	1.97	0.63
1:0:111:C:O2'	29:1:20:ARG:HG2	1.99	0.63
29:1:25:LYS:CD	30:2:49:GLU:H	2.06	0.63
1:0:1766:U:O2	1:0:1778:A:H5'	1.99	0.63
9:F:60:VAL:HG12	9:F:60:VAL:O	1.99	0.63
1:0:877:G:H5'	1:0:878:G:OP1	1.98	0.63
8:E:68:HIS:O	8:E:72:MET:HG3	1.99	0.63
22:T:115:GLU:HG3	22:T:116:ASP:N	2.13	0.63
1:0:289:G:N2	1:0:363:A:H2	1.94	0.62
1:0:1119:G:H22	1:0:1246:A:H2	1.39	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
39:O:7132:HOH:O	27:Y:155:ARG:HD2	1.98	0.62
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.28	0.62
9:F:48:VAL:HG23	9:F:74:PHE:HB3	1.81	0.62
6:C:139:VAL:HG13	39:C:9251:HOH:O	1.99	0.62
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.79	0.62
5:B:215:VAL:HB	5:B:234:ARG:HH12	1.64	0.62
5:B:98:THR:HG21	5:B:127:GLN:OE1	1.99	0.62
4:A:179:MET:HA	4:A:179:MET:CE	2.30	0.62
1:O:2769:C:C2'	1:O:2770:G:H5'	2.29	0.62
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.30	0.62
1:O:1119:G:H8	12:J:52:GLN:HE22	1.46	0.62
1:O:2426:G:H1'	39:O:6634:HOH:O	1.98	0.62
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.80	0.62
1:O:2896:A:N3	1:O:2896:A:H2'	2.15	0.62
7:D:170:TYR:O	7:D:171:ASP:HB3	1.99	0.62
1:O:1700:C:H5''	1:O:1701:A:OP2	1.99	0.62
14:L:91:VAL:HG13	14:L:120:LEU:HD23	1.81	0.62
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.98	0.62
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.81	0.62
1:O:2827:A:H2'	1:O:2828:G:O4'	1.99	0.62
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.80	0.62
22:T:38:ARG:NH1	39:T:6217:HOH:O	2.33	0.62
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.63	0.62
1:O:1183:C:H2'	39:O:6785:HOH:O	2.00	0.62
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.79	0.62
1:O:2769:C:O2'	1:O:2770:G:H5'	2.00	0.62
9:F:21:GLU:O	9:F:24:ARG:HG3	2.00	0.62
7:D:146:LYS:NZ	16:N:107:ASN:HD21	1.98	0.62
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.82	0.62
1:O:1426:C:H2'	39:O:3214:HOH:O	1.98	0.62
7:D:136:ARG:NH1	7:D:157:LEU:HA	2.13	0.61
29:1:10:LYS:HG3	39:1:9488:HOH:O	1.99	0.61
1:O:1181:A:H5'	32:I:94:GLU:OE2	1.99	0.61
1:O:2064:U:H5'	1:O:2652:U:H4'	1.81	0.61
16:N:139:TRP:CE3	16:N:139:TRP:HA	2.35	0.61
15:M:59:GLY:HA3	15:M:141:ILE:HD12	1.82	0.61
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.81	0.61
1:O:757:C:OP1	14:L:27:ARG:HD2	2.00	0.61
17:O:87:THR:O	17:O:91:GLN:HG3	2.00	0.61
1:O:1377:C:H5'	1:O:1377:C:C6	2.36	0.61
39:9:4350:HOH:O	19:Q:25:PRO:HB2	1.99	0.61
1:O:1528:A:H2'	1:O:1529:G:O4'	2.01	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:275:GLY:O	5:B:291:ASP:HA	2.01	0.61
1:0:1666:C:O2'	1:0:1667:A:H5''	1.99	0.61
1:0:1209:C:H2'	1:0:1210:G:H8	1.65	0.61
15:M:79:ALA:HB3	15:M:81:ARG:NH1	2.15	0.61
1:0:2468:A:H61	31:3:48:ASN:HD21	1.46	0.61
8:E:100:ASP:HB2	39:E:2789:HOH:O	2.01	0.61
1:0:381:G:H5''	39:0:4905:HOH:O	1.99	0.61
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.16	0.61
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.30	0.61
18:P:64:GLU:HG2	39:P:163:HOH:O	2.00	0.61
6:C:194:PHE:CD2	6:C:234:VAL:HG11	2.34	0.61
15:M:27:ARG:HH12	15:M:44:THR:CG2	2.14	0.61
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.00	0.61
6:C:79:ARG:O	6:C:87:ARG:HG2	2.00	0.61
1:0:343:C:O2'	1:0:344:C:H5'	1.99	0.61
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.30	0.61
1:0:2769:C:H2'	1:0:2770:G:O4'	2.00	0.61
7:D:159:PRO:O	7:D:163:VAL:HG23	1.99	0.61
1:0:2003:U:H4'	1:0:2004:U:H5	1.65	0.61
1:0:380:A:OP2	15:M:9:ARG:HD2	2.01	0.61
7:D:84:LEU:HA	7:D:87:ALA:HB3	1.83	0.61
1:0:2507:G:H2'	1:0:2510:C:H42	1.66	0.60
18:P:115:SER:N	18:P:118:GLN:HE21	1.93	0.60
6:C:246:ARG:CB	6:C:246:ARG:HH11	2.13	0.60
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.31	0.60
18:P:89:ASN:OD1	18:P:92:GLU:HB2	2.00	0.60
17:O:59:VAL:HG23	17:O:111:VAL:HG22	1.83	0.60
39:0:7025:HOH:O	27:Y:141:THR:HG23	2.01	0.60
39:0:5188:HOH:O	4:A:206:ARG:HD3	1.99	0.60
1:0:1184:C:H1'	39:0:7950:HOH:O	2.00	0.60
32:I:129:VAL:O	32:I:129:VAL:HG12	2.00	0.60
1:0:221:G:H5''	39:0:6299:HOH:O	2.00	0.60
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.01	0.60
1:0:541:C:H2'	1:0:542:A:H5''	1.83	0.60
1:0:1116:U:H3	1:0:1246:A:H62	1.49	0.60
11:H:27:LYS:N	11:H:59:HIS:HD2	1.99	0.60
1:0:56:G:H5''	24:V:50:ARG:HH12	1.64	0.60
39:0:9975:HOH:O	29:1:1:THR:HA	2.00	0.60
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.00	0.60
1:0:1175:G:H1'	1:0:1193:A:H2'	1.83	0.60
7:D:138:GLY:N	39:D:7597:HOH:O	2.35	0.60
26:X:31:ILE:O	26:X:35:GLU:HG3	2.02	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:S:51:GLN:NE2	21:S:53:ASN:HD21	1.92	0.60
6:C:107:ARG:HH11	6:C:107:ARG:HB3	1.64	0.60
1:O:308:U:H5'	22:T:97:ARG:NH2	2.16	0.60
9:F:58:GLU:HG3	9:F:61:MET:CE	2.32	0.60
15:M:27:ARG:NH1	15:M:44:THR:CG2	2.64	0.60
24:V:55:ARG:O	24:V:59:ILE:HG12	2.02	0.60
1:O:138:U:H5''	1:O:139:C:OP2	2.02	0.60
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.31	0.60
1:O:338:C:H4'	6:C:174:ILE:CD1	2.31	0.60
5:B:40:GLY:HA3	39:B:9642:HOH:O	2.01	0.60
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.16	0.60
8:E:34:TRP:O	12:J:127:ILE:HD11	2.02	0.60
1:O:1119:G:H2'	12:J:52:GLN:HE22	1.65	0.60
6:C:77:ALA:O	6:C:78:ARG:HG3	2.01	0.59
5:B:307:ARG:HB3	39:B:9647:HOH:O	2.01	0.59
11:H:21:THR:O	11:H:120:ILE:HD12	2.02	0.59
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.02	0.59
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.32	0.59
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.02	0.59
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.84	0.59
1:O:1681:G:H5''	1:O:1682:A:H5'	1.82	0.59
1:O:272:A:H5'	1:O:273:G:OP2	2.02	0.59
25:W:139:GLY:O	25:W:141:HIS:HD2	1.85	0.59
1:O:1118:A:H8	1:O:1119:G:H5''	1.67	0.59
9:F:46:GLU:OE1	9:F:100:ASP:HA	2.02	0.59
1:O:883:U:H2'	1:O:883:U:O2	2.02	0.59
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.84	0.59
6:C:2:GLN:HB3	39:C:9189:HOH:O	2.02	0.59
1:O:2718:C:H6	1:O:2718:C:H5'	1.68	0.59
1:O:2073:G:OP2	1:O:2490:A:H5'	2.02	0.59
13:K:30:LYS:O	13:K:55:VAL:HG13	2.02	0.59
4:A:211:LYS:CG	4:A:212:PRO:HD2	2.29	0.59
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.03	0.59
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.84	0.59
1:O:474:C:O3'	6:C:73:LEU:HD21	2.03	0.59
17:O:45:LEU:HD11	17:O:88:LYS:HD2	1.84	0.59
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.84	0.59
4:A:209:PRO:O	4:A:211:LYS:N	2.34	0.59
31:3:6:ARG:NH1	31:3:21:GLU:HG3	2.17	0.59
1:O:447:A:P	22:T:1:SER:HB2	2.43	0.59
8:E:81:GLU:HG2	8:E:134:SER:CB	2.33	0.59
23:U:39:ASN:ND2	23:U:44:ARG:HH11	2.00	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:524:A:H5''	20:R:29:LYS:HD3	1.84	0.59
4:A:94:LEU:HD12	4:A:98:GLU:HB2	1.85	0.59
8:E:107:PHE:O	8:E:110:GLU:HG3	2.03	0.59
22:T:49:GLU:CB	22:T:59:GLU:HG2	2.33	0.59
18:P:9:LEU:O	18:P:13:VAL:HG12	2.03	0.59
5:B:305:ASP:O	5:B:306:LYS:HB2	2.03	0.59
6:C:236:THR:H	6:C:239:ALA:HB3	1.68	0.59
1:0:558:C:H2'	1:0:559:U:C5'	2.32	0.59
17:O:32:ARG:NE	17:O:35:LYS:HD2	2.18	0.59
15:M:27:ARG:NH1	15:M:44:THR:HG21	2.17	0.59
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.85	0.58
1:0:95:A:H5''	1:0:97:G:O4'	2.03	0.58
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.68	0.58
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.85	0.58
1:0:475:G:C5'	6:C:73:LEU:HD23	2.33	0.58
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.86	0.58
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.28	0.58
17:O:97:SER:OG	17:O:100:GLN:HG3	2.03	0.58
1:0:2563:U:H2'	1:0:2565:C:O5'	2.02	0.58
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.85	0.58
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.19	0.58
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.03	0.58
24:V:8:ILE:HA	24:V:11:MET:CE	2.33	0.58
1:0:1352:A:O2'	1:0:1353:C:OP1	2.20	0.58
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.68	0.58
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.85	0.58
1:0:1182:C:H1'	1:0:1192:A:H8	1.67	0.58
32:I:125:ALA:O	32:I:129:VAL:HG23	2.03	0.58
39:O:7389:HOH:O	15:M:178:LYS:HB2	2.03	0.58
15:M:60:VAL:C	15:M:61:ILE:HD12	2.22	0.58
1:0:69:A:H5'	1:0:69:A:C8	2.39	0.58
25:W:64:THR:O	25:W:68:THR:HG22	2.04	0.58
24:V:8:ILE:HG21	24:V:59:ILE:HG13	1.85	0.58
5:B:145:HIS:HD2	5:B:146:THR:O	1.86	0.58
7:D:75:LEU:HD22	7:D:79:MET:HB3	1.85	0.58
14:L:104:ASP:HB2	39:L:9461:HOH:O	2.04	0.58
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.86	0.58
14:L:80:ASP:CB	14:L:90:ARG:HB3	2.32	0.58
16:N:176:ARG:HG3	16:N:180:LEU:HD13	1.86	0.58
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.86	0.58
26:X:37:LEU:HD13	26:X:85:VAL:CG2	2.30	0.58
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.19	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1218:U:H2'	1:0:1219:U:C6	2.39	0.58
2:9:3054:A:H2	39:9:3535:HOH:O	1.85	0.58
20:R:39:THR:HB	20:R:42:GLU:HG3	1.84	0.58
1:0:558:C:O2'	1:0:559:U:H5''	2.04	0.58
10:G:20:VAL:O	10:G:24:VAL:HG23	2.03	0.58
1:0:248:A:H5'	1:0:249:G:OP2	2.04	0.58
1:0:2878:U:H2'	1:0:2879:A:O4'	2.04	0.58
15:M:164:THR:HG22	15:M:167:GLY:H	1.69	0.57
7:D:57:THR:HG23	7:D:63:ILE:CA	2.33	0.57
4:A:206:ARG:HD3	4:A:206:ARG:H	1.67	0.57
12:J:130:VAL:HG12	12:J:131:THR:N	2.19	0.57
39:0:8128:HOH:O	31:3:60:LYS:HG3	2.03	0.57
8:E:88:TYR:CE1	8:E:92:PRO:HA	2.39	0.57
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.18	0.57
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.39	0.57
1:0:1979:G:O2'	1:0:1980:U:OP1	2.20	0.57
10:G:12:ILE:HD12	39:G:692:HOH:O	2.04	0.57
11:H:154:TYR:HB2	39:H:9557:HOH:O	2.04	0.57
31:3:62:THR:HB	39:3:9481:HOH:O	2.03	0.57
7:D:13:MET:HA	7:D:137:PRO:HG2	1.86	0.57
11:H:166:SER:CB	11:H:167:PRO:HD3	2.35	0.57
24:V:64:GLY:O	24:V:65:ASP:HB2	2.03	0.57
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.33	0.57
15:M:182:LYS:O	15:M:194:ALA:HB2	2.05	0.57
5:B:185:GLY:HA2	39:B:9631:HOH:O	2.03	0.57
1:0:1625:U:H4'	39:0:5245:HOH:O	2.05	0.57
9:F:91:VAL:CG1	9:F:92:GLY:H	2.07	0.57
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.39	0.57
1:0:960:G:H4'	39:0:7917:HOH:O	2.03	0.57
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.31	0.57
14:L:80:ASP:HB3	14:L:90:ARG:HB3	1.87	0.57
5:B:72:THR:HB	39:B:9603:HOH:O	2.04	0.57
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.87	0.57
21:S:77:VAL:O	21:S:80:ARG:HG2	2.05	0.57
13:K:58:THR:HG22	13:K:59:LYS:HG3	1.85	0.57
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.69	0.57
1:0:2866:U:H4'	1:0:2867:G:H5'	1.85	0.57
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.34	0.57
7:D:23:VAL:HG21	7:D:45:THR:CG2	2.35	0.57
1:0:2726:U:O2'	26:X:22:ASN:ND2	2.38	0.57
1:0:1878:G:O2'	1:0:1879:U:OP2	2.22	0.57
32:I:134:SER:O	32:I:135:LEU:HD23	2.05	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.05	0.57
1:0:1185:U:H4'	32:I:123:ASN:HB3	1.87	0.57
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.19	0.57
1:0:475:G:H5'	6:C:73:LEU:HD23	1.86	0.57
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.87	0.57
7:D:25:MET:SD	7:D:40:ILE:HD11	2.44	0.57
27:Y:115:ARG:NE	39:Y:9353:HOH:O	2.38	0.57
1:0:241:A:C2	1:0:378:A:H4'	2.40	0.57
23:U:52:THR:HG22	23:U:54:THR:N	2.20	0.57
1:0:1819:G:H2'	1:0:1820:G:H4'	1.86	0.57
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.34	0.57
1:0:121:U:OP2	30:2:10:ARG:NH2	2.32	0.56
5:B:310:ARG:HD2	39:B:9590:HOH:O	2.04	0.56
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.86	0.56
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.05	0.56
11:H:158:THR:HB	11:H:159:PRO:HD3	1.87	0.56
28:Z:17:ARG:HD3	39:Z:9218:HOH:O	2.05	0.56
39:0:3159:HOH:O	18:P:81:LYS:HG2	2.04	0.56
7:D:135:VAL:HG22	7:D:136:ARG:H	1.70	0.56
7:D:136:ARG:HB3	7:D:137:PRO:HD2	1.88	0.56
1:0:2717:C:O2'	1:0:2718:C:H5''	2.03	0.56
1:0:545:G:C8	1:0:545:G:H5'	2.36	0.56
1:0:2644:C:O2'	1:0:2645:U:H5'	2.05	0.56
32:I:113:HIS:N	32:I:114:PRO:HD2	2.21	0.56
15:M:57:LYS:HE2	15:M:140:ALA:O	2.05	0.56
1:0:1853:C:OP1	4:A:231:LYS:HG3	2.05	0.56
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.86	0.56
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.69	0.56
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.86	0.56
24:V:39:ALA:N	24:V:40:PRO:CD	2.68	0.56
1:0:2851:G:O2'	1:0:2852:A:H5'	2.06	0.56
18:P:40:VAL:O	18:P:44:VAL:HG23	2.05	0.56
1:0:2781:U:H1'	8:E:139:GLU:OE2	2.04	0.56
1:0:164:G:H4'	14:L:30:ARG:HD3	1.87	0.56
32:I:89:SER:HB2	32:I:95:ASP:HB2	1.88	0.56
4:A:26:ASP:O	4:A:28:GLU:N	2.38	0.56
15:M:99:ARG:HH21	15:M:170:ASN:ND2	1.96	0.56
15:M:107:ARG:NH1	15:M:107:ARG:HG3	2.21	0.56
1:0:1328:A:OP1	27:Y:169:ARG:HD2	2.06	0.56
11:H:166:SER:HB2	11:H:167:PRO:CD	2.36	0.56
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.16	0.56
11:H:170:ASN:N	11:H:170:ASN:ND2	2.54	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:80:ARG:HB2	5:B:145:HIS:CE1	2.41	0.56
8:E:101:GLU:HB2	8:E:116:THR:O	2.04	0.56
14:L:136:ALA:HB3	39:L:9471:HOH:O	2.05	0.56
8:E:11:VAL:HG12	8:E:12:ASP:N	2.20	0.56
16:N:154:LEU:HG	16:N:155:GLU:H	1.70	0.56
1:O:926:A:O2'	14:L:41:HIS:HD2	1.89	0.56
5:B:85:ARG:NH1	39:B:9632:HOH:O	2.38	0.56
6:C:16:VAL:HG12	6:C:17:ASP:H	1.70	0.56
5:B:234:ARG:HH11	5:B:234:ARG:HB3	1.69	0.56
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.88	0.56
23:U:17:THR:CG2	23:U:18:GLY:N	2.69	0.56
2:9:3007:G:H5'	39:9:5071:HOH:O	2.06	0.56
9:F:46:GLU:O	9:F:73:PRO:HD2	2.05	0.56
5:B:96:PRO:HG3	39:B:9632:HOH:O	2.05	0.56
12:J:39:VAL:HG11	12:J:107:ASN:CG	2.27	0.56
16:N:22:GLN:HG2	16:N:26:LEU:HD22	1.88	0.56
5:B:91:PRO:O	12:J:144:THR:HG21	2.06	0.56
39:K:7438:HOH:O	23:U:20:MET:HE1	2.05	0.56
1:O:2812:A:C2	1:O:2814:A:N6	2.65	0.56
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.69	0.56
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.35	0.56
16:N:176:ARG:O	16:N:180:LEU:HD13	2.05	0.56
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.88	0.56
1:O:625:U:H5''	1:O:1044:C:N4	2.21	0.56
2:9:3002:U:OP2	2:9:3003:A:H5'	2.06	0.56
6:C:236:THR:HA	39:C:9254:HOH:O	2.05	0.56
16:N:82:TYR:OH	16:N:176:ARG:NH1	2.39	0.56
9:F:1:PRO:H3	9:F:4:VAL:HG23	1.71	0.56
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.41	0.56
39:O:5303:HOH:O	16:N:21:HIS:HD2	1.90	0.55
1:O:2748:G:H1'	39:O:8464:HOH:O	2.04	0.55
1:O:93:C:H5''	24:V:1:THR:HB	1.88	0.55
1:O:797:A:H4'	28:Z:10:ARG:N	2.21	0.55
1:O:2780:C:H1'	8:E:143:GLN:HE21	1.72	0.55
14:L:148:GLU:HB2	39:L:9487:HOH:O	2.05	0.55
18:P:143:ALA:HA	39:P:162:HOH:O	2.07	0.55
1:O:1165:G:H1'	1:O:1174:A:H1'	1.87	0.55
1:O:2502:C:C2'	1:O:2503:A:H5'	2.36	0.55
1:O:2265:U:H2'	1:O:2266:A:C8	2.42	0.55
19:Q:11:ARG:HD3	39:Q:5620:HOH:O	2.06	0.55
16:N:139:TRP:HE3	16:N:139:TRP:HA	1.70	0.55
1:O:1787:C:OP1	18:P:68:LYS:HE2	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2670:G:O2'	1:0:2671:U:H5'	2.06	0.55
1:0:1244:U:H2'	12:J:47:THR:HG21	1.88	0.55
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.37	0.55
1:0:447:A:OP2	22:T:1:SER:HB2	2.07	0.55
5:B:297:VAL:HB	39:B:9603:HOH:O	2.06	0.55
5:B:138:GLY:O	5:B:139:ASP:O	2.24	0.55
7:D:59:GLY:O	7:D:61:PHE:N	2.40	0.55
11:H:167:PRO:O	11:H:168:ALA:HB2	2.07	0.55
16:N:143:ARG:NH2	16:N:169:PRO:HB2	2.21	0.55
32:I:138:THR:HG22	32:I:139:ILE:N	2.22	0.55
1:0:949:U:O2'	19:Q:40:HIS:HE1	1.89	0.55
1:0:960:G:H3'	1:0:960:G:N3	2.22	0.55
1:0:1946:C:H2'	1:0:1971:G:C8	2.42	0.55
5:B:5:ARG:HH11	5:B:8:LYS:CE	2.17	0.55
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.89	0.55
1:0:516:A:H5'	39:0:6210:HOH:O	2.06	0.55
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.22	0.55
2:9:3020:G:O2'	2:9:3021:G:H5'	2.06	0.55
6:C:170:ASP:O	6:C:171:GLU:HG3	2.07	0.55
22:T:89:ARG:O	22:T:89:ARG:HG3	2.07	0.55
1:0:1299:G:H5'	39:0:4667:HOH:O	2.06	0.55
22:T:40:VAL:HG22	22:T:41:ARG:N	2.22	0.55
1:0:2406:U:H1'	39:0:7222:HOH:O	2.06	0.55
1:0:1462:C:H2'	1:0:1463:A:C8	2.42	0.55
13:K:109:LEU:HD13	13:K:113:ILE:CD1	2.36	0.54
25:W:88:THR:CG2	25:W:89:ASP:H	2.20	0.54
1:0:119:A:H2'	1:0:120:A:H5''	1.89	0.54
1:0:2252:A:H2'	1:0:2253:G:O4'	2.06	0.54
27:Y:133:HIS:HD2	39:Y:9380:HOH:O	1.90	0.54
1:0:1552:G:N2	1:0:1634:G:H1'	2.23	0.54
5:B:58:PRO:HA	5:B:63:GLU:OE1	2.06	0.54
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.89	0.54
1:0:2073:G:H3'	39:0:4424:HOH:O	2.07	0.54
1:0:2419:U:H5''	1:0:2420:G:H5'	1.88	0.54
16:N:154:LEU:O	16:N:155:GLU:CB	2.55	0.54
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.08	0.54
1:0:1384:C:H5'	26:X:30:MET:HG2	1.88	0.54
1:0:475:G:OP1	6:C:73:LEU:HD22	2.07	0.54
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.73	0.54
39:0:5272:HOH:O	28:Z:13:ARG:HD3	2.07	0.54
6:C:129:HIS:HD2	6:C:165:ASP:OD2	1.90	0.54
17:O:25:VAL:HG23	17:O:26:TRP:H	1.72	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:69:A:H5'	1:0:69:A:H8	1.73	0.54
1:0:151:A:H2'	1:0:152:A:O4'	2.07	0.54
1:0:156:C:H5''	15:M:171:ARG:CD	2.28	0.54
30:2:48:ASP:O	30:2:49:GLU:HB2	2.06	0.54
6:C:107:ARG:HH11	6:C:107:ARG:CB	2.20	0.54
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.89	0.54
25:W:149:LEU:HG	25:W:153:MET:CE	2.38	0.54
13:K:87:ARG:CZ	39:K:4854:HOH:O	2.54	0.54
1:0:1187:U:O2'	1:0:1189:A:H2	1.91	0.54
1:0:2533:C:C6	1:0:2533:C:H5'	2.42	0.54
11:H:136:ALA:HB3	11:H:146:VAL:HG21	1.88	0.54
5:B:258:GLY:H	5:B:260:HIS:CE1	2.25	0.54
5:B:140:LEU:HD23	39:B:9580:HOH:O	2.08	0.54
5:B:195:ARG:HD2	5:B:324:ASP:OD1	2.07	0.54
1:0:2362:A:H2'	1:0:2363:G:C8	2.43	0.54
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.22	0.54
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.90	0.54
1:0:969:G:H1	1:0:999:C:H42	1.54	0.54
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.89	0.54
1:0:1278:A:H4'	1:0:1279:U:C4	2.42	0.54
28:Z:72:GLU:OE1	28:Z:77:LYS:HE2	2.07	0.54
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.90	0.54
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.38	0.54
20:R:29:LYS:NZ	39:R:9449:HOH:O	2.39	0.54
2:9:3029:C:C2'	2:9:3030:C:H5'	2.37	0.54
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.22	0.54
10:G:67:LEU:O	10:G:71:LEU:HG	2.07	0.54
5:B:18:ARG:HE	5:B:256:GLN:NE2	2.06	0.54
9:F:57:GLU:O	9:F:61:MET:HG3	2.07	0.54
1:0:2851:G:H2'	1:0:2852:A:H5'	1.90	0.54
4:A:94:LEU:N	4:A:94:LEU:HD23	2.22	0.54
22:T:75:GLU:O	22:T:76:ASP:HB2	2.08	0.54
1:0:1595:G:O2'	1:0:1596:U:H5'	2.08	0.54
1:0:185:G:H4'	1:0:186:A:H4'	1.90	0.54
16:N:110:THR:HB	16:N:113:SER:OG	2.08	0.54
12:J:45:VAL:HG11	12:J:121:LEU:CD2	2.38	0.54
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.37	0.54
1:0:1778:A:H2'	1:0:1779:A:H5'	1.89	0.54
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.08	0.54
16:N:114:LYS:O	16:N:118:ILE:HG13	2.07	0.53
15:M:164:THR:CG2	15:M:166:ALA:H	2.21	0.53
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.89	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:M:27:ARG:NH2	15:M:44:THR:HG23	2.22	0.53
1:0:1789:G:O6	18:P:73:HIS:HE1	1.91	0.53
1:0:2908:A:H2'	1:0:2909:G:O4'	2.06	0.53
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.23	0.53
11:H:27:LYS:H	11:H:59:HIS:CD2	2.18	0.53
32:I:92:PRO:C	32:I:94:GLU:H	2.11	0.53
1:0:1189:A:H1'	1:0:1209:C:O4'	2.08	0.53
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.07	0.53
1:0:2346:C:H4'	7:D:52:THR:CG2	2.38	0.53
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.43	0.53
18:P:103:THR:O	18:P:107:GLU:HG3	2.08	0.53
6:C:214:THR:HG23	39:C:9240:HOH:O	2.08	0.53
31:3:55:VAL:HG22	39:3:9444:HOH:O	2.07	0.53
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.22	0.53
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.90	0.53
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.74	0.53
1:0:1201:C:H5''	39:0:6774:HOH:O	2.08	0.53
6:C:98:ARG:NH1	39:C:9160:HOH:O	2.41	0.53
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.90	0.53
19:Q:75:ILE:HD13	19:Q:84:ILE:HD11	1.90	0.53
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.91	0.53
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.37	0.53
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.09	0.53
1:0:2817:G:P	39:0:8491:HOH:O	2.67	0.53
15:M:64:ARG:HD2	39:M:9386:HOH:O	2.08	0.53
7:D:23:VAL:CG2	7:D:73:VAL:HB	2.38	0.53
27:Y:96:GLU:O	27:Y:235:GLU:HA	2.09	0.53
4:A:33:GLU:CD	4:A:33:GLU:H	2.10	0.53
1:0:2645:U:OP2	1:0:2645:U:C6	2.62	0.53
30:2:5:LYS:O	30:2:9:LYS:HG3	2.08	0.53
13:K:99:ASP:OD1	13:K:101:ASN:N	2.41	0.53
1:0:500:G:H21	20:R:98:ASN:HD21	1.55	0.53
1:0:558:C:H2'	1:0:559:U:H5''	1.89	0.53
32:I:100:LEU:O	32:I:139:ILE:HG23	2.09	0.53
25:W:4:LEU:O	25:W:32:CYS:HA	2.09	0.53
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.39	0.53
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.08	0.53
1:0:2783:A:H5''	39:0:5797:HOH:O	2.07	0.53
5:B:264:GLU:HG2	5:B:267:LYS:CE	2.26	0.53
11:H:30:GLN:H	11:H:66:ARG:HH11	1.57	0.53
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.91	0.53
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.38	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:D:35:ALA:O	7:D:38:GLU:HG3	2.08	0.53
4:A:132:ASP:OD1	4:A:133:ARG:N	2.41	0.53
1:0:1119:G:N2	1:0:1246:A:N1	2.57	0.53
1:0:656:G:H5'	17:O:3:THR:CG2	2.37	0.53
2:9:3029:C:O3'	7:D:138:GLY:HA2	2.09	0.53
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.91	0.53
5:B:41:PHE:CG	5:B:79:MET:HE2	2.44	0.53
11:H:40:ALA:HB1	11:H:137:TYR:CE2	2.44	0.53
1:0:1943:C:H4'	4:A:211:LYS:O	2.09	0.53
16:N:152:GLU:C	16:N:154:LEU:H	2.12	0.53
5:B:214:PRO:HD2	39:B:9524:HOH:O	2.09	0.53
1:0:2807:U:P	5:B:27:ASN:HD21	2.32	0.53
1:0:1400:C:H4'	26:X:56:GLU:HG2	1.90	0.53
1:0:299:U:H5'	39:O:7830:HOH:O	2.09	0.53
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.08	0.53
1:0:775:G:OP1	29:1:16:HIS:HE1	1.92	0.53
31:3:48:ASN:ND2	31:3:50:GLY:H	2.07	0.53
26:X:43:VAL:HG12	26:X:44:ASP:N	2.23	0.53
1:0:541:C:H2'	1:0:542:A:H5'	1.90	0.52
1:0:2661:U:H3	1:0:2812:A:H62	1.57	0.52
1:0:1641:A:C2'	1:0:1642:A:H5'	2.38	0.52
15:M:79:ALA:HB3	15:M:81:ARG:HH12	1.74	0.52
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.06	0.52
4:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.91	0.52
12:J:8:ALA:HA	12:J:35:THR:HG22	1.90	0.52
1:0:2472:C:O2'	1:0:2634:G:H4'	2.08	0.52
1:0:2100:A:H4'	6:C:64:GLY:O	2.08	0.52
17:O:22:GLY:HA2	39:O:2823:HOH:O	2.08	0.52
5:B:190:MET:CE	5:B:194:PHE:HD1	2.22	0.52
14:L:97:VAL:HG12	14:L:98:GLU:O	2.09	0.52
1:0:441:A:H1'	1:0:442:A:N7	2.23	0.52
26:X:22:ASN:O	26:X:25:ARG:HG3	2.09	0.52
11:H:28:ILE:HG23	39:H:9546:HOH:O	2.09	0.52
22:T:40:VAL:HG22	22:T:41:ARG:H	1.74	0.52
1:0:447:A:OP1	22:T:2:LYS:HG2	2.09	0.52
25:W:130:HIS:O	25:W:136:GLY:HA3	2.09	0.52
8:E:133:VAL:HG12	8:E:141:VAL:HG13	1.92	0.52
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.44	0.52
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.57	0.52
1:0:1328:A:C8	27:Y:169:ARG:HD3	2.45	0.52
30:2:36:ASN:HB3	30:2:39:ARG:HG3	1.91	0.52
1:0:291:C:H2'	1:0:292:G:O4'	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:9:3050:G:H5''	16:N:159:TYR:HE1	1.74	0.52
24:V:5:VAL:HG23	39:V:2271:HOH:O	2.09	0.52
15:M:30:GLU:O	15:M:34:GLU:HG3	2.09	0.52
13:K:87:ARG:NH1	39:K:4066:HOH:O	2.43	0.52
6:C:107:ARG:NE	39:C:9263:HOH:O	2.36	0.52
1:0:1167:G:H4'	32:I:135:LEU:CD2	2.40	0.52
23:U:9:CYS:O	23:U:52:THR:HG23	2.10	0.52
25:W:29:VAL:O	25:W:30:ASN:HB2	2.10	0.52
2:9:3076:G:C3'	2:9:3077:A:H5''	2.32	0.52
5:B:8:LYS:HG3	5:B:220:VAL:HG12	1.92	0.52
24:V:1:THR:HG22	24:V:48:GLU:OE1	2.10	0.52
30:2:20:ARG:HD2	30:2:39:ARG:NH2	2.24	0.52
39:0:4582:HOH:O	22:T:82:THR:HA	2.09	0.52
1:0:446:G:OP2	22:T:6:LYS:NZ	2.39	0.52
16:N:37:ARG:NE	39:N:9333:HOH:O	2.42	0.52
1:0:1189:A:O2'	1:0:1208:C:H2'	2.10	0.52
17:O:38:ARG:NH1	39:O:7674:HOH:O	2.43	0.52
13:K:55:VAL:CG1	13:K:56:SER:N	2.72	0.52
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.92	0.52
24:V:1:THR:HG23	24:V:2:VAL:N	2.19	0.52
1:0:2064:U:H5'	1:0:2652:U:O3'	2.10	0.52
1:0:848:C:H5'	39:0:7771:HOH:O	2.10	0.52
1:0:407:A:H2'	1:0:408:A:C8	2.45	0.52
1:0:407:A:H5'	39:0:6572:HOH:O	2.10	0.52
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.57	0.52
1:0:1080:C:H4'	1:0:1081:A:OP1	2.09	0.52
1:0:1555:G:H4'	1:0:1630:A:H2	1.75	0.52
18:P:14:LEU:O	18:P:16:VAL:HG23	2.10	0.52
18:P:16:VAL:HG13	18:P:20:ARG:NH1	2.24	0.52
1:0:2636:C:H3'	1:0:2637:A:C5'	2.40	0.51
17:O:25:VAL:HG11	17:O:111:VAL:HG11	1.93	0.51
19:Q:75:ILE:CD1	19:Q:84:ILE:HD11	2.40	0.51
1:0:2748:G:H8	39:0:8086:HOH:O	1.92	0.51
28:Z:37:HIS:O	28:Z:45:ASP:HA	2.10	0.51
8:E:69:ILE:HA	8:E:72:MET:CE	2.40	0.51
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.76	0.51
1:0:1363:G:OP1	6:C:76:ARG:NH2	2.43	0.51
1:0:1451:C:H5'	1:0:1505:U:C5	2.45	0.51
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.92	0.51
1:0:1626:A:H2'	1:0:1627:G:O4'	2.10	0.51
11:H:2:PRO:HD2	11:H:5:MET:SD	2.49	0.51
1:0:2133:U:H4'	1:0:2134:G:H5'	1.91	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:G:64:ASN:N	10:G:64:ASN:HD22	2.07	0.51
1:0:1189:A:H1'	1:0:1209:C:C1'	2.40	0.51
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.46	0.51
1:0:622:G:P	27:Y:148:GLY:HA3	2.49	0.51
1:0:1771:U:H5'	28:Z:20:ARG:HH21	1.76	0.51
4:A:149:ASP:OD1	4:A:151:GLN:HB2	2.09	0.51
1:0:2250:G:OP1	4:A:31:LYS:HD3	2.10	0.51
6:C:142:ASP:OD1	6:C:237:GLU:HB3	2.11	0.51
5:B:267:LYS:HE3	5:B:300:SER:O	2.10	0.51
22:T:71:VAL:HG13	22:T:91:LEU:O	2.11	0.51
1:0:2717:C:H2'	1:0:2718:C:C5'	2.37	0.51
10:G:12:ILE:N	10:G:13:PRO:CD	2.74	0.51
25:W:5:VAL:O	25:W:52:VAL:HG22	2.10	0.51
32:I:131:THR:O	32:I:135:LEU:HG	2.10	0.51
1:0:1218:U:H2'	1:0:1219:U:H6	1.74	0.51
12:J:131:THR:HG22	12:J:133:GLY:N	2.26	0.51
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.91	0.51
1:0:2795:C:O2'	1:0:2796:U:H5'	2.10	0.51
1:0:316:A:H5'	22:T:54:ASP:OD2	2.09	0.51
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.91	0.51
22:T:61:GLU:HG3	39:T:3851:HOH:O	2.09	0.51
1:0:1882:C:OP1	4:A:192:VAL:HG23	2.09	0.51
5:B:53:LEU:CD1	5:B:327:VAL:HG22	2.41	0.51
4:A:100:PRO:HG2	4:A:103:VAL:CG2	2.40	0.51
1:0:2502:C:H2'	1:0:2503:A:H5'	1.91	0.51
7:D:81:GLU:O	7:D:85:GLN:HG3	2.10	0.51
11:H:45:VAL:HA	11:H:167:PRO:O	2.10	0.51
20:R:106:GLY:HA2	20:R:109:MET:CE	2.41	0.51
1:0:1118:A:C8	1:0:1119:G:H5''	2.45	0.51
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.43	0.51
1:0:602:A:O2'	1:0:605:C:H4'	2.10	0.51
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.39	0.51
25:W:80:ASP:O	25:W:84:VAL:HG23	2.09	0.51
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.40	0.51
1:0:2769:C:H2'	1:0:2770:G:C5'	2.40	0.51
18:P:16:VAL:HG12	18:P:17:GLY:N	2.25	0.51
1:0:485:A:N3	1:0:487:G:H5''	2.25	0.51
1:0:65:C:O2'	1:0:66:G:H5'	2.10	0.51
1:0:2632:G:H5''	4:A:210:GLY:HA3	1.92	0.51
39:O:5855:HOH:O	25:W:122:ARG:NH2	2.36	0.51
6:C:242:GLU:HG3	39:C:9186:HOH:O	2.10	0.51
1:0:2747:C:H4'	39:O:8486:HOH:O	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:16:VAL:HG12	6:C:17:ASP:N	2.26	0.51
1:O:797:A:C5'	28:Z:10:ARG:N	2.72	0.51
32:I:78:LEU:HD12	32:I:112:LYS:NZ	2.26	0.51
6:C:46:TYR:CE2	6:C:98:ARG:NH1	2.79	0.51
12:J:131:THR:HG22	12:J:134:GLU:H	1.74	0.51
4:A:125:ASN:CB	4:A:158:VAL:HG12	2.40	0.51
13:K:115:ARG:HG3	13:K:116:GLU:N	2.26	0.51
25:W:38:THR:HG22	25:W:39:ASP:N	2.25	0.51
1:O:621:C:H5'	27:Y:132:ASP:OD2	2.11	0.51
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.25	0.51
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.92	0.51
1:O:1972:U:H2'	1:O:1973:A:C5'	2.41	0.51
39:O:4127:HOH:O	18:P:91:LYS:HD3	2.11	0.51
1:O:120:A:H5'	29:1:20:ARG:HH21	1.76	0.51
1:O:709:G:O2'	17:O:25:VAL:HG12	2.09	0.51
13:K:49:LEU:HD22	13:K:117:VAL:CG2	2.41	0.51
27:Y:216:ARG:HD2	39:Y:9367:HOH:O	2.10	0.51
30:2:41:HIS:HD2	30:2:44:ARG:H	1.58	0.51
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.75	0.51
1:O:644:G:O2'	14:L:4:LYS:HE3	2.11	0.51
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.26	0.51
25:W:5:VAL:O	25:W:52:VAL:CG2	2.59	0.51
1:O:2416:G:O2'	16:N:25:ARG:HG2	2.10	0.51
14:L:57:VAL:HG12	14:L:57:VAL:O	2.10	0.51
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.46	0.51
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.92	0.50
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.92	0.50
23:U:9:CYS:HA	23:U:52:THR:HG23	1.92	0.50
7:D:36:ASN:HA	39:D:7500:HOH:O	2.11	0.50
1:O:564:G:H1'	39:O:6848:HOH:O	2.09	0.50
16:N:162:ASP:HA	39:N:9330:HOH:O	2.11	0.50
13:K:13:GLU:OE1	13:K:44:LEU:HD12	2.10	0.50
1:O:371:U:H2'	1:O:372:A:C8	2.46	0.50
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.85	0.50
6:C:118:THR:O	6:C:136:VAL:HG13	2.10	0.50
8:E:69:ILE:HA	8:E:72:MET:HE3	1.93	0.50
2:9:3050:G:H5''	16:N:159:TYR:CE1	2.47	0.50
7:D:51:ARG:HD3	39:D:7636:HOH:O	2.11	0.50
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.51	0.50
1:O:1506:U:H6	1:O:1506:U:H5'	1.76	0.50
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.93	0.50
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.12	0.50
1:0:1687:C:O2	29:1:9:GLY:HA2	2.11	0.50
1:0:20:G:H21	20:R:117:HIS:HD2	1.58	0.50
1:0:2480:G:H3'	39:0:4777:HOH:O	2.11	0.50
8:E:20:ILE:CD1	8:E:33:LEU:HD12	2.42	0.50
1:0:1184:C:H4'	32:I:126:LYS:HB3	1.92	0.50
1:0:2704:C:O2	8:E:110:GLU:HB3	2.11	0.50
2:9:3049:G:O2'	2:9:3050:G:H5'	2.11	0.50
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.25	0.50
12:J:54:VAL:O	12:J:58:GLU:HG3	2.11	0.50
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.45	0.50
1:0:2825:C:H4'	1:0:2826:G:O5'	2.12	0.50
27:Y:209:VAL:HG12	27:Y:214:ARG:HG3	1.93	0.50
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.11	0.50
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.94	0.50
25:W:65:VAL:HA	25:W:68:THR:HG22	1.92	0.50
1:0:2912:C:H2'	1:0:2913:A:O4'	2.12	0.50
5:B:264:GLU:CG	5:B:267:LYS:HE2	2.28	0.50
1:0:2726:U:O2	1:0:2749:U:O5'	2.30	0.50
4:A:36:ASP:O	4:A:38:ILE:N	2.42	0.50
15:M:68:ARG:HD3	15:M:68:ARG:O	2.11	0.50
32:I:91:GLU:HB2	32:I:95:ASP:OD2	2.12	0.50
7:D:50:VAL:O	7:D:71:ALA:HA	2.11	0.50
11:H:148:GLU:HA	11:H:148:GLU:OE1	2.12	0.50
1:0:558:C:H2'	1:0:559:U:H5'	1.94	0.50
15:M:107:ARG:NH1	39:M:9378:HOH:O	2.44	0.50
8:E:7:ILE:HD11	8:E:11:VAL:O	2.11	0.50
1:0:894:A:N1	6:C:87:ARG:NH2	2.59	0.50
1:0:625:U:H5'	39:0:3793:HOH:O	2.12	0.50
1:0:2816:A:H2'	39:0:8491:HOH:O	2.12	0.50
1:0:1406:A:H4'	1:0:1407:A:H5''	1.94	0.50
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.47	0.50
7:D:37:ALA:O	7:D:40:ILE:HG12	2.11	0.50
1:0:2032:U:H2'	1:0:2033:G:H5'	1.92	0.50
31:3:35:TRP:HD1	39:3:9487:HOH:O	1.94	0.50
1:0:1701:A:H5'	39:0:6821:HOH:O	2.11	0.49
12:J:70:PHE:CG	12:J:70:PHE:O	2.65	0.49
27:Y:144:ARG:CG	27:Y:144:ARG:NH1	2.69	0.49
17:O:25:VAL:HG11	17:O:111:VAL:CG1	2.42	0.49
11:H:157:ILE:HD11	11:H:161:CYS:SG	2.52	0.49
1:0:2032:U:H2'	1:0:2033:G:C5'	2.42	0.49
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	1.92	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.32	0.49
1:0:1926:G:H2'	1:0:1927:A:C8	2.47	0.49
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.12	0.49
13:K:14:LYS:HG3	13:K:32:ILE:O	2.12	0.49
1:0:870:G:OP2	4:A:3:ARG:HD3	2.12	0.49
15:M:98:GLN:O	15:M:102:GLU:HG3	2.11	0.49
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.11	0.49
1:0:1435:U:H5'	39:0:3214:HOH:O	2.12	0.49
1:0:136:C:H2'	1:0:137:U:O4'	2.12	0.49
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.43	0.49
5:B:81:ALA:O	5:B:186:GLY:HA3	2.11	0.49
1:0:329:A:OP2	6:C:206:ASN:HB2	2.13	0.49
18:P:125:LYS:HB3	18:P:130:GLU:HG3	1.93	0.49
19:Q:30:VAL:HG12	19:Q:30:VAL:O	2.12	0.49
1:0:1118:A:C8	1:0:1118:A:C3'	2.91	0.49
1:0:1667:A:C8	1:0:1667:A:H5'	2.38	0.49
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.41	0.49
7:D:170:TYR:O	7:D:171:ASP:CB	2.60	0.49
9:F:16:ALA:HA	9:F:111:ILE:HD13	1.94	0.49
1:0:1773:G:C8	28:Z:16:ALA:HA	2.47	0.49
1:0:1736:A:H1'	39:0:8155:HOH:O	2.12	0.49
7:D:135:VAL:HG22	7:D:136:ARG:N	2.27	0.49
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.53	0.49
6:C:246:ARG:NH1	39:C:9174:HOH:O	2.44	0.49
1:0:1666:C:H2'	1:0:1667:A:C5'	2.42	0.49
4:A:105:VAL:HG12	4:A:106:CYS:N	2.27	0.49
32:I:105:VAL:HG11	32:I:129:VAL:CG2	2.42	0.49
12:J:39:VAL:HG13	12:J:106:GLY:O	2.12	0.49
1:0:666:A:H2'	1:0:667:C:O4'	2.13	0.49
22:T:88:PRO:HB3	39:T:6320:HOH:O	2.13	0.49
31:3:3:MET:O	31:3:90:PHE:HA	2.12	0.49
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.94	0.49
6:C:19:PRO:HG2	6:C:22:PHE:CE1	2.48	0.49
1:0:2748:G:OP1	1:0:2749:U:H5''	2.12	0.49
32:I:129:VAL:HG13	32:I:139:ILE:HD11	1.95	0.49
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.94	0.49
13:K:49:LEU:HD12	13:K:80:ILE:HD13	1.94	0.49
12:J:15:ARG:NH1	12:J:43:ARG:NH1	2.61	0.49
25:W:137:GLN:NE2	25:W:141:HIS:HE1	1.95	0.49
24:V:8:ILE:HA	24:V:11:MET:HE2	1.95	0.49
1:0:2895:C:H4'	39:X:4132:HOH:O	2.12	0.49
1:0:653:C:H2'	1:0:654:A:C8	2.48	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.94	0.49
6:C:25:PRO:HG2	39:C:9123:HOH:O	2.12	0.49
7:D:23:VAL:O	7:D:23:VAL:HG23	2.13	0.49
2:9:3057:A:C8	7:D:141:VAL:HG21	2.47	0.49
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.41	0.49
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.11	0.49
1:0:399:C:H5'	15:M:179:GLY:O	2.12	0.49
1:0:2365:G:H5''	39:Q:6597:HOH:O	2.10	0.49
6:C:153:VAL:O	6:C:157:LEU:HG	2.13	0.49
15:M:69:LYS:HG3	15:M:126:GLN:CA	2.42	0.49
6:C:194:PHE:CE2	6:C:234:VAL:HG11	2.48	0.49
20:R:39:THR:HG23	20:R:107:GLU:O	2.13	0.49
1:0:1573:A:H2'	1:0:1574:C:O4'	2.12	0.49
27:Y:145:LYS:HE2	39:Y:9403:HOH:O	2.13	0.49
13:K:23:ASN:HD21	13:K:107:THR:HB	1.77	0.49
1:0:328:U:O4'	6:C:202:THR:HG22	2.13	0.49
12:J:142:ASN:O	12:J:144:THR:N	2.46	0.49
11:H:78:GLY:C	11:H:80:GLU:H	2.16	0.49
10:G:14:GLU:HB3	39:G:4173:HOH:O	2.13	0.49
14:L:89:PHE:CD1	14:L:89:PHE:N	2.81	0.49
22:T:69:LYS:O	22:T:71:VAL:HG23	2.13	0.49
25:W:84:VAL:HG12	39:W:6679:HOH:O	2.11	0.49
21:S:57:THR:CG2	21:S:58:MET:N	2.75	0.49
5:B:190:MET:CE	5:B:194:PHE:CD1	2.96	0.49
24:V:64:GLY:O	24:V:65:ASP:CB	2.60	0.49
7:D:104:PHE:CE2	7:D:166:ILE:HD13	2.48	0.49
15:M:61:ILE:N	15:M:61:ILE:HD12	2.27	0.49
1:0:1853:C:O2'	4:A:217:ARG:NH2	2.46	0.49
39:O:3561:HOH:O	26:X:23:HIS:HD2	1.95	0.49
9:F:29:VAL:HG12	9:F:98:VAL:HA	1.94	0.49
1:0:2626:C:H2'	1:0:2627:G:C8	2.48	0.49
1:0:2456:A:H2'	1:0:2457:U:C6	2.48	0.49
1:0:1165:G:O3'	1:0:1174:A:H4'	2.13	0.48
5:B:62:ARG:CA	5:B:65:MET:HE3	2.43	0.48
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.27	0.48
5:B:17:LYS:O	5:B:260:HIS:HD2	1.95	0.48
1:0:2908:A:C2'	1:0:2909:G:H5'	2.42	0.48
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.48	0.48
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.77	0.48
12:J:50:GLU:O	12:J:54:VAL:HG23	2.13	0.48
18:P:121:ASP:O	18:P:125:LYS:HG3	2.13	0.48
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:M:169:ARG:NH2	39:M:9352:HOH:O	2.46	0.48
13:K:125:ALA:C	13:K:127:ALA:H	2.15	0.48
1:O:449:A:C8	6:C:43:LYS:HG2	2.48	0.48
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.93	0.48
13:K:87:ARG:NE	39:K:4854:HOH:O	2.46	0.48
1:O:1209:C:H2'	1:O:1210:G:C8	2.48	0.48
32:I:139:ILE:HG22	32:I:140:GLU:N	2.29	0.48
7:D:24:HIS:HB2	7:D:72:LYS:HB3	1.94	0.48
4:A:39:ALA:HB3	4:A:61:GLU:OE2	2.14	0.48
1:O:737:A:H2'	1:O:738:G:O4'	2.13	0.48
6:C:140:VAL:HG12	6:C:141:SER:N	2.28	0.48
20:R:96:VAL:HG13	20:R:106:GLY:HA3	1.95	0.48
1:O:558:C:C2'	1:O:559:U:C5'	2.91	0.48
1:O:656:G:C5'	17:O:3:THR:HG22	2.40	0.48
10:G:12:ILE:HG13	39:G:6833:HOH:O	2.12	0.48
14:L:91:VAL:CG1	14:L:120:LEU:HD23	2.43	0.48
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.94	0.48
1:O:1675:C:H5''	30:2:5:LYS:HD2	1.95	0.48
1:O:371:U:H2'	1:O:372:A:H8	1.77	0.48
24:V:43:PRO:O	24:V:46:ILE:HG22	2.12	0.48
1:O:1198:U:H2'	1:O:1200:A:OP2	2.13	0.48
39:O:4965:HOH:O	15:M:83:SER:HB3	2.13	0.48
5:B:7:ARG:HG2	5:B:7:ARG:HH11	1.78	0.48
26:X:72:VAL:CG2	26:X:85:VAL:HG12	2.37	0.48
1:O:1603:A:H5''	1:O:1605:G:H5'	1.95	0.48
1:O:1972:U:H2'	1:O:1973:A:H5'	1.96	0.48
23:U:20:MET:CG	23:U:28:THR:HG23	2.44	0.48
14:L:145:LEU:O	14:L:148:GLU:HG3	2.13	0.48
14:L:97:VAL:O	14:L:100:ALA:HB2	2.13	0.48
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.77	0.48
4:A:135:VAL:HG21	4:A:147:ARG:NH1	2.28	0.48
14:L:72:ASN:HB2	39:L:9480:HOH:O	2.13	0.48
1:O:951:A:C2'	1:O:952:G:H5'	2.43	0.48
26:X:43:VAL:CG1	26:X:44:ASP:N	2.76	0.48
1:O:204:A:C2'	1:O:205:U:H5'	2.44	0.48
5:B:294:TYR:HE2	39:B:9644:HOH:O	1.95	0.48
11:H:75:LYS:O	11:H:75:LYS:HG2	2.13	0.48
1:O:1242:A:C5'	12:J:82:THR:HG23	2.36	0.48
6:C:107:ARG:NH1	39:C:9235:HOH:O	2.47	0.48
11:H:29:ALA:C	11:H:30:GLN:HG3	2.33	0.48
18:P:16:VAL:HG13	18:P:20:ARG:CZ	2.43	0.48
1:O:776:A:OP1	29:1:28:HIS:HE1	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:820:G:O2'	1:0:856:G:H4'	2.14	0.48
32:I:128:VAL:C	32:I:130:GLY:H	2.16	0.48
1:0:2837:U:H2'	39:0:7353:HOH:O	2.13	0.48
12:J:52:GLN:HG3	12:J:53:ILE:N	2.28	0.48
39:9:5071:HOH:O	16:N:18:THR:HG21	2.12	0.48
1:0:1462:C:H2'	1:0:1463:A:H8	1.78	0.48
7:D:82:GLU:HA	7:D:85:GLN:HE21	1.78	0.48
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.49	0.48
5:B:75:GLU:C	5:B:77:PRO:HD3	2.33	0.48
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.29	0.48
1:0:1056:U:H2'	1:0:1057:A:O4'	2.13	0.48
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.95	0.48
2:9:3092:G:H2'	2:9:3093:A:C8	2.49	0.48
11:H:116:ALA:O	11:H:117:PHE:C	2.52	0.48
7:D:25:MET:CE	7:D:37:ALA:HB1	2.40	0.48
4:A:88:ILE:HG22	4:A:88:ILE:O	2.13	0.48
15:M:187:LEU:HD22	15:M:194:ALA:HB3	1.95	0.48
1:0:1159:G:H1	1:0:1208:C:H42	1.62	0.48
1:0:2820:A:H2'	1:0:2821:C:C6	2.47	0.48
32:I:78:LEU:HD12	32:I:112:LYS:HZ2	1.77	0.48
1:0:249:G:O2'	1:0:250:C:H5'	2.14	0.48
19:Q:3:SER:HB3	39:Q:5998:HOH:O	2.13	0.48
1:0:482:G:H4'	1:0:508:A:N1	2.29	0.48
31:3:65:THR:CG2	31:3:67:LEU:HG	2.42	0.48
11:H:1:LYS:HE2	11:H:1:LYS:HA	1.95	0.48
1:0:2072:G:H3'	1:0:2073:G:C5'	2.44	0.48
5:B:84:LEU:HB2	5:B:182:VAL:HG21	1.96	0.48
1:0:2421:G:H2'	39:0:4671:HOH:O	2.12	0.48
13:K:28:GLU:OE2	13:K:58:THR:HG21	2.14	0.48
2:9:3024:U:H3'	2:9:3025:G:H5'	1.95	0.48
1:0:2348:C:H1'	7:D:131:THR:HG21	1.96	0.48
1:0:90:A:H2'	1:0:91:G:O4'	2.14	0.48
25:W:142:ASP:HB3	25:W:145:GLY:H	1.79	0.48
20:R:132:ARG:NH2	39:R:9492:HOH:O	2.47	0.48
23:U:47:ARG:HG2	39:U:4381:HOH:O	2.14	0.48
12:J:103:VAL:HG12	39:J:5907:HOH:O	2.14	0.48
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.49	0.48
4:A:223:ARG:NE	39:A:9560:HOH:O	2.46	0.48
20:R:18:LEU:HB2	20:R:143:VAL:HG13	1.95	0.48
17:O:57:THR:HB	17:O:111:VAL:HG23	1.96	0.48
1:0:1634:G:H3'	39:0:4492:HOH:O	2.13	0.48
31:3:17:HIS:O	31:3:18:GLN:HG3	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2414:A:H2'	1:0:2415:A:C8	2.49	0.48
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.96	0.48
1:0:1942:A:H3'	39:0:7839:HOH:O	2.14	0.48
1:0:834:G:H4'	1:0:835:U:OP2	2.14	0.48
14:L:10:SER:O	14:L:11:ARG:HB3	2.13	0.48
14:L:21:ARG:N	39:L:9424:HOH:O	2.46	0.48
13:K:81:ARG:HD3	13:K:87:ARG:CZ	2.44	0.47
4:A:51:ARG:NH1	4:A:120:ARG:O	2.47	0.47
1:0:2363:G:O2'	19:Q:11:ARG:HG3	2.14	0.47
32:I:72:VAL:HG11	32:I:111:GLN:O	2.13	0.47
4:A:194:MET:CE	4:A:199:HIS:HB2	2.44	0.47
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.29	0.47
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.17	0.47
17:O:80:ASP:OD1	17:O:81:PHE:N	2.47	0.47
1:0:1236:A:H2'	1:0:1237:U:O4'	2.14	0.47
1:0:1477:C:H5'	1:0:1868:G:C5'	2.44	0.47
1:0:1290:G:H3'	39:0:5735:HOH:O	2.13	0.47
1:0:1333:U:H2'	1:0:1334:C:C6	2.49	0.47
1:0:2587:OMU:H6	1:0:2587:OMU:O5'	2.13	0.47
7:D:172:VAL:HG12	7:D:173:GLU:N	2.28	0.47
27:Y:122:ARG:NH2	39:Y:9333:HOH:O	2.47	0.47
1:0:1750:C:H4'	39:0:7969:HOH:O	2.15	0.47
5:B:254:GLN:HG2	5:B:255:GLY:H	1.79	0.47
25:W:110:GLN:HE21	25:W:110:GLN:HA	1.77	0.47
4:A:179:MET:HA	4:A:179:MET:HE3	1.97	0.47
7:D:99:ASP:O	7:D:159:PRO:HG3	2.14	0.47
1:0:1044:C:H5''	39:0:9647:HOH:O	2.13	0.47
17:O:98:LEU:O	17:O:102:ILE:HG13	2.15	0.47
1:0:2911:C:O2'	1:0:2912:C:H5'	2.14	0.47
12:J:88:PRO:O	12:J:94:GLY:HA3	2.15	0.47
1:0:2505:G:C2'	1:0:2506:A:H5'	2.45	0.47
22:T:71:VAL:CG1	22:T:72:ILE:N	2.77	0.47
4:A:36:ASP:HB2	4:A:85:SER:H	1.80	0.47
32:I:113:HIS:N	32:I:114:PRO:CD	2.78	0.47
3:4:75:C:H2'	3:4:76:PPU:C8	2.44	0.47
8:E:125:GLU:HB2	8:E:132:THR:HG23	1.97	0.47
7:D:44:ILE:HG23	7:D:45:THR:HG23	1.97	0.47
1:0:1973:A:H5'	1:0:1973:A:C8	2.40	0.47
5:B:41:PHE:CG	5:B:190:MET:HE3	2.49	0.47
2:9:3008:G:O6	16:N:11:ARG:NH1	2.43	0.47
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.14	0.47
10:G:24:VAL:O	10:G:28:GLU:HB2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:26:ASP:CG	4:A:26:ASP:O	2.53	0.47
1:0:926:A:O2'	14:L:41:HIS:CD2	2.67	0.47
1:0:449:A:N7	6:C:43:LYS:HG2	2.29	0.47
1:0:2711:U:H1'	39:0:4046:HOH:O	2.13	0.47
39:0:4783:HOH:O	27:Y:186:ARG:HD2	2.15	0.47
1:0:317:A:H5''	22:T:52:ARG:HD2	1.96	0.47
6:C:236:THR:HG22	6:C:239:ALA:CB	2.45	0.47
21:S:57:THR:HG22	21:S:58:MET:N	2.29	0.47
7:D:76:ARG:O	7:D:77:ASP:HB2	2.14	0.47
1:0:1181:A:N1	1:0:1192:A:O2'	2.47	0.47
16:N:170:GLU:HA	16:N:173:ASP:OD2	2.15	0.47
1:0:1167:G:H4'	32:I:135:LEU:HD22	1.97	0.47
9:F:101:ALA:HA	39:F:5413:HOH:O	2.15	0.47
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.45	0.47
17:O:39:THR:O	17:O:115:ARG:NH2	2.47	0.47
7:D:27:ILE:HD11	7:D:37:ALA:HB3	1.96	0.47
8:E:20:ILE:HD12	8:E:33:LEU:HD12	1.95	0.47
1:0:1119:G:H8	12:J:52:GLN:NE2	2.09	0.47
22:T:96:VAL:HG13	22:T:97:ARG:N	2.29	0.47
14:L:73:VAL:HG23	14:L:74:THR:N	2.24	0.47
1:0:396:U:H1'	39:0:8194:HOH:O	2.15	0.47
7:D:166:ILE:HB	39:D:6326:HOH:O	2.14	0.47
1:0:709:G:O2'	17:O:25:VAL:CG1	2.62	0.47
17:O:25:VAL:HG23	17:O:26:TRP:N	2.29	0.47
24:V:8:ILE:HA	24:V:11:MET:HE3	1.96	0.47
14:L:145:LEU:O	14:L:145:LEU:HD23	2.15	0.47
1:0:2456:A:H2'	1:0:2457:U:H6	1.80	0.47
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.44	0.47
1:0:2541:U:H3	1:0:2618:G:H1	1.61	0.47
1:0:1482:A:O2'	1:0:1483:C:H5'	2.15	0.47
26:X:34:ARG:NH1	26:X:48:VAL:O	2.45	0.47
8:E:1:PRO:HG2	8:E:59:MET:SD	2.55	0.47
1:0:1234:U:N3	5:B:244:PRO:HB3	2.30	0.47
1:0:1066:U:H2'	1:0:1067:A:C8	2.49	0.47
4:A:121:ALA:O	4:A:124:VAL:HG22	2.14	0.47
5:B:280:VAL:HG13	5:B:333:GLU:O	2.14	0.47
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.15	0.47
20:R:119:VAL:CG1	20:R:119:VAL:O	2.62	0.47
25:W:4:LEU:HD11	25:W:45:VAL:HG12	1.97	0.47
4:A:131:HIS:O	4:A:132:ASP:HB2	2.14	0.47
16:N:93:GLN:HE21	16:N:127:LEU:CD1	2.27	0.47
1:0:1503:U:H2'	1:0:1504:A:O4'	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:171:VAL:HG23	5:B:172:SER:N	2.30	0.47
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.80	0.47
26:X:7:GLU:HA	26:X:74:ALA:O	2.14	0.47
15:M:164:THR:CG2	15:M:165:GLY:N	2.78	0.47
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.96	0.47
11:H:169:GLY:HA3	39:H:9555:HOH:O	2.13	0.47
24:V:39:ALA:C	24:V:41:GLU:H	2.19	0.47
8:E:23:GLU:HG2	8:E:28:SER:CB	2.44	0.47
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.97	0.47
1:O:2890:A:H1'	23:U:56:ARG:CZ	2.45	0.47
2:9:3041:C:O4'	7:D:50:VAL:HG22	2.14	0.47
1:O:68:U:H4'	39:O:7269:HOH:O	2.14	0.47
1:O:1684:A:H1'	30:2:43:ARG:HH22	1.79	0.47
1:O:920:C:H4'	1:O:921:G:C2	2.50	0.47
1:O:1342:C:C2'	1:O:1343:C:H5'	2.45	0.47
6:C:154:VAL:O	6:C:158:GLU:HG3	2.15	0.47
6:C:168:ARG:NH2	6:C:190:ALA:O	2.48	0.47
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.96	0.47
4:A:109:GLU:HG2	4:A:116:GLY:N	2.30	0.47
11:H:28:ILE:HG21	11:H:31:HIS:CE1	2.50	0.47
39:9:5537:HOH:O	16:N:110:THR:HG22	2.16	0.47
25:W:88:THR:CG2	25:W:89:ASP:N	2.72	0.47
4:A:39:ALA:O	4:A:61:GLU:HG3	2.14	0.47
1:O:1350:U:H2'	1:O:1351:G:O4'	2.15	0.47
1:O:2531:U:O2'	1:O:2532:A:H5'	2.14	0.47
20:R:46:TYR:O	20:R:50:VAL:HG23	2.14	0.47
7:D:128:LEU:HB2	39:D:6007:HOH:O	2.14	0.47
1:O:2299:G:O6	19:Q:1:PRO:HA	2.15	0.47
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.97	0.46
1:O:541:C:C2'	1:O:542:A:C5'	2.92	0.46
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.96	0.46
2:9:3039:U:C2'	2:9:3040:C:OP1	2.63	0.46
22:T:96:VAL:CG1	22:T:97:ARG:N	2.78	0.46
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.16	0.46
1:O:88:G:H2'	1:O:89:G:C8	2.49	0.46
1:O:2353:A:H4'	1:O:2354:A:O5'	2.15	0.46
1:O:1714:C:O2'	1:O:1715:C:H5'	2.15	0.46
1:O:1098:A:H2'	1:O:1099:G:O4'	2.15	0.46
2:9:3107:C:H5	39:9:3167:HOH:O	1.97	0.46
23:U:17:THR:CG2	23:U:18:GLY:H	2.28	0.46
11:H:59:HIS:HA	11:H:62:LEU:HD23	1.95	0.46
20:R:61:GLN:NE2	39:R:9449:HOH:O	2.48	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.62	0.46
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.50	0.46
32:I:124:ALA:O	32:I:128:VAL:HG23	2.15	0.46
20:R:132:ARG:CZ	39:R:9492:HOH:O	2.63	0.46
20:R:114:VAL:HA	20:R:144:GLU:O	2.15	0.46
16:N:89:GLY:O	16:N:92:ALA:HB3	2.15	0.46
6:C:219:ASN:O	6:C:222:ASP:OD1	2.33	0.46
10:G:19:GLU:HG2	10:G:66:LEU:HD13	1.98	0.46
9:F:31:LYS:HE3	39:F:2623:HOH:O	2.15	0.46
1:O:244:C:OP2	9:F:38:LYS:HE3	2.15	0.46
26:X:45:GLU:HG3	39:X:6178:HOH:O	2.14	0.46
14:L:101:ASP:C	14:L:103:ALA:H	2.19	0.46
5:B:41:PHE:HA	5:B:79:MET:HE2	1.97	0.46
2:9:3051:A:H5'	16:N:160:SER:HB2	1.96	0.46
24:V:56:ILE:HG22	24:V:60:GLN:NE2	2.31	0.46
1:O:2769:C:H2'	1:O:2770:G:H5'	1.96	0.46
30:2:36:ASN:HB3	30:2:39:ARG:NE	2.30	0.46
1:O:1067:A:H5'	39:O:4933:HOH:O	2.15	0.46
1:O:794:U:H3	1:O:819:A:H61	1.62	0.46
20:R:69:LYS:HB2	20:R:72:VAL:HG23	1.97	0.46
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.97	0.46
20:R:84:ALA:O	20:R:88:PHE:HD1	1.98	0.46
1:O:2712:G:H5'	39:K:4183:HOH:O	2.16	0.46
6:C:5:ILE:HG13	6:C:15:GLU:HA	1.97	0.46
4:A:34:ASP:OD1	4:A:35:GLY:N	2.49	0.46
22:T:20:HIS:HB3	22:T:41:ARG:HD2	1.96	0.46
8:E:81:GLU:HG2	8:E:134:SER:HB2	1.97	0.46
14:L:145:LEU:C	14:L:145:LEU:HD23	2.35	0.46
1:O:316:A:N3	1:O:336:G:O2'	2.43	0.46
1:O:2824:C:H5''	1:O:2825:C:H5'	1.97	0.46
24:V:42:ASN:O	24:V:44:GLY:N	2.48	0.46
1:O:1669:A:H2'	1:O:1670:G:C8	2.51	0.46
1:O:497:A:H2'	1:O:498:A:C5'	2.45	0.46
1:O:2338:G:H2'	7:D:129:ASP:OD1	2.16	0.46
1:O:259:G:H21	15:M:58:GLN:NE2	2.14	0.46
5:B:36:PRO:HA	5:B:167:GLY:O	2.16	0.46
4:A:203:GLY:HA2	39:A:9534:HOH:O	2.14	0.46
16:N:43:VAL:CG1	16:N:118:ILE:HD11	2.46	0.46
39:9:4707:HOH:O	16:N:147:ILE:HD12	2.15	0.46
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.15	0.46
1:O:368:C:H2'	1:O:369:G:H5'	1.97	0.46
1:O:2591:C:H2'	1:O:2592:G:O4'	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2852:A:H5''	39:0:5799:HOH:O	2.15	0.46
1:0:2676:C:H6	1:0:2676:C:H5''	1.81	0.46
1:0:2779:G:H21	8:E:143:GLN:NE2	2.13	0.46
11:H:47:ILE:HD12	11:H:146:VAL:CG1	2.45	0.46
1:0:952:G:N3	1:0:2302:A:H2'	2.31	0.46
1:0:1940:C:H4'	39:0:7839:HOH:O	2.15	0.46
16:N:87:LEU:HD21	16:N:91:ARG:NH2	2.30	0.46
1:0:2906:A:H5'	1:0:2907:C:O4'	2.15	0.46
7:D:21:VAL:HG23	7:D:80:ALA:HB1	1.97	0.46
7:D:96:SER:C	7:D:98:PHE:H	2.18	0.46
1:0:2831:C:O3'	20:R:71:LYS:HE2	2.16	0.46
9:F:65:GLU:O	9:F:69:GLU:HG2	2.16	0.46
20:R:122:GLN:HB3	20:R:138:SER:HB2	1.95	0.46
7:D:27:ILE:HG22	7:D:28:GLY:N	2.29	0.46
23:U:17:THR:HG22	23:U:18:GLY:H	1.79	0.46
1:0:1666:C:C2'	1:0:1667:A:C5'	2.94	0.46
1:0:2346:C:O5'	1:0:2346:C:H6	1.98	0.46
2:9:3054:A:O2'	2:9:3055:U:H5'	2.15	0.46
39:0:3175:HOH:O	25:W:119:HIS:HE1	1.98	0.46
1:0:1748:U:H4'	39:0:8016:HOH:O	2.15	0.46
21:S:2:TRP:CH2	21:S:31:ARG:HB2	2.51	0.46
12:J:92:GLN:HB3	39:J:1405:HOH:O	2.15	0.46
1:0:2401:A:H2'	1:0:2402:A:C8	2.51	0.46
5:B:175:LEU:O	5:B:175:LEU:HD23	2.16	0.46
12:J:76:ASP:HA	39:J:5907:HOH:O	2.14	0.46
5:B:307:ARG:CG	5:B:307:ARG:HH11	2.21	0.46
5:B:41:PHE:HA	5:B:79:MET:CE	2.45	0.46
39:0:7645:HOH:O	29:1:1:THR:HB	2.15	0.46
23:U:49:LEU:HG	39:U:3805:HOH:O	2.15	0.46
30:2:22:PRO:HG2	30:2:25:VAL:HG21	1.97	0.46
9:F:12:LEU:CD2	9:F:111:ILE:HG23	2.46	0.46
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.51	0.46
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.51	0.46
27:Y:212:ARG:HD2	39:Y:9399:HOH:O	2.15	0.46
13:K:7:ASP:OD2	13:K:81:ARG:NH2	2.48	0.46
39:0:7912:HOH:O	22:T:9:LYS:HG3	2.14	0.46
1:0:1185:U:OP1	32:I:126:LYS:HD3	2.15	0.46
1:0:137:U:H2'	1:0:139:C:C5	2.51	0.46
1:0:2320:U:H4'	1:0:2321:A:O4'	2.15	0.46
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.97	0.46
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.98	0.46
14:L:134:GLU:HG3	39:L:9454:HOH:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:1120:U:H5''	1:O:1120:U:C6	2.51	0.46
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.46	0.46
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.97	0.46
1:O:1667:A:H2'	1:O:1668:U:C6	2.51	0.46
11:H:119:LYS:HB2	11:H:119:LYS:HE3	1.75	0.46
1:O:1168:C:H5''	32:I:87:THR:HG23	1.98	0.46
4:A:126:ALA:HB1	4:A:138:VAL:CG1	2.46	0.46
1:O:2453:G:H5''	39:L:9437:HOH:O	2.15	0.46
1:O:424:C:H2'	1:O:425:U:C6	2.50	0.46
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.78	0.46
7:D:154:LYS:HD2	7:D:154:LYS:N	2.31	0.46
25:W:139:GLY:O	25:W:141:HIS:CD2	2.68	0.46
6:C:78:ARG:CG	6:C:78:ARG:NH1	2.75	0.46
30:2:49:GLU:HB2	39:2:131:HOH:O	2.15	0.46
4:A:105:VAL:HG13	4:A:155:THR:O	2.15	0.46
5:B:97:LEU:O	5:B:98:THR:HG23	2.16	0.46
32:I:75:THR:CA	32:I:112:LYS:HZ3	2.28	0.46
1:O:470:U:O2'	29:1:16:HIS:CD2	2.65	0.46
1:O:999:C:H2'	1:O:1000:C:O4'	2.16	0.46
16:N:74:PRO:HG2	16:N:159:TYR:CE1	2.51	0.46
31:3:65:THR:HG23	31:3:67:LEU:HG	1.98	0.46
7:D:95:THR:OG1	7:D:174:VAL:HG22	2.16	0.46
1:O:2515:C:H2'	1:O:2516:G:O4'	2.15	0.46
16:N:132:ASN:O	16:N:135:VAL:HG12	2.15	0.46
1:O:432:G:O2'	1:O:433:C:H5'	2.16	0.46
15:M:47:ASP:CG	15:M:48:LYS:N	2.70	0.46
22:T:47:THR:HB	22:T:100:ASP:HB3	1.97	0.46
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.49	0.46
1:O:2635:A:C2'	1:O:2636:C:H5'	2.46	0.45
4:A:33:GLU:OE1	4:A:33:GLU:N	2.31	0.45
2:9:3049:G:H2'	2:9:3050:G:O4'	2.17	0.45
7:D:167:GLU:C	7:D:169:THR:H	2.20	0.45
1:O:2329:C:O2'	1:O:2330:U:H5'	2.16	0.45
1:O:2649:A:H5'	1:O:2649:A:H8	1.81	0.45
15:M:43:PRO:HG3	15:M:62:VAL:HG21	1.97	0.45
11:H:69:ALA:HB2	11:H:153:ALA:HB2	1.98	0.45
1:O:588:G:O6	25:W:154:ARG:NH1	2.50	0.45
25:W:48:VAL:CG1	25:W:48:VAL:O	2.64	0.45
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.27	0.45
27:Y:154:ARG:NH1	27:Y:155:ARG:HG2	2.24	0.45
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.98	0.45
1:O:834:G:H3'	1:O:835:U:H4'	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1342:C:O2'	1:0:1343:C:H5'	2.16	0.45
5:B:36:PRO:HB3	5:B:174:ARG:CB	2.47	0.45
15:M:72:ALA:HB2	15:M:93:ARG:HG2	1.98	0.45
1:0:1306:U:OP1	6:C:184:ARG:HD2	2.17	0.45
1:0:2612:A:H4'	39:0:4284:HOH:O	2.15	0.45
1:0:256:C:H2'	1:0:257:G:O4'	2.16	0.45
25:W:85:ALA:HB2	25:W:91:ASP:O	2.16	0.45
1:0:263:U:O4'	9:F:59:ILE:HD13	2.16	0.45
9:F:70:LYS:C	9:F:72:VAL:H	2.20	0.45
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.16	0.45
15:M:74:LYS:HG2	15:M:75:ARG:N	2.30	0.45
12:J:47:THR:HG22	12:J:48:GLY:N	2.32	0.45
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.45	0.45
1:0:120:A:H2'	1:0:120:A:N3	2.32	0.45
4:A:65:ARG:C	4:A:66:ARG:HG3	2.36	0.45
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.98	0.45
6:C:19:PRO:HG2	6:C:22:PHE:CD1	2.51	0.45
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.49	0.45
1:0:286:U:H2'	1:0:287:C:C6	2.52	0.45
4:A:207:GLN:O	4:A:208:HIS:HB3	2.16	0.45
1:0:1751:G:C2'	1:0:1752:G:H5''	2.43	0.45
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.49	0.45
20:R:119:VAL:HG12	20:R:119:VAL:O	2.17	0.45
1:0:426:G:H2'	1:0:427:C:O4'	2.16	0.45
15:M:184:ARG:HG3	15:M:185:PRO:HA	1.99	0.45
1:0:702:G:O2'	1:0:703:G:H5'	2.17	0.45
1:0:1441:G:O2'	1:0:1442:A:H5'	2.17	0.45
23:U:4:ARG:HH11	23:U:4:ARG:HG2	1.81	0.45
1:0:288:A:H2'	1:0:289:G:C8	2.50	0.45
9:F:60:VAL:HG13	9:F:63:ILE:HG13	1.97	0.45
24:V:39:ALA:O	24:V:41:GLU:N	2.42	0.45
1:0:319:A:H4'	1:0:338:C:C5	2.51	0.45
5:B:146:THR:C	5:B:148:PRO:HD3	2.37	0.45
1:0:64:G:H2'	1:0:65:C:O4'	2.17	0.45
1:0:284:C:H4'	1:0:285:A:H8	1.82	0.45
39:0:4996:HOH:O	4:A:11:ARG:CZ	2.64	0.45
1:0:1131:G:H5'	2:9:3091:C:O4'	2.16	0.45
1:0:363:A:H1'	39:0:5847:HOH:O	2.15	0.45
16:N:64:SER:C	16:N:66:LEU:H	2.20	0.45
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.23	0.45
5:B:41:PHE:CD2	5:B:190:MET:HE3	2.52	0.45
1:0:338:C:H4'	6:C:174:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:H:40:ALA:HB1	11:H:137:TYR:CD2	2.52	0.45
1:0:2415:A:H2'	1:0:2416:G:H5'	1.98	0.45
9:F:99:THR:HG23	9:F:99:THR:O	2.17	0.45
13:K:98:VAL:CG2	13:K:102:GLU:C	2.85	0.45
15:M:114:VAL:O	15:M:158:ARG:HD3	2.17	0.45
7:D:10:PHE:CG	7:D:11:HIS:N	2.84	0.45
24:V:12:THR:OG1	24:V:13:PRO:HD2	2.16	0.45
29:1:25:LYS:HD2	30:2:48:ASP:CA	2.46	0.45
28:Z:42:CYS:SG	28:Z:59:TYR:HD2	2.40	0.45
12:J:75:PRO:HD3	12:J:136:SER:OG	2.16	0.45
1:0:1203:G:O2'	1:0:1204:C:H5'	2.17	0.45
7:D:170:TYR:CD1	7:D:170:TYR:N	2.85	0.45
1:0:1167:G:H2'	1:0:1168:C:O4'	2.16	0.45
1:0:2402:A:O2'	1:0:2403:C:H5'	2.17	0.45
32:I:101:SER:OG	32:I:104:GLN:HG3	2.16	0.45
1:0:1252:A:H2'	1:0:1253:C:O4'	2.16	0.45
1:0:2019:A:H5'	39:0:5123:HOH:O	2.16	0.45
25:W:125:HIS:HE1	39:W:3071:HOH:O	1.99	0.45
1:0:506:G:N2	1:0:509:A:H5"	2.21	0.45
14:L:67:ARG:HG2	14:L:67:ARG:HH11	1.81	0.45
27:Y:144:ARG:NH1	39:Y:9374:HOH:O	2.50	0.45
8:E:101:GLU:OE2	8:E:115:ARG:HD3	2.17	0.45
4:A:101:GLU:HB3	4:A:129:LEU:O	2.15	0.45
1:0:432:G:H2'	1:0:433:C:H6	1.82	0.45
7:D:10:PHE:CD1	7:D:11:HIS:N	2.85	0.45
25:W:78:ASP:OD2	25:W:79:VAL:N	2.50	0.45
16:N:83:LEU:HD13	16:N:175:LEU:CD2	2.41	0.45
1:0:1592:G:O2'	1:0:1593:C:O4'	2.32	0.45
1:0:2072:G:C6	1:0:2533:C:H1'	2.52	0.45
14:L:143:THR:CG2	14:L:144:ASP:N	2.80	0.45
1:0:1734:C:OP1	5:B:234:ARG:NH1	2.50	0.45
7:D:82:GLU:HA	7:D:85:GLN:NE2	2.32	0.45
1:0:1484:G:H2'	39:0:9723:HOH:O	2.16	0.45
1:0:1086:A:C6	25:W:11:VAL:HG11	2.52	0.45
6:C:150:THR:HA	6:C:203:ALA:O	2.17	0.45
1:0:542:A:H2'	1:0:543:G:O4'	2.17	0.45
24:V:56:ILE:HG22	24:V:60:GLN:HE21	1.80	0.45
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.98	0.45
1:0:2883:A:H2'	1:0:2884:G:O4'	2.17	0.45
25:W:11:VAL:O	25:W:12:ASN:HB2	2.17	0.45
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.16	0.45
39:0:4690:HOH:O	5:B:216:LYS:HE2	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2102:G:H5''	1:0:2538:A:C2	2.51	0.45
1:0:2724:U:H2'	1:0:2725:G:O4'	2.17	0.45
1:0:1724:U:H5''	39:0:4333:HOH:O	2.16	0.45
6:C:72:LYS:HG2	6:C:77:ALA:HA	1.99	0.44
1:0:362:G:H2'	1:0:363:A:C8	2.52	0.44
25:W:13:MET:HE1	25:W:18:GLN:CA	2.41	0.44
2:9:3044:A:O4'	7:D:76:ARG:NE	2.50	0.44
2:9:3028:U:H2'	2:9:3029:C:C6	2.52	0.44
1:0:1527:A:H1'	1:0:1528:A:C8	2.52	0.44
1:0:1175:G:H2'	1:0:1176:C:O4'	2.17	0.44
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.82	0.44
1:0:407:A:H8	39:0:5045:HOH:O	2.00	0.44
1:0:2541:U:H1'	3:4:76:PPU:O2'	2.17	0.44
39:0:9836:HOH:O	4:A:11:ARG:HD3	2.17	0.44
25:W:19:ASP:O	25:W:23:MET:HG3	2.17	0.44
9:F:14:ASP:O	9:F:18:GLU:HG3	2.17	0.44
1:0:366:U:H2'	1:0:367:G:O4'	2.17	0.44
7:D:25:MET:HE1	7:D:37:ALA:O	2.17	0.44
30:2:48:ASP:O	30:2:49:GLU:CB	2.65	0.44
1:0:1189:A:H1'	1:0:1209:C:H1'	1.99	0.44
16:N:86:LEU:HD21	16:N:180:LEU:HD12	1.99	0.44
1:0:317:A:OP1	22:T:52:ARG:O	2.35	0.44
10:G:19:GLU:HG2	10:G:66:LEU:CD1	2.47	0.44
1:0:220:C:H1'	39:0:6313:HOH:O	2.17	0.44
5:B:321:PRO:HA	39:B:9653:HOH:O	2.17	0.44
1:0:1380:U:O4	1:0:2043:U:H4'	2.17	0.44
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.99	0.44
39:9:3472:HOH:O	16:N:41:LYS:HD3	2.16	0.44
22:T:64:ASN:HB3	22:T:73:HIS:HB2	1.98	0.44
26:X:37:LEU:HD11	26:X:85:VAL:HG11	1.99	0.44
26:X:74:ALA:CB	26:X:85:VAL:HG13	2.25	0.44
26:X:30:MET:CE	26:X:58:ALA:HB3	2.43	0.44
14:L:143:THR:O	14:L:147:GLU:HG3	2.18	0.44
7:D:78:GLU:O	7:D:82:GLU:HG3	2.18	0.44
13:K:49:LEU:HD22	13:K:117:VAL:HG21	2.00	0.44
1:0:2894:C:O2'	1:0:2895:C:H5'	2.17	0.44
20:R:113:HIS:HE1	20:R:144:GLU:OE1	1.99	0.44
5:B:321:PRO:HG3	39:B:9599:HOH:O	2.17	0.44
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.81	0.44
1:0:2243:C:H5''	39:0:4351:HOH:O	2.18	0.44
4:A:56:ALA:O	4:A:68:ILE:HG22	2.17	0.44
12:J:74:ARG:HH12	12:J:76:ASP:CB	2.31	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1202:A:H2'	1:0:1203:G:O4'	2.18	0.44
24:V:8:ILE:CG2	24:V:59:ILE:HG13	2.46	0.44
16:N:171:HIS:CE1	39:N:9363:HOH:O	2.70	0.44
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.53	0.44
5:B:243:ASN:HA	5:B:244:PRO:C	2.37	0.44
39:0:9728:HOH:O	5:B:229:ARG:HD2	2.16	0.44
39:M:9334:HOH:O	31:3:46:ILE:HB	2.17	0.44
15:M:49:ALA:C	15:M:54:TYR:HB3	2.38	0.44
1:0:870:G:C3'	1:0:871:G:H5''	2.48	0.44
28:Z:10:ARG:HA	39:Z:9214:HOH:O	2.16	0.44
28:Z:11:SER:O	28:Z:14:PHE:HB2	2.17	0.44
23:U:52:THR:HG22	23:U:54:THR:H	1.80	0.44
10:G:27:ILE:HD13	10:G:71:LEU:HD23	1.98	0.44
7:D:51:ARG:HH11	7:D:68:PRO:HB3	1.83	0.44
26:X:20:GLU:HG3	26:X:21:PRO:CD	2.48	0.44
18:P:97:ARG:HD2	39:P:159:HOH:O	2.17	0.44
1:0:806:A:H2'	1:0:807:A:O4'	2.17	0.44
8:E:15:GLN:NE2	8:E:40:VAL:O	2.51	0.44
9:F:60:VAL:HG13	9:F:63:ILE:CG1	2.48	0.44
1:0:1180:U:O2'	32:I:92:PRO:HD2	2.18	0.44
32:I:105:VAL:HG11	32:I:129:VAL:HG22	1.99	0.44
1:0:664:U:O4	1:0:681:G:H5''	2.18	0.44
6:C:233:THR:HG22	6:C:234:VAL:N	2.32	0.44
23:U:44:ARG:HB3	39:U:3805:HOH:O	2.17	0.44
17:O:78:ALA:C	17:O:98:LEU:HD13	2.38	0.44
1:0:1200:A:H3'	39:0:6312:HOH:O	2.18	0.44
1:0:2649:A:C8	1:0:2649:A:H5'	2.53	0.44
32:I:85:PHE:CD1	32:I:98:ALA:HB2	2.53	0.44
1:0:1902:G:H2'	1:0:1903:U:O4'	2.17	0.44
1:0:308:U:C4	1:0:342:C:H1'	2.53	0.44
1:0:56:G:C5'	24:V:50:ARG:HH12	2.30	0.44
1:0:1878:G:O2'	1:0:1879:U:P	2.75	0.44
32:I:113:HIS:HE1	32:I:121:LEU:HD22	1.83	0.44
8:E:7:ILE:HA	8:E:8:PRO:HD3	1.92	0.44
12:J:42:GLU:O	12:J:131:THR:HG23	2.18	0.44
1:0:2663:U:O2	39:0:8491:HOH:O	2.21	0.44
4:A:96:LEU:O	4:A:131:HIS:HE1	2.00	0.44
1:0:398:U:H2'	1:0:399:C:C6	2.53	0.44
7:D:154:LYS:HD2	7:D:154:LYS:H	1.83	0.44
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.99	0.44
1:0:2104:C:O2	1:0:2485:A:N1	2.50	0.44
23:U:14:GLU:OE1	23:U:15:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1295:G:H4'	39:L:9490:HOH:O	2.18	0.44
4:A:36:ASP:O	4:A:36:ASP:CG	2.55	0.44
18:P:13:VAL:HG21	18:P:41:ARG:HG2	2.00	0.44
1:0:475:G:H5'	6:C:73:LEU:CD2	2.48	0.44
25:W:149:LEU:HG	25:W:153:MET:HE2	1.99	0.44
1:0:968:G:O2'	1:0:969:G:H5'	2.17	0.44
2:9:3052:A:H2'	2:9:3053:G:O4'	2.18	0.44
1:0:2549:C:H1'	5:B:248:ARG:NH2	2.33	0.44
1:0:1201:C:C2'	1:0:1202:A:H5'	2.42	0.44
6:C:27:ARG:HG2	6:C:30:LEU:HG	1.98	0.44
15:M:69:LYS:HG2	15:M:127:LYS:HG3	2.00	0.44
7:D:167:GLU:OE2	7:D:173:GLU:HG2	2.18	0.44
1:0:125:U:H2'	39:0:4367:HOH:O	2.18	0.44
21:S:33:SER:OG	21:S:36:GLU:HG3	2.18	0.44
11:H:67:LEU:O	11:H:71:ARG:HB2	2.18	0.44
5:B:238:ASN:ND2	5:B:240:GLY:H	2.03	0.43
6:C:127:ARG:CZ	6:C:225:PRO:HG2	2.46	0.43
6:C:115:LEU:O	6:C:118:THR:HB	2.18	0.43
4:A:36:ASP:C	4:A:38:ILE:H	2.21	0.43
14:L:80:ASP:HB2	14:L:90:ARG:HB3	2.00	0.43
16:N:154:LEU:HD11	16:N:157:PRO:HA	2.00	0.43
7:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.66	0.43
1:0:710:G:H5'	17:O:25:VAL:HG13	1.99	0.43
1:0:2044:G:OP1	26:X:23:HIS:HE1	2.01	0.43
1:0:1741:U:H3'	39:0:3379:HOH:O	2.18	0.43
1:0:1163:G:H2'	1:0:1164:U:C5	2.53	0.43
5:B:23:THR:HA	5:B:24:PRO:HD3	1.87	0.43
11:H:54:THR:O	11:H:55:VAL:HG13	2.17	0.43
1:0:1299:G:N2	39:0:5261:HOH:O	2.51	0.43
5:B:85:ARG:HB2	5:B:99:GLU:HG2	1.99	0.43
1:0:1406:A:H4'	1:0:1407:A:C5'	2.48	0.43
20:R:114:VAL:HG13	20:R:114:VAL:O	2.18	0.43
7:D:94:ALA:HA	7:D:174:VAL:O	2.17	0.43
1:0:1314:U:H2'	39:0:6429:HOH:O	2.17	0.43
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.47	0.43
5:B:16:ARG:NE	39:B:9556:HOH:O	2.39	0.43
5:B:115:VAL:HA	5:B:116:PRO:HD3	1.92	0.43
11:H:154:TYR:HA	11:H:157:ILE:HG12	2.00	0.43
4:A:217:ARG:CG	4:A:217:ARG:HH11	2.32	0.43
1:0:2435:U:H1'	39:0:5996:HOH:O	2.18	0.43
1:0:603:A:H5''	1:0:604:G:OP1	2.17	0.43
2:9:3014:G:H2'	2:9:3015:C:H5'	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:223:ARG:CZ	39:A:9560:HOH:O	2.66	0.43
1:O:1878:G:H5''	39:O:3406:HOH:O	2.18	0.43
4:A:179:MET:HG2	4:A:186:TRP:HB2	1.99	0.43
20:R:39:THR:HB	20:R:42:GLU:CG	2.47	0.43
1:O:1817:U:O2	18:P:81:LYS:NZ	2.47	0.43
18:P:143:ALA:HB2	39:P:186:HOH:O	2.18	0.43
18:P:121:ASP:OD1	18:P:125:LYS:HE3	2.17	0.43
7:D:128:LEU:C	7:D:128:LEU:HD23	2.39	0.43
2:9:3058:G:H1'	39:9:3839:HOH:O	2.17	0.43
1:O:1966:U:H2'	1:O:1967:U:H2'	2.01	0.43
1:O:2090:G:H2'	1:O:2091:G:C8	2.53	0.43
7:D:88:LEU:N	7:D:89:PRO:CD	2.80	0.43
1:O:1654:U:H2'	4:A:47:HIS:CD2	2.54	0.43
1:O:2506:A:O2'	1:O:2507:G:O5'	2.37	0.43
1:O:1473:U:O2'	1:O:1474:C:H5''	2.19	0.43
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.33	0.43
39:K:1387:HOH:O	23:U:20:MET:HE3	2.19	0.43
1:O:1250:C:O2'	1:O:1251:C:H5'	2.19	0.43
13:K:113:ILE:HD12	13:K:128:ALA:HB2	1.99	0.43
1:O:1603:A:H5'	1:O:1605:G:C4'	2.48	0.43
2:9:3039:U:HO2'	2:9:3042:C:H5	1.61	0.43
11:H:169:GLY:C	11:H:170:ASN:HD22	2.21	0.43
4:A:53:ALA:HB3	39:A:9594:HOH:O	2.17	0.43
11:H:47:ILE:HD12	11:H:146:VAL:HG13	2.00	0.43
1:O:2587:OMU:H2'	1:O:2589:U:H5''	1.99	0.43
1:O:1291:A:H2	39:O:5858:HOH:O	2.01	0.43
5:B:277:GLU:N	5:B:278:PRO:HD2	2.33	0.43
1:O:1119:G:C8	12:J:52:GLN:NE2	2.87	0.43
6:C:246:ARG:NE	39:C:9228:HOH:O	2.43	0.43
6:C:157:LEU:HD22	6:C:162:VAL:CG1	2.49	0.43
14:L:144:ASP:HA	14:L:147:GLU:OE1	2.19	0.43
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.53	0.43
8:E:84:MET:HE3	8:E:131:LEU:HD13	2.00	0.43
1:O:2252:A:C5	1:O:2253:G:H1'	2.53	0.43
11:H:146:VAL:HG22	39:H:9543:HOH:O	2.18	0.43
7:D:173:GLU:O	7:D:174:VAL:C	2.57	0.43
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.54	0.43
1:O:2453:G:H4'	14:L:50:GLY:C	2.38	0.43
1:O:1470:A:OP1	15:M:93:ARG:HD2	2.17	0.43
4:A:82:VAL:HG13	4:A:93:THR:HB	1.99	0.43
1:O:793:A:H5''	18:P:83:LYS:HG2	2.01	0.43
21:S:8:PRO:HD2	24:V:32:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2300:A:H4'	1:0:2301:A:O5'	2.19	0.43
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.59	0.43
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.18	0.43
1:0:1131:G:C6	1:0:1230:A:C4	3.06	0.43
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.55	0.43
13:K:22:ASP:O	13:K:110:LYS:HE3	2.18	0.43
5:B:71:VAL:HG11	5:B:296:LEU:HD22	2.00	0.43
17:O:73:ASP:HA	17:O:92:VAL:O	2.19	0.43
9:F:26:THR:HG21	9:F:102:GLY:C	2.39	0.43
22:T:71:VAL:HG12	22:T:72:ILE:H	1.79	0.43
7:D:57:THR:HA	39:D:5728:HOH:O	2.19	0.43
20:R:104:PHE:CB	20:R:109:MET:HE1	2.49	0.43
14:L:6:ARG:NH2	39:L:9444:HOH:O	2.51	0.43
8:E:8:PRO:HB2	8:E:11:VAL:HG23	2.01	0.43
7:D:99:ASP:HB3	7:D:103:ASN:H	1.83	0.43
1:0:447:A:O2'	1:0:448:G:H5'	2.19	0.43
1:0:1594:C:O2'	1:0:1607:A:H4'	2.18	0.43
12:J:39:VAL:CG1	12:J:40:ASN:N	2.82	0.43
1:0:920:C:H5''	1:0:921:G:O5'	2.19	0.43
15:M:58:GLN:HG3	39:M:9404:HOH:O	2.18	0.43
1:0:391:U:OP2	15:M:84:LYS:NZ	2.48	0.43
2:9:3031:C:H2'	2:9:3032:G:O4'	2.19	0.43
1:0:2791:U:H1'	1:0:2792:A:H5''	2.01	0.43
1:0:123:U:O2'	1:0:124:C:H5'	2.18	0.43
1:0:2256:G:C2'	1:0:2257:G:H5'	2.49	0.43
1:0:810:G:H1'	39:O:7750:HOH:O	2.19	0.43
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.19	0.43
16:N:36:ALA:N	39:N:9333:HOH:O	2.52	0.43
7:D:60:GLU:O	7:D:60:GLU:HG3	2.19	0.43
4:A:33:GLU:O	4:A:34:ASP:HB2	2.18	0.43
16:N:167:ASP:C	16:N:168:LEU:HG	2.39	0.43
20:R:18:LEU:HG	20:R:91:LEU:HD13	2.01	0.43
6:C:46:TYR:CE1	6:C:92:PRO:HB3	2.54	0.43
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.33	0.43
15:M:77:HIS:HD2	15:M:79:ALA:O	2.01	0.43
1:0:949:U:C4'	19:Q:95:GLU:HA	2.46	0.43
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.48	0.43
7:D:18:ILE:HD13	7:D:84:LEU:CD1	2.49	0.43
17:O:26:TRP:HB2	39:O:3062:HOH:O	2.19	0.43
30:2:20:ARG:HG3	30:2:21:VAL:N	2.34	0.43
1:0:2540:G:O2'	1:0:2541:U:H5''	2.19	0.43
32:I:101:SER:H	32:I:104:GLN:NE2	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:200:PRO:HB3	6:C:212:VAL:HG23	2.01	0.43
1:O:2016:U:H2'	1:O:2017:U:O4'	2.19	0.43
7:D:37:ALA:HA	39:D:5583:HOH:O	2.19	0.42
9:F:80:GLN:HB3	39:F:2563:HOH:O	2.17	0.42
1:O:2645:U:OP2	1:O:2645:U:H6	2.02	0.42
1:O:1878:G:H4'	39:O:4709:HOH:O	2.19	0.42
14:L:92:ASP:HA	14:L:121:ILE:HB	2.00	0.42
29:1:10:LYS:N	39:1:9488:HOH:O	2.49	0.42
6:C:57:PRO:HG2	6:C:73:LEU:HD13	2.01	0.42
18:P:141:ILE:C	18:P:143:ALA:H	2.22	0.42
15:M:169:ARG:NH1	39:M:9372:HOH:O	2.52	0.42
1:O:497:A:H2'	1:O:498:A:H5'	2.01	0.42
1:O:2831:C:H2'	1:O:2832:C:H5'	2.00	0.42
16:N:119:GLN:O	16:N:123:ILE:HG13	2.18	0.42
1:O:672:G:O6	6:C:213:ALA:HB1	2.19	0.42
8:E:112:ALA:HA	8:E:113:PRO:HD3	1.89	0.42
5:B:265:LEU:HD21	5:B:316:ARG:HD3	2.01	0.42
1:O:360:A:H2'	1:O:361:C:O4'	2.19	0.42
16:N:36:ALA:HB1	16:N:118:ILE:HD12	2.01	0.42
16:N:37:ARG:CZ	39:N:9333:HOH:O	2.67	0.42
12:J:74:ARG:NH1	12:J:105:LEU:HD11	2.33	0.42
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	2.01	0.42
27:Y:115:ARG:CZ	39:Y:9353:HOH:O	2.67	0.42
5:B:41:PHE:CB	5:B:190:MET:HE3	2.50	0.42
4:A:179:MET:HG2	4:A:186:TRP:HB3	2.01	0.42
11:H:151:ARG:HA	11:H:154:TYR:CE2	2.54	0.42
31:3:73:GLU:HG2	31:3:73:GLU:O	2.18	0.42
1:O:935:G:H4'	17:O:38:ARG:HH12	1.84	0.42
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.54	0.42
1:O:263:U:C2	9:F:59:ILE:CD1	3.02	0.42
1:O:2256:G:O2'	1:O:2257:G:H5'	2.20	0.42
1:O:2356:A:H2'	1:O:2357:G:O4'	2.18	0.42
26:X:8:ARG:NH1	39:X:2479:HOH:O	2.51	0.42
1:O:195:C:H2'	1:O:196:G:H5'	2.01	0.42
1:O:2310:G:OP2	11:H:115:ALA:HA	2.18	0.42
1:O:2715:G:N2	5:B:264:GLU:OE1	2.53	0.42
8:E:18:LEU:HD13	8:E:34:TRP:CG	2.54	0.42
1:O:1701:A:P	39:O:4968:HOH:O	2.77	0.42
2:9:3040:C:N4	7:D:53:LYS:HE3	2.34	0.42
1:O:2270:G:C4'	4:A:223:ARG:HH12	2.28	0.42
16:N:137:ALA:HB1	16:N:141:ARG:HD3	2.01	0.42
13:K:98:VAL:HG22	13:K:102:GLU:C	2.39	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:J:63:ILE:CG2	12:J:64:GLY:N	2.82	0.42
15:M:36:ALA:O	15:M:65:VAL:HA	2.19	0.42
22:T:117:ASP:OD1	22:T:118:SER:N	2.51	0.42
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.90	0.42
1:O:1826:C:O2'	1:O:1827:G:H5'	2.19	0.42
6:C:236:THR:O	6:C:237:GLU:C	2.57	0.42
1:O:2718:C:H5'	1:O:2718:C:C6	2.51	0.42
1:O:2636:C:C3'	1:O:2637:A:C5'	2.96	0.42
4:A:94:LEU:HB2	4:A:95:PRO:HD2	2.00	0.42
32:I:72:VAL:HG13	32:I:73:PRO:HD2	2.01	0.42
5:B:333:GLU:HB2	39:U:3564:HOH:O	2.18	0.42
1:O:2241:C:O2'	1:O:2242:U:H5'	2.19	0.42
1:O:2067:A:H2'	1:O:2068:G:O4'	2.19	0.42
4:A:164:ARG:CZ	39:A:9575:HOH:O	2.67	0.42
1:O:612:U:H2'	1:O:613:C:C6	2.55	0.42
9:F:5:ASP:O	9:F:119:ARG:NH1	2.52	0.42
16:N:108:SER:HA	16:N:109:PRO:HD3	1.82	0.42
6:C:1:MET:HG2	6:C:2:GLN:HE21	1.84	0.42
12:J:47:THR:CG2	12:J:48:GLY:N	2.83	0.42
4:A:201:PHE:HB3	39:A:9621:HOH:O	2.19	0.42
1:O:2821:C:H4'	5:B:116:PRO:HG3	2.01	0.42
39:O:5543:HOH:O	11:H:58:ARG:HG3	2.18	0.42
21:S:29:ASP:OD2	21:S:31:ARG:NH1	2.51	0.42
26:X:20:GLU:HG3	26:X:21:PRO:HD2	2.00	0.42
2:9:3052:A:O2'	2:9:3053:G:H5'	2.20	0.42
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.55	0.42
1:O:522:U:O2'	1:O:1366:C:H5'	2.18	0.42
1:O:1369:A:H4'	20:R:64:SER:OG	2.19	0.42
26:X:73:ARG:HH12	26:X:88:GLU:HA	1.85	0.42
27:Y:115:ARG:HH11	27:Y:115:ARG:CB	2.29	0.42
1:O:2704:C:H2'	1:O:2705:U:O4'	2.20	0.42
2:9:3024:U:H3'	2:9:3025:G:C5'	2.50	0.42
1:O:424:C:H2'	1:O:425:U:H6	1.84	0.42
1:O:2324:G:N2	1:O:2377:U:H1'	2.34	0.42
5:B:69:VAL:HA	5:B:70:PRO:HD3	1.86	0.42
32:I:76:ALA:O	32:I:80:LYS:HG3	2.20	0.42
6:C:124:VAL:HA	6:C:230:GLY:O	2.18	0.42
1:O:130:C:H2'	39:O:3769:HOH:O	2.18	0.42
1:O:1705:C:O2	1:O:2735:U:H5''	2.20	0.42
1:O:2838:A:H2'	1:O:2839:C:C6	2.55	0.42
39:O:9737:HOH:O	15:M:82:ARG:HD2	2.19	0.42
1:O:1603:A:H5''	1:O:1604:G:H3'	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:W:110:GLN:NE2	25:W:110:GLN:CA	2.82	0.42
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	2.02	0.42
1:O:1298:U:H2'	1:O:1299:G:C8	2.53	0.42
1:O:1878:G:O2'	1:O:1879:U:C6	2.70	0.42
6:C:194:PHE:CD2	6:C:234:VAL:CG1	3.01	0.42
7:D:18:ILE:HG12	7:D:134:LEU:CD2	2.49	0.42
1:O:185:G:C4'	1:O:186:A:H4'	2.49	0.42
17:O:14:LEU:HG	17:O:102:ILE:HD11	2.01	0.42
26:X:23:HIS:CD2	26:X:24:LYS:HG3	2.55	0.42
11:H:76:GLU:C	11:H:77:LEU:HD23	2.40	0.42
1:O:2880:A:H2'	1:O:2881:C:H5'	2.02	0.42
27:Y:163:THR:HB	39:Y:9398:HOH:O	2.20	0.42
14:L:61:ALA:HB2	14:L:105:TYR:CZ	2.54	0.42
1:O:1759:A:N3	1:O:1818:C:H2'	2.35	0.42
5:B:87:TYR:OH	5:B:163:GLU:OE2	2.30	0.42
1:O:2676:C:H4'	12:J:70:PHE:HD1	1.78	0.42
14:L:94:ARG:NH1	14:L:143:THR:HG21	2.35	0.42
6:C:194:PHE:HA	6:C:234:VAL:HG13	2.02	0.42
7:D:18:ILE:HD13	7:D:84:LEU:HD12	2.01	0.42
5:B:24:PRO:HG3	5:B:204:GLY:HA2	2.00	0.42
1:O:1654:U:H2'	4:A:47:HIS:HD2	1.83	0.42
1:O:1419:U:H2'	1:O:1685:A:C2	2.54	0.42
1:O:1992:U:OP2	13:K:66:ARG:HD2	2.19	0.42
19:Q:33:PHE:HE2	19:Q:93:ARG:HG3	1.85	0.42
11:H:66:ARG:HD3	39:H:9546:HOH:O	2.20	0.42
1:O:1244:U:C6	12:J:47:THR:HG22	2.54	0.42
4:A:36:ASP:OD2	4:A:85:SER:HB2	2.20	0.42
5:B:84:LEU:HD13	5:B:84:LEU:O	2.19	0.42
32:I:80:LYS:HD3	32:I:86:GLU:O	2.19	0.42
9:F:20:LEU:O	9:F:23:ALA:HB3	2.20	0.42
11:H:144:GLU:HG2	39:H:9535:HOH:O	2.19	0.42
1:O:912:A:C4	1:O:1294:A:C2	3.06	0.42
1:O:2568:A:H2'	1:O:2569:A:O4'	2.19	0.42
1:O:1909:A:N1	1:O:2128:G:H1'	2.35	0.42
2:9:3005:G:OP1	16:N:17:ARG:NH2	2.52	0.42
1:O:1287:A:O4'	25:W:117:ARG:HD3	2.20	0.42
6:C:123:LEU:HA	6:C:123:LEU:HD23	1.92	0.42
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.23	0.42
7:D:60:GLU:O	7:D:61:PHE:C	2.57	0.42
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.19	0.42
1:O:2635:A:HO2'	1:O:2636:C:H5'	1.84	0.42
1:O:308:U:H5'	22:T:97:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1980:U:O2	1:0:2008:U:H4'	2.20	0.42
16:N:152:GLU:HA	16:N:152:GLU:OE1	2.20	0.42
5:B:301:VAL:HG11	5:B:309:VAL:HG11	2.02	0.42
2:9:3003:A:OP2	2:9:3025:G:N2	2.52	0.42
10:G:23:ILE:O	10:G:27:ILE:HG13	2.20	0.42
9:F:28:ALA:CB	9:F:99:THR:HG23	2.49	0.42
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.55	0.42
1:0:2697:A:H2'	1:0:2698:G:O4'	2.20	0.42
1:0:2508:C:H2'	39:0:7270:HOH:O	2.18	0.42
25:W:41:TYR:HA	25:W:44:MET:HE3	2.02	0.42
11:H:45:VAL:HG13	39:H:9525:HOH:O	2.19	0.41
27:Y:155:ARG:HH21	27:Y:157:ILE:HD11	1.85	0.41
32:I:138:THR:HG22	32:I:139:ILE:H	1.84	0.41
20:R:16:ALA:HB1	20:R:94:ASN:HD22	1.85	0.41
10:G:64:ASN:N	10:G:64:ASN:ND2	2.67	0.41
12:J:71:TYR:CG	12:J:72:PRO:HD2	2.55	0.41
1:0:1476:A:O2'	1:0:1477:C:H5'	2.20	0.41
16:N:93:GLN:HE21	16:N:127:LEU:HD12	1.84	0.41
1:0:1149:U:H5''	1:0:1151:G:O4'	2.20	0.41
1:0:2015:A:H2'	1:0:2016:U:O4'	2.20	0.41
1:0:87:C:C2	30:2:30:ASP:OD2	2.72	0.41
1:0:1768:C:H2'	1:0:1769:C:O4'	2.19	0.41
1:0:2388:C:H5'	19:Q:83:THR:O	2.20	0.41
1:0:462:A:H2'	39:0:5457:HOH:O	2.20	0.41
11:H:29:ALA:CB	11:H:66:ARG:HH12	2.20	0.41
6:C:127:ARG:HD3	6:C:129:HIS:CE1	2.53	0.41
6:C:132:ASP:HB2	6:C:161:ASP:HB3	2.02	0.41
1:0:2896:A:H5''	39:X:5399:HOH:O	2.21	0.41
4:A:94:LEU:HG	4:A:99:ILE:HD11	2.02	0.41
1:0:920:C:OP1	14:L:37:LYS:NZ	2.51	0.41
24:V:29:ASN:O	24:V:33:VAL:HG23	2.20	0.41
26:X:80:GLU:HG2	26:X:80:GLU:O	2.20	0.41
11:H:63:GLU:HA	39:H:9546:HOH:O	2.19	0.41
1:0:1878:G:O2'	1:0:1879:U:C5	2.68	0.41
16:N:49:THR:HG22	16:N:56:ASP:CB	2.50	0.41
4:A:57:ALA:HA	4:A:67:LEU:HD23	2.02	0.41
1:0:2866:U:C4	23:U:50:GLU:HB3	2.55	0.41
8:E:102:VAL:HG13	8:E:116:THR:HG23	2.02	0.41
39:0:5855:HOH:O	25:W:119:HIS:CG	2.73	0.41
1:0:2337:G:O3'	7:D:97:GLN:HA	2.20	0.41
1:0:2256:G:H2'	1:0:2257:G:C5'	2.51	0.41
6:C:166:ILE:HD11	6:C:207:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:9:3064:C:C2'	2:9:3065:A:H5'	2.49	0.41
21:S:42:GLU:O	21:S:46:ASP:HA	2.21	0.41
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.50	0.41
1:0:349:U:O2'	1:0:350:C:H5'	2.21	0.41
1:0:2506:A:O2'	1:0:2507:G:P	2.79	0.41
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.42	0.41
5:B:217:ARG:CG	5:B:257:THR:HG22	2.48	0.41
12:J:19:MET:HE2	12:J:79:PHE:HA	2.02	0.41
17:O:45:LEU:HD12	17:O:88:LYS:HD2	2.02	0.41
14:L:92:ASP:HB3	14:L:95:ASP:OD2	2.21	0.41
1:0:883:U:C2'	1:0:883:U:O2	2.66	0.41
20:R:39:THR:HG22	20:R:41:GLY:N	2.36	0.41
1:0:314:G:N2	1:0:316:A:H3'	2.35	0.41
21:S:38:ALA:O	21:S:42:GLU:HG3	2.20	0.41
22:T:78:THR:HB	22:T:87:VAL:O	2.21	0.41
1:0:583:G:H2'	1:0:584:U:C6	2.56	0.41
1:0:2101:A:H2'	6:C:63:SER:OG	2.20	0.41
9:F:79:GLN:HB2	9:F:82:ASP:OD2	2.20	0.41
1:0:932:U:H2'	1:0:933:C:C6	2.56	0.41
12:J:75:PRO:HB3	12:J:132:LEU:HB3	2.02	0.41
16:N:66:LEU:HG	16:N:175:LEU:HD21	2.02	0.41
1:0:506:G:H22	1:0:509:A:H5'	1.79	0.41
1:0:936:C:OP1	17:O:35:LYS:NZ	2.46	0.41
32:I:135:LEU:HB2	32:I:137:VAL:HG23	2.02	0.41
1:0:2503:A:OP1	11:H:151:ARG:NH2	2.46	0.41
12:J:39:VAL:HG11	12:J:107:ASN:CB	2.50	0.41
1:0:2265:U:H2'	1:0:2266:A:H8	1.82	0.41
1:0:500:G:O2'	20:R:94:ASN:ND2	2.53	0.41
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.51	0.41
27:Y:107:PRO:HD3	27:Y:182:PHE:CE1	2.56	0.41
1:0:414:C:H5'	39:O:3274:HOH:O	2.20	0.41
15:M:167:GLY:O	15:M:171:ARG:HG3	2.20	0.41
7:D:139:TYR:CE2	7:D:143:LYS:HE3	2.56	0.41
1:0:1881:A:OP1	4:A:199:HIS:HE1	2.03	0.41
28:Z:10:ARG:HG3	28:Z:11:SER:N	2.36	0.41
5:B:16:ARG:NH2	39:B:9556:HOH:O	2.43	0.41
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.54	0.41
5:B:62:ARG:CB	5:B:65:MET:HE3	2.50	0.41
23:U:9:CYS:CA	23:U:52:THR:HG23	2.51	0.41
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.20	0.41
1:0:1787:C:H4'	1:0:2883:A:O4'	2.20	0.41
1:0:1279:U:O2	1:0:1279:U:H2'	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1363:G:P	6:C:76:ARG:HH22	2.43	0.41
1:0:2338:G:OP1	7:D:97:GLN:HG2	2.21	0.41
1:0:611:U:H2'	1:0:612:U:C6	2.56	0.41
1:0:1304:U:H2'	1:0:1305:C:C6	2.56	0.41
15:M:159:VAL:HG13	15:M:160:PHE:N	2.36	0.41
22:T:18:GLU:O	22:T:21:LYS:HG2	2.21	0.41
1:0:177:A:H2'	1:0:178:U:O4'	2.20	0.41
8:E:20:ILE:HD12	8:E:33:LEU:CD1	2.50	0.41
1:0:1181:A:H4'	32:I:92:PRO:HG2	2.02	0.41
1:0:2564:G:OP2	1:0:2565:C:H5''	2.20	0.41
9:F:111:ILE:O	9:F:115:VAL:HG23	2.19	0.41
1:0:2443:C:H5'	14:L:57:VAL:HG21	2.03	0.41
1:0:2456:A:H5'	39:0:6254:HOH:O	2.20	0.41
12:J:63:ILE:HG22	12:J:64:GLY:N	2.35	0.41
29:1:42:SER:HB2	39:1:9465:HOH:O	2.20	0.41
1:0:1162:G:H1'	32:I:117:LEU:HD11	2.02	0.41
7:D:22:VAL:HG22	7:D:74:THR:HG22	2.02	0.41
1:0:2784:A:H1'	8:E:60:SER:OG	2.21	0.41
1:0:2281:C:C2'	1:0:2282:U:H5'	2.50	0.41
7:D:135:VAL:HG21	7:D:139:TYR:CG	2.54	0.41
25:W:125:HIS:HD2	25:W:127:GLY:N	2.02	0.41
1:0:559:U:H2'	1:0:560:C:O4'	2.21	0.41
14:L:144:ASP:O	14:L:147:GLU:HB2	2.21	0.41
8:E:7:ILE:CD1	8:E:12:ASP:HA	2.48	0.41
15:M:27:ARG:HH22	15:M:44:THR:HG23	1.85	0.41
4:A:65:ARG:HH11	4:A:65:ARG:HG2	1.86	0.41
5:B:104:GLU:HB2	39:B:9631:HOH:O	2.20	0.41
1:0:960:G:N3	1:0:960:G:C2'	2.84	0.41
25:W:119:HIS:HD2	25:W:120:PRO:O	2.04	0.41
16:N:77:ASN:OD1	16:N:79:PRO:HD2	2.21	0.41
1:0:1163:G:H5'	32:I:115:ASP:O	2.21	0.41
4:A:52:SER:HB2	4:A:164:ARG:HH11	1.86	0.41
2:9:3064:C:H2'	2:9:3065:A:H5'	2.02	0.41
1:0:1132:A:N6	1:0:1229:C:H2'	2.36	0.41
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.39	0.41
1:0:2283:G:C6	11:H:113:MET:HB3	2.56	0.41
4:A:194:MET:HE1	4:A:199:HIS:HB2	2.02	0.41
23:U:14:GLU:O	23:U:17:THR:HB	2.21	0.41
4:A:36:ASP:CB	4:A:85:SER:H	2.33	0.41
1:0:553:G:P	27:Y:204:ARG:NH2	2.86	0.41
9:F:60:VAL:O	9:F:60:VAL:CG1	2.68	0.41
4:A:103:VAL:O	4:A:105:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:D:56:ARG:N	39:D:6752:HOH:O	2.52	0.41
24:V:59:ILE:O	24:V:63:GLU:HG2	2.20	0.41
4:A:94:LEU:HD12	4:A:98:GLU:CB	2.51	0.41
1:0:185:G:O3'	1:0:186:A:H4'	2.21	0.41
25:W:38:THR:HG22	25:W:40:ALA:H	1.85	0.41
1:0:2365:G:H4'	19:Q:45:PRO:O	2.21	0.41
26:X:23:HIS:NE2	26:X:24:LYS:HD2	2.36	0.41
1:0:855:U:H4'	1:0:856:G:O4'	2.20	0.41
31:3:24:LYS:HA	31:3:67:LEU:HD23	2.02	0.41
1:0:2094:G:O6	1:0:2649:A:H2	2.03	0.41
4:A:68:ILE:HG12	4:A:69:LEU:N	2.35	0.41
5:B:277:GLU:N	5:B:278:PRO:CD	2.84	0.41
1:0:1755:A:H2'	1:0:1756:G:O4'	2.21	0.41
1:0:2699:A:H2'	1:0:2700:G:O4'	2.20	0.41
1:0:1754:A:H2'	1:0:1755:A:O4'	2.20	0.41
22:T:85:GLU:HG2	22:T:86:GLU:N	2.36	0.41
20:R:33:ARG:NH1	39:R:9452:HOH:O	2.45	0.41
1:0:517:U:H1'	39:0:8147:HOH:O	2.20	0.41
22:T:27:LEU:HD23	22:T:98:VAL:HB	2.02	0.41
13:K:38:SER:O	39:K:4183:HOH:O	2.22	0.41
1:0:2748:G:H4'	1:0:2749:U:C5'	2.51	0.41
15:M:68:ARG:NH2	15:M:73:ARG:HD3	2.36	0.41
1:0:1352:A:HO2'	1:0:1353:C:P	2.44	0.41
16:N:176:ARG:HG3	16:N:180:LEU:CD1	2.51	0.41
13:K:115:ARG:CG	13:K:116:GLU:N	2.84	0.41
14:L:93:VAL:HG12	14:L:97:VAL:HG23	2.02	0.41
1:0:830:G:O2'	1:0:831:U:H5'	2.21	0.41
1:0:941:G:C5	1:0:942:U:C4	3.09	0.41
4:A:171:LYS:NZ	39:A:9514:HOH:O	2.54	0.41
4:A:173:GLY:O	4:A:176:HIS:HB3	2.20	0.41
22:T:14:ALA:HA	22:T:15:PRO:HD3	1.95	0.41
12:J:80:LYS:HE2	12:J:98:PHE:CE1	2.56	0.41
18:P:131:PHE:CE1	18:P:137:LEU:HD13	2.56	0.41
1:0:17:G:H2'	1:0:18:C:C6	2.56	0.41
1:0:2681:A:H4'	1:0:2682:C:H5'	2.03	0.41
16:N:37:ARG:HD3	36:N:9307:CL:CL	2.58	0.40
2:9:3056:A:HO2'	7:D:155:HIS:CE1	2.39	0.40
1:0:2748:G:H4'	1:0:2749:U:H5'	2.02	0.40
1:0:2523:U:O2'	1:0:2524:G:H5'	2.22	0.40
20:R:13:THR:CG2	20:R:14:ALA:N	2.84	0.40
18:P:37:ARG:O	18:P:41:ARG:HG3	2.20	0.40
1:0:380:A:H2'	39:0:7729:HOH:O	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:E:126:ILE:HB	8:E:131:LEU:CD2	2.51	0.40
25:W:149:LEU:HG	25:W:153:MET:HE1	2.03	0.40
1:O:2807:U:OP2	5:B:28:SER:HB2	2.21	0.40
12:J:54:VAL:HG11	12:J:138:THR:HG21	2.02	0.40
6:C:133:ARG:NH1	39:C:9216:HOH:O	2.54	0.40
27:Y:177:LYS:HD3	27:Y:181:GLY:O	2.21	0.40
17:O:112:ARG:HE	17:O:112:ARG:HB2	1.77	0.40
26:X:9:VAL:HG13	26:X:88:GLU:CD	2.41	0.40
6:C:162:VAL:CG2	6:C:232:LEU:HD21	2.48	0.40
4:A:186:TRP:CG	4:A:187:PRO:HA	2.57	0.40
1:O:1044:C:H3'	1:O:1045:G:H5''	2.03	0.40
16:N:112:GLY:HA2	16:N:137:ALA:N	2.36	0.40
31:3:55:VAL:HB	31:3:56:PRO:HD2	2.03	0.40
1:O:1745:G:H22	1:O:2033:G:H5'	1.86	0.40
1:O:951:A:O2'	1:O:952:G:H5'	2.21	0.40
6:C:133:ARG:HG3	6:C:133:ARG:HH11	1.85	0.40
1:O:1131:G:H4'	2:9:3091:C:O4'	2.21	0.40
39:9:1361:HOH:O	16:N:41:LYS:HE3	2.21	0.40
21:S:81:ILE:HG22	24:V:29:ASN:OD1	2.21	0.40
1:O:2611:G:H5'	1:O:2613:G:C8	2.56	0.40
1:O:294:C:H2'	1:O:295:C:O4'	2.21	0.40
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.93	0.40
11:H:39:ASP:HB3	11:H:41:ASP:OD2	2.21	0.40
14:L:77:ALA:C	14:L:79:ASP:H	2.25	0.40
1:O:2754:G:H2'	1:O:2755:G:O4'	2.21	0.40
22:T:106:GLU:HG3	39:T:4913:HOH:O	2.21	0.40
5:B:255:GLY:O	5:B:257:THR:HG23	2.20	0.40
1:O:644:G:N3	1:O:644:G:H5'	2.37	0.40
17:O:97:SER:H	17:O:100:GLN:NE2	2.20	0.40
32:I:99:ASP:HA	32:I:138:THR:O	2.21	0.40
24:V:60:GLN:O	24:V:65:ASP:N	2.54	0.40
1:O:1168:C:H5''	32:I:87:THR:CG2	2.51	0.40
5:B:305:ASP:O	5:B:306:LYS:CB	2.67	0.40
20:R:39:THR:CG2	20:R:107:GLU:O	2.70	0.40
1:O:2428:G:N7	31:3:60:LYS:NZ	2.68	0.40
1:O:921:G:H4'	1:O:924:G:N1	2.36	0.40
1:O:1099:G:OP1	25:W:129:LYS:HE3	2.22	0.40
1:O:1657:A:H2'	1:O:1658:A:C8	2.56	0.40
1:O:629:A:H2'	1:O:630:A:O4'	2.22	0.40
39:O:6895:HOH:O	4:A:205:GLY:HA3	2.22	0.40
4:A:192:VAL:HG13	4:A:208:HIS:N	2.37	0.40
1:O:1972:U:C2'	1:O:1973:A:H5''	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:41:PHE:CD1	5:B:79:MET:CE	3.04	0.40
1:0:2565:C:H4'	39:0:5409:HOH:O	2.22	0.40
20:R:16:ALA:CB	20:R:94:ASN:HD22	2.34	0.40
1:0:1477:C:H5'	1:0:1868:G:H5'	2.04	0.40
27:Y:95:THR:N	27:Y:236:VAL:O	2.54	0.40
1:0:2499:U:H2'	1:0:2500:C:H6	1.86	0.40
23:U:35:LYS:HE2	23:U:51:TRP:CZ2	2.57	0.40
6:C:140:VAL:CG1	6:C:141:SER:N	2.85	0.40
7:D:40:ILE:HG13	7:D:41:LEU:N	2.37	0.40
7:D:28:GLY:CA	7:D:69:ILE:HG23	2.37	0.40
1:0:1117:A:C2	1:0:1244:U:C2	3.10	0.40
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.68	0.40
1:0:370:G:O2'	1:0:371:U:H5'	2.21	0.40
1:0:204:A:H2'	1:0:205:U:H5'	2.02	0.40
1:0:920:C:H5'	1:0:921:G:C4	2.56	0.40
25:W:91:ASP:HB2	39:W:5425:HOH:O	2.22	0.40
1:0:1864:C:C5	15:M:75:ARG:HD2	2.57	0.40
1:0:285:A:H2'	1:0:286:U:O4'	2.21	0.40
12:J:64:GLY:HA3	36:J:9321:CL:CL	2.58	0.40
1:0:582:C:O2'	1:0:583:G:H5'	2.22	0.40
1:0:2038:A:O2'	1:0:2039:A:H5'	2.21	0.40
7:D:49:PRO:HB3	39:D:5828:HOH:O	2.21	0.40
1:0:226:A:H1'	1:0:393:G:C5	2.56	0.40
4:A:166:ASP:HA	39:A:9607:HOH:O	2.20	0.40
19:Q:62:THR:O	19:Q:64:GLU:HG2	2.22	0.40
1:0:2374:A:H2'	1:0:2375:G:C8	2.57	0.40
28:Z:39:CYS:SG	28:Z:41:ASN:HB3	2.60	0.40
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.56	0.40
1:0:2857:C:H2'	1:0:2858:U:C6	2.57	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	
4	A	235/240 (98%)	208 (88%)	25 (11%)	2 (1%)	25	21
5	B	335/338 (99%)	315 (94%)	16 (5%)	4 (1%)	19	14
6	C	244/246 (99%)	225 (92%)	19 (8%)	0	100	100
7	D	134/177 (76%)	107 (80%)	16 (12%)	11 (8%)	1	0
8	E	170/178 (96%)	164 (96%)	6 (4%)	0	100	100
9	F	117/120 (98%)	105 (90%)	8 (7%)	4 (3%)	6	2
10	G	25/348 (7%)	25 (100%)	0	0	100	100
11	H	156/171 (91%)	137 (88%)	15 (10%)	4 (3%)	8	4
12	J	140/145 (97%)	132 (94%)	5 (4%)	3 (2%)	11	5
13	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
14	L	141/165 (86%)	119 (84%)	20 (14%)	2 (1%)	16	12
15	M	192/195 (98%)	183 (95%)	8 (4%)	1 (0%)	38	38
16	N	184/187 (98%)	165 (90%)	12 (6%)	7 (4%)	5	2
17	O	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
18	P	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
19	Q	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	25	21
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	58 (92%)	4 (6%)	1 (2%)	14	9
25	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
26	X	80/92 (87%)	72 (90%)	8 (10%)	0	100	100
27	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
28	Z	71/83 (86%)	62 (87%)	6 (8%)	3 (4%)	4	1
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
31	3	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
32	I	68/162 (42%)	56 (82%)	10 (15%)	2 (3%)	7	3
All	All	3705/4431 (84%)	3432 (93%)	228 (6%)	45 (1%)	19	14

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	27	LEU
5	B	139	ASP
11	H	166	SER
11	H	168	ALA
12	J	143	LYS
14	L	80	ASP
16	N	154	LEU
16	N	184	ILE
28	Z	81	ARG
4	A	37	VAL
7	D	27	ILE
7	D	60	GLU
7	D	61	PHE
7	D	97	GLN
7	D	171	ASP
9	F	101	ALA
22	T	53	GLY
24	V	43	PRO
28	Z	20	ARG
28	Z	21	VAL
7	D	28	GLY
7	D	56	ARG
11	H	16	ARG
11	H	81	GLY
12	J	5	GLU
12	J	65	ASN
14	L	102	ASP
16	N	65	ASP
16	N	155	GLU
16	N	164	ASP
16	N	167	ASP
5	B	34	GLY
5	B	185	GLY
7	D	16	PRO
7	D	137	PRO
7	D	173	GLU
9	F	71	GLY
32	I	132	CYS
7	D	164	ALA
15	M	83	SER
16	N	160	SER
32	I	129	VAL
9	F	100	ASP

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Mol	Chain	Res	Type
9	F	27	GLY
5	B	2	GLN

### 5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/182 (98%)	168 (94%)	11 (6%)	26	28
5	B	282/283 (100%)	265 (94%)	17 (6%)	27	29
6	C	193/193 (100%)	176 (91%)	17 (9%)	14	13
7	D	117/148 (79%)	111 (95%)	6 (5%)	33	38
8	E	152/156 (97%)	147 (97%)	5 (3%)	50	60
9	F	93/94 (99%)	92 (99%)	1 (1%)	84	92
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	128 (97%)	4 (3%)	53	64
12	J	118/121 (98%)	111 (94%)	7 (6%)	28	30
13	K	106/106 (100%)	102 (96%)	4 (4%)	44	53
14	L	113/127 (89%)	110 (97%)	3 (3%)	57	68
15	M	158/159 (99%)	153 (97%)	5 (3%)	51	62
16	N	149/150 (99%)	144 (97%)	5 (3%)	49	59
17	O	93/94 (99%)	91 (98%)	2 (2%)	64	76
18	P	113/117 (97%)	111 (98%)	2 (2%)	71	82
19	Q	79/80 (99%)	76 (96%)	3 (4%)	44	53
20	R	117/122 (96%)	115 (98%)	2 (2%)	73	84
21	S	71/74 (96%)	71 (100%)	0	100	100
22	T	105/106 (99%)	101 (96%)	4 (4%)	44	53
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	68	79
25	W	130/130 (100%)	125 (96%)	5 (4%)	44	53
26	X	66/74 (89%)	62 (94%)	4 (6%)	26	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	Y	120/196 (61%)	107 (89%)	13 (11%)	9	8
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	61	73
31	3	79/79 (100%)	78 (99%)	1 (1%)	80	89
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2970 (96%)	123 (4%)	42	51

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	36	ASP
4	A	78	ASP
4	A	94	LEU
4	A	131	HIS
4	A	151	GLN
4	A	153	ARG
4	A	165	THR
4	A	179	MET
4	A	206	ARG
4	A	217	ARG
5	B	7	ARG
5	B	11	LEU
5	B	27	ASN
5	B	56	ASP
5	B	82	VAL
5	B	149	ASP
5	B	175	LEU
5	B	180	ASP
5	B	190	MET
5	B	234	ARG
5	B	251	VAL
5	B	254	GLN
5	B	264	GLU
5	B	265	LEU
5	B	277	GLU
5	B	307	ARG
5	B	312	ARG
6	C	2	GLN

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Mol	Chain	Res	Type
6	C	67	GLN
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	101	ASP
6	C	136	VAL
6	C	162	VAL
6	C	187	ARG
6	C	214	THR
6	C	222	ASP
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
6	C	243	VAL
6	C	246	ARG
7	D	24	HIS
7	D	50	VAL
7	D	61	PHE
7	D	133	ASN
7	D	137	PRO
7	D	170	TYR
8	E	7	ILE
8	E	102	VAL
8	E	108	LEU
8	E	155	ASN
8	E	164	ASP
9	F	12	LEU
11	H	84	LYS
11	H	154	TYR
11	H	159	PRO
11	H	170	ASN
12	J	52	GLN
12	J	70	PHE
12	J	74	ARG
12	J	79	PHE
12	J	107	ASN
12	J	127	ILE
12	J	131	THR
13	K	4	LEU
13	K	10	GLN
13	K	49	LEU

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Mol	Chain	Res	Type
13	K	84	ASP
14	L	35	ARG
14	L	43	HIS
14	L	89	PHE
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
16	N	12	ARG
16	N	26	LEU
16	N	49	THR
16	N	65	ASP
16	N	139	TRP
17	O	3	THR
17	O	111	VAL
18	P	81	LYS
18	P	98	ILE
19	Q	16	ASN
19	Q	57	ASP
19	Q	95	GLU
20	R	82	GLU
20	R	132	ARG
22	T	39	ASN
22	T	73	HIS
22	T	89	ARG
22	T	96	VAL
24	V	65	ASP
25	W	26	ILE
25	W	35	VAL
25	W	52	VAL
25	W	142	ASP
25	W	146	ILE
26	X	8	ARG
26	X	79	GLU
26	X	82	GLU
26	X	85	VAL
27	Y	103	THR
27	Y	108	ASP
27	Y	141	THR
27	Y	144	ARG
27	Y	154	ARG

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Mol	Chain	Res	Type
27	Y	163	THR
27	Y	186	ARG
27	Y	189	ASN
27	Y	200	THR
27	Y	203	VAL
27	Y	204	ARG
27	Y	220	GLU
27	Y	235	GLU
30	2	18	ASN
31	3	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	47	HIS
4	A	199	HIS
5	B	27	ASN
5	B	145	HIS
5	B	221	GLN
5	B	238	ASN
5	B	256	GLN
5	B	260	HIS
5	B	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	129	HIS
7	D	47	GLN
7	D	85	GLN
7	D	103	ASN
7	D	133	ASN
8	E	106	ASN
8	E	143	GLN
10	G	64	ASN
11	H	31	HIS
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	170	ASN
12	J	25	GLN
12	J	52	GLN
12	J	107	ASN
12	J	126	ASN

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Mol	Chain	Res	Type
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	77	HIS
15	M	143	ASN
15	M	170	ASN
16	N	93	GLN
16	N	107	ASN
16	N	153	GLN
17	O	100	GLN
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS
18	P	88	GLN
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
21	S	53	ASN
22	T	37	GLN
22	T	39	ASN
22	T	43	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	60	GLN
25	W	12	ASN
25	W	27	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	22	ASN
27	Y	133	HIS

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Mol	Chain	Res	Type
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	30	GLN
31	3	48	ASN
32	I	104	GLN
32	I	113	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	232 (8%)	35 (1%)
2	9	121/122 (99%)	16 (13%)	2 (1%)
3	4	1/3 (33%)	0	0
All	All	2867/3047 (94%)	248 (8%)	37 (1%)

All (248) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A

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Mol	Chain	Res	Type
1	0	169	A
1	0	170	U
1	0	186	A
1	0	191	A
1	0	192	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	498	A
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U

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Mol	Chain	Res	Type
1	0	702	G
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	846	A
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	875	A
1	0	877	G
1	0	878	G
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1100	G
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1164	U
1	0	1165	G
1	0	1166	A

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Mol	Chain	Res	Type
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1331	A
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1564	C
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G

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Mol	Chain	Res	Type
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2354	A

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Mol	Chain	Res	Type
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2465	A
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2645	U
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C

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Mol	Chain	Res	Type
1	0	2852	A
1	0	2853	U
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3040	C
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (37) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1232	A
1	0	1237	U
1	0	1246	A

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Mol	Chain	Res	Type
1	0	1352	A
1	0	1506	U
1	0	1563	G
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1752	G
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2320	U
1	0	2467	A
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2761	A
1	0	2791	U
1	0	2852	A
2	9	3043	G
2	9	3065	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	OMU	0	2587	1	20,22,23	0.79	1 (5%)	24,31,34	0.85	0
1	OMG	0	2588	1,3	24,26,27	0.83	0	32,38,41	5.07	4 (12%)
1	UR3	0	2619	1	20,22,23	0.79	0	23,32,35	0.81	0
1	PSU	0	2621	1	19,21,22	1.30	3 (15%)	23,30,33	1.08	2 (8%)
1	1MA	0	628	1	23,25,26	0.81	0	32,37,40	1.00	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PPU	4	76	1,3	38,40,41	1.07	2 (5%)	54,57,60	0.92	2 (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
1	OMU	0	2587	1	-	0/8/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/10/27/28	0/1/3/3
1	UR3	0	2619	1	-	0/6/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/8/25/26	0/2/2/2
1	1MA	0	628	1	-	1/8/25/26	0/1/3/3
3	PPU	4	76	1,3	-	0/26/43/44	0/2/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	76	PPU	OC-CM	-5.02	1.26	1.42
1	0	2621	PSU	C2-N1	3.39	1.43	1.37
1	0	2621	PSU	C6-N1	2.75	1.34	1.32
1	0	2621	PSU	P-OP1	2.61	1.49	1.46
1	0	2587	OMU	P-OP1	2.44	1.49	1.46
3	4	76	PPU	P-OP1	2.34	1.49	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	C6-C5-N7	-28.02	130.37	134.14
3	4	76	PPU	C2-N1-C6	3.45	119.00	111.53
1	0	2588	OMG	C6-N1-C2	3.30	125.29	119.51
1	0	628	1MA	C2-N3-C4	-3.12	110.90	116.23
3	4	76	PPU	C4'-C3'-N3'	-2.49	108.25	113.69
1	0	2621	PSU	C5-C4-N3	-2.34	114.59	118.86
1	0	2588	OMG	C2-N3-C4	-2.29	111.87	115.09
1	0	2621	PSU	C5-C1'-C2'	-2.14	111.83	115.61
1	0	2588	OMG	N2-C2-N1	-2.01	115.65	117.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	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 312 ligands modelled in this entry, 312 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	0	2754/2922 (94%)	-0.17	96 (3%) 42 42	26, 46, 90, 148	0
2	9	122/122 (100%)	0.08	5 (4%) 35 36	39, 62, 87, 147	0
3	4	3/3 (100%)	-0.02	0 100 100	52, 52, 57, 62	0
4	A	237/240 (98%)	0.40	15 (6%) 19 19	30, 52, 82, 104	0
5	B	337/338 (99%)	0.12	5 (1%) 70 71	31, 50, 72, 85	0
6	C	246/246 (100%)	-0.02	3 (1%) 75 76	28, 47, 68, 81	0
7	D	140/177 (79%)	1.63	44 (31%) 1 1	56, 90, 119, 127	0
8	E	172/178 (96%)	0.66	19 (11%) 6 6	42, 60, 78, 83	0
9	F	119/120 (99%)	1.09	29 (24%) 1 1	47, 71, 99, 108	0
10	G	29/348 (8%)	2.38	15 (51%) 0 0	68, 89, 97, 98	0
11	H	160/171 (93%)	0.63	19 (11%) 5 5	44, 60, 92, 99	0
12	J	142/145 (97%)	-0.03	4 (2%) 50 51	36, 47, 66, 86	0
13	K	132/132 (100%)	-0.23	1 (0%) 83 85	34, 45, 66, 69	0
14	L	145/165 (87%)	0.73	25 (17%) 2 2	30, 64, 110, 119	0
15	M	194/195 (99%)	0.43	11 (5%) 23 23	35, 46, 67, 79	0
16	N	186/187 (99%)	0.79	30 (16%) 2 2	44, 62, 104, 112	0
17	O	115/116 (99%)	0.07	2 (1%) 67 68	41, 53, 66, 74	0
18	P	143/149 (95%)	0.17	4 (2%) 50 51	40, 51, 65, 78	0
19	Q	95/96 (98%)	0.04	3 (3%) 45 46	41, 47, 63, 74	0
20	R	150/155 (96%)	-0.09	1 (0%) 84 86	31, 44, 62, 70	0
21	S	81/85 (95%)	0.37	6 (7%) 14 14	43, 62, 82, 95	0
22	T	119/120 (99%)	0.58	10 (8%) 11 10	43, 56, 79, 107	0
23	U	53/66 (80%)	0.35	3 (5%) 23 23	42, 51, 67, 75	0
24	V	65/71 (91%)	2.02	23 (35%) 1 0	54, 78, 111, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	-0.00	2 (1%) 74 74	36, 48, 69, 78	0
26	X	82/92 (89%)	0.52	7 (8%) 11 10	41, 53, 79, 97	0
27	Y	142/241 (58%)	0.12	8 (5%) 24 23	31, 43, 62, 82	0
28	Z	73/83 (87%)	1.07	20 (27%) 1 1	49, 73, 86, 92	0
29	1	56/57 (98%)	-0.46	0 100 100	30, 35, 42, 50	0
30	2	46/50 (92%)	0.69	7 (15%) 3 3	38, 58, 73, 83	0
31	3	92/92 (100%)	0.19	4 (4%) 34 34	37, 55, 68, 79	0
32	I	70/162 (43%)	4.93	60 (85%) 0 0	107, 120, 137, 139	0
All	All	6654/7478 (88%)	0.21	481 (7%) 15 15	26, 51, 95, 148	0

All (481) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	16.1
24	V	1	THR	15.2
7	D	63	ILE	12.9
32	I	133	THR	12.6
24	V	39	ALA	11.6
16	N	166	ALA	11.0
32	I	76	ALA	10.3
32	I	137	VAL	10.1
32	I	96	PHE	10.0
24	V	40	PRO	9.8
32	I	79	ILE	9.7
15	M	70	GLY	9.3
32	I	85	PHE	8.8
7	D	57	THR	8.6
32	I	75	THR	8.3
32	I	88	GLY	8.2
7	D	10	PHE	8.1
1	0	1951	G	8.1
32	I	89	SER	8.0
2	9	3001	U	7.9
4	A	37	VAL	7.8
30	2	49	GLU	7.7
32	I	111	GLN	7.4
32	I	116	LEU	7.2
24	V	38	GLY	7.1
28	Z	22	SER	7.1

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Mol	Chain	Res	Type	RSRZ
32	I	72	VAL	7.1
32	I	107	GLN	7.0
7	D	61	PHE	7.0
32	I	132	CYS	6.9
32	I	102	VAL	6.9
1	0	282	C	6.8
32	I	98	ALA	6.8
22	T	119	ALA	6.6
32	I	113	HIS	6.6
32	I	118	SER	6.5
32	I	109	ALA	6.4
10	G	24	VAL	6.2
7	D	69	ILE	6.1
7	D	170	TYR	6.0
14	L	80	ASP	6.0
1	0	1173	A	6.0
22	T	118	SER	5.9
32	I	77	GLU	5.9
1	0	1199	A	5.9
32	I	91	GLU	5.9
17	O	22	GLY	5.9
32	I	97	VAL	5.8
32	I	93	GLN	5.8
22	T	116	ASP	5.8
32	I	81	ASP	5.8
14	L	82	ALA	5.8
10	G	27	ILE	5.7
32	I	87	THR	5.7
32	I	121	LEU	5.7
2	9	3024	U	5.6
12	J	70	PHE	5.6
2	9	3002	U	5.5
26	X	88	GLU	5.5
14	L	81	VAL	5.4
1	0	2237	G	5.4
1	0	280	C	5.3
10	G	23	ILE	5.3
11	H	111	ASP	5.3
32	I	78	LEU	5.2
32	I	74	PRO	5.2
22	T	115	GLU	5.2
1	0	1172	G	5.2

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Mol	Chain	Res	Type	RSRZ
32	I	86	GLU	5.1
16	N	183	ASP	5.1
1	O	1950	G	5.1
24	V	37	GLY	5.1
28	Z	11	SER	5.1
1	O	2004	U	5.1
24	V	36	ALA	5.0
1	O	2637	A	5.0
28	Z	20	ARG	4.9
7	D	66	GLY	4.9
32	I	114	PRO	4.9
32	I	104	GLN	4.8
32	I	117	LEU	4.8
1	O	514	G	4.8
26	X	80	GLU	4.8
1	O	497	A	4.8
1	O	285	A	4.7
1	O	2508	C	4.7
32	I	129	VAL	4.7
7	D	64	ARG	4.7
14	L	130	ARG	4.7
8	E	45	ASP	4.6
16	N	184	ILE	4.5
1	O	1177	A	4.5
32	I	108	ILE	4.5
9	F	108	VAL	4.5
1	O	1202	A	4.5
9	F	119	ARG	4.5
14	L	91	VAL	4.5
1	O	1948	G	4.4
2	9	3023	U	4.4
1	O	10	U	4.4
17	O	23	GLY	4.4
16	N	161	GLY	4.3
24	V	43	PRO	4.3
2	9	3122	C	4.3
28	Z	45	ASP	4.3
7	D	90	LEU	4.3
32	I	103	ASP	4.3
32	I	119	TYR	4.3
10	G	26	MET	4.3
4	A	35	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
28	Z	19	GLY	4.3
1	0	2748	G	4.2
9	F	99	THR	4.2
32	I	105	VAL	4.2
7	D	44	ILE	4.2
9	F	117	GLU	4.2
4	A	133	ARG	4.2
26	X	85	VAL	4.1
1	0	1965	C	4.1
8	E	10	ASP	4.1
4	A	237	GLY	4.1
11	H	171	ALA	4.1
24	V	2	VAL	4.1
4	A	32	VAL	4.1
28	Z	24	ARG	4.1
23	U	47	ARG	4.0
32	I	126	LYS	4.0
30	2	35	ARG	4.0
9	F	100	ASP	4.0
1	0	970	U	4.0
28	Z	25	ARG	4.0
14	L	99	GLU	3.9
9	F	28	ALA	3.9
1	0	1171	A	3.9
28	Z	12	GLY	3.9
11	H	37	GLN	3.9
32	I	134	SER	3.9
7	D	62	ASP	3.9
24	V	3	LEU	3.9
1	0	2344	G	3.9
9	F	22	VAL	3.9
4	A	97	ALA	3.9
7	D	65	GLU	3.9
1	0	1200	A	3.9
1	0	2238	A	3.9
21	S	81	ILE	3.8
10	G	69	ARG	3.8
1	0	960	G	3.8
7	D	53	LYS	3.8
1	0	272	A	3.8
24	V	10	ASP	3.8
32	I	125	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	0	1163	G	3.8
32	I	106	LYS	3.8
12	J	4	ALA	3.7
15	M	74	LYS	3.7
8	E	100	ASP	3.7
1	0	1192	A	3.7
32	I	110	GLU	3.7
24	V	59	ILE	3.7
1	0	999	C	3.7
9	F	90	GLU	3.7
32	I	84	GLY	3.6
7	D	11	HIS	3.6
1	0	1169	U	3.6
15	M	71	SER	3.6
25	W	86	GLU	3.6
7	D	56	ARG	3.6
9	F	110	ASP	3.6
19	Q	17	LYS	3.6
1	0	1947	G	3.6
7	D	26	GLY	3.5
4	A	31	LYS	3.5
16	N	175	LEU	3.5
4	A	82	VAL	3.5
22	T	117	ASP	3.5
5	B	57	GLU	3.5
7	D	27	ILE	3.5
9	F	103	GLU	3.5
7	D	107	GLY	3.4
8	E	154	ILE	3.4
16	N	95	ALA	3.4
24	V	41	GLU	3.4
32	I	140	GLU	3.4
21	S	20	PHE	3.4
28	Z	14	PHE	3.4
4	A	36	ASP	3.4
6	C	61	PHE	3.4
32	I	120	ASP	3.4
1	0	138	U	3.4
5	B	1	PRO	3.4
1	0	1164	U	3.4
27	Y	95	THR	3.3
16	N	155	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
21	S	2	TRP	3.3
7	D	154	LYS	3.3
9	F	98	VAL	3.3
1	0	288	A	3.3
24	V	63	GLU	3.3
27	Y	236	VAL	3.3
32	I	115	ASP	3.3
16	N	165	ALA	3.3
8	E	126	ILE	3.3
14	L	75	LEU	3.3
1	0	969	G	3.3
19	Q	95	GLU	3.2
32	I	135	LEU	3.2
28	Z	16	ALA	3.2
16	N	152	GLU	3.2
28	Z	23	ARG	3.2
32	I	122	THR	3.2
1	0	279	C	3.2
1	0	358	G	3.2
8	E	99	GLY	3.2
7	D	35	ALA	3.1
7	D	171	ASP	3.1
32	I	99	ASP	3.1
32	I	138	THR	3.1
1	0	362	G	3.1
14	L	79	ASP	3.1
7	D	134	LEU	3.1
32	I	123	ASN	3.1
27	Y	108	ASP	3.1
9	F	106	ALA	3.1
10	G	66	LEU	3.1
16	N	163	PHE	3.1
16	N	162	ASP	3.1
8	E	124	VAL	3.1
1	0	1525	G	3.1
9	F	16	ALA	3.1
32	I	139	ILE	3.1
1	0	1168	C	3.1
1	0	2747	C	3.1
16	N	68	GLU	3.0
14	L	150	GLN	3.0
7	D	70	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
31	3	41	GLU	3.0
16	N	178	THR	3.0
8	E	87	PHE	3.0
1	0	281	U	3.0
1	0	1000	C	3.0
26	X	7	GLU	3.0
7	D	88	LEU	3.0
30	2	27	LEU	3.0
10	G	63	ARG	3.0
1	0	289	G	3.0
24	V	5	VAL	3.0
28	Z	31	SER	3.0
11	H	83	TYR	3.0
1	0	1279	U	3.0
11	H	35	ARG	3.0
9	F	118	LEU	3.0
9	F	25	ASP	3.0
1	0	2511	A	3.0
1	0	1966	U	3.0
1	0	284	C	2.9
11	H	143	ALA	2.9
7	D	51	ARG	2.9
16	N	154	LEU	2.9
4	A	38	ILE	2.9
10	G	12	ILE	2.9
7	D	25	MET	2.9
1	0	293	A	2.9
16	N	180	LEU	2.8
1	0	291	C	2.8
25	W	76	ASP	2.8
11	H	149	ALA	2.8
11	H	73	LEU	2.8
10	G	22	ALA	2.8
14	L	105	TYR	2.8
24	V	8	ILE	2.8
1	0	1203	G	2.8
30	2	39	ARG	2.8
9	F	107	ASP	2.8
1	0	2345	A	2.8
27	Y	216	ARG	2.8
1	0	370	G	2.8
14	L	148	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
16	N	185	GLU	2.8
15	M	132	ILE	2.8
16	N	156	GLU	2.7
1	O	716	G	2.7
15	M	75	ARG	2.7
11	H	32	LYS	2.7
14	L	142	LEU	2.7
27	Y	102	LEU	2.7
7	D	18	ILE	2.7
9	F	49	PHE	2.7
26	X	77	PHE	2.7
11	H	74	ILE	2.7
1	O	1198	U	2.7
11	H	140	VAL	2.7
32	I	100	LEU	2.7
9	F	101	ALA	2.7
6	C	132	ASP	2.7
10	G	15	TRP	2.7
1	O	1174	A	2.7
15	M	88	VAL	2.6
10	G	65	THR	2.6
19	Q	18	PRO	2.6
11	H	141	GLU	2.6
14	L	147	GLU	2.6
28	Z	59	TYR	2.6
16	N	137	ALA	2.6
4	A	85	SER	2.6
14	L	145	LEU	2.6
16	N	164	ASP	2.6
1	O	1175	G	2.6
9	F	79	GLN	2.6
1	O	128	A	2.6
1	O	735	C	2.6
14	L	60	GLU	2.6
22	T	106	GLU	2.6
13	K	132	VAL	2.6
14	L	101	ASP	2.6
32	I	73	PRO	2.6
7	D	166	ILE	2.6
18	P	141	ILE	2.6
15	M	49	ALA	2.6
8	E	123	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	0	363	A	2.6
1	0	368	C	2.6
7	D	52	THR	2.6
9	F	26	THR	2.6
6	C	143	ASP	2.5
11	H	39	ASP	2.5
4	A	236	GLY	2.5
30	2	26	MET	2.5
8	E	6	GLU	2.5
1	0	1201	C	2.5
7	D	23	VAL	2.5
8	E	11	VAL	2.5
7	D	68	PRO	2.5
28	Z	36	ASP	2.5
21	S	45	TYR	2.5
24	V	12	THR	2.5
16	N	138	ASP	2.5
1	0	1165	G	2.5
9	F	29	VAL	2.5
32	I	83	ALA	2.5
28	Z	37	HIS	2.5
10	G	21	ASP	2.5
9	F	27	GLY	2.5
1	0	369	G	2.5
1	0	1190	G	2.5
1	0	290	C	2.5
8	E	125	GLU	2.5
28	Z	21	VAL	2.5
16	N	134	ASP	2.5
14	L	90	ARG	2.5
15	M	87	GLY	2.4
10	G	64	ASN	2.4
28	Z	34	ASN	2.4
1	0	87	C	2.4
31	3	62	THR	2.4
11	H	78	GLY	2.4
11	H	137	TYR	2.4
28	Z	18	TYR	2.4
5	B	104	GLU	2.4
7	D	135	VAL	2.4
8	E	97	VAL	2.4
11	H	146	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	0	1181	A	2.4
11	H	82	ASP	2.4
28	Z	10	ARG	2.4
1	0	1949	G	2.4
1	0	1967	U	2.4
1	0	295	C	2.4
4	A	33	GLU	2.4
7	D	92	GLU	2.4
5	B	2	GLN	2.4
1	0	1170	U	2.4
24	V	14	ALA	2.4
16	N	149	GLU	2.4
16	N	174	GLU	2.4
7	D	55	LYS	2.3
1	0	372	A	2.3
1	0	2103	A	2.3
16	N	158	LEU	2.3
4	A	86	ALA	2.3
16	N	145	ALA	2.3
32	I	92	PRO	2.3
11	H	138	CYS	2.3
7	D	12	GLU	2.3
26	X	66	THR	2.3
31	3	92	GLU	2.3
7	D	93	LEU	2.3
24	V	49	LEU	2.3
9	F	115	VAL	2.3
21	S	78	ALA	2.3
1	0	1929	G	2.3
7	D	172	VAL	2.3
14	L	100	ALA	2.3
12	J	5	GLU	2.3
14	L	141	GLU	2.3
21	S	19	ASP	2.3
7	D	157	LEU	2.3
8	E	4	GLU	2.3
16	N	72	GLU	2.3
24	V	33	VAL	2.3
14	L	102	ASP	2.3
8	E	15	GLN	2.3
27	Y	235	GLU	2.2
1	0	1665	G	2.2

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Mol	Chain	Res	Type	RSRZ
1	0	2507	G	2.2
7	D	165	PHE	2.2
7	D	54	ALA	2.2
15	M	79	ALA	2.2
18	P	67	LYS	2.2
7	D	81	GLU	2.2
8	E	129	GLU	2.2
32	I	112	LYS	2.2
14	L	76	LEU	2.2
14	L	97	VAL	2.2
1	0	2769	C	2.2
8	E	128	GLY	2.2
18	P	135	ALA	2.2
32	I	124	ALA	2.2
27	Y	234	VAL	2.2
9	F	21	GLU	2.2
24	V	46	ILE	2.2
1	0	2241	C	2.2
14	L	89	PHE	2.2
9	F	102	GLY	2.2
1	0	1904	A	2.2
24	V	52	ALA	2.2
7	D	67	ASP	2.2
16	N	177	GLU	2.2
22	T	103	LEU	2.2
7	D	85	GLN	2.2
31	3	56	PRO	2.2
15	M	164	THR	2.2
32	I	80	LYS	2.2
1	0	1964	U	2.2
1	0	1189	A	2.2
15	M	159	VAL	2.2
1	0	736	A	2.1
27	Y	96	GLU	2.1
8	E	127	ASP	2.1
1	0	1197	G	2.1
1	0	1970	G	2.1
18	P	18	LYS	2.1
7	D	58	VAL	2.1
1	0	278	A	2.1
1	0	1919	A	2.1
11	H	154	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
12	J	46	ILE	2.1
14	L	119	THR	2.1
1	0	2250	G	2.1
9	F	19	ALA	2.1
1	0	1633	C	2.1
9	F	17	LEU	2.1
24	V	28	LEU	2.1
26	X	10	VAL	2.1
10	G	25	GLU	2.1
24	V	6	GLN	2.1
28	Z	33	MET	2.1
1	0	292	G	2.1
4	A	209	PRO	2.1
1	0	2645	U	2.1
16	N	181	ASP	2.1
23	U	45	GLU	2.1
9	F	12	LEU	2.1
10	G	67	LEU	2.1
16	N	168	LEU	2.1
1	0	1195	G	2.1
1	0	1523	G	2.1
20	R	96	VAL	2.1
1	0	1180	U	2.1
14	L	55	GLN	2.0
22	T	57	GLY	2.0
30	2	44	ARG	2.0
22	T	112	LEU	2.0
5	B	119	HIS	2.0
1	0	296	G	2.0
8	E	118	ILE	2.0
9	F	69	GLU	2.0
22	T	104	GLU	2.0
30	2	24	TRP	2.0
16	N	147	ILE	2.0
23	U	53	ASP	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
1	UR3	0	2619	21/22	0.15	-0.07	45,45,49,50	0
3	PPU	4	76	37/38	0.14	-0.12	48,54,66,71	0
1	1MA	0	628	23/24	0.12	-0.45	29,33,36,37	0
1	OMG	0	2588	24/25	0.11	-0.47	30,35,40,41	0
1	OMU	0	2587	21/22	0.10	-0.97	33,36,38,39	0
1	PSU	0	2621	20/21	0.10	-1.14	37,40,50,51	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
37	SR	0	9601	1/1	0.68	1125.00	200,200,200,200	0
37	SR	0	9501	1/1	0.34	461.00	200,200,200,200	0
35	NA	0	9152	1/1	0.66	191.08	78,78,78,78	0
35	NA	0	9179	1/1	1.28	129.10	100,100,100,100	0
37	SR	0	9547	1/1	1.19	105.44	200,200,200,200	0
35	NA	B	9161	1/1	0.76	89.60	62,62,62,62	0
35	NA	0	9118	1/1	0.20	57.27	60,60,60,60	0
33	MG	0	8092	1/1	0.65	55.50	81,81,81,81	0
33	MG	0	8047	1/1	0.47	55.20	91,91,91,91	0
37	SR	0	9500	1/1	1.46	54.79	200,200,200,200	0
35	NA	0	9125	1/1	0.68	52.04	115,115,115,115	0
33	MG	0	8022	1/1	0.77	41.43	74,74,74,74	0
35	NA	0	9158	1/1	0.31	40.91	63,63,63,63	0
35	NA	0	9184	1/1	0.70	38.54	102,102,102,102	0
33	MG	0	8084	1/1	0.76	30.59	74,74,74,74	0
35	NA	0	9149	1/1	0.21	28.30	42,42,42,42	0
33	MG	0	8082	1/1	0.24	26.98	107,107,107,107	0
33	MG	0	8108	1/1	0.26	26.50	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
33	MG	0	8094	1/1	0.21	24.98	67,67,67,67	0
35	NA	0	9120	1/1	0.25	21.59	64,64,64,64	0
36	CL	0	9322	1/1	0.23	21.34	53,53,53,53	0
35	NA	0	9173	1/1	0.34	20.97	70,70,70,70	0
33	MG	0	8085	1/1	0.29	20.96	91,91,91,91	0
33	MG	0	8013	1/1	0.35	20.27	22,22,22,22	0
37	SR	0	9626	1/1	0.28	19.77	128,128,128,128	0
33	MG	0	8025	1/1	0.34	18.98	25,25,25,25	0
35	NA	0	9170	1/1	0.38	18.62	94,94,94,94	0
33	MG	0	8024	1/1	1.64	18.49	77,77,77,77	0
35	NA	0	9164	1/1	0.28	18.40	59,59,59,59	0
33	MG	0	8040	1/1	0.37	17.79	100,100,100,100	0
37	SR	B	9521	1/1	0.50	17.54	199,199,199,199	0
35	NA	R	9186	1/1	0.43	17.29	69,69,69,69	0
33	MG	0	8072	1/1	0.27	17.04	96,96,96,96	0
35	NA	0	9129	1/1	0.20	16.70	85,85,85,85	0
33	MG	0	8107	1/1	0.20	15.30	67,67,67,67	0
33	MG	0	8059	1/1	0.28	15.10	78,78,78,78	0
33	MG	0	8052	1/1	0.34	14.50	68,68,68,68	0
35	NA	0	9182	1/1	0.26	13.60	78,78,78,78	0
35	NA	0	9111	1/1	0.12	13.56	57,57,57,57	0
35	NA	0	9172	1/1	0.40	13.49	70,70,70,70	0
33	MG	0	8012	1/1	0.26	13.32	41,41,41,41	0
37	SR	0	9539	1/1	0.21	12.85	162,162,162,162	0
35	NA	0	9175	1/1	0.26	11.41	52,52,52,52	0
35	NA	0	9171	1/1	0.22	11.33	61,61,61,61	0
35	NA	0	9106	1/1	0.21	10.78	37,37,37,37	0
33	MG	0	8118	1/1	0.18	10.28	76,76,76,76	0
37	SR	0	9482	1/1	0.20	9.99	102,102,102,102	0
33	MG	0	8038	1/1	0.22	9.87	20,20,20,20	0
35	NA	0	9185	1/1	0.28	9.63	46,46,46,46	0
35	NA	0	9107	1/1	0.25	9.60	61,61,61,61	0
33	MG	0	8001	1/1	0.25	9.17	20,20,20,20	0
33	MG	0	8008	1/1	0.19	9.16	17,17,17,17	0
35	NA	0	9102	1/1	0.21	8.93	57,57,57,57	0
33	MG	0	8089	1/1	0.12	8.50	54,54,54,54	0
37	SR	0	9406	1/1	0.16	8.27	38,38,38,38	0
33	MG	0	8060	1/1	0.30	8.25	71,71,71,71	0
35	NA	0	9169	1/1	0.45	8.14	104,104,104,104	0
33	MG	0	8114	1/1	0.19	7.98	63,63,63,63	0
33	MG	0	8103	1/1	0.16	7.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	K	0	9001	1/1	0.36	7.16	116,116,116,116	0
33	MG	0	8041	1/1	0.17	6.67	50,50,50,50	0
33	MG	K	8069	1/1	0.20	6.35	29,29,29,29	0
35	NA	0	9122	1/1	0.34	6.31	96,96,96,96	0
33	MG	0	8090	1/1	0.51	6.19	80,80,80,80	0
33	MG	0	8065	1/1	0.41	6.13	93,93,93,93	0
35	NA	0	9157	1/1	0.13	6.08	47,47,47,47	0
33	MG	0	8029	1/1	0.21	5.97	33,33,33,33	0
33	MG	0	8061	1/1	0.13	5.74	95,95,95,95	0
35	NA	9	9183	1/1	0.19	5.72	66,66,66,66	0
33	MG	0	8051	1/1	0.17	5.44	26,26,26,26	0
33	MG	0	8021	1/1	0.17	5.24	55,55,55,55	0
37	SR	0	9474	1/1	0.11	5.18	112,112,112,112	0
35	NA	0	9177	1/1	0.20	5.06	63,63,63,63	0
37	SR	0	9432	1/1	0.11	5.03	62,62,62,62	0
33	MG	0	8026	1/1	0.15	4.95	27,27,27,27	0
33	MG	0	8045	1/1	0.30	4.81	84,84,84,84	0
35	NA	0	9165	1/1	0.30	4.57	47,47,47,47	0
35	NA	0	9178	1/1	0.19	4.39	51,51,51,51	0
33	MG	0	8014	1/1	0.34	4.26	73,73,73,73	0
35	NA	0	9101	1/1	0.14	4.22	47,47,47,47	0
35	NA	0	9132	1/1	0.19	4.12	51,51,51,51	0
33	MG	9	8095	1/1	0.19	4.09	46,46,46,46	0
33	MG	0	8017	1/1	0.13	3.82	28,28,28,28	0
37	SR	0	9405	1/1	0.14	3.75	60,60,60,60	0
33	MG	0	8027	1/1	0.18	3.75	39,39,39,39	0
35	NA	0	9116	1/1	0.18	3.72	58,58,58,58	0
33	MG	0	8058	1/1	0.25	3.48	45,45,45,45	0
35	NA	0	9141	1/1	0.14	3.35	62,62,62,62	0
36	CL	0	9316	1/1	0.21	3.33	69,69,69,69	0
37	SR	0	9452	1/1	0.17	3.13	114,114,114,114	0
33	MG	A	8066	1/1	0.17	3.02	53,53,53,53	0
35	NA	0	9163	1/1	0.16	2.60	66,66,66,66	0
35	NA	0	9156	1/1	0.12	2.57	53,53,53,53	0
35	NA	0	9154	1/1	0.16	2.40	59,59,59,59	0
33	MG	0	8101	1/1	0.14	2.34	59,59,59,59	0
33	MG	0	8056	1/1	0.20	2.26	46,46,46,46	0
37	SR	0	9408	1/1	0.13	2.15	39,39,39,39	0
35	NA	0	9155	1/1	0.27	2.05	55,55,55,55	0
33	MG	B	8055	1/1	0.20	2.03	108,108,108,108	0
33	MG	0	8002	1/1	0.15	2.02	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8057	1/1	0.20	2.01	85,85,85,85	0
33	MG	0	8080	1/1	0.16	1.94	47,47,47,47	0
37	SR	0	9529	1/1	0.15	1.82	138,138,138,138	0
37	SR	0	9515	1/1	0.15	1.57	87,87,87,87	0
33	MG	0	8104	1/1	0.23	1.38	76,76,76,76	0
37	SR	S	9470	1/1	0.12	1.38	100,100,100,100	0
35	NA	0	9128	1/1	0.12	1.20	45,45,45,45	0
35	NA	0	9174	1/1	0.10	1.18	65,65,65,65	0
36	CL	A	9309	1/1	0.20	1.08	68,68,68,68	0
35	NA	0	9117	1/1	0.16	1.02	39,39,39,39	0
33	MG	0	8097	1/1	0.13	0.97	62,62,62,62	0
33	MG	0	8074	1/1	0.19	0.93	23,23,23,23	0
37	SR	0	9407	1/1	0.11	0.90	43,43,43,43	0
33	MG	0	8020	1/1	0.15	0.87	37,37,37,37	0
33	MG	0	8070	1/1	0.14	0.86	26,26,26,26	0
33	MG	0	8015	1/1	0.12	0.83	34,34,34,34	0
35	NA	0	9140	1/1	0.18	0.77	60,60,60,60	0
33	MG	0	8050	1/1	0.14	0.75	93,93,93,93	0
33	MG	0	8028	1/1	0.12	0.73	37,37,37,37	0
35	NA	C	9104	1/1	0.17	0.69	34,34,34,34	0
37	SR	H	9486	1/1	0.16	0.62	109,109,109,109	0
37	SR	A	9437	1/1	0.13	0.58	67,67,67,67	0
33	MG	0	8076	1/1	0.11	0.54	61,61,61,61	0
33	MG	0	8003	1/1	0.15	0.49	32,32,32,32	0
33	MG	0	8091	1/1	0.11	0.46	45,45,45,45	0
35	NA	M	9147	1/1	0.16	0.33	43,43,43,43	0
35	NA	0	9166	1/1	0.10	0.30	67,67,67,67	0
35	NA	0	9113	1/1	0.11	0.25	65,65,65,65	0
36	CL	B	9319	1/1	0.11	0.21	52,52,52,52	0
35	NA	0	9139	1/1	0.15	0.17	52,52,52,52	0
35	NA	0	9136	1/1	0.10	-0.13	34,34,34,34	0
33	MG	0	8079	1/1	0.10	-0.16	34,34,34,34	0
35	NA	0	9162	1/1	0.11	-0.17	58,58,58,58	0
37	SR	F	9595	1/1	0.14	-0.22	105,105,105,105	0
33	MG	0	8004	1/1	0.09	-0.23	30,30,30,30	0
33	MG	0	8102	1/1	0.10	-0.27	56,56,56,56	0
37	SR	0	9537	1/1	0.12	-0.28	154,154,154,154	0
33	MG	0	8054	1/1	0.11	-0.37	58,58,58,58	0
34	K	0	9002	1/1	0.12	-0.37	89,89,89,89	0
35	NA	0	9126	1/1	0.10	-0.38	59,59,59,59	0
35	NA	0	9110	1/1	0.11	-0.43	46,46,46,46	0
36	CL	J	9301	1/1	0.10	-0.45	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	S	9112	1/1	0.11	-0.45	59,59,59,59	0
33	MG	0	8093	1/1	0.11	-0.52	42,42,42,42	0
33	MG	0	8096	1/1	0.12	-0.58	46,46,46,46	0
37	SR	0	9477	1/1	0.10	-0.61	84,84,84,84	0
33	MG	0	8046	1/1	0.09	-0.62	40,40,40,40	0
33	MG	0	8099	1/1	0.11	-0.70	59,59,59,59	0
37	SR	0	9509	1/1	0.11	-0.70	81,81,81,81	0
35	NA	0	9181	1/1	0.09	-0.70	50,50,50,50	0
37	SR	R	9418	1/1	0.11	-0.74	54,54,54,54	0
37	SR	0	9414	1/1	0.10	-0.76	52,52,52,52	0
33	MG	0	8063	1/1	0.11	-0.76	70,70,70,70	0
37	SR	0	9417	1/1	0.09	-0.77	59,59,59,59	0
35	NA	R	9137	1/1	0.10	-0.78	36,36,36,36	0
37	SR	0	9433	1/1	0.09	-0.81	76,76,76,76	0
37	SR	0	9590	1/1	0.12	-0.85	178,178,178,178	0
37	SR	1	9419	1/1	0.10	-0.85	40,40,40,40	0
38	CD	U	9201	1/1	0.10	-0.86	48,48,48,48	0
36	CL	M	9318	1/1	0.15	-0.87	41,41,41,41	0
35	NA	J	9146	1/1	0.10	-0.90	55,55,55,55	0
33	MG	0	8088	1/1	0.08	-0.90	45,45,45,45	0
37	SR	0	9430	1/1	0.10	-0.93	44,44,44,44	0
37	SR	A	9497	1/1	0.07	-1.00	91,91,91,91	0
35	NA	0	9114	1/1	0.09	-1.07	46,46,46,46	0
37	SR	0	9440	1/1	0.03	-1.08	61,61,61,61	0
35	NA	0	9168	1/1	0.09	-1.08	57,57,57,57	0
36	CL	R	9306	1/1	0.10	-1.10	44,44,44,44	0
33	MG	0	8042	1/1	0.09	-1.11	60,60,60,60	0
35	NA	0	9124	1/1	0.06	-1.12	47,47,47,47	0
38	CD	Z	9203	1/1	0.07	-1.12	78,78,78,78	0
37	SR	0	9413	1/1	0.09	-1.13	44,44,44,44	0
35	NA	0	9134	1/1	0.07	-1.18	51,51,51,51	0
33	MG	T	8073	1/1	0.12	-1.20	46,46,46,46	0
37	SR	0	9420	1/1	0.10	-1.22	56,56,56,56	0
37	SR	L	9409	1/1	0.09	-1.26	40,40,40,40	0
33	MG	0	8030	1/1	0.09	-1.27	39,39,39,39	0
37	SR	0	9450	1/1	0.07	-1.31	62,62,62,62	0
37	SR	0	9475	1/1	0.08	-1.32	77,77,77,77	0
37	SR	0	9421	1/1	0.07	-1.33	64,64,64,64	0
36	CL	J	9321	1/1	0.04	-1.38	53,53,53,53	0
35	NA	0	9127	1/1	0.10	-1.42	57,57,57,57	0
35	NA	0	9105	1/1	0.09	-1.49	43,43,43,43	0
35	NA	D	9151	1/1	0.15	-1.50	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	CL	J	9302	1/1	0.05	-1.50	48,48,48,48	0
37	SR	0	9545	1/1	0.03	-1.51	79,79,79,79	0
37	SR	0	9415	1/1	0.09	-1.51	50,50,50,50	0
37	SR	0	9568	1/1	0.08	-1.52	75,75,75,75	0
37	SR	0	9504	1/1	0.08	-1.57	105,105,105,105	0
35	NA	0	9108	1/1	0.08	-1.60	35,35,35,35	0
37	SR	0	9451	1/1	0.08	-1.61	62,62,62,62	0
37	SR	0	9447	1/1	0.07	-1.61	67,67,67,67	0
38	CD	O	9205	1/1	0.07	-1.62	75,75,75,75	0
37	SR	0	9534	1/1	0.09	-1.65	100,100,100,100	0
37	SR	0	9410	1/1	0.11	-1.68	37,37,37,37	0
35	NA	R	9138	1/1	0.07	-1.69	56,56,56,56	0
37	SR	0	9490	1/1	0.08	-1.69	109,109,109,109	0
35	NA	0	9159	1/1	0.09	-1.73	46,46,46,46	0
37	SR	0	9462	1/1	0.09	-1.75	64,64,64,64	0
37	SR	0	9488	1/1	0.07	-1.75	76,76,76,76	0
37	SR	0	9424	1/1	0.11	-1.76	45,45,45,45	0
38	CD	3	9204	1/1	0.04	-1.79	60,60,60,60	0
36	CL	0	9315	1/1	0.08	-1.79	58,58,58,58	0
37	SR	0	9416	1/1	0.09	-1.82	43,43,43,43	0
37	SR	0	9517	1/1	0.06	-1.86	91,91,91,91	0
36	CL	0	9311	1/1	0.06	-1.91	57,57,57,57	0
36	CL	O	9308	1/1	0.06	-1.94	60,60,60,60	0
33	MG	0	8068	1/1	0.10	-1.96	46,46,46,46	0
35	NA	0	9160	1/1	0.08	-1.97	39,39,39,39	0
37	SR	0	9530	1/1	0.10	-1.99	84,84,84,84	0
35	NA	Q	9148	1/1	0.07	-1.99	44,44,44,44	0
37	SR	0	9422	1/1	0.08	-2.11	54,54,54,54	0
37	SR	0	9467	1/1	0.07	-2.17	67,67,67,67	0
37	SR	0	9431	1/1	0.10	-2.25	55,55,55,55	0
37	SR	0	9446	1/1	0.06	-2.27	83,83,83,83	0
36	CL	L	9310	1/1	0.08	-2.33	54,54,54,54	0
33	MG	0	8067	1/1	0.09	-2.41	42,42,42,42	0
35	NA	0	9115	1/1	0.07	-2.42	39,39,39,39	0
36	CL	0	9314	1/1	0.08	-2.46	45,45,45,45	0
37	SR	0	9505	1/1	0.10	-2.49	85,85,85,85	0
33	MG	0	8019	1/1	0.07	-2.50	58,58,58,58	0
33	MG	0	8036	1/1	0.08	-2.50	60,60,60,60	0
33	MG	Y	8109	1/1	0.08	-2.51	41,41,41,41	0
37	SR	A	9436	1/1	0.04	-2.58	61,61,61,61	0
37	SR	0	9423	1/1	0.07	-2.60	54,54,54,54	0
33	MG	0	8116	1/1	0.06	-2.62	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	9468	1/1	0.04	-2.64	113,113,113,113	0
33	MG	0	8032	1/1	0.07	-2.65	43,43,43,43	0
35	NA	0	9130	1/1	0.07	-2.66	49,49,49,49	0
37	SR	0	9443	1/1	0.08	-2.68	57,57,57,57	0
37	SR	0	9461	1/1	0.04	-2.74	76,76,76,76	0
37	SR	0	9427	1/1	0.09	-2.76	52,52,52,52	0
37	SR	0	9483	1/1	0.07	-2.77	68,68,68,68	0
37	SR	0	9449	1/1	0.07	-2.78	59,59,59,59	0
37	SR	0	9428	1/1	0.03	-2.79	49,49,49,49	0
37	SR	3	9439	1/1	0.04	-2.81	63,63,63,63	0
37	SR	0	9425	1/1	0.09	-2.81	55,55,55,55	0
36	CL	0	9303	1/1	0.09	-2.88	46,46,46,46	0
36	CL	K	9312	1/1	0.05	-2.90	46,46,46,46	0
37	SR	1	9460	1/1	0.07	-2.94	52,52,52,52	0
37	SR	0	9448	1/1	0.04	-2.94	60,60,60,60	0
35	NA	0	9143	1/1	0.07	-3.00	43,43,43,43	0
37	SR	0	9455	1/1	0.06	-3.07	67,67,67,67	0
38	CD	1	9202	1/1	0.04	-3.07	51,51,51,51	0
33	MG	0	8115	1/1	0.08	-3.19	56,56,56,56	0
37	SR	0	9444	1/1	0.03	-3.20	50,50,50,50	0
37	SR	0	9581	1/1	0.06	-3.27	121,121,121,121	0
36	CL	0	9313	1/1	0.08	-3.47	51,51,51,51	0
35	NA	0	9123	1/1	0.08	-3.51	41,41,41,41	0
37	SR	0	9532	1/1	0.07	-3.56	103,103,103,103	0
37	SR	0	9442	1/1	0.07	-3.58	59,59,59,59	0
37	SR	0	9473	1/1	0.03	-3.65	69,69,69,69	0
36	CL	3	9304	1/1	0.06	-3.71	55,55,55,55	0
36	CL	0	9305	1/1	0.06	-3.72	54,54,54,54	0
33	MG	0	8039	1/1	0.06	-3.75	65,65,65,65	0
35	NA	0	9131	1/1	0.06	-3.78	48,48,48,48	0
37	SR	0	9566	1/1	0.04	-3.82	77,77,77,77	0
33	MG	0	8037	1/1	0.08	-3.84	39,39,39,39	0
37	SR	0	9434	1/1	0.08	-3.92	55,55,55,55	0
36	CL	N	9307	1/1	0.11	-4.05	52,52,52,52	0
37	SR	0	9560	1/1	0.06	-4.12	97,97,97,97	0
37	SR	0	9508	1/1	0.05	-4.17	80,80,80,80	0
33	MG	0	8112	1/1	0.05	-4.19	43,43,43,43	0
33	MG	0	8075	1/1	0.07	-4.21	36,36,36,36	0
33	MG	0	8044	1/1	0.06	-4.27	39,39,39,39	0
37	SR	0	9411	1/1	0.11	-4.30	40,40,40,40	0
33	MG	0	8098	1/1	0.06	-4.36	39,39,39,39	0
33	MG	0	8005	1/1	0.06	-4.36	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	9426	1/1	0.06	-4.40	67,67,67,67	0
37	SR	0	9456	1/1	0.06	-4.66	69,69,69,69	0
37	SR	0	9465	1/1	0.06	-4.72	100,100,100,100	0
37	SR	0	9435	1/1	0.07	-4.77	65,65,65,65	0
37	SR	0	9457	1/1	0.06	-4.98	47,47,47,47	0
37	SR	0	9469	1/1	0.04	-5.04	79,79,79,79	0
37	SR	0	9506	1/1	0.03	-5.18	66,66,66,66	0
33	MG	0	8117	1/1	0.07	-5.22	43,43,43,43	0
37	SR	0	9498	1/1	0.04	-5.28	59,59,59,59	0
36	CL	0	9317	1/1	0.06	-5.41	50,50,50,50	0
33	MG	0	8009	1/1	0.09	-5.43	28,28,28,28	0
33	MG	0	8110	1/1	0.05	-5.48	36,36,36,36	0
37	SR	0	9466	1/1	0.03	-5.49	84,84,84,84	0
33	MG	0	8043	1/1	0.07	-5.51	49,49,49,49	0
33	MG	0	8031	1/1	0.06	-5.51	50,50,50,50	0
37	SR	0	9489	1/1	0.04	-5.66	85,85,85,85	0
35	NA	0	9135	1/1	0.07	-5.68	50,50,50,50	0
35	NA	0	9167	1/1	0.07	-5.69	56,56,56,56	0
37	SR	0	9429	1/1	0.07	-5.72	60,60,60,60	0
37	SR	0	9480	1/1	0.04	-5.78	87,87,87,87	0
36	CL	Y	9320	1/1	0.04	-6.00	43,43,43,43	0
37	SR	0	9478	1/1	0.06	-6.03	70,70,70,70	0
37	SR	9	9588	1/1	0.08	-6.24	114,114,114,114	0
37	SR	0	9441	1/1	0.05	-6.36	60,60,60,60	0
35	NA	0	9150	1/1	0.09	-6.64	38,38,38,38	0
37	SR	0	9438	1/1	0.04	-6.67	63,63,63,63	0
33	MG	0	8113	1/1	0.08	-6.85	50,50,50,50	0
37	SR	0	9459	1/1	0.07	-8.09	101,101,101,101	0
37	SR	0	9629	1/1	0.05	-8.17	65,65,65,65	0
33	MG	0	8106	1/1	0.03	-8.19	43,43,43,43	0
37	SR	B	9458	1/1	0.04	-8.23	68,68,68,68	0
37	SR	0	9445	1/1	0.05	-9.00	56,56,56,56	0
37	SR	0	9412	1/1	0.10	-9.84	42,42,42,42	0
37	SR	0	9454	1/1	0.03	-10.03	74,74,74,74	0
37	SR	9	9503	1/1	0.03	-11.45	114,114,114,114	0
37	SR	9	9481	1/1	0.04	-11.62	80,80,80,80	0
37	SR	0	9453	1/1	0.04	-11.65	69,69,69,69	0
37	SR	0	9585	1/1	0.05	-12.01	83,83,83,83	0
37	SR	0	9570	1/1	0.03	-13.68	98,98,98,98	0
37	SR	0	9464	1/1	0.03	-13.82	74,74,74,74	0
37	SR	0	9495	1/1	0.07	-14.37	88,88,88,88	0
33	MG	0	8083	1/1	0.07	-14.71	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	9522	1/1	0.04	-18.57	104,104,104,104	0
37	SR	0	9484	1/1	0.11	-	147,147,147,147	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.