



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 08:08 PM GMT

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

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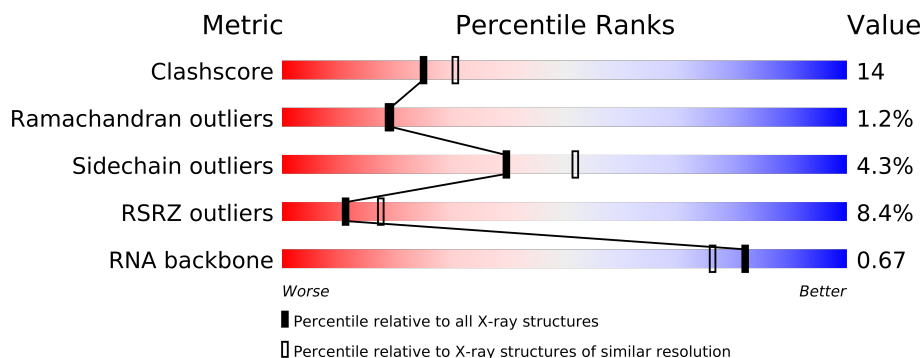
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)
RNA backbone	1838	1081 (3.00-1.60)

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	5	
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	8008	-	X
33	MG	0	8012	-	X
33	MG	0	8013	-	X
33	MG	0	8017	-	X
33	MG	0	8020	-	X
33	MG	0	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	8029	-	X
33	MG	0	8038	-	X
33	MG	0	8040	-	X
33	MG	0	8047	-	X
33	MG	0	8050	-	X
33	MG	0	8051	-	X
33	MG	0	8052	-	X
33	MG	0	8057	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
33	MG	0	8058	-	X
33	MG	0	8059	-	X
33	MG	0	8061	-	X
33	MG	0	8065	-	X
33	MG	0	8070	-	X
33	MG	0	8072	-	X
33	MG	0	8076	-	X
33	MG	0	8080	-	X
33	MG	0	8082	-	X
33	MG	0	8084	-	X
33	MG	0	8085	-	X
33	MG	0	8089	-	X
33	MG	0	8092	-	X
33	MG	0	8094	-	X
33	MG	0	8099	-	X
33	MG	0	8102	-	X
33	MG	0	8103	-	X
33	MG	0	8107	-	X
33	MG	0	8108	-	X
33	MG	0	8114	-	X
33	MG	9	8095	-	X
33	MG	B	8055	-	X
33	MG	K	8069	-	X
34	K	0	9001	-	X
35	NA	0	9102	-	X
35	NA	0	9106	-	X
35	NA	0	9107	-	X
35	NA	0	9110	-	X
35	NA	0	9111	-	X
35	NA	0	9115	-	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	9127	-	X
35	NA	0	9129	-	X
35	NA	0	9132	-	X
35	NA	0	9135	-	X
35	NA	0	9140	-	X
35	NA	0	9149	-	X
35	NA	0	9150	-	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	9156	-	X
35	NA	0	9157	-	X
35	NA	0	9160	-	X
35	NA	0	9161	-	X
35	NA	0	9162	-	X
35	NA	0	9163	-	X
35	NA	0	9164	-	X
35	NA	0	9165	-	X
35	NA	0	9168	-	X
35	NA	0	9170	-	X
35	NA	0	9171	-	X
35	NA	0	9172	-	X
35	NA	0	9173	-	X
35	NA	0	9174	-	X
35	NA	0	9175	-	X
35	NA	0	9177	-	X
35	NA	0	9178	-	X
35	NA	0	9179	-	X
35	NA	0	9184	-	X
35	NA	0	9185	-	X
35	NA	3	9169	-	X
35	NA	9	9183	-	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	9434	-	X
37	SR	0	9452	-	X
37	SR	0	9477	-	X
37	SR	0	9482	-	X
37	SR	0	9484	-	X
37	SR	0	9500	-	X
37	SR	0	9501	-	X
37	SR	0	9515	-	X
37	SR	0	9539	-	X
37	SR	0	9547	-	X
37	SR	0	9601	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
37	SR	O	9626	-	X
37	SR	B	9521	-	X

## 2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:



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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Q	95	Total	C	N	O	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	87	Total	Mg	0	0
			87	87		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	64	Total	Na	0	0
			64	64		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	D	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	3	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	3	Total 3	Na 3	0	0
35	9	1	Total 1	Na 1	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	10	Total 10	Cl 10	0	0
36	J	3	Total 3	Cl 3	0	0
36	B	1	Total 1	Cl 1	0	0
36	A	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	98	Total 98	Sr 98	0	0
37	1	2	Total 2	Sr 2	0	0

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

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

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

- Molecule 39 is water.

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

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

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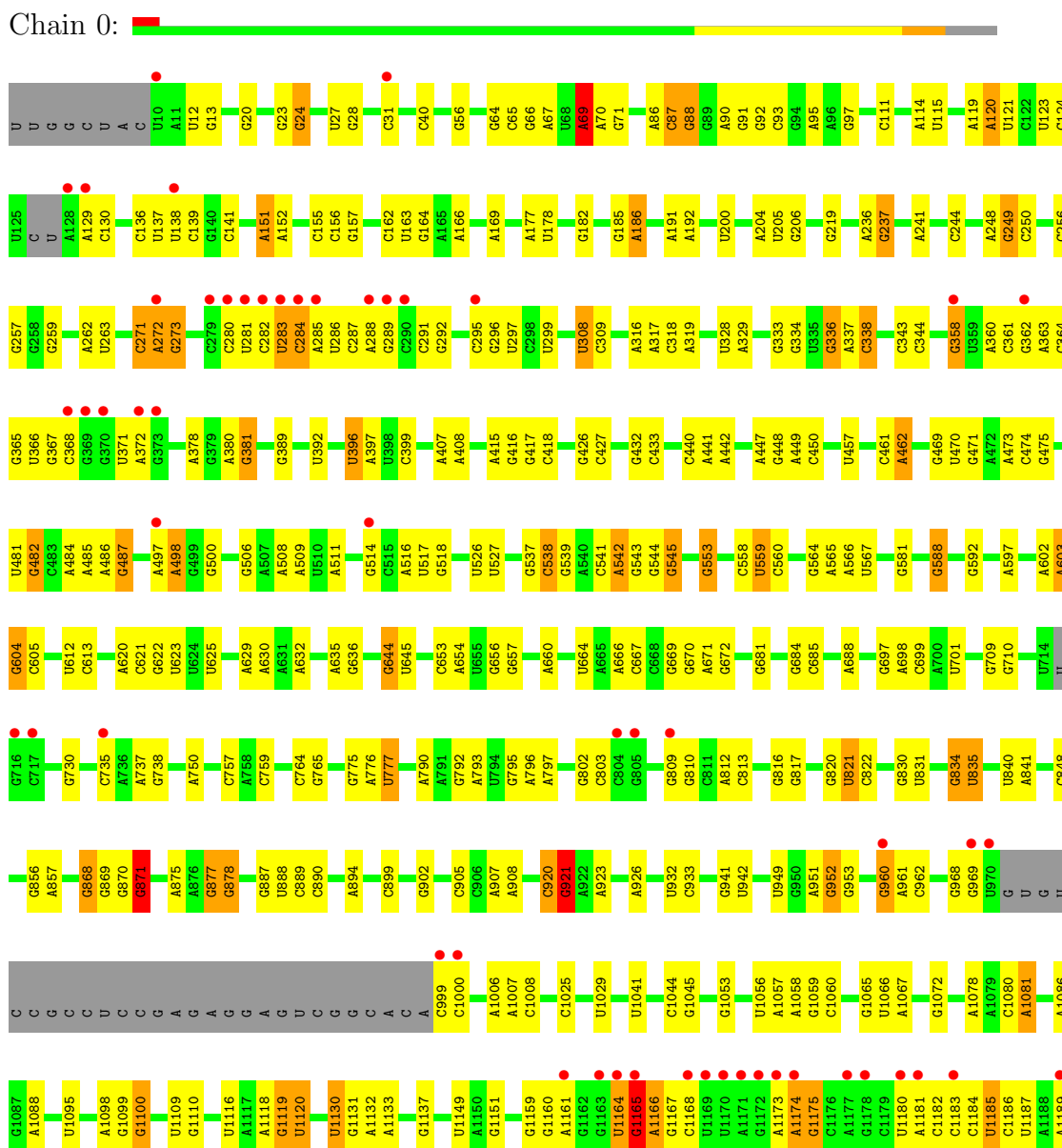
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	24	Total 24	O 24	0	0
39	Y	96	Total 96	O 96	0	0
39	Z	31	Total 31	O 31	0	0
39	1	50	Total 50	O 50	0	0
39	2	40	Total 40	O 40	0	0
39	3	67	Total 67	O 67	0	0
39	I	7	Total 7	O 7	0	0



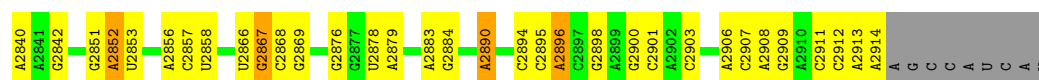
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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

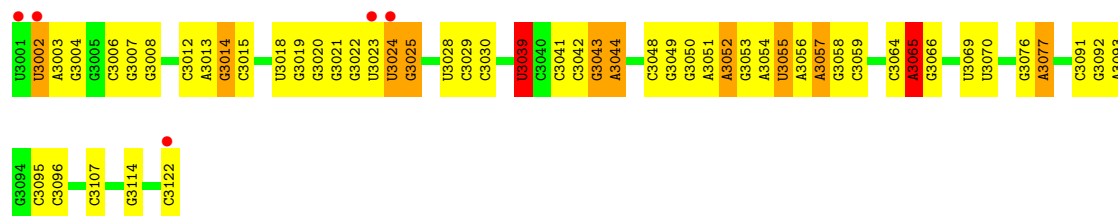


U2749	A2511	G2412	G2272	G2134	U1996	U1879	U1766	U1654	C1477	G1299	G1190
G2750	A2521	A2413	A2291	A2135	U2003	C1882	A1767	G1655	U1478	G1311	A1191
G2754	G2524	A2414	A2302	G2136	U2004	G1902	C1768	A1656	C1495	G1314	A1192
G2755	G2525	G2415	C2309	C	G2005	U1903	C1769	G1660	G1496	U1314	A1193
G2756	G2526	G2416	C	U	A2007	A1919	A1778	A1659	A1501	A1328	G1194
A2761	U2531	G2417	C	G	U2008	C1920	A1779	G1666	A1502	G1332	G1195
C2762	A2532	G2418	C	G	A2011	U1921	C1786	U1667	U1503	A1331	C1196
C2765	G2533	G2419	A	U	G2012	A1922	C1787	U1668	A1504	U1333	U1198
C2768	G2534	G2420	G	C	G2013	G1926	U1788	U1668	U1505	C1334	A1200
C2769	U2535	G2421	U	C	G2014	G1927	G1789	G1681	U1506	C1335	C1201
G2770	G2536	G2422	C	C	A2015	A1927	G1794	A1682	G1523	G1360	G1202
G2771	G2537	G2423	A	G	U2016	G1928	G1795	G1683	U1524	G1360	G1203
G2772	A2538	U2435	C	A	U2017	G1929	A1796	A1684	U1525	G1360	C1204
G2773	U2541	G2443	A	U	U2032	U1937	A1797	A1685	A1526	A1342	U1205
G2774	U2542	G2444	G	U	G2033	U1938	C1798	A1686	A1527	C1343	U1206
G2775	G2543	G2445	U	U	U2034	U1939	C1799	C1687	A1528	U1360	A1207
G2776	G2544	G2446	G	C	C2035	G1940	G1809	C1692	G1552	G1351	C1208
G2777	G2545	G2447	A	C	C2036	A1941	G1810	C1700	G1553	A1352	G1210
G2778	G2546	G2448	A	G	U2042	A1942	C1811	A1701	G1554	C1353	G1211
G2779	G2547	G2449	U	A	U2043	C1943	G1812	U1702	G1555	G1360	C1212
G2780	G2548	G2450	C	U	G2044	G1946	G1813	A1710	A1559	G1360	G1216
G2781	G2549	G2451	C	U	G2045	G1947	G1814	A1711	U	G1360	G1217
G2782	G2550	G2452	U	A	A2053	G1948	G1815	A1712	U1561	G1360	U1218
G2783	G2551	G2453	C	G	G2054	U1949	A1821	C1714	U1562	G1360	U1219
G2784	G2552	G2454	C	U	G2055	G1950	A1822	C1715	C1562	A1372	G1226
G2785	G2553	G2455	C	U	C2061	G1951	A1823	A1716	G1563	G1377	G1226
G2786	G2554	G2456	C	G	U2062	U1952	A1824	A1717	C1564	C1378	C1229
G2787	G2555	G2457	C	A	U2063	U1953	G1834	A1718	A1573	A1230	A1230
G2788	G2556	G2458	U	G	U2064	U1954	U1835	G1719	C1574	A1231	A1231
G2789	G2557	G2459	C	C	U2065	U1955	U1836	U1722	G1592	A1406	A1232
G2790	G2558	G2460	C	A	A2067	U1956	G1837	G1723	C1593	A1407	A1233
G2791	G2559	G2461	C	U	G2068	U1957	U1838	U1724	C1594	U1408	U1234
G2792	G2560	G2462	C	A	G2069	U1958	U1839	C1725	C1595	G1409	G1235
G2793	G2561	G2463	C	C	U2070	U1959	U1840	G1730	G1596	U1419	U1236
G2794	G2562	G2464	C	U	A2071	U1960	U1841	C1731	U1597	U1419	C1238
G2795	G2563	G2465	C	C	A2072	U1961	U1842	A1732	A1598	U1422	G1239
G2796	G2564	G2466	C	A	U2073	U1962	G1843	A1733	A1603	A1242	A1242
G2797	G2565	G2467	C	C	G2074	U1963	G1844	A1734	G1604	C1243	C1243
G2798	G2566	G2468	C	G	A2075	U1964	G1845	G1735	G1605	C1246	U1244
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G2800	G2568	G2470	C	C	A2077	U1966	U1847	U1741	A1615	U1435	A1252
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G2810	G2578	G2480	C	C	U2087	U1976	G1857	G1761	U1635	C1474	U1298
G2811	G2579	G2481	C	U	A2088	U1977	G1858	G1762	U1636	C1474	U1298
G2812	G2580	G2482	C	C	G2089	U1978	G1859	G1763	U1637	C1474	U1298
G2813	G2581	G2483	C	A	U2090	U1979	G1860	G1764	U1638	C1474	U1298
G2814	G2582	G2484	C	C	A2091	U1980	G1861	G1765	U1639	C1474	U1298
G2815	G2583	G2485	C	U	A2092	U1981	G1862	G1766	U1640	C1474	U1298
G2816	G2584	G2486	C	C	U2093	U1982	G1863	G1767	U1641	C1474	U1298
G2817	G2585	G2487	C	A	U2094	U1983	G1864	G1768	U1642	C1474	U1298
G2818	G2586	G2488	C	C	A2095	U1984	G1865	G1769	U1643	C1474	U1298
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G2820	G2588	G2490	C	C	A2097	U1986	G1867	G1771	U1645	C1474	U1298
G2821	G2589	G2491	C	A	U2098	U1987	G1868	G1772	U1646	C1474	U1298
G2822	G2590	G2492	C	C	A2099	U1988	G1869	G1773	U1647	C1474	U1298
G2823	G2591	G2493	C	U	U2100	U1989	G1870	G1774	U1648	C1474	U1298
G2824	G2592	G2494	C	C	A2101	U1990	G1871	G1775	U1649	C1474	U1298
G2825	G2593	G2495	C	A	U2102	U1991	G1872	G1776	U1650	C1474	U1298
G2826	G2594	G2496	C	C	G2103	U1992	G1873	G1777	U1651	C1474	U1298
G2827	G2595	G2497	C	U	U2104	U1993	G1874	G1778	U1652	C1474	U1298
G2828	G2596	G2498	C	C	G2105	U1994	G1875	G1779	U1653	C1474	U1298
G2829	G2597	G2499	C	A	U2106	U1995	G1876	G1780	U1654	C1474	U1298
G2830	G2598	G2500	C	C	A2107	U1996	G1877	G1781	U1655	C1474	U1298
G2831	G2599	G2501	C	U	U2108	U1997	G1878	G1782	U1656	C1474	U1298
G2832	G2600	G2502	C	C	G2109	U1998	G1879	G1783	U1657	C1474	U1298
G2833	G2601	G2503	C	A	U2110	U1999	G1880	G1784	U1658	C1474	U1298
G2834	G2602	G2504	C	C	A2111	U2000	G1881	G1785	U1659	C1474	U1298
G2835	G2603	G2505	C	U	U2112	U2001	G1882	G1786	U1660	C1474	U1298
G2836	G2604	G2506	C	C	G2113	U2002	G1883	G1787	U1661	C1474	U1298
G2837	G2605	G2507	C	A	U2114	U2003	G1884	G1788	U1662	C1474	U1298
G2838	G2606	G2508	C	C	G2115	U2004	G1885	G1789	U1663	C1474	U1298
G2839	G2607	G2509	C	U	U2116	U2005	G1886	G1790	U1664	C1474	U1298
G2840	G2608	G2510	C	C	G2117	U2006	G1887	G1791	U1665	C1474	U1298
G2841	G2609	G2511	C	A	U2118	U2007	G1888	G1792	U1666	C1474	U1298
G2842	G2610	G2512	C	C	A2119	U2008	G1889	G1793	U1667	C1474	U1298
G2843	G2611	G2513	C	U	U2119	U2009	G1890	G1794	U1668	C1474	U1298
G2844	G2612	G2514	C	C	G2120	U2010	G1891	G1795	U1669	C1474	U1298
G2845	G2613	G2515	C	A	U2121	U2011	G1892	G1796	U1670	C1474	U1298
G2846	G2614	G2516	C	C	G2122	U2012	G1893	G1797	U1671	C1474	U1298
G2847	G2615	G2517	C	U	U2123	U2013	G1894	G1798	U1672	C1474	U1298
G2848	G2616	G2518	C	C	A2124	U2014	G1895	G1799	U1673	C1474	U1298
G2849	G2617	G2519	C	A	U2125	U2015	G1896	G1800	U1674	C1474	U1298
G2850	G2618	G2520	C	C	G2126	U2016	G1897	G1801	U1675	C1474	U1298
G2851	G2619	G2521	C	U	U2127	U2017	G1898	G1802	U1676	C1474	U1298
G2852	G2620	G2522	C	C	A2127	U2018	G1899	G1803	U1677	C1474	U1298
G2853	G2621	G2523	C	A	U2128	U2019	G1900	G1804	U1678	C1474	U1298
G2854	G2622	G2524	C	C	G2129	U2020	G1901	G1805	U1679	C1474	U1298
G2855	G2623	G2525	C	U	U2130	U2021	G1902	G1806	U1680	C1474	U1298
G2856	G2624	G2526	C	C	A2131	U2022	G1903	G1807	U1681	C1474	U1298
G2857	G2625	G2527	C	A	U2132	U2023	G1904	G1808	U1682	C1474	U1298
G2858	G2626	G2528	C	C	G2133	U2024	G1905	G1809	U1683	C1474	U1298
G2859	G2627	G2529	C	U	U2134	U2025	G1906	G1810	U1684	C1474	U1298
G2860	G2628	G2530	C	C	A2135	U2026	G1907	G1811	U1685	C1474	U1298
G2861	G2629	G2531	C	A	U2136	U2027	G1908	G1812	U1686	C1474	U1298
G2862	G2630	G2532	C	C	G2137	U2028	G1909	G1813	U1687	C1474	U1298
G2863	G2631	G2533	C	U	U2138	U2029	G1910	G1814	U1688	C1474	U1298
G2864	G2632	G2534	C	C	A2139	U2030	G1911	G1815	U1689	C1474	U1298
G2865	G2633	G2535	C	A	U2139	U2031	G1912	G1816	U1690	C1474	U1298
G2866	G2634	G2536	C	C	G2140	U2032	G1913	G1817	U1691	C1474	U1298
G2867	G2635	G2537	C	U	U2141	U2033	G1914	G1818	U1692	C1474	U1298
G2868	G2636	G2538	C	C	A2141	U2034	G1915	G1819	U1693	C1474	U1298
G2869	G2637	G2539	C	A	U2142	U2035	G1916	G1820	U1694	C1474	U1298
G2870	G2638	G2540	C	C	G2143	U2036	G1917	G1821	U1695	C1474	U1298
G2871	G2639	G2541	C	U	U2144	U2037	G1918	G1822	U1696	C1474	U1298
G2872	G2640	G2542	C	C	A2144	U2038	G1919	G1823	U1697	C1474	U1298
G2873	G2641	G2543	C	A	U2145	U2039	G1920	G1824	U1698	C1474	U1298



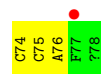
- Molecule 2: 5S ribosomal RNA

Chain 9:



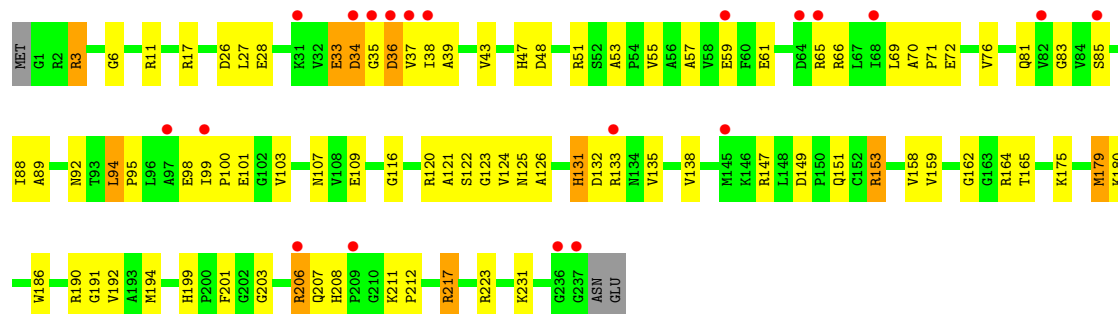
- Molecule 3: 5'-R(\*CP\*CP\*(DA)\*(PHE)\*(ACA))-3'

Chain 4:



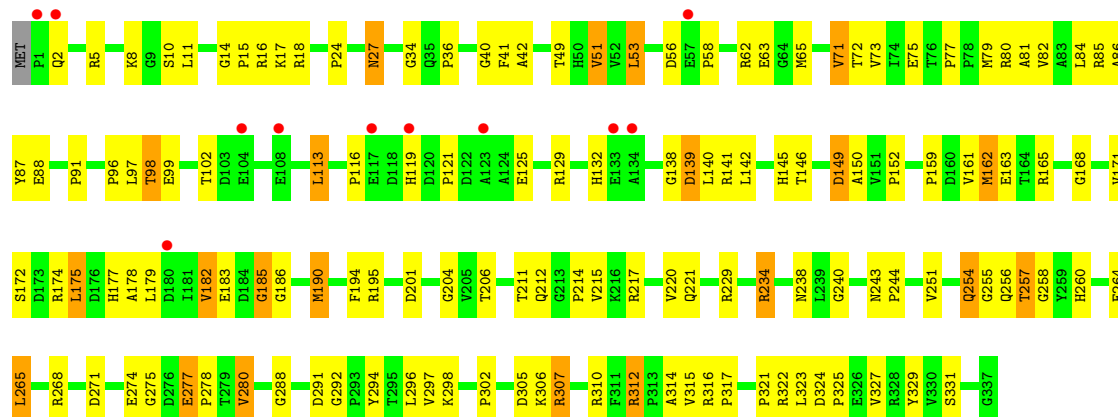
- Molecule 4: 50S ribosomal protein L2P

Chain A:



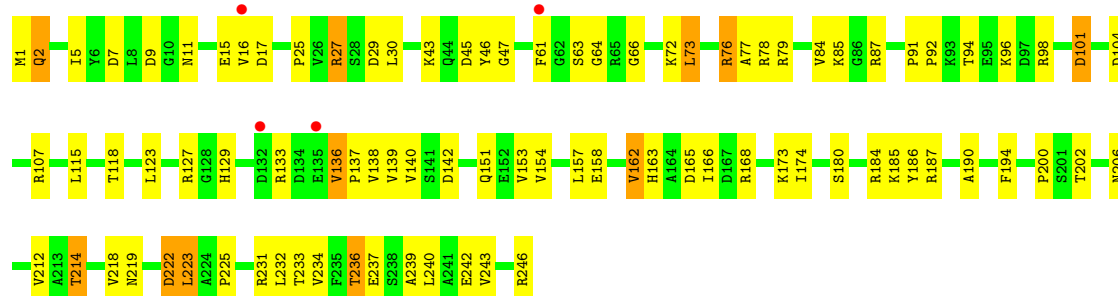
- Molecule 5: 50S ribosomal protein L3P

Chain B: 



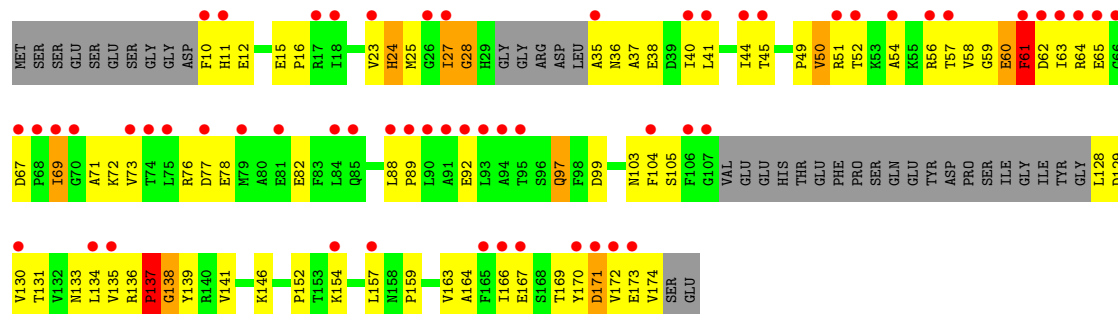
- Molecule 6: 50S ribosomal protein L4E

Chain C:



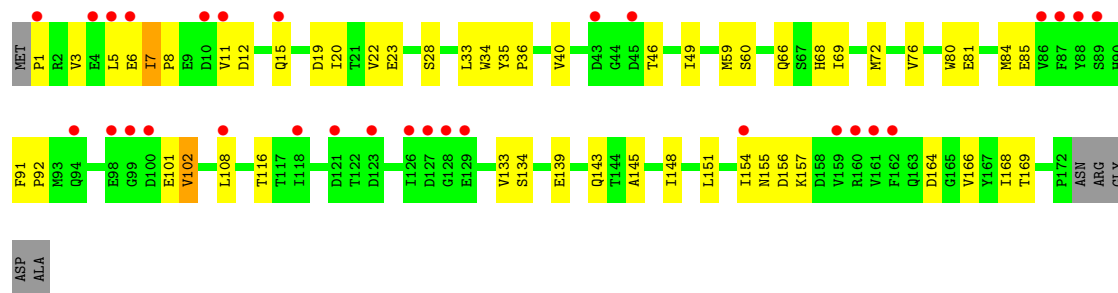
• Molecule 7: 50S ribosomal protein L5P

Chain D:



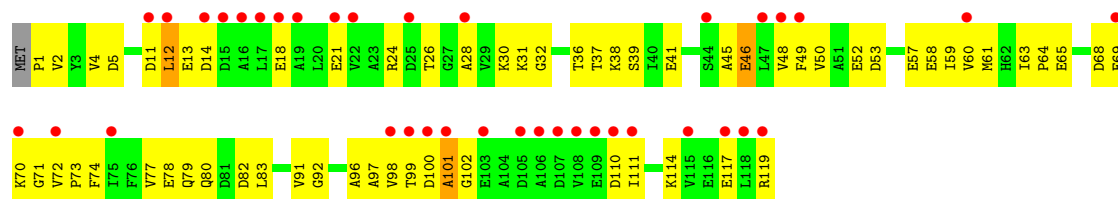
• Molecule 8: 50S ribosomal protein L6P

Chain E:



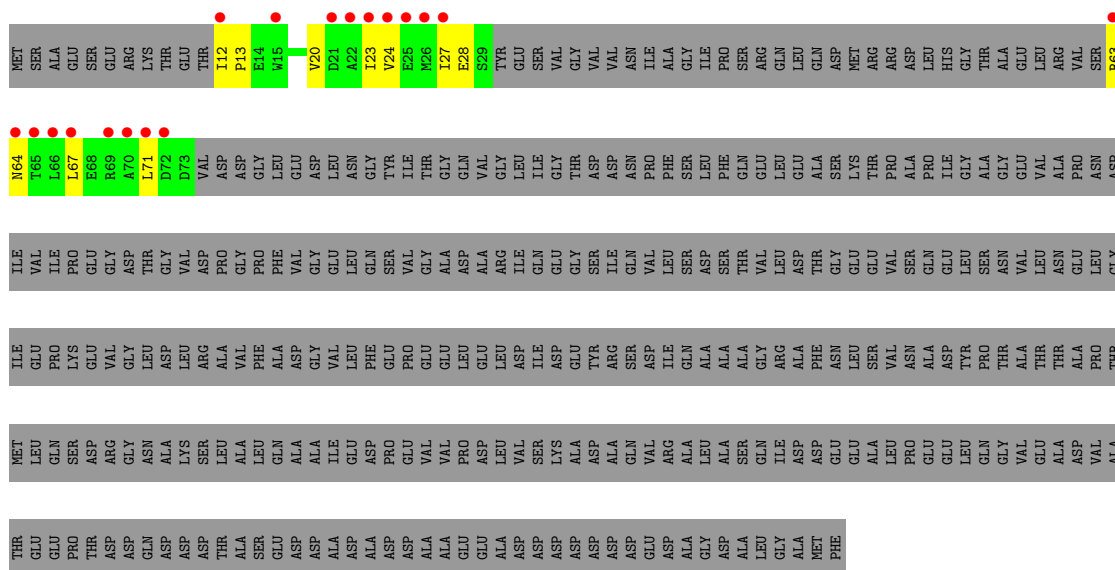
• Molecule 9: 50S ribosomal protein L7AE

Chain F:



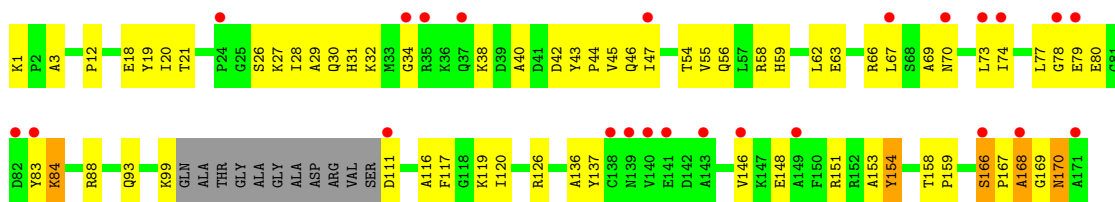
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

Chain G:



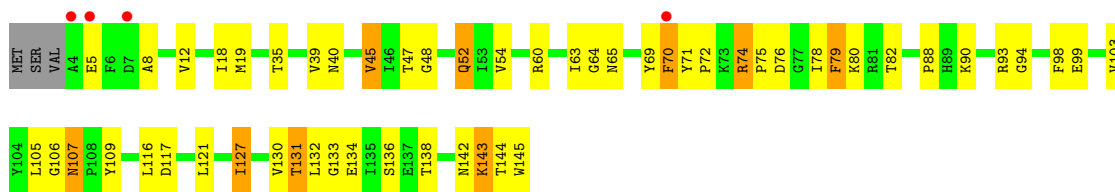
• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

Chain H:



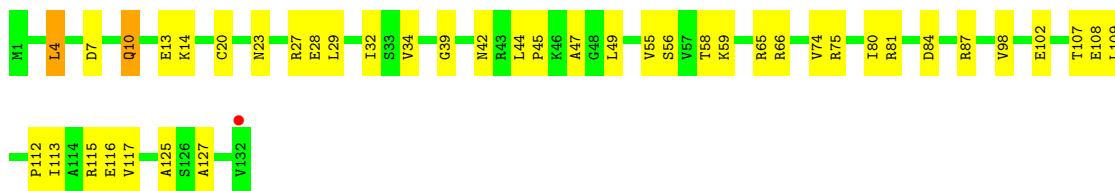
• Molecule 12: 50S ribosomal protein L13P

Chain J:



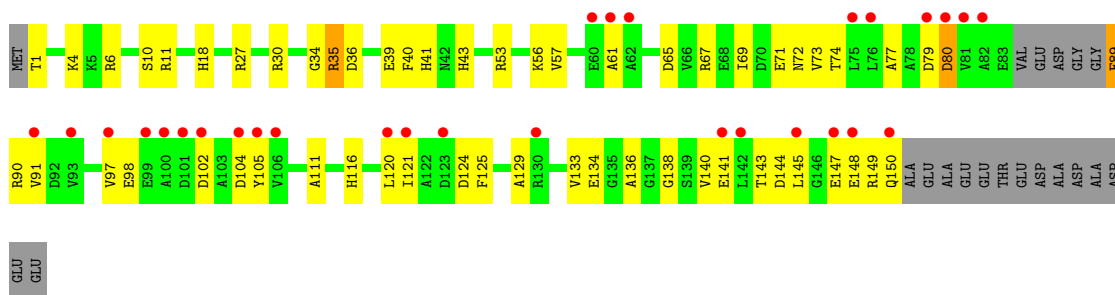
• Molecule 13: 50S ribosomal protein L14P

Chain K:



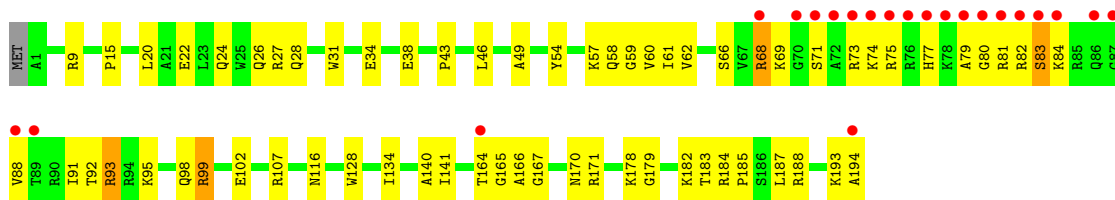
• Molecule 14: 50S ribosomal protein L15P

Chain L:



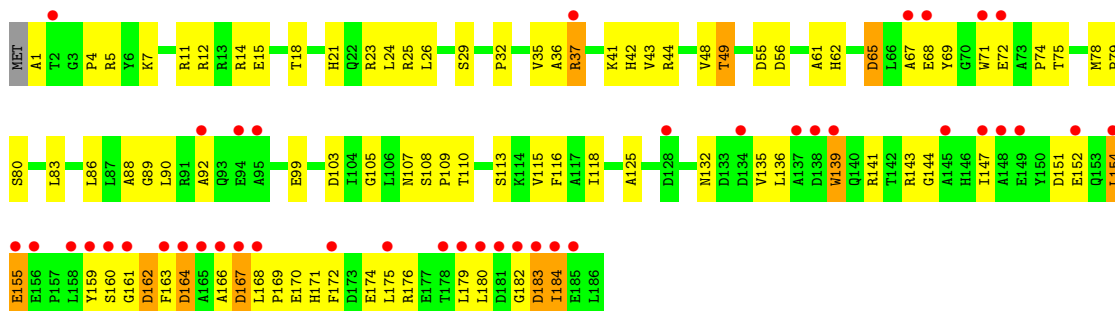
• Molecule 15: 50S Ribosomal Protein L15E

Chain M:



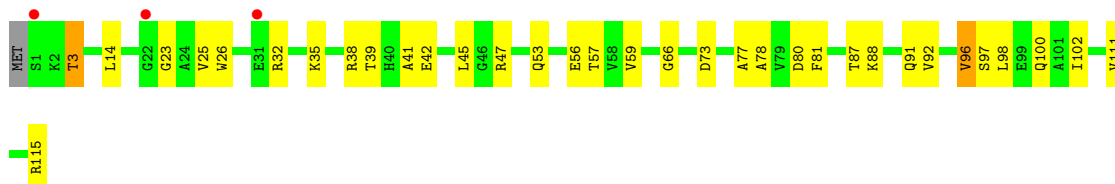
• Molecule 16: 50S ribosomal protein L18P

Chain N:



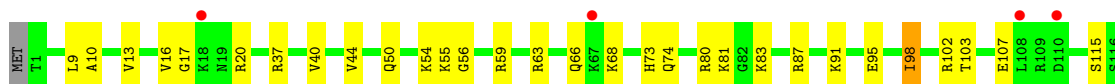
• Molecule 17: 50S ribosomal protein L18e

Chain O:



• Molecule 18: 50S ribosomal protein L19E

Chain P:





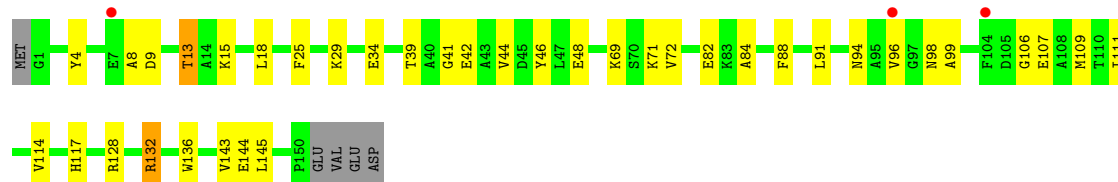
- Molecule 19: 50S ribosomal protein L21e

Chain Q:



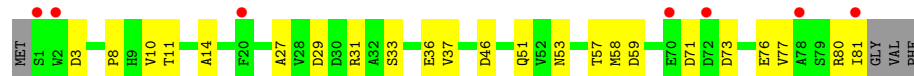
- Molecule 20: 50S ribosomal protein L22P

Chain R:



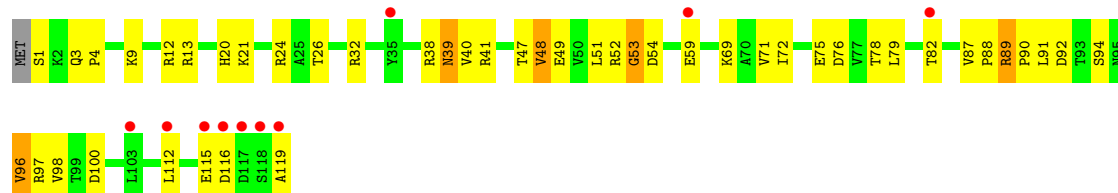
- Molecule 21: 50S ribosomal protein L23P

Chain S:



- Molecule 22: 50S ribosomal protein L24P

Chain T:



- Molecule 23: 50S ribosomal protein L24E

Chain U:



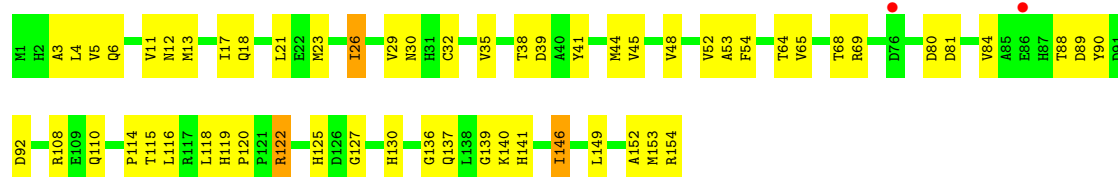
- Molecule 24: 50S ribosomal protein L29P

Chain V:



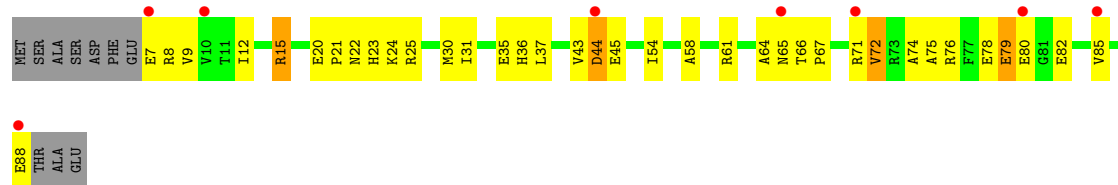
- Molecule 25: 50S ribosomal protein L30P

Chain W: 



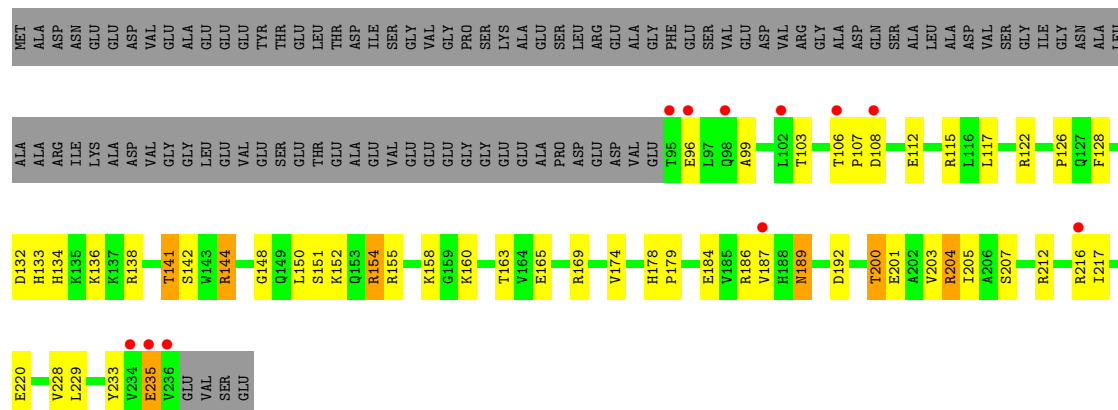
- Molecule 26: 50S ribosomal protein L31e

Chain X: 



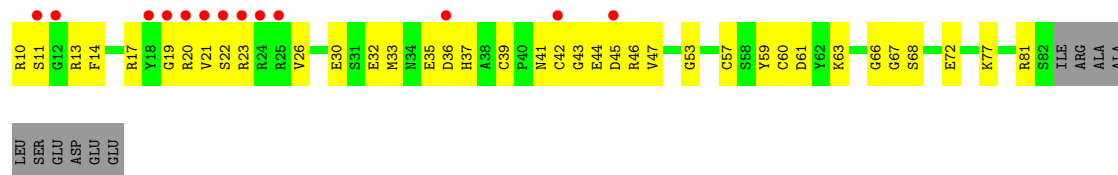
- Molecule 27: 50S ribosomal protein L32E

Chain Y: 



- Molecule 28: 50S ribosomal protein L37Ae

Chain Z: 



- Molecule 29: 50S ribosomal protein L37e

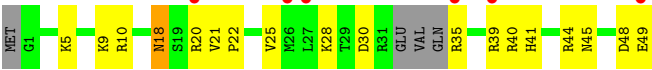
Chain 1: 



- Molecule 30: 50S ribosomal protein L39e

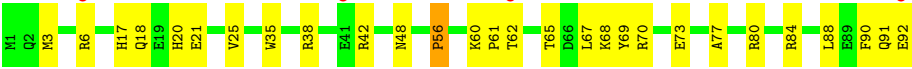


Chain 2: 



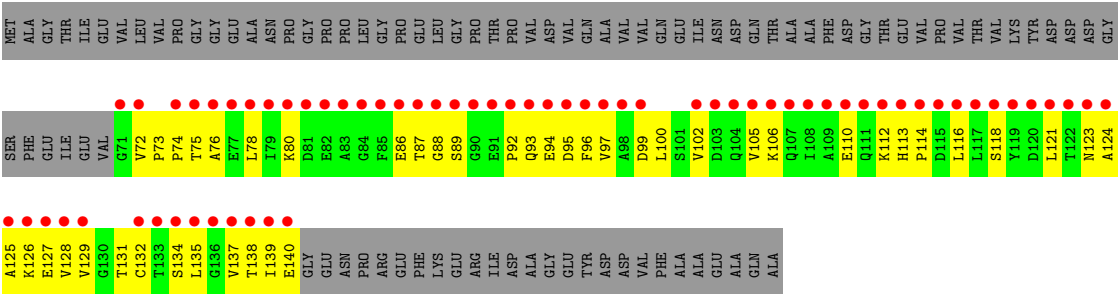
• Molecule 31: 50S ribosomal protein L44E

Chain 3: 



• Molecule 32: 50S RIBOSOMAL PROTEIN L11P

Chain I: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.87Å 298.57Å 575.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.5 (50.00-2.30) 89.6 (49.73-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.218 , 0.250 0.208 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 797435 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	99036	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, ACA, CD, OMU, UR3, 1MA, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	0	0.37	0/65959	0.70	26/102870 (0.0%)
2	9	0.33	0/2905	0.71	1/4528 (0.0%)
3	4	0.52	0/75	0.73	0/110
4	A	0.34	0/1786	0.66	0/2408
5	B	0.33	0/2690	0.66	0/3652
6	C	0.38	0/1884	0.64	1/2551 (0.0%)
7	D	0.29	0/1111	0.54	0/1498
8	E	0.32	0/1382	0.57	0/1880
9	F	0.31	0/901	0.54	0/1224
10	G	0.27	0/241	0.47	0/324
11	H	0.33	0/1287	0.64	0/1725
12	J	0.35	0/1136	0.61	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.33	0/1130	0.64	0/1509
15	M	0.34	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.60	0/1999
17	O	0.33	0/874	0.59	1/1181 (0.1%)
18	P	0.34	0/1147	0.56	0/1528
19	Q	0.35	0/749	0.69	0/1005
20	R	0.35	0/1172	0.67	0/1578
21	S	0.32	0/648	0.58	1/875 (0.1%)
22	T	0.31	0/958	0.63	0/1289
23	U	0.35	0/417	0.58	0/562
24	V	0.27	0/502	0.53	0/675
25	W	0.34	0/1219	0.60	0/1655
26	X	0.33	0/664	0.60	0/895
27	Y	0.36	0/1146	0.65	0/1536
28	Z	0.34	0/589	0.61	0/787
29	1	0.43	0/438	0.66	0/578
30	2	0.35	0/401	0.60	0/529
31	3	0.38	0/771	0.58	0/1024
32	I	0.28	0/526	0.50	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.36	0/98767	0.67	30/147687 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	39
2	9	0	2
All	All	1	41

There are no bond length outliers.

All (30) bond angle outliers are listed below:

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

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

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (41) planarity outliers are listed below:

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

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

## 5.2 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	29813	722	0
2	9	2600	0	1326	50	0
3	4	73	0	44	2	0
4	A	1753	0	1766	101	0
5	B	2625	0	2532	145	0
6	C	1859	0	1816	106	0
7	D	1094	0	1085	79	0
8	E	1357	0	1266	45	0
9	F	890	0	843	57	0
10	G	240	0	231	11	0
11	H	1266	0	1268	68	0
12	J	1120	0	1098	68	0
13	K	992	0	1031	53	0
14	L	1118	0	1076	61	0
15	M	1560	0	1568	63	0
16	N	1445	0	1401	97	0
17	O	865	0	873	40	0
18	P	1136	0	1123	35	0
19	Q	735	0	729	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	R	1149	0	1122	37	0
21	S	641	0	605	16	0
22	T	950	0	923	47	0
23	U	410	0	364	26	0
24	V	499	0	511	38	0
25	W	1196	0	1137	82	0
26	X	654	0	653	35	0
27	Y	1130	0	1133	57	0
28	Z	578	0	539	28	0
29	1	431	0	426	22	0
30	2	396	0	413	26	0
31	3	755	0	728	26	0
32	I	519	0	500	51	0
33	0	87	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	64	0	0	0	0
35	3	1	0	0	0	0
35	9	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	0	98	0	0	0	0
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	5769	0	0	106	0
39	1	50	0	0	2	0
39	2	40	0	0	3	0
39	3	67	0	0	4	0
39	9	140	0	0	6	0
39	A	121	0	0	11	0
39	B	144	0	0	18	0
39	C	177	0	0	18	0
39	D	48	0	0	10	0
39	E	44	0	0	1	0
39	F	27	0	0	4	0
39	G	17	0	0	1	0
39	H	69	0	0	7	0
39	I	7	0	0	1	0
39	J	52	0	0	4	0
39	K	57	0	0	6	0
39	L	81	0	0	14	0
39	M	130	0	0	3	0
39	N	61	0	0	9	0
39	O	40	0	0	5	0
39	P	64	0	0	2	0
39	Q	49	0	0	5	0
39	R	82	0	0	3	0
39	S	32	0	0	1	0
39	T	37	0	0	3	0
39	U	29	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	V	14	0	0	2	0
39	W	69	0	0	5	0
39	X	24	0	0	6	0
39	Y	96	0	0	9	0
39	Z	31	0	0	2	0
All	All	99036	0	59943	2083	0

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 (2083) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.29	1.14
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.29	1.10
6:C:236:THR:HG22	6:C:239:ALA:H	1.19	1.07
1:O:656:G:H5'	17:O:3:THR:HG22	1.38	1.05
1:O:1160:G:H5'	1:O:1161:A:H5'	1.40	1.04
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.72	1.03
2:9:3076:G:H3'	2:9:3077:A:H5''	1.41	1.02
9:F:91:VAL:HG12	9:F:92:GLY:H	1.25	1.00
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.42	0.99
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.38	0.99
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.45	0.98
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.78	0.97
18:P:115:SER:H	18:P:118:GLN:HE21	1.12	0.96
1:O:156:C:H5''	15:M:171:ARG:HD3	1.47	0.95
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.32	0.94
13:K:39:GLY:HA2	39:K:4183:HOH:O	1.68	0.94
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.29	0.93
7:D:57:THR:HG23	7:D:63:ILE:HA	1.51	0.93
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.15	0.93
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.51	0.93
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.34	0.92
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.50	0.92
21:S:57:THR:HG22	21:S:59:ASP:H	1.34	0.92
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.52	0.91
2:9:3056:A:H2'	2:9:3057:A:H5''	1.52	0.89
1:O:2506:A:HO2'	1:O:2507:G:H8	0.92	0.89
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.54	0.89
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.53	0.89
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.21	0.89
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.55	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2717:C:H2'	1:0:2718:C:H5''	1.54	0.89
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.53	0.88
1:0:1593:C:OP1	18:P:117:SER:HB3	1.74	0.88
13:K:10:GLN:H	13:K:10:GLN:HE21	0.89	0.88
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.56	0.88
13:K:10:GLN:N	13:K:10:GLN:HE21	1.71	0.88
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.37	0.87
1:0:542:A:H5'	1:0:542:A:H8	1.40	0.87
1:0:2717:C:C2'	1:0:2718:C:H5''	2.04	0.87
13:K:10:GLN:H	13:K:10:GLN:NE2	1.73	0.87
4:A:81:GLN:HB2	4:A:92:ASN:ND2	1.89	0.87
5:B:238:ASN:HD22	5:B:240:GLY:H	1.17	0.87
1:0:1603:A:H5'	1:0:1605:G:O4'	1.74	0.87
6:C:1:MET:HG2	6:C:2:GLN:H	1.40	0.87
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.57	0.87
1:0:1242:A:H5'	12:J:82:THR:HG23	1.55	0.86
1:0:1372:A:H3'	39:0:7681:HOH:O	1.75	0.86
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.57	0.86
1:0:288:A:H61	1:0:364:C:H42	1.21	0.86
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.57	0.86
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.40	0.86
16:N:144:GLY:O	16:N:147:ILE:HG22	1.76	0.86
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.58	0.85
1:0:2812:A:H2	1:0:2814:A:H62	1.21	0.85
7:D:25:MET:HE2	7:D:41:LEU:HG	1.58	0.84
7:D:58:VAL:HB	7:D:62:ASP:HB3	1.58	0.84
1:0:1835:U:H5	1:0:1840:A:N7	1.75	0.84
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.59	0.84
1:0:2541:U:H3	1:0:2618:G:H1	1.24	0.84
18:P:115:SER:OG	18:P:118:GLN:HG3	1.77	0.83
1:0:2073:G:H5''	39:0:4410:HOH:O	1.77	0.83
1:0:289:G:H22	1:0:363:A:H2	1.22	0.83
25:W:122:ARG:NH2	25:W:154:ARG:HG2	1.93	0.83
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.80	0.83
2:9:3039:U:H1'	2:9:3044:A:H61	1.43	0.83
15:M:164:THR:HG22	15:M:166:ALA:H	1.43	0.83
16:N:113:SER:HB2	39:N:9356:HOH:O	1.77	0.83
1:0:2840:A:OP1	5:B:211:THR:HG23	1.78	0.82
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.26	0.82
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.61	0.82
24:V:1:THR:HG23	24:V:2:VAL:H	1.44	0.82
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.61	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:W:88:THR:HB	39:W:6679:HOH:O	1.80	0.82
4:A:206:ARG:HD3	4:A:206:ARG:H	1.44	0.81
1:O:2506:A:O2'	1:O:2507:G:H8	1.62	0.81
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.62	0.81
39:O:5402:HOH:O	12:J:47:THR:HB	1.80	0.81
1:O:560:C:H42	1:O:597:A:H61	1.25	0.81
1:O:1116:U:HO2'	1:O:1118:A:H2	0.82	0.81
4:A:192:VAL:HB	39:A:9578:HOH:O	1.79	0.81
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.95	0.81
5:B:162:MET:CE	5:B:310:ARG:HD3	2.09	0.81
4:A:211:LYS:HG2	4:A:212:PRO:HD2	1.60	0.81
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.60	0.81
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.11	0.80
1:O:1377:C:H6	1:O:1377:C:H5'	1.44	0.80
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.63	0.80
4:A:192:VAL:HG22	39:A:9618:HOH:O	1.81	0.80
1:O:1041:U:H5'	39:L:9489:HOH:O	1.80	0.80
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.64	0.80
25:W:125:HIS:HD2	25:W:127:GLY:H	1.30	0.80
1:O:1474:C:H6	1:O:1474:C:H5'	1.46	0.79
25:W:13:MET:HE1	25:W:18:GLN:HA	1.63	0.79
31:3:65:THR:HG22	31:3:67:LEU:HG	1.64	0.79
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.64	0.79
1:O:1116:U:O2'	1:O:1118:A:H2	1.64	0.79
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.65	0.79
1:O:2005:G:H3'	1:O:2005:G:OP2	1.83	0.78
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.14	0.78
1:O:1165:G:H4'	1:O:1174:A:O2'	1.84	0.78
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.66	0.78
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.13	0.78
1:O:2054:A:N3	20:R:128:ARG:NH2	2.32	0.78
30:2:41:HIS:H	30:2:45:ASN:HD22	1.32	0.78
5:B:58:PRO:HA	5:B:63:GLU:OE1	1.83	0.78
18:P:115:SER:H	18:P:118:GLN:NE2	1.82	0.78
1:O:381:G:H5''	39:M:9376:HOH:O	1.85	0.78
6:C:236:THR:HG22	6:C:239:ALA:N	1.97	0.77
9:F:91:VAL:HG12	9:F:92:GLY:N	1.99	0.77
18:P:115:SER:N	18:P:118:GLN:HE21	1.82	0.77
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.66	0.77
1:O:1701:A:H4'	1:O:1702:U:H5''	1.66	0.77
1:O:1205:U:H2'	1:O:1206:U:H5''	1.67	0.77
1:O:2635:A:O2'	1:O:2636:C:H5'	1.85	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.50	0.76
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.66	0.76
1:0:1166:A:H61	1:0:1180:U:H3	1.31	0.76
5:B:53:LEU:HD11	5:B:327:VAL:HG22	1.65	0.76
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.13	0.76
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.20	0.76
1:0:962:C:H1'	16:N:5:ARG:NH1	2.00	0.76
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.68	0.76
1:0:545:G:H8	1:0:545:G:H5'	1.49	0.76
1:0:559:U:H5'	1:0:559:U:H6	1.51	0.76
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.68	0.76
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.20	0.76
16:N:37:ARG:HG3	36:N:9307:CL:CL	2.23	0.76
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.86	0.75
1:0:2534:C:H1'	39:0:4089:HOH:O	1.86	0.75
13:K:107:THR:HG22	13:K:108:GLU:HG3	1.68	0.75
1:0:1119:G:N2	1:0:1246:A:C2	2.53	0.75
1:0:1206:U:H6	1:0:1206:U:H5'	1.51	0.75
1:0:871:G:H8	1:0:871:G:H5''	1.49	0.75
1:0:1175:G:H1'	1:0:1193:A:H2'	1.67	0.75
4:A:199:HIS:HD2	4:A:201:PHE:H	1.33	0.75
6:C:236:THR:CG2	6:C:239:ALA:H	1.99	0.75
4:A:191:GLY:HA2	4:A:194:MET:CE	2.17	0.75
4:A:33:GLU:CD	4:A:33:GLU:H	1.89	0.75
8:E:15:GLN:HG2	8:E:19:ASP:O	1.85	0.75
1:0:544:G:H2'	1:0:545:G:H5''	1.69	0.75
39:0:6067:HOH:O	5:B:298:LYS:HG2	1.86	0.75
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.52	0.75
1:0:871:G:C8	1:0:871:G:C5'	2.69	0.75
5:B:179:LEU:O	5:B:183:GLU:HG2	1.86	0.74
16:N:110:THR:HB	16:N:113:SER:OG	1.87	0.74
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.69	0.74
32:I:99:ASP:OD1	32:I:138:THR:HB	1.88	0.74
13:K:32:ILE:HD11	13:K:56:SER:HB2	1.69	0.74
27:Y:154:ARG:HH12	27:Y:155:ARG:HG3	1.53	0.74
9:F:96:ALA:HA	39:F:3111:HOH:O	1.88	0.74
14:L:73:VAL:HG23	14:L:74:THR:H	1.52	0.74
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.85	0.74
1:0:871:G:H8	1:0:871:G:C5'	2.01	0.74
1:0:1973:A:H5'	1:0:1973:A:H8	1.52	0.74
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.51	0.74
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.02	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1159:G:H21	1:0:1189:A:H8	1.36	0.73
9:F:46:GLU:OE1	9:F:100:ASP:HA	1.89	0.73
1:0:656:G:C5'	17:O:3:THR:HG22	2.17	0.73
1:0:1667:A:H8	1:0:1667:A:H5'	1.54	0.73
11:H:27:LYS:H	11:H:59:HIS:HD2	1.35	0.73
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.03	0.73
1:0:656:G:H5'	17:O:3:THR:CG2	2.17	0.73
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.70	0.73
1:0:2491:G:H1'	39:0:7375:HOH:O	1.88	0.73
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.70	0.73
1:0:506:G:H22	1:0:509:A:C5'	2.02	0.73
1:0:2851:G:C2'	1:0:2852:A:H5'	2.18	0.73
21:S:57:THR:HG22	21:S:59:ASP:N	2.02	0.72
16:N:80:SER:HB2	39:N:9335:HOH:O	1.89	0.72
1:0:1299:G:O6	14:L:6:ARG:HD3	1.89	0.72
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.70	0.72
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.71	0.72
13:K:58:THR:HG22	13:K:59:LYS:HG3	1.70	0.72
1:0:2749:U:H5'	39:0:8471:HOH:O	1.89	0.72
1:0:1160:G:C5'	1:0:1161:A:H5'	2.15	0.72
1:0:481:U:H5''	39:0:6188:HOH:O	1.89	0.72
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.71	0.72
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.70	0.72
1:0:1118:A:H3'	1:0:1118:A:H8	1.55	0.72
1:0:1116:U:O2'	1:0:1118:A:C2	2.41	0.72
5:B:141:ARG:HD2	5:B:163:GLU:OE2	1.90	0.72
2:9:3014:G:H8	2:9:3014:G:H5'	1.55	0.71
4:A:94:LEU:HD12	4:A:98:GLU:HB2	1.71	0.71
27:Y:165:GLU:HB3	39:Y:9394:HOH:O	1.90	0.71
1:0:541:C:H2'	1:0:542:A:H5''	1.72	0.71
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.04	0.71
11:H:30:GLN:H	11:H:66:ARG:NH1	1.87	0.71
4:A:35:GLY:O	4:A:36:ASP:HB3	1.89	0.71
10:G:12:ILE:N	10:G:13:PRO:HD3	2.06	0.71
1:0:1700:C:H5''	1:0:1701:A:OP2	1.91	0.71
32:I:110:GLU:HA	32:I:113:HIS:CE1	2.25	0.71
1:0:506:G:H22	1:0:509:A:H5''	1.54	0.71
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.05	0.71
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.73	0.71
20:R:99:ALA:HB1	20:R:109:MET:CE	2.19	0.71
1:0:541:C:C2'	1:0:542:A:H5''	2.20	0.71
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.71	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:F:13:GLU:OE2	9:F:78:GLU:HG2	1.90	0.71
23:U:17:THR:HG22	23:U:18:GLY:N	2.06	0.71
14:L:80:ASP:HB2	14:L:90:ARG:O	1.91	0.71
1:0:1166:A:H1'	1:0:1192:A:C2	2.26	0.70
12:J:45:VAL:HG11	12:J:121:LEU:HD22	1.73	0.70
26:X:71:ARG:HD3	39:X:2171:HOH:O	1.90	0.70
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.91	0.70
2:9:3039:U:H1'	2:9:3044:A:N6	2.06	0.70
1:0:2716:G:H5''	5:B:206:THR:HG21	1.73	0.70
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.06	0.70
1:0:2765:C:H4'	39:0:6067:HOH:O	1.92	0.70
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.21	0.70
18:P:91:LYS:O	18:P:95:GLU:HG3	1.91	0.70
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.72	0.70
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.73	0.70
1:0:949:U:H4'	19:Q:95:GLU:HA	1.72	0.70
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.92	0.70
4:A:48:ASP:HB3	39:A:9587:HOH:O	1.91	0.70
1:0:2586:U:H3	1:0:2592:G:H22	1.39	0.70
1:0:2042:U:H1'	39:0:7798:HOH:O	1.90	0.70
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.22	0.70
1:0:1979:G:H2'	39:0:3890:HOH:O	1.90	0.70
1:0:1838:U:O2'	1:0:2644:C:H5'	1.91	0.70
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.72	0.70
6:C:2:GLN:HB3	39:C:9191:HOH:O	1.90	0.70
1:0:1878:G:H1'	39:0:6649:HOH:O	1.90	0.70
1:0:796:A:HO2'	28:Z:10:ARG:N	1.89	0.70
1:0:470:U:O2'	29:1:16:HIS:HD2	1.75	0.70
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.73	0.70
6:C:194:PHE:CD2	6:C:234:VAL:HG11	2.26	0.70
15:M:69:LYS:O	15:M:73:ARG:NH2	2.25	0.70
1:0:2073:G:OP2	1:0:2490:A:H5'	1.92	0.70
1:0:1183:C:N4	1:0:1184:C:H41	1.90	0.70
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.74	0.70
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.92	0.70
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.21	0.69
39:0:7927:HOH:O	5:B:211:THR:HG21	1.92	0.69
27:Y:141:THR:HG23	39:Y:9389:HOH:O	1.92	0.69
1:0:1118:A:H3'	1:0:1118:A:C8	2.27	0.69
1:0:1206:U:H2'	1:0:1207:A:O4'	1.92	0.69
24:V:39:ALA:N	24:V:40:PRO:HD2	2.08	0.69
5:B:307:ARG:NH1	5:B:307:ARG:HG3	2.02	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.07	0.69
25:W:125:HIS:CD2	25:W:127:GLY:H	2.11	0.69
14:L:148:GLU:HB2	39:L:9485:HOH:O	1.91	0.69
2:9:3029:C:O3'	7:D:138:GLY:HA2	1.92	0.69
6:C:1:MET:HG2	6:C:2:GLN:N	2.08	0.69
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.23	0.69
4:A:51:ARG:HB2	39:A:9587:HOH:O	1.90	0.69
39:O:8484:HOH:O	5:B:2:GLN:HG3	1.91	0.69
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.23	0.69
1:O:280:C:H2'	1:O:281:U:O4'	1.93	0.69
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.75	0.69
1:O:282:C:H1'	1:O:368:C:N4	2.07	0.69
2:9:3056:A:C2'	2:9:3057:A:H5''	2.23	0.69
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.75	0.69
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.08	0.69
18:P:9:LEU:O	18:P:13:VAL:HG12	1.93	0.69
1:O:2578:G:H5'	1:O:2578:G:H8	1.57	0.69
22:T:9:LYS:HE3	22:T:13:ARG:CZ	2.22	0.68
1:O:1666:C:H2'	1:O:1667:A:H5'	1.75	0.68
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.75	0.68
1:O:2468:A:H61	31:3:48:ASN:HD21	1.38	0.68
1:O:2533:C:H5'	1:O:2533:C:H6	1.57	0.68
29:1:18:LYS:HB2	30:2:49:GLU:HG2	1.76	0.68
9:F:37:THR:O	9:F:41:GLU:HG3	1.94	0.68
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.94	0.68
1:O:1160:G:H5'	1:O:1161:A:C5'	2.19	0.68
26:X:9:VAL:HG22	26:X:88:GLU:OE2	1.94	0.68
5:B:140:LEU:HA	39:B:9576:HOH:O	1.91	0.68
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.57	0.68
17:O:32:ARG:HD3	17:O:32:ARG:O	1.93	0.68
1:O:541:C:H2'	1:O:542:A:C5'	2.23	0.68
1:O:2890:A:H1'	23:U:56:ARG:NH2	2.08	0.68
1:O:93:C:H5''	24:V:1:THR:HB	1.76	0.68
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.74	0.68
5:B:125:GLU:O	5:B:129:ARG:HG3	1.94	0.68
4:A:81:GLN:HB2	4:A:92:ASN:HD21	1.57	0.68
1:O:111:C:O2'	29:1:20:ARG:HG2	1.94	0.68
20:R:39:THR:HB	20:R:42:GLU:HG3	1.74	0.68
25:W:88:THR:HG22	25:W:89:ASP:N	2.09	0.67
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.75	0.67
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.75	0.67
17:O:32:ARG:NE	17:O:35:LYS:HD2	2.08	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1474:C:C6	1:0:1474:C:H5'	2.28	0.67
1:0:281:U:H2'	1:0:282:C:O4'	1.94	0.67
27:Y:144:ARG:CZ	39:Y:9412:HOH:O	2.42	0.67
32:I:89:SER:HB2	32:I:95:ASP:HB2	1.76	0.67
6:C:78:ARG:HH11	6:C:78:ARG:HG3	1.59	0.67
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.08	0.67
1:0:2346:C:O2'	7:D:52:THR:HG21	1.94	0.67
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.77	0.67
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.77	0.67
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.95	0.67
14:L:143:THR:HG22	14:L:144:ASP:N	2.09	0.67
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.76	0.67
1:0:1209:C:H2'	1:0:1210:G:H8	1.60	0.67
1:0:1184:C:H4'	32:I:126:LYS:HB3	1.77	0.67
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.95	0.66
1:0:553:G:P	27:Y:204:ARG:HH22	2.18	0.66
11:H:166:SER:CB	11:H:167:PRO:CD	2.73	0.66
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.76	0.66
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.25	0.66
1:0:1189:A:H3'	39:0:8231:HOH:O	1.95	0.66
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.94	0.66
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.76	0.66
5:B:102:THR:HG23	5:B:182:VAL:HG12	1.78	0.66
24:V:12:THR:HG22	24:V:15:GLU:CG	2.24	0.66
4:A:69:LEU:HD23	4:A:107:ASN:HB2	1.76	0.66
5:B:275:GLY:O	5:B:291:ASP:HA	1.95	0.66
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.25	0.66
25:W:80:ASP:O	25:W:84:VAL:HG23	1.94	0.66
1:0:380:A:OP2	15:M:9:ARG:HD2	1.96	0.66
1:0:797:A:C4'	28:Z:10:ARG:N	2.59	0.66
29:1:25:LYS:HD2	30:2:49:GLU:N	2.11	0.66
1:0:657:G:OP1	6:C:27:ARG:NH2	2.26	0.66
5:B:102:THR:HG21	5:B:182:VAL:O	1.96	0.66
1:0:2779:G:H21	8:E:143:GLN:NE2	1.94	0.66
1:0:544:G:C2'	1:0:545:G:H5''	2.25	0.66
2:9:3013:A:O2'	2:9:3014:G:H5''	1.95	0.66
8:E:68:HIS:O	8:E:72:MET:HG3	1.94	0.66
15:M:80:GLY:O	15:M:81:ARG:HD2	1.95	0.66
5:B:8:LYS:HG3	5:B:220:VAL:HG12	1.78	0.65
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.77	0.65
11:H:170:ASN:HD22	11:H:170:ASN:N	1.95	0.65
1:0:871:G:C8	1:0:871:G:H5'	2.30	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.10	0.65
1:O:338:C:H4'	6:C:174:ILE:CD1	2.26	0.65
7:D:154:LYS:HD2	7:D:154:LYS:H	1.61	0.65
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.45	0.65
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.11	0.65
19:Q:25:PRO:HB2	39:Q:4350:HOH:O	1.96	0.65
1:O:2363:G:O2'	19:Q:11:ARG:HG3	1.97	0.65
14:L:91:VAL:HG13	14:L:120:LEU:HD23	1.78	0.65
12:J:93:ARG:NH1	12:J:93:ARG:HB3	2.08	0.65
7:D:65:GLU:HA	39:D:6752:HOH:O	1.97	0.65
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.78	0.65
1:O:1244:U:OP1	12:J:18:ILE:HD13	1.97	0.65
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.78	0.65
16:N:164:ASP:CG	16:N:167:ASP:HA	2.15	0.65
12:J:19:MET:CE	12:J:132:LEU:HD11	2.26	0.65
1:O:709:G:O2'	17:O:25:VAL:HG12	1.96	0.65
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.43	0.65
1:O:1426:C:H2'	39:O:3209:HOH:O	1.96	0.65
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.25	0.65
1:O:1641:A:H2'	1:O:1642:A:H5'	1.78	0.65
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.26	0.65
1:O:447:A:P	22:T:1:SER:HB2	2.37	0.65
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.26	0.65
29:I:25:LYS:HD2	30:2:49:GLU:H	1.60	0.65
22:T:26:THR:HA	22:T:39:ASN:HB3	1.79	0.65
9:F:77:VAL:HG21	9:F:83:LEU:HD13	1.77	0.65
21:S:51:GLN:NE2	21:S:53:ASN:HD21	1.94	0.64
4:A:199:HIS:CD2	4:A:201:PHE:H	2.13	0.64
15:M:107:ARG:NH1	15:M:107:ARG:HG3	2.11	0.64
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.62	0.64
1:O:1184:C:H1'	39:O:7937:HOH:O	1.95	0.64
24:V:56:ILE:O	24:V:60:GLN:HG3	1.96	0.64
7:D:159:PRO:O	7:D:163:VAL:HG23	1.96	0.64
23:U:47:ARG:HG3	39:U:4381:HOH:O	1.97	0.64
1:O:2718:C:H6	1:O:2718:C:H5'	1.63	0.64
1:O:2661:U:H3	1:O:2812:A:H62	1.44	0.64
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.79	0.64
1:O:1201:C:H2'	1:O:1202:A:H5'	1.79	0.64
23:U:52:THR:HG22	23:U:54:THR:N	2.13	0.64
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.27	0.64
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.19	0.64
1:O:1205:U:H2'	1:O:1206:U:C5'	2.27	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
32:I:105:VAL:HG11	32:I:129:VAL:HG22	1.80	0.64
1:O:2780:C:H1'	8:E:143:GLN:HE21	1.62	0.64
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.27	0.64
1:O:2420:G:O2'	1:O:2421:G:H5'	1.97	0.64
28:Z:17:ARG:HD3	39:Z:9219:HOH:O	1.97	0.64
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.33	0.64
1:O:962:C:H1'	16:N:5:ARG:HH12	1.63	0.64
5:B:62:ARG:HA	5:B:65:MET:CE	2.28	0.64
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.44	0.64
25:W:48:VAL:HG12	25:W:48:VAL:O	1.98	0.64
22:T:71:VAL:HG12	22:T:72:ILE:N	2.13	0.64
26:X:25:ARG:HD3	26:X:64:ALA:O	1.98	0.64
22:T:38:ARG:NH1	39:T:6217:HOH:O	2.31	0.64
25:W:13:MET:CE	25:W:17:ILE:HG22	2.28	0.64
1:O:1205:U:C2'	1:O:1206:U:H5''	2.27	0.64
8:E:8:PRO:HB2	8:E:11:VAL:HG23	1.80	0.64
1:O:1119:G:H22	1:O:1246:A:H2	1.40	0.63
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.96	0.63
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.80	0.63
1:O:2507:G:H2'	1:O:2510:C:H42	1.62	0.63
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.34	0.63
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.26	0.63
1:O:1666:C:O2'	1:O:1667:A:H5''	1.98	0.63
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.79	0.63
16:N:132:ASN:O	16:N:135:VAL:HG12	1.97	0.63
1:O:2896:A:N3	1:O:2896:A:H2'	2.14	0.63
6:C:139:VAL:HG13	39:C:9254:HOH:O	1.98	0.63
15:M:164:THR:HG22	15:M:166:ALA:N	2.11	0.63
32:I:125:ALA:O	32:I:129:VAL:HG23	1.99	0.63
1:O:2748:G:H2'	39:O:8049:HOH:O	1.99	0.63
16:N:23:ARG:HH11	16:N:23:ARG:HG2	1.63	0.63
1:O:1168:C:H5''	32:I:87:THR:HG23	1.81	0.63
1:O:1687:C:O2	29:1:9:GLY:HA2	1.99	0.63
11:H:59:HIS:HA	11:H:62:LEU:HD23	1.79	0.63
1:O:1182:C:H1'	1:O:1192:A:H8	1.63	0.63
27:Y:144:ARG:HG3	27:Y:144:ARG:HH11	1.63	0.63
1:O:1563:G:H4'	39:O:4808:HOH:O	1.98	0.63
14:L:40:PHE:HB3	39:L:9458:HOH:O	1.99	0.63
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.62	0.63
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.81	0.63
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.29	0.63
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1766:U:O2	1:0:1778:A:H5'	1.99	0.63
5:B:254:GLN:HG2	5:B:255:GLY:N	2.13	0.63
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.29	0.62
16:N:164:ASP:OD1	16:N:167:ASP:HA	1.99	0.62
1:0:1377:C:H5'	1:0:1377:C:C6	2.30	0.62
7:D:138:GLY:N	39:D:7597:HOH:O	2.32	0.62
15:M:79:ALA:HB3	15:M:81:ARG:NH1	2.14	0.62
6:C:236:THR:HG21	39:C:9180:HOH:O	1.98	0.62
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.29	0.62
11:H:27:LYS:N	11:H:59:HIS:HD2	1.98	0.62
24:V:56:ILE:HG22	24:V:60:GLN:HE21	1.63	0.62
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.82	0.62
1:0:2878:U:H2'	1:0:2879:A:O4'	1.99	0.62
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.26	0.62
1:0:1116:U:H3	1:0:1246:A:H62	1.47	0.62
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.80	0.62
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.29	0.62
12:J:74:ARG:NH1	12:J:105:LEU:HD11	2.14	0.62
11:H:166:SER:CB	11:H:167:PRO:HD3	2.30	0.62
11:H:154:TYR:HB2	39:H:9555:HOH:O	1.99	0.62
7:D:170:TYR:O	7:D:171:ASP:HB3	1.99	0.62
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.63	0.62
2:9:3020:G:O2'	2:9:3021:G:H5'	1.99	0.62
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.48	0.61
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.11	0.61
32:I:92:PRO:C	32:I:94:GLU:H	2.02	0.61
1:0:282:C:O2'	1:0:283:U:H5'	2.00	0.61
24:V:43:PRO:O	24:V:46:ILE:HG22	2.00	0.61
5:B:215:VAL:HB	5:B:234:ARG:HH12	1.65	0.61
16:N:143:ARG:HH21	16:N:169:PRO:HB2	1.65	0.61
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.82	0.61
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.29	0.61
1:0:396:U:O2'	1:0:418:C:H4'	2.00	0.61
4:A:121:ALA:O	4:A:124:VAL:HG22	2.01	0.61
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.81	0.61
1:0:902:G:N7	14:L:18:HIS:HD2	1.98	0.61
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.15	0.61
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.16	0.61
1:0:2502:C:H2'	1:0:2503:A:H5'	1.82	0.61
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.31	0.61
22:T:115:GLU:HG3	22:T:116:ASP:N	2.16	0.61
25:W:84:VAL:HG12	39:W:6679:HOH:O	2.00	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:U:17:THR:CG2	23:U:18:GLY:N	2.64	0.61
24:V:64:GLY:O	24:V:65:ASP:HB2	2.00	0.61
1:0:156:C:H5''	15:M:171:ARG:CD	2.27	0.61
1:0:1118:A:H62	1:0:1244:U:H3	1.47	0.61
1:0:1701:A:H4'	1:0:1702:U:C5'	2.31	0.61
32:I:102:VAL:O	32:I:106:LYS:HG3	2.00	0.61
25:W:52:VAL:HG22	25:W:53:ALA:H	1.64	0.61
24:V:39:ALA:C	24:V:41:GLU:H	2.03	0.61
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.65	0.61
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.24	0.61
6:C:107:ARG:NE	39:C:9264:HOH:O	2.31	0.61
14:L:133:VAL:HA	39:L:9470:HOH:O	2.01	0.61
1:0:164:G:H4'	14:L:30:ARG:HD3	1.82	0.61
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.64	0.60
22:T:48:VAL:HG22	22:T:96:VAL:HG22	1.82	0.60
1:0:2769:C:H2'	1:0:2770:G:O4'	1.99	0.60
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.65	0.60
1:0:2064:U:H5'	1:0:2652:U:H4'	1.82	0.60
25:W:130:HIS:O	25:W:136:GLY:HA3	2.01	0.60
16:N:110:THR:HB	16:N:113:SER:HG	1.64	0.60
6:C:16:VAL:HG12	6:C:17:ASP:H	1.65	0.60
32:I:138:THR:HG22	32:I:139:ILE:H	1.65	0.60
1:0:2851:G:H2'	1:0:2852:A:H5'	1.82	0.60
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.83	0.60
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.02	0.60
1:0:1528:A:H2'	1:0:1529:G:O4'	2.02	0.60
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.82	0.60
6:C:118:THR:O	6:C:136:VAL:HG13	2.00	0.60
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.04	0.60
29:1:10:LYS:HG3	39:1:9488:HOH:O	2.00	0.60
6:C:236:THR:HA	39:C:9257:HOH:O	2.00	0.60
7:D:25:MET:SD	7:D:40:ILE:HD11	2.42	0.60
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.66	0.60
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.65	0.60
4:A:125:ASN:CB	4:A:158:VAL:HG12	2.31	0.60
1:0:681:G:N3	1:0:681:G:H5'	2.17	0.60
5:B:16:ARG:NH1	39:B:9615:HOH:O	2.33	0.60
1:0:1201:C:H5''	39:0:6761:HOH:O	2.02	0.60
2:9:3029:C:H2'	2:9:3030:C:H5'	1.83	0.60
12:J:131:THR:HG22	12:J:134:GLU:H	1.65	0.60
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.07	0.60
11:H:166:SER:HB2	11:H:167:PRO:CD	2.32	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2748:G:H5'	39:0:8049:HOH:O	2.00	0.60
27:Y:187:VAL:HG12	27:Y:205:ILE:HA	1.83	0.60
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.84	0.60
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.84	0.60
2:9:3014:G:C8	2:9:3014:G:H5'	2.35	0.60
18:P:40:VAL:O	18:P:44:VAL:HG23	2.01	0.60
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.02	0.60
32:I:134:SER:O	32:I:135:LEU:HD23	2.02	0.60
1:0:960:G:H4'	39:0:7904:HOH:O	2.00	0.60
1:0:2291:A:C8	1:0:2309:C:H5'	2.37	0.60
1:0:1555:G:H4'	1:0:1630:A:H2	1.67	0.60
6:C:140:VAL:HB	39:C:9257:HOH:O	2.01	0.59
1:0:380:A:H2'	39:0:7718:HOH:O	2.01	0.59
17:O:32:ARG:HH21	17:O:35:LYS:HZ1	1.50	0.59
1:0:2502:C:C2'	1:0:2503:A:H5'	2.32	0.59
1:0:272:A:H5'	1:0:273:G:OP2	2.02	0.59
12:J:74:ARG:O	12:J:78:ILE:HG12	2.02	0.59
32:I:78:LEU:HD12	32:I:112:LYS:NZ	2.16	0.59
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.84	0.59
1:0:263:U:O4'	9:F:59:ILE:HD13	2.02	0.59
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.83	0.59
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.37	0.59
14:L:35:ARG:HB2	14:L:35:ARG:HH11	1.67	0.59
9:F:91:VAL:CG1	9:F:92:GLY:H	2.08	0.59
5:B:85:ARG:NH1	39:B:9633:HOH:O	2.35	0.59
17:O:42:GLU:HB2	39:O:2176:HOH:O	2.02	0.59
5:B:297:VAL:HB	39:B:9604:HOH:O	2.01	0.59
15:M:77:HIS:HD2	15:M:79:ALA:O	1.85	0.59
1:0:834:G:H4'	1:0:835:U:OP2	2.03	0.59
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.02	0.59
1:0:542:A:H5'	1:0:542:A:C8	2.28	0.59
7:D:136:ARG:HH12	7:D:157:LEU:HA	1.65	0.59
14:L:73:VAL:HG23	14:L:74:THR:N	2.17	0.59
16:N:176:ARG:HG3	16:N:180:LEU:HD13	1.84	0.59
5:B:96:PRO:HG3	39:B:9633:HOH:O	2.00	0.59
24:V:1:THR:HG23	24:V:2:VAL:N	2.16	0.59
16:N:154:LEU:O	16:N:155:GLU:HB3	2.03	0.59
1:0:2100:A:H4'	6:C:64:GLY:O	2.02	0.59
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.68	0.59
32:I:113:HIS:N	32:I:114:PRO:HD2	2.18	0.59
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.33	0.59
1:0:2795:C:O2'	1:0:2796:U:H5'	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2003:U:H4'	1:0:2004:U:H5	1.68	0.59
1:0:516:A:H5'	39:0:6188:HOH:O	2.03	0.59
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.33	0.59
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.84	0.59
1:0:870:G:H2'	1:0:871:G:H5''	1.85	0.59
39:0:9698:HOH:O	5:B:214:PRO:HD2	2.03	0.59
1:0:316:A:N3	1:0:336:G:O2'	2.35	0.59
21:S:51:GLN:HE21	21:S:53:ASN:ND2	1.95	0.59
23:U:14:GLU:OE1	23:U:15:PRO:HD2	2.03	0.59
1:0:2851:G:O2'	1:0:2852:A:H5'	2.03	0.59
14:L:35:ARG:HB2	14:L:35:ARG:NH1	2.18	0.59
1:0:1328:A:OP1	27:Y:169:ARG:HD2	2.02	0.59
1:0:1819:G:H2'	1:0:1820:G:H4'	1.84	0.59
1:0:2676:C:H4'	12:J:70:PHE:CD1	2.38	0.59
13:K:23:ASN:HD21	13:K:107:THR:HB	1.68	0.58
9:F:46:GLU:O	9:F:73:PRO:HD2	2.03	0.58
9:F:58:GLU:CD	15:M:27:ARG:HH22	2.05	0.58
39:0:9972:HOH:O	29:1:1:THR:HA	2.03	0.58
5:B:88:GLU:HB3	5:B:97:LEU:HD12	1.84	0.58
1:0:2505:G:O2'	1:0:2506:A:H5'	2.04	0.58
4:A:33:GLU:O	4:A:34:ASP:HB2	2.03	0.58
16:N:69:TYR:HE2	16:N:184:ILE:HG13	1.67	0.58
7:D:59:GLY:O	7:D:61:PHE:N	2.36	0.58
1:0:545:G:C8	1:0:545:G:H5'	2.35	0.58
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.03	0.58
15:M:68:ARG:NH2	15:M:73:ARG:HD3	2.18	0.58
24:V:39:ALA:N	24:V:40:PRO:CD	2.66	0.58
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.19	0.58
39:0:3154:HOH:O	18:P:81:LYS:HG2	2.03	0.58
1:0:20:G:H21	20:R:117:HIS:HD2	1.48	0.58
1:0:289:G:N2	1:0:363:A:H2	1.96	0.58
11:H:63:GLU:HA	39:H:9544:HOH:O	2.03	0.58
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.32	0.58
14:L:143:THR:HG22	14:L:144:ASP:H	1.68	0.58
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.39	0.58
1:0:877:G:H5'	1:0:878:G:OP1	2.03	0.58
1:0:969:G:H1	1:0:999:C:H42	1.49	0.58
1:0:2726:U:O2'	26:X:22:ASN:ND2	2.37	0.58
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.69	0.58
16:N:169:PRO:O	16:N:172:PHE:HB3	2.03	0.58
1:0:2426:G:H1'	39:0:6621:HOH:O	2.03	0.58
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.39	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.33	0.58
1:0:625:U:H5'	39:0:3784:HOH:O	2.04	0.58
11:H:111:ASP:HA	39:H:9510:HOH:O	2.02	0.58
1:0:558:C:C2'	1:0:559:U:H5''	2.34	0.58
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.03	0.58
6:C:236:THR:H	6:C:239:ALA:HB3	1.68	0.58
20:R:96:VAL:HG13	20:R:106:GLY:HA3	1.86	0.58
8:E:20:ILE:HD12	8:E:33:LEU:HD12	1.86	0.58
5:B:238:ASN:ND2	5:B:240:GLY:H	1.95	0.58
10:G:20:VAL:O	10:G:24:VAL:HG23	2.03	0.58
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.04	0.58
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.85	0.58
14:L:104:ASP:HB2	39:L:9460:HOH:O	2.03	0.58
5:B:238:ASN:HD22	5:B:240:GLY:N	1.95	0.58
1:0:1181:A:H5'	32:I:94:GLU:OE2	2.04	0.58
1:0:1352:A:O2'	1:0:1353:C:OP1	2.20	0.58
1:0:1384:C:H5'	26:X:30:MET:HG2	1.85	0.57
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.04	0.57
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.51	0.57
4:A:26:ASP:O	4:A:28:GLU:N	2.36	0.57
24:V:55:ARG:O	24:V:59:ILE:HG12	2.04	0.57
1:0:558:C:O2'	1:0:559:U:H5''	2.04	0.57
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.04	0.57
1:0:447:A:OP2	22:T:1:SER:HB2	2.04	0.57
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.69	0.57
17:O:57:THR:O	17:O:111:VAL:HG23	2.03	0.57
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.39	0.57
39:0:9983:HOH:O	4:A:180:LYS:HG2	2.04	0.57
5:B:195:ARG:HG2	5:B:323:LEU:HD22	1.86	0.57
32:I:78:LEU:HD12	32:I:112:LYS:HZ2	1.68	0.57
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.86	0.57
26:X:31:ILE:O	26:X:35:GLU:HG3	2.05	0.57
16:N:170:GLU:O	16:N:174:GLU:HG3	2.04	0.57
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.37	0.57
1:0:2726:U:O2	1:0:2749:U:O5'	2.22	0.57
27:Y:203:VAL:CG1	27:Y:228:VAL:HG22	2.35	0.57
7:D:172:VAL:HG12	7:D:173:GLU:N	2.18	0.57
9:F:21:GLU:O	9:F:24:ARG:HG3	2.05	0.57
5:B:185:GLY:HA2	39:B:9632:HOH:O	2.04	0.57
14:L:67:ARG:O	14:L:71:GLU:HG3	2.04	0.57
1:0:1552:G:N2	1:0:1634:G:H1'	2.19	0.57
6:C:236:THR:HG22	6:C:239:ALA:CB	2.34	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:558:C:H2'	1:0:559:U:C5'	2.34	0.57
1:0:1943:C:H4'	4:A:211:LYS:O	2.05	0.57
31:3:3:MET:HB2	31:3:88:LEU:HD11	1.85	0.57
14:L:136:ALA:HB3	39:L:9470:HOH:O	2.03	0.57
1:0:2421:G:H1'	39:0:4289:HOH:O	2.03	0.57
1:0:1066:U:H2'	1:0:1067:A:C8	2.40	0.57
31:3:62:THR:HB	39:3:9482:HOH:O	2.04	0.57
15:M:164:THR:CG2	15:M:165:GLY:N	2.68	0.57
1:0:1189:A:O2'	1:0:1208:C:H2'	2.04	0.57
1:0:308:U:H5'	22:T:97:ARG:NH2	2.19	0.57
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.70	0.57
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.88	0.57
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.05	0.57
1:0:871:G:C8	1:0:871:G:H5''	2.34	0.57
10:G:12:ILE:N	10:G:13:PRO:CD	2.68	0.57
1:0:1218:U:H2'	1:0:1219:U:C6	2.40	0.57
14:L:36:ASP:HB2	39:L:9433:HOH:O	2.05	0.57
39:9:4707:HOH:O	16:N:147:ILE:HD12	2.05	0.57
12:J:39:VAL:HG13	12:J:106:GLY:O	2.05	0.57
1:0:256:C:H2'	1:0:257:G:O4'	2.05	0.57
7:D:146:LYS:NZ	16:N:107:ASN:HD21	2.02	0.57
17:O:39:THR:O	17:O:115:ARG:NH2	2.37	0.57
4:A:33:GLU:CD	4:A:33:GLU:N	2.57	0.56
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.04	0.56
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.70	0.56
6:C:214:THR:HG23	39:C:9242:HOH:O	2.03	0.56
1:0:138:U:H5''	1:0:139:C:OP2	2.04	0.56
21:S:77:VAL:O	21:S:80:ARG:HG2	2.05	0.56
1:0:244:C:OP2	9:F:38:LYS:HE3	2.05	0.56
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.85	0.56
18:P:16:VAL:HG12	18:P:17:GLY:N	2.20	0.56
8:E:34:TRP:O	12:J:127:ILE:HD11	2.05	0.56
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.87	0.56
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.85	0.56
2:9:3002:U:OP2	2:9:3003:A:H5'	2.06	0.56
13:K:55:VAL:HG12	13:K:56:SER:N	2.19	0.56
1:0:775:G:OP1	29:1:16:HIS:HE1	1.89	0.56
6:C:194:PHE:HA	6:C:234:VAL:HG13	1.86	0.56
15:M:182:LYS:O	15:M:194:ALA:HB2	2.06	0.56
1:0:1634:G:H3'	39:0:4478:HOH:O	2.05	0.56
1:0:2563:U:H2'	1:0:2565:C:O5'	2.05	0.56
5:B:145:HIS:HD2	5:B:146:THR:O	1.89	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:M:60:VAL:C	15:M:61:ILE:HD12	2.25	0.56
25:W:65:VAL:HA	25:W:68:THR:HG22	1.87	0.56
11:H:56:GLN:HE22	11:H:93:GLN:HG2	1.70	0.56
9:F:1:PRO:H3	9:F:4:VAL:HG23	1.71	0.56
11:H:148:GLU:HA	11:H:148:GLU:OE1	2.05	0.56
25:W:88:THR:HG22	25:W:89:ASP:H	1.69	0.56
5:B:51:VAL:HG23	5:B:329:TYR:O	2.06	0.56
2:9:3014:G:O2'	16:N:1:ALA:HB2	2.05	0.56
1:0:2064:U:H5'	1:0:2652:U:O3'	2.05	0.56
1:0:2032:U:H2'	1:0:2033:G:C5'	2.35	0.56
1:0:151:A:H2'	1:0:152:A:O4'	2.05	0.56
1:0:432:G:O2'	1:0:433:C:H5'	2.06	0.56
23:U:5:GLU:HG2	23:U:10:GLY:O	2.05	0.56
5:B:264:GLU:OE2	5:B:302:PRO:HD3	2.05	0.56
6:C:154:VAL:O	6:C:158:GLU:HG3	2.06	0.56
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.88	0.56
25:W:4:LEU:HD11	25:W:45:VAL:HG12	1.87	0.56
22:T:49:GLU:CB	22:T:59:GLU:HG2	2.34	0.56
26:X:25:ARG:HG2	39:X:5356:HOH:O	2.06	0.56
12:J:107:ASN:HD22	12:J:109:TYR:H	1.53	0.56
1:0:185:G:H4'	1:0:186:A:H4'	1.87	0.56
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.35	0.56
1:0:1118:A:H8	1:0:1119:G:H5''	1.71	0.56
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.35	0.56
32:I:138:THR:HG22	32:I:139:ILE:N	2.20	0.56
1:0:1187:U:O2'	1:0:1189:A:H2	1.89	0.56
1:0:316:A:H5'	22:T:54:ASP:OD2	2.03	0.56
10:G:24:VAL:O	10:G:28:GLU:HB2	2.05	0.56
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.70	0.56
23:U:39:ASN:ND2	23:U:44:ARG:HH11	2.03	0.56
1:0:558:C:H2'	1:0:559:U:H5'	1.88	0.56
6:C:162:VAL:HG22	6:C:232:LEU:HD21	1.88	0.56
39:O:9738:HOH:O	15:M:82:ARG:HD2	2.06	0.56
39:9:1361:HOH:O	16:N:41:LYS:HE3	2.05	0.56
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.88	0.55
12:J:107:ASN:ND2	12:J:109:TYR:H	2.04	0.55
4:A:135:VAL:HG11	4:A:147:ARG:NH1	2.21	0.55
10:G:67:LEU:O	10:G:71:LEU:HG	2.05	0.55
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.88	0.55
2:9:3076:G:C3'	2:9:3077:A:H5''	2.27	0.55
5:B:53:LEU:CD1	5:B:327:VAL:HG22	2.36	0.55
9:F:58:GLU:HA	9:F:61:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:X:61:ARG:HB2	26:X:65:ASN:HB2	1.87	0.55
1:0:1736:A:H1'	39:0:8143:HOH:O	2.07	0.55
4:A:36:ASP:OD2	4:A:85:SER:HB2	2.06	0.55
1:0:1926:G:H2'	1:0:1927:A:C8	2.41	0.55
30:2:49:GLU:HB2	39:2:131:HOH:O	2.06	0.55
4:A:89:ALA:HB3	39:A:9608:HOH:O	2.05	0.55
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.36	0.55
13:K:4:LEU:CD2	13:K:116:GLU:HB3	2.35	0.55
1:0:1778:A:H2'	1:0:1779:A:H5'	1.88	0.55
5:B:305:ASP:O	5:B:306:LYS:HB2	2.07	0.55
1:0:2456:A:H2'	1:0:2457:U:C6	2.42	0.55
1:0:291:C:H2'	1:0:292:G:O4'	2.06	0.55
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.41	0.55
15:M:71:SER:HB2	15:M:92:THR:HG22	1.89	0.55
1:0:475:G:H5'	6:C:73:LEU:HD23	1.87	0.55
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.88	0.55
12:J:75:PRO:HD3	12:J:136:SER:OG	2.05	0.55
10:G:12:ILE:HD12	39:G:692:HOH:O	2.06	0.55
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.21	0.55
14:L:57:VAL:HG12	14:L:57:VAL:O	2.07	0.55
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.87	0.55
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.17	0.55
1:0:1973:A:H5'	1:0:1973:A:C8	2.39	0.55
1:0:960:G:N3	1:0:960:G:H2'	2.21	0.55
1:0:1789:G:O6	18:P:73:HIS:HE1	1.89	0.55
6:C:246:ARG:NH1	6:C:246:ARG:HB3	2.22	0.55
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.88	0.55
8:E:20:ILE:CD1	8:E:33:LEU:HD12	2.37	0.55
4:A:194:MET:HE1	4:A:199:HIS:HB2	1.88	0.55
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.05	0.55
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.05	0.55
1:0:625:U:H5''	1:0:1044:C:N4	2.21	0.55
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.37	0.55
1:0:441:A:H1'	1:0:442:A:N7	2.21	0.55
7:D:135:VAL:HG22	7:D:136:ARG:H	1.72	0.55
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.89	0.55
2:9:3051:A:H5'	16:N:160:SER:HB3	1.89	0.55
39:0:8105:HOH:O	31:3:60:LYS:HG3	2.06	0.55
5:B:307:ARG:HB3	39:B:9650:HOH:O	2.06	0.54
1:0:1882:C:OP1	4:A:192:VAL:HG23	2.07	0.54
1:0:1183:C:H2'	39:0:6772:HOH:O	2.07	0.54
15:M:68:ARG:HD3	15:M:68:ARG:O	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:258:GLY:H	5:B:260:HIS:CE1	2.25	0.54
9:F:60:VAL:HG12	9:F:60:VAL:O	2.06	0.54
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.72	0.54
1:0:2769:C:O2'	1:0:2770:G:H5'	2.07	0.54
16:N:11:ARG:O	16:N:15:GLU:HG3	2.07	0.54
2:9:3051:A:H5'	16:N:160:SER:CB	2.37	0.54
22:T:78:THR:HB	22:T:87:VAL:O	2.08	0.54
1:0:2827:A:H2'	1:0:2828:G:O4'	2.06	0.54
1:0:2866:U:H4'	1:0:2867:G:H5'	1.89	0.54
16:N:115:VAL:HG22	39:N:9356:HOH:O	2.07	0.54
32:I:139:ILE:HG22	32:I:140:GLU:N	2.23	0.54
1:0:1189:A:H1'	1:0:1209:C:O4'	2.07	0.54
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.37	0.54
1:0:2591:C:H2'	1:0:2592:G:O4'	2.07	0.54
12:J:107:ASN:HD22	12:J:107:ASN:C	2.11	0.54
1:0:2533:C:C6	1:0:2533:C:H5'	2.42	0.54
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.21	0.54
11:H:21:THR:O	11:H:120:ILE:HD12	2.08	0.54
16:N:154:LEU:HG	16:N:155:GLU:H	1.71	0.54
23:U:14:GLU:O	23:U:17:THR:HB	2.08	0.54
1:0:1878:G:O2'	1:0:1879:U:OP2	2.25	0.54
1:0:797:A:H4'	28:Z:10:ARG:N	2.22	0.54
5:B:72:THR:HB	39:B:9604:HOH:O	2.07	0.54
1:0:474:C:O3'	6:C:73:LEU:HD21	2.07	0.54
1:0:1681:G:H5''	1:0:1682:A:H5'	1.89	0.54
26:X:43:VAL:HG12	26:X:44:ASP:N	2.23	0.54
1:0:1626:A:H2'	1:0:1627:G:O4'	2.08	0.54
5:B:40:GLY:HA3	39:B:9645:HOH:O	2.08	0.54
1:0:2717:C:O2'	1:0:2718:C:H5''	2.07	0.54
1:0:1666:C:H2'	1:0:1667:A:C5'	2.36	0.54
1:0:2769:C:C2'	1:0:2770:G:H5'	2.38	0.54
7:D:50:VAL:O	7:D:71:ALA:HA	2.07	0.54
1:0:1350:U:H2'	1:0:1351:G:O4'	2.07	0.54
1:0:2670:G:O2'	1:0:2671:U:H5'	2.08	0.54
28:Z:72:GLU:OE1	28:Z:77:LYS:HE2	2.07	0.54
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.40	0.54
11:H:46:GLN:NE2	11:H:137:TYR:HE2	2.05	0.54
1:0:1209:C:H2'	1:0:1210:G:C8	2.42	0.54
25:W:4:LEU:O	25:W:32:CYS:HA	2.08	0.54
5:B:62:ARG:HA	5:B:65:MET:HE2	1.90	0.54
5:B:254:GLN:HG3	39:B:9530:HOH:O	2.08	0.54
17:O:59:VAL:HG23	17:O:111:VAL:CG2	2.37	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.88	0.54
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.42	0.54
12:J:8:ALA:HA	12:J:35:THR:HG22	1.90	0.54
1:0:1595:G:O2'	1:0:1596:U:H5'	2.08	0.54
22:T:12:ARG:NH1	39:T:3035:HOH:O	2.40	0.54
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.90	0.53
15:M:59:GLY:HA3	15:M:141:ILE:HD12	1.89	0.53
5:B:17:LYS:O	5:B:260:HIS:HD2	1.91	0.53
1:0:1406:A:H4'	1:0:1407:A:H5''	1.90	0.53
5:B:56:ASP:OD1	5:B:322:ARG:HB3	2.08	0.53
1:0:1625:U:H4'	39:0:5232:HOH:O	2.08	0.53
1:0:2817:G:P	39:0:8476:HOH:O	2.66	0.53
1:0:949:U:O2'	19:Q:40:HIS:HE1	1.91	0.53
23:U:49:LEU:HG	39:U:3805:HOH:O	2.07	0.53
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.08	0.53
6:C:107:ARG:HH11	6:C:107:ARG:HB3	1.71	0.53
5:B:195:ARG:HD2	5:B:324:ASP:OD1	2.07	0.53
1:0:2265:U:H2'	1:0:2266:A:C8	2.43	0.53
39:0:7381:HOH:O	15:M:178:LYS:HB2	2.07	0.53
31:3:3:MET:O	31:3:90:PHE:HA	2.09	0.53
5:B:51:VAL:HG23	5:B:327:VAL:HG13	1.90	0.53
1:0:2645:U:OP2	1:0:2645:U:C6	2.61	0.53
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.21	0.53
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.44	0.53
1:0:2894:C:O2'	1:0:2895:C:H5'	2.08	0.53
12:J:47:THR:HG22	12:J:48:GLY:N	2.23	0.53
7:D:172:VAL:HG12	7:D:173:GLU:H	1.74	0.53
24:V:42:ASN:HB3	39:V:7247:HOH:O	2.08	0.53
30:2:18:ASN:ND2	30:2:40:ARG:H	2.06	0.53
7:D:92:GLU:HB2	39:D:3862:HOH:O	2.07	0.53
31:3:65:THR:HG23	31:3:88:LEU:HD22	1.91	0.53
5:B:51:VAL:HG22	5:B:53:LEU:HD13	1.90	0.53
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.38	0.53
1:0:1168:C:H5''	32:I:87:THR:CG2	2.38	0.53
1:0:1419:U:H2'	1:0:1685:A:C2	2.43	0.53
6:C:25:PRO:HG2	39:C:9126:HOH:O	2.08	0.53
26:X:7:GLU:HA	26:X:74:ALA:O	2.09	0.53
5:B:86:ALA:HA	39:B:9576:HOH:O	2.09	0.53
1:0:2676:C:H6	1:0:2676:C:H5''	1.73	0.53
1:0:2456:A:H2'	1:0:2457:U:H6	1.73	0.53
11:H:136:ALA:HB3	11:H:146:VAL:HG21	1.90	0.53
12:J:103:VAL:HG12	39:J:5907:HOH:O	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:18:ARG:HE	5:B:256:GLN:NE2	2.06	0.53
4:A:203:GLY:HA2	39:A:9531:HOH:O	2.08	0.53
1:0:951:A:C2'	1:0:952:G:H5'	2.38	0.53
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.90	0.53
14:L:80:ASP:CB	14:L:90:ARG:HB3	2.38	0.53
6:C:233:THR:HG22	6:C:234:VAL:N	2.23	0.53
22:T:89:ARG:O	22:T:89:ARG:HG3	2.09	0.53
1:0:2320:U:H4'	1:0:2321:A:O4'	2.08	0.53
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.08	0.53
1:0:1501:A:OP2	18:P:37:ARG:HD2	2.08	0.53
1:0:2912:C:H2'	1:0:2913:A:O4'	2.09	0.53
13:K:55:VAL:CG1	13:K:56:SER:N	2.72	0.53
11:H:45:VAL:HA	11:H:167:PRO:O	2.09	0.53
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.90	0.53
5:B:62:ARG:HA	5:B:65:MET:HE3	1.90	0.53
6:C:246:ARG:NH1	39:C:9176:HOH:O	2.40	0.53
18:P:103:THR:O	18:P:107:GLU:HG3	2.08	0.53
29:I:21:ARG:HD2	29:I:37:CYS:SG	2.48	0.53
1:0:1724:U:H5''	39:0:4320:HOH:O	2.08	0.53
23:U:4:ARG:HH11	23:U:4:ARG:HG2	1.74	0.53
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.41	0.52
24:V:56:ILE:HG22	24:V:60:GLN:NE2	2.24	0.52
1:0:2419:U:H5''	1:0:2420:G:H5'	1.91	0.52
5:B:321:PRO:HA	39:B:9655:HOH:O	2.09	0.52
15:M:107:ARG:NH1	39:M:9383:HOH:O	2.42	0.52
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.91	0.52
1:0:564:G:H1'	39:0:6837:HOH:O	2.09	0.52
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.22	0.52
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.74	0.52
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.90	0.52
1:0:248:A:H5'	1:0:249:G:OP2	2.10	0.52
10:G:64:ASN:N	10:G:64:ASN:HD22	2.05	0.52
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.33	0.52
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.70	0.52
7:D:136:ARG:HB3	7:D:137:PRO:HD2	1.90	0.52
20:R:18:LEU:HB2	20:R:143:VAL:HG13	1.91	0.52
4:A:69:LEU:HD23	4:A:107:ASN:CB	2.40	0.52
1:0:2508:C:H2'	39:0:7264:HOH:O	2.09	0.52
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.09	0.52
6:C:127:ARG:CZ	6:C:225:PRO:HG2	2.39	0.52
32:I:129:VAL:O	32:I:129:VAL:HG12	2.10	0.52
14:L:145:LEU:O	14:L:148:GLU:HG3	2.08	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:121:U:OP2	30:2:10:ARG:NH2	2.38	0.52
17:O:59:VAL:CG2	17:O:111:VAL:HG21	2.39	0.52
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.91	0.52
1:0:848:C:H5'	39:0:7760:HOH:O	2.10	0.52
4:A:109:GLU:HG2	4:A:116:GLY:N	2.25	0.52
1:0:2541:U:O2	1:0:2618:G:N2	2.43	0.52
32:I:106:LYS:O	32:I:110:GLU:HG3	2.09	0.52
1:0:119:A:H2'	1:0:120:A:H5''	1.92	0.52
4:A:88:ILE:HG22	4:A:88:ILE:O	2.09	0.52
16:N:154:LEU:O	16:N:155:GLU:CB	2.58	0.52
1:0:2816:A:H2'	39:0:8476:HOH:O	2.10	0.52
14:L:97:VAL:HG12	14:L:98:GLU:O	2.09	0.52
1:0:1234:U:N3	5:B:244:PRO:HB3	2.25	0.52
16:N:162:ASP:HA	39:N:9331:HOH:O	2.10	0.52
22:T:69:LYS:O	22:T:71:VAL:HG23	2.10	0.52
14:L:91:VAL:CG1	14:L:120:LEU:HD23	2.39	0.52
1:0:1527:A:H1'	1:0:1528:A:C8	2.45	0.52
4:A:179:MET:HA	4:A:179:MET:CE	2.39	0.52
1:0:1462:C:H2'	1:0:1463:A:C8	2.45	0.52
24:V:8:ILE:HG21	24:V:59:ILE:HG13	1.91	0.52
15:M:164:THR:HG22	15:M:165:GLY:N	2.23	0.52
15:M:98:GLN:O	15:M:102:GLU:HG3	2.10	0.52
4:A:94:LEU:HB2	4:A:95:PRO:HD2	1.90	0.52
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.45	0.52
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.08	0.52
1:0:2896:A:H5''	39:X:5399:HOH:O	2.09	0.52
1:0:1218:U:H2'	1:0:1219:U:H6	1.74	0.52
25:W:38:THR:HG22	25:W:39:ASP:N	2.24	0.52
21:S:33:SER:OG	21:S:36:GLU:HG3	2.10	0.52
12:J:80:LYS:NZ	39:J:7377:HOH:O	2.42	0.52
1:0:737:A:H2'	1:0:738:G:O4'	2.09	0.52
5:B:41:PHE:CD2	5:B:190:MET:HE3	2.45	0.52
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.91	0.52
1:0:1211:G:O2'	1:0:1212:C:H5'	2.10	0.52
1:0:2101:A:H2'	6:C:63:SER:OG	2.10	0.52
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.91	0.52
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.92	0.52
16:N:152:GLU:C	16:N:154:LEU:H	2.13	0.52
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.25	0.52
16:N:42:HIS:CE1	16:N:75:THR:HG1	2.28	0.52
17:O:97:SER:OG	17:O:100:GLN:HG3	2.10	0.52
1:0:1946:C:H2'	1:0:1971:G:C8	2.45	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.10	0.52
15:M:99:ARG:NH2	15:M:170:ASN:HD22	2.00	0.51
1:0:1741:U:H3'	39:0:3369:HOH:O	2.09	0.51
6:C:142:ASP:OD1	6:C:237:GLU:HB3	2.10	0.51
16:N:49:THR:HG22	16:N:56:ASP:CB	2.40	0.51
16:N:18:THR:HG21	39:N:9346:HOH:O	2.08	0.51
15:M:24:GLN:O	15:M:28:GLN:HG3	2.11	0.51
20:R:44:VAL:O	20:R:48:GLU:HG3	2.10	0.51
6:C:163:HIS:HD2	39:C:9243:HOH:O	1.92	0.51
7:D:57:THR:HG23	7:D:63:ILE:CA	2.31	0.51
1:0:1835:U:C5	1:0:1840:A:N7	2.67	0.51
15:M:79:ALA:HB3	15:M:81:ARG:HH12	1.72	0.51
9:F:48:VAL:HG23	9:F:74:PHE:HB3	1.92	0.51
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.46	0.51
15:M:15:PRO:HA	15:M:20:LEU:HD23	1.92	0.51
1:0:1477:C:H5'	1:0:1868:G:C5'	2.40	0.51
7:D:23:VAL:CG2	7:D:73:VAL:HB	2.41	0.51
25:W:110:GLN:HE21	25:W:110:GLN:HA	1.76	0.51
4:A:36:ASP:O	4:A:38:ILE:N	2.42	0.51
1:0:776:A:OP1	29:1:28:HIS:HE1	1.92	0.51
1:0:284:C:H4'	1:0:285:A:H8	1.74	0.51
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.92	0.51
6:C:115:LEU:O	6:C:118:THR:HB	2.10	0.51
39:0:8484:HOH:O	5:B:2:GLN:CG	2.53	0.51
12:J:39:VAL:HG11	12:J:107:ASN:CG	2.30	0.51
1:0:2032:U:H2'	1:0:2033:G:H5''	1.92	0.51
1:0:1363:G:OP1	6:C:76:ARG:NH2	2.43	0.51
1:0:407:A:H5'	39:0:6556:HOH:O	2.10	0.51
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.92	0.51
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.92	0.51
18:P:55:LYS:HG2	18:P:56:GLY:N	2.25	0.51
20:R:29:LYS:NZ	39:R:9449:HOH:O	2.44	0.51
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.25	0.51
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.92	0.51
5:B:62:ARG:HG2	5:B:65:MET:HE3	1.92	0.51
1:0:2883:A:H2'	1:0:2884:G:O4'	2.11	0.51
1:0:2717:C:H2'	1:0:2718:C:C5'	2.35	0.51
4:A:36:ASP:C	4:A:38:ILE:H	2.14	0.51
16:N:86:LEU:HD21	16:N:180:LEU:HD12	1.92	0.51
1:0:1067:A:H5'	39:0:4922:HOH:O	2.10	0.51
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.25	0.51
1:0:2443:C:H5'	14:L:57:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.76	0.51
1:0:2626:C:H2'	1:0:2627:G:C8	2.46	0.51
1:0:1919:A:H4'	39:0:5416:HOH:O	2.10	0.51
11:H:54:THR:O	11:H:55:VAL:HG13	2.11	0.51
1:0:559:U:H2'	1:0:560:C:O4'	2.11	0.51
22:T:40:VAL:HG22	22:T:41:ARG:N	2.26	0.51
8:E:11:VAL:HG12	8:E:12:ASP:N	2.26	0.51
1:0:2524:G:H21	1:0:2526:C:N4	2.08	0.51
1:0:1966:U:H2'	1:0:1967:U:H2'	1.93	0.51
19:Q:3:SER:HB3	39:Q:5998:HOH:O	2.11	0.51
1:0:2711:U:H1'	39:0:4035:HOH:O	2.09	0.51
1:0:1278:A:H4'	1:0:1279:U:C4	2.46	0.51
1:0:69:A:H5'	1:0:69:A:C8	2.45	0.51
6:C:142:ASP:CG	6:C:237:GLU:HB3	2.31	0.51
13:K:7:ASP:OD2	13:K:81:ARG:NH2	2.44	0.51
9:F:58:GLU:HA	9:F:61:MET:HG3	1.93	0.51
1:0:1333:U:H2'	1:0:1334:C:C6	2.46	0.51
21:S:57:THR:CG2	21:S:58:MET:N	2.74	0.50
5:B:41:PHE:CG	5:B:79:MET:HE2	2.46	0.50
8:E:7:ILE:HD11	8:E:11:VAL:C	2.32	0.50
12:J:99:GLU:HA	39:J:7377:HOH:O	2.09	0.50
1:0:1853:C:OP1	4:A:231:LYS:HG3	2.12	0.50
1:0:2821:C:H4'	5:B:116:PRO:HG3	1.92	0.50
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.93	0.50
26:X:7:GLU:HA	26:X:75:ALA:HA	1.92	0.50
15:M:167:GLY:O	15:M:171:ARG:HG3	2.11	0.50
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.26	0.50
1:0:1165:G:H1'	1:0:1174:A:H1'	1.94	0.50
2:9:3008:G:O6	16:N:11:ARG:NH1	2.39	0.50
1:0:1363:G:P	6:C:76:ARG:HH22	2.35	0.50
11:H:116:ALA:O	11:H:117:PHE:C	2.50	0.50
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.41	0.50
1:0:90:A:H2'	1:0:91:G:O4'	2.11	0.50
9:F:26:THR:HG21	9:F:102:GLY:C	2.32	0.50
26:X:78:GLU:HG2	26:X:79:GLU:OE2	2.11	0.50
5:B:175:LEU:O	5:B:175:LEU:HD23	2.11	0.50
6:C:16:VAL:HG12	6:C:17:ASP:N	2.25	0.50
1:0:1198:U:H2'	1:0:1200:A:OP2	2.11	0.50
7:D:104:PHE:CE2	7:D:166:ILE:HD13	2.46	0.50
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.92	0.50
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.75	0.50
1:0:475:G:C5'	6:C:73:LEU:HD23	2.42	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:926:A:O2'	14:L:41:HIS:HD2	1.94	0.50
31:3:35:TRP:HB2	39:3:9488:HOH:O	2.09	0.50
1:0:1120:U:H5''	1:0:1120:U:C6	2.46	0.50
1:0:362:G:H2'	1:0:363:A:C8	2.46	0.50
5:B:310:ARG:HD2	39:B:9588:HOH:O	2.10	0.50
1:0:2812:A:C2	1:0:2814:A:N6	2.68	0.50
1:0:1118:A:C8	1:0:1118:A:C3'	2.89	0.50
23:U:9:CYS:O	23:U:52:THR:HG23	2.10	0.50
1:0:474:C:O3'	6:C:73:LEU:CD2	2.60	0.50
1:0:485:A:N3	1:0:487:G:H5''	2.26	0.50
7:D:51:ARG:HD3	39:D:7636:HOH:O	2.11	0.50
1:0:1592:G:O2'	1:0:1593:C:O4'	2.29	0.50
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.11	0.50
32:I:100:LEU:O	32:I:139:ILE:HG23	2.11	0.50
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.77	0.50
6:C:162:VAL:CG2	6:C:232:LEU:HD21	2.42	0.50
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.85	0.50
25:W:119:HIS:HD2	25:W:120:PRO:O	1.94	0.50
1:0:1119:G:H8	12:J:52:GLN:NE2	2.10	0.50
1:0:1979:G:O2'	1:0:1980:U:OP1	2.30	0.50
1:0:1167:G:H2'	1:0:1168:C:O4'	2.11	0.50
1:0:482:G:H4'	1:0:508:A:N1	2.27	0.50
1:0:1252:A:H2'	1:0:1253:C:O4'	2.12	0.50
7:D:10:PHE:CE1	7:D:11:HIS:HB3	2.47	0.50
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.41	0.50
12:J:76:ASP:HA	39:J:5907:HOH:O	2.11	0.50
1:0:1972:U:H2'	1:0:1973:A:H5'	1.94	0.50
1:0:447:A:O2'	1:0:448:G:H5'	2.12	0.50
39:K:7438:HOH:O	23:U:20:MET:HE1	2.11	0.50
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.92	0.50
24:V:59:ILE:O	24:V:63:GLU:HG2	2.11	0.50
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.24	0.50
1:0:1189:A:H1'	1:0:1209:C:C1'	2.41	0.50
11:H:3:ALA:CA	11:H:58:ARG:HH12	2.24	0.50
1:0:2815:G:OP2	12:J:99:GLU:HG2	2.12	0.50
1:0:920:C:H5''	1:0:921:G:O5'	2.12	0.50
1:0:87:C:H2'	30:2:28:LYS:O	2.12	0.50
7:D:167:GLU:C	7:D:169:THR:H	2.14	0.50
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.94	0.49
2:9:3044:A:O4'	7:D:76:ARG:NE	2.44	0.49
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.47	0.49
4:A:65:ARG:C	4:A:66:ARG:HG3	2.32	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:O:78:ALA:C	17:O:98:LEU:HD13	2.32	0.49
1:O:1477:C:O2'	1:O:1478:U:H5'	2.12	0.49
1:O:1942:A:H3'	39:O:7828:HOH:O	2.12	0.49
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.93	0.49
1:O:1132:A:N6	1:O:1229:C:H2'	2.27	0.49
1:O:155:C:OP2	15:M:188:ARG:HD3	2.11	0.49
1:O:1119:G:N2	1:O:1246:A:N1	2.60	0.49
11:H:40:ALA:HB1	11:H:137:TYR:CE2	2.47	0.49
1:O:1159:G:H1	1:O:1208:C:H42	1.60	0.49
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.11	0.49
2:9:3054:A:H2	39:9:3535:HOH:O	1.94	0.49
1:O:1921:A:O2'	1:O:1922:A:H5'	2.12	0.49
1:O:449:A:N7	6:C:43:LYS:HG2	2.26	0.49
1:O:1119:G:H8	12:J:52:GLN:HE22	1.59	0.49
11:H:27:LYS:H	11:H:59:HIS:CD2	2.23	0.49
16:N:183:ASP:O	16:N:184:ILE:O	2.30	0.49
11:H:73:LEU:HD21	11:H:146:VAL:HA	1.95	0.49
1:O:894:A:N1	6:C:87:ARG:NH2	2.61	0.49
4:A:132:ASP:OD1	4:A:133:ARG:N	2.42	0.49
1:O:317:A:OP1	22:T:52:ARG:O	2.30	0.49
1:O:1666:C:C2'	1:O:1667:A:C5'	2.91	0.49
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.93	0.49
11:H:169:GLY:HA3	39:H:9553:HOH:O	2.11	0.49
1:O:292:G:H2'	1:O:358:G:N2	2.27	0.49
6:C:219:ASN:O	6:C:222:ASP:OD1	2.30	0.49
5:B:49:THR:CG2	5:B:280:VAL:HG23	2.43	0.49
1:O:821:U:H2'	1:O:822:C:H6	1.77	0.49
26:X:30:MET:HE1	26:X:58:ALA:CB	2.40	0.49
32:I:74:PRO:C	32:I:112:LYS:HZ1	2.15	0.49
4:A:131:HIS:O	4:A:132:ASP:HB2	2.11	0.49
1:O:2786:G:H2'	39:O:7679:HOH:O	2.12	0.49
16:N:167:ASP:C	16:N:168:LEU:HG	2.33	0.49
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.77	0.49
1:O:2453:G:H5''	39:L:9438:HOH:O	2.11	0.49
1:O:820:G:O2'	1:O:856:G:H4'	2.13	0.49
31:3:70:ARG:HB3	39:3:9504:HOH:O	2.13	0.49
4:A:33:GLU:OE1	4:A:33:GLU:N	2.45	0.49
1:O:1667:A:H2'	1:O:1668:U:C6	2.48	0.49
1:O:470:U:O2'	29:1:16:HIS:CD2	2.62	0.49
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.94	0.49
4:A:223:ARG:CZ	39:A:9556:HOH:O	2.60	0.49
1:O:951:A:O2'	1:O:952:G:H5'	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:204:A:C2'	1:0:205:U:H5'	2.43	0.49
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.12	0.49
39:0:9730:HOH:O	5:B:229:ARG:HD2	2.13	0.49
25:W:115:THR:HB	39:W:6871:HOH:O	2.12	0.49
6:C:107:ARG:CB	6:C:107:ARG:HH11	2.25	0.49
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.24	0.49
24:V:39:ALA:O	24:V:41:GLU:N	2.41	0.49
20:R:39:THR:HB	20:R:42:GLU:CG	2.42	0.49
6:C:200:PRO:HB3	6:C:212:VAL:HG23	1.95	0.49
7:D:128:LEU:HB2	39:D:6007:HOH:O	2.13	0.49
1:0:2090:G:H2'	1:0:2091:G:C8	2.47	0.49
5:B:113:LEU:HD21	5:B:161:VAL:HG21	1.95	0.49
23:U:17:THR:CG2	23:U:18:GLY:H	2.25	0.49
1:0:1878:G:O2'	1:0:1879:U:C6	2.62	0.49
23:U:52:THR:HG22	23:U:54:THR:H	1.76	0.49
1:0:2895:C:H4'	39:X:4132:HOH:O	2.13	0.49
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.94	0.49
12:J:142:ASN:O	12:J:144:THR:N	2.45	0.49
1:0:299:U:H5'	39:0:7818:HOH:O	2.12	0.49
12:J:45:VAL:HG11	12:J:121:LEU:CD2	2.42	0.49
2:9:3028:U:H2'	2:9:3029:C:C6	2.47	0.49
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.13	0.49
9:F:14:ASP:O	9:F:18:GLU:HG3	2.12	0.49
5:B:81:ALA:O	5:B:186:GLY:HA3	2.12	0.49
1:0:2365:G:H5''	39:Q:6597:HOH:O	2.11	0.49
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.95	0.49
2:9:3004:G:H21	16:N:44:ARG:NH1	2.10	0.49
16:N:37:ARG:NH2	16:N:105:GLY:HA3	2.27	0.48
25:W:52:VAL:HG22	25:W:53:ALA:N	2.27	0.48
7:D:146:LYS:NZ	16:N:107:ASN:ND2	2.61	0.48
18:P:16:VAL:HG13	18:P:20:ARG:NH1	2.28	0.48
7:D:35:ALA:O	7:D:38:GLU:HG3	2.13	0.48
1:0:392:U:H5''	15:M:193:LYS:HB3	1.95	0.48
1:0:399:C:H5'	15:M:179:GLY:O	2.13	0.48
17:O:41:ALA:HA	39:O:5104:HOH:O	2.12	0.48
13:K:125:ALA:C	13:K:127:ALA:H	2.15	0.48
1:0:1654:U:H2'	4:A:47:HIS:HD2	1.76	0.48
24:V:29:ASN:O	24:V:33:VAL:HG23	2.13	0.48
7:D:57:THR:HA	39:D:5728:HOH:O	2.13	0.48
31:3:20:HIS:HA	31:3:70:ARG:O	2.13	0.48
1:0:1180:U:H2'	1:0:1181:A:C8	2.47	0.48
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:H:169:GLY:C	11:H:170:ASN:HD22	2.15	0.48
11:H:170:ASN:ND2	11:H:170:ASN:N	2.57	0.48
24:V:64:GLY:O	24:V:65:ASP:CB	2.59	0.48
12:J:131:THR:HB	12:J:134:GLU:OE1	2.13	0.48
12:J:70:PHE:CG	12:J:70:PHE:O	2.65	0.48
1:O:2507:G:H2'	1:O:2510:C:N4	2.28	0.48
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.94	0.48
1:O:541:C:H2'	1:O:542:A:H5'	1.94	0.48
16:N:1:ALA:HB3	39:N:9368:HOH:O	2.13	0.48
27:Y:203:VAL:HG12	27:Y:228:VAL:HG22	1.94	0.48
16:N:24:LEU:HD13	19:Q:26:PRO:HB3	1.94	0.48
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.94	0.48
1:O:1654:U:H2'	4:A:47:HIS:CD2	2.48	0.48
1:O:1056:U:H2'	1:O:1057:A:O4'	2.12	0.48
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.29	0.48
39:O:5842:HOH:O	25:W:122:ARG:NH2	2.47	0.48
1:O:1299:G:H5'	39:O:4654:HOH:O	2.13	0.48
1:O:2748:G:H4'	1:O:2749:U:C5'	2.43	0.48
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.48	0.48
1:O:1745:G:H22	1:O:2033:G:H5'	1.78	0.48
1:O:475:G:OP1	6:C:73:LEU:HD22	2.13	0.48
21:S:33:SER:O	21:S:37:VAL:HG23	2.13	0.48
1:O:2414:A:H2'	1:O:2415:A:C8	2.49	0.48
1:O:2253:G:O2'	1:O:2254:G:H5'	2.14	0.48
1:O:2649:A:H5'	1:O:2649:A:H8	1.78	0.48
22:T:71:VAL:CG1	22:T:72:ILE:N	2.76	0.48
25:W:122:ARG:NH2	39:W:5817:HOH:O	2.46	0.48
32:I:131:THR:O	32:I:135:LEU:HG	2.13	0.48
4:A:179:MET:HG2	4:A:186:TRP:CB	2.44	0.48
9:F:11:ASP:O	9:F:14:ASP:HB2	2.14	0.48
1:O:603:A:H5''	1:O:604:G:OP1	2.12	0.48
1:O:1902:G:H2'	1:O:1903:U:O4'	2.14	0.48
15:M:99:ARG:HH21	15:M:170:ASN:ND2	2.02	0.48
17:O:59:VAL:HG21	17:O:111:VAL:HG21	1.95	0.48
15:M:57:LYS:HE2	15:M:140:ALA:O	2.13	0.48
11:H:34:GLY:HA3	11:H:84:LYS:HA	1.94	0.48
2:9:3039:U:O2'	2:9:3042:C:C5	2.65	0.48
1:O:558:C:C2'	1:O:559:U:C5'	2.92	0.48
7:D:136:ARG:NH1	7:D:157:LEU:HA	2.27	0.48
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.48	0.48
31:3:6:ARG:NH1	31:3:21:GLU:HB2	2.28	0.48
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2831:C:O3'	20:R:71:LYS:HE2	2.14	0.48
39:0:4952:HOH:O	15:M:83:SER:HB3	2.14	0.48
1:0:1203:G:O2'	1:0:1204:C:H5'	2.13	0.48
12:J:19:MET:HE2	12:J:79:PHE:HA	1.94	0.48
32:I:105:VAL:HG11	32:I:129:VAL:CG2	2.44	0.48
4:A:53:ALA:HB3	39:A:9587:HOH:O	2.14	0.48
30:2:10:ARG:HD2	30:2:49:GLU:OE2	2.13	0.48
11:H:146:VAL:HG22	39:H:9541:HOH:O	2.14	0.48
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.96	0.48
25:W:29:VAL:O	25:W:30:ASN:HB2	2.14	0.48
22:T:71:VAL:HG13	22:T:91:LEU:O	2.13	0.48
2:9:3057:A:C8	7:D:141:VAL:HG21	2.48	0.48
4:A:26:ASP:CG	4:A:26:ASP:O	2.53	0.48
1:0:137:U:H2'	1:0:139:C:C5	2.48	0.48
1:0:932:U:H2'	1:0:933:C:C6	2.49	0.48
25:W:149:LEU:HG	25:W:153:MET:CE	2.44	0.48
1:0:343:C:O2'	1:0:344:C:H5'	2.12	0.48
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.95	0.48
1:0:2781:U:H1'	8:E:139:GLU:OE2	2.14	0.48
16:N:36:ALA:HB1	16:N:118:ILE:HD12	1.95	0.48
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.94	0.48
1:0:500:G:H21	20:R:98:ASN:HD21	1.60	0.48
25:W:139:GLY:O	25:W:141:HIS:HD2	1.95	0.48
7:D:49:PRO:HA	7:D:73:VAL:HG22	1.96	0.48
25:W:88:THR:CG2	25:W:89:ASP:N	2.75	0.48
12:J:75:PRO:HB3	12:J:132:LEU:HB3	1.95	0.48
32:I:113:HIS:N	32:I:114:PRO:CD	2.77	0.48
22:T:48:VAL:HG23	22:T:98:VAL:HA	1.96	0.48
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.14	0.48
1:0:2681:A:H4'	1:0:2682:C:H5'	1.96	0.48
6:C:61:PHE:HB3	39:C:9250:HOH:O	2.12	0.48
1:0:329:A:OP2	6:C:206:ASN:HB2	2.14	0.48
17:O:80:ASP:OD1	17:O:81:PHE:N	2.46	0.48
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.96	0.48
1:0:1130:U:H2'	1:0:1131:G:O4'	2.14	0.48
6:C:153:VAL:O	6:C:157:LEU:HG	2.14	0.48
39:9:5851:HOH:O	16:N:115:VAL:HG13	2.13	0.47
1:0:2748:G:C5'	39:0:8049:HOH:O	2.59	0.47
8:E:7:ILE:HD11	8:E:11:VAL:O	2.14	0.47
1:0:2003:U:H4'	1:0:2004:U:C5	2.46	0.47
6:C:157:LEU:HD13	6:C:166:ILE:HD11	1.95	0.47
27:Y:150:LEU:HB3	39:Y:9358:HOH:O	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.49	0.47
15:M:43:PRO:HG3	15:M:62:VAL:HG21	1.96	0.47
2:9:3049:G:H5''	39:9:4707:HOH:O	2.14	0.47
1:0:1118:A:C8	1:0:1119:G:H5''	2.48	0.47
1:0:757:C:OP1	14:L:27:ARG:HD2	2.13	0.47
1:0:486:A:H1'	39:0:7288:HOH:O	2.13	0.47
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.77	0.47
11:H:79:GLU:C	11:H:80:GLU:HG3	2.35	0.47
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.95	0.47
27:Y:122:ARG:NH2	39:Y:9335:HOH:O	2.48	0.47
1:0:1506:U:H6	1:0:1506:U:H5'	1.79	0.47
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.80	0.47
1:0:2072:G:H3'	1:0:2073:G:C5'	2.44	0.47
5:B:36:PRO:HB3	5:B:174:ARG:CB	2.44	0.47
10:G:27:ILE:HD13	10:G:71:LEU:HD23	1.97	0.47
17:O:14:LEU:HG	17:O:102:ILE:HD11	1.97	0.47
24:V:5:VAL:HG23	39:V:2271:HOH:O	2.13	0.47
1:0:1451:C:H5'	1:0:1505:U:C5	2.49	0.47
1:0:2825:C:H4'	1:0:2826:G:O5'	2.14	0.47
2:9:3092:G:H2'	2:9:3093:A:C8	2.50	0.47
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.52	0.47
17:O:32:ARG:HB2	39:O:4656:HOH:O	2.13	0.47
8:E:101:GLU:HB2	8:E:116:THR:O	2.14	0.47
5:B:254:GLN:NE2	39:B:9589:HOH:O	2.46	0.47
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.95	0.47
1:0:1755:A:H2'	1:0:1756:G:O4'	2.14	0.47
1:0:830:G:O2'	1:0:831:U:H5'	2.14	0.47
9:F:117:GLU:C	9:F:119:ARG:H	2.18	0.47
11:H:167:PRO:O	11:H:168:ALA:HB2	2.14	0.47
32:I:89:SER:CB	32:I:95:ASP:HB2	2.44	0.47
11:H:20:ILE:HG23	11:H:120:ILE:CD1	2.43	0.47
1:0:1406:A:H4'	1:0:1407:A:C5'	2.44	0.47
1:0:952:G:N3	1:0:2302:A:H2'	2.29	0.47
9:F:5:ASP:O	9:F:119:ARG:NH1	2.47	0.47
8:E:22:VAL:HG12	8:E:76:VAL:HG11	1.97	0.47
2:9:3058:G:H1'	39:D:3839:HOH:O	2.14	0.47
1:0:2102:G:H5''	1:0:2538:A:C2	2.50	0.47
1:0:2908:A:H2'	1:0:2909:G:O4'	2.13	0.47
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.21	0.47
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.78	0.47
1:0:542:A:H2'	1:0:543:G:O4'	2.15	0.47
5:B:162:MET:HE3	5:B:310:ARG:HD3	1.90	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:588:G:O6	25:W:154:ARG:NH1	2.48	0.47
9:F:68:ASP:C	9:F:70:LYS:H	2.18	0.47
1:0:2852:A:H5''	39:0:5787:HOH:O	2.14	0.47
13:K:28:GLU:OE2	13:K:58:THR:HG21	2.15	0.47
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.45	0.47
1:0:2032:U:C2'	1:0:2033:G:H5''	2.44	0.47
6:C:46:TYR:CE2	6:C:98:ARG:NH1	2.82	0.47
1:0:1525:G:H5'	1:0:1526:A:OP2	2.15	0.47
6:C:242:GLU:HB2	39:C:9188:HOH:O	2.14	0.47
5:B:24:PRO:HG3	5:B:204:GLY:HA2	1.95	0.47
1:0:2509:A:H2'	1:0:2510:C:O4'	2.15	0.47
16:N:74:PRO:HG2	16:N:159:TYR:CE1	2.49	0.47
2:9:3042:C:H5'	2:9:3043:G:OP2	2.14	0.47
20:R:9:ASP:O	20:R:13:THR:HB	2.14	0.47
4:A:94:LEU:N	4:A:94:LEU:HD23	2.30	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.72	0.47
5:B:41:PHE:CG	5:B:190:MET:HE3	2.49	0.47
8:E:102:VAL:HG13	8:E:116:THR:HG23	1.95	0.47
8:E:69:ILE:HA	8:E:72:MET:CE	2.44	0.47
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.96	0.47
12:J:130:VAL:HG12	12:J:131:THR:H	1.80	0.47
1:0:2819:C:O4'	5:B:96:PRO:HB2	2.14	0.47
12:J:39:VAL:HG11	12:J:107:ASN:CB	2.44	0.47
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.96	0.47
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.97	0.47
1:0:1120:U:H6	1:0:1120:U:H5''	1.80	0.47
1:0:87:C:C2	30:2:30:ASP:OD2	2.68	0.47
1:0:2649:A:C8	1:0:2649:A:H5'	2.49	0.47
1:0:603:A:H4'	1:0:604:G:O5'	2.14	0.47
8:E:1:PRO:HG2	8:E:59:MET:SD	2.54	0.47
9:F:101:ALA:HA	39:F:5413:HOH:O	2.15	0.47
13:K:13:GLU:OE1	13:K:44:LEU:HD12	2.14	0.47
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.49	0.47
1:0:645:U:OP2	14:L:4:LYS:HE2	2.13	0.47
1:0:1603:A:H5''	1:0:1605:G:H5'	1.96	0.47
1:0:380:A:H4'	1:0:381:G:OP1	2.15	0.47
1:0:870:G:OP2	4:A:3:ARG:HD3	2.15	0.47
1:0:506:G:H22	1:0:509:A:H5'	1.75	0.47
1:0:2644:C:O2'	1:0:2645:U:H5'	2.14	0.47
1:0:894:A:C2	6:C:87:ARG:NH2	2.83	0.47
11:H:158:THR:HB	11:H:159:PRO:HD3	1.97	0.47
1:0:1422:U:H2'	1:0:1423:C:C6	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2837:U:H2'	39:0:7345:HOH:O	2.14	0.47
8:E:80:TRP:O	8:E:134:SER:HA	2.14	0.47
1:0:2712:G:H5'	39:K:4183:HOH:O	2.14	0.47
1:0:1181:A:N1	1:0:1192:A:O2'	2.46	0.47
1:0:1972:U:H2'	1:0:1973:A:C5'	2.45	0.47
9:F:28:ALA:CB	9:F:99:THR:HG23	2.45	0.47
5:B:190:MET:CE	5:B:194:PHE:CD1	2.98	0.47
1:0:2346:C:H6	1:0:2346:C:O5'	1.96	0.47
16:N:69:TYR:CE2	16:N:184:ILE:HG13	2.48	0.47
14:L:35:ARG:HD3	14:L:35:ARG:C	2.36	0.47
1:0:1836:A:H1'	29:1:1:THR:O	2.14	0.47
1:0:241:A:C2	1:0:378:A:H4'	2.50	0.47
7:D:99:ASP:O	7:D:159:PRO:HG3	2.14	0.47
1:0:1352:A:HO2'	1:0:1353:C:P	2.36	0.47
12:J:80:LYS:HE2	12:J:98:PHE:CZ	2.50	0.47
2:9:3091:C:H2'	2:9:3092:G:O4'	2.15	0.47
4:A:126:ALA:HB1	4:A:138:VAL:CG1	2.45	0.47
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.50	0.47
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.97	0.47
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.30	0.47
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.96	0.47
14:L:61:ALA:HB2	14:L:105:TYR:CZ	2.50	0.47
2:9:3039:U:HO2'	2:9:3042:C:H5	1.55	0.46
1:0:1201:C:C2'	1:0:1202:A:H5'	2.45	0.46
9:F:99:THR:O	9:F:100:ASP:HB2	2.15	0.46
30:2:22:PRO:HG2	30:2:25:VAL:HG21	1.97	0.46
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.49	0.46
1:0:2252:A:H2'	1:0:2253:G:O4'	2.16	0.46
16:N:67:ALA:HA	16:N:71:TRP:HB3	1.97	0.46
17:O:73:ASP:HA	17:O:92:VAL:O	2.14	0.46
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.80	0.46
5:B:14:GLY:HA2	5:B:15:PRO:C	2.35	0.46
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.45	0.46
2:9:3049:G:O2'	2:9:3050:G:H5'	2.14	0.46
31:3:70:ARG:CG	31:3:77:ALA:HB2	2.42	0.46
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.98	0.46
14:L:145:LEU:O	14:L:145:LEU:HD23	2.15	0.46
39:0:4570:HOH:O	22:T:82:THR:HA	2.15	0.46
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	1.96	0.46
1:0:1331:A:OP2	27:Y:142:SER:OG	2.32	0.46
39:0:5295:HOH:O	16:N:21:HIS:HD2	1.97	0.46
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.51	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2338:G:H2'	7:D:129:ASP:OD1	2.15	0.46
1:0:1095:U:O2	25:W:120:PRO:HG2	2.16	0.46
7:D:135:VAL:HG22	7:D:136:ARG:N	2.29	0.46
4:A:194:MET:CE	4:A:199:HIS:HB2	2.45	0.46
1:0:2748:G:H4'	1:0:2749:U:H5'	1.95	0.46
11:H:66:ARG:HD3	39:H:9544:HOH:O	2.14	0.46
1:0:2346:C:H4'	7:D:52:THR:CG2	2.46	0.46
5:B:277:GLU:N	5:B:278:PRO:HD2	2.30	0.46
23:U:6:CYS:HB2	23:U:32:CYS:HB3	1.97	0.46
17:O:38:ARG:NH1	39:O:7674:HOH:O	2.47	0.46
13:K:14:LYS:HG3	13:K:32:ILE:O	2.15	0.46
39:O:6852:HOH:O	8:E:35:TYR:HB2	2.16	0.46
1:0:2635:A:C2'	1:0:2636:C:H5'	2.45	0.46
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.16	0.46
14:L:143:THR:CG2	14:L:144:ASP:N	2.76	0.46
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.81	0.46
1:0:709:G:O2'	17:O:25:VAL:CG1	2.61	0.46
1:0:1435:U:H5'	39:O:3209:HOH:O	2.14	0.46
11:H:47:ILE:HD12	11:H:146:VAL:CG1	2.45	0.46
1:0:407:A:H2'	1:0:408:A:C8	2.51	0.46
1:0:920:C:H4'	1:0:921:G:C2	2.51	0.46
1:0:1748:U:H4'	39:O:7993:HOH:O	2.14	0.46
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.15	0.46
27:Y:133:HIS:HD2	39:Y:9382:HOH:O	1.97	0.46
1:0:1098:A:H2'	1:0:1099:G:O4'	2.15	0.46
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.80	0.46
25:W:88:THR:CG2	25:W:89:ASP:H	2.28	0.46
14:L:134:GLU:HG3	39:L:9453:HOH:O	2.15	0.46
5:B:81:ALA:HB1	5:B:142:LEU:HD13	1.97	0.46
1:0:2906:A:H5'	1:0:2907:C:O4'	2.15	0.46
7:D:36:ASN:HB3	39:D:1655:HOH:O	2.16	0.46
1:0:653:C:H2'	1:0:654:A:C8	2.51	0.46
1:0:333:G:O2'	1:0:334:G:H5'	2.16	0.46
14:L:89:PHE:CD1	14:L:89:PHE:N	2.83	0.46
2:9:3024:U:H3'	2:9:3025:G:H5'	1.97	0.46
13:K:87:ARG:NH1	39:K:4066:HOH:O	2.49	0.46
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.44	0.46
32:I:89:SER:HB3	32:I:97:VAL:CG2	2.46	0.46
1:0:2362:A:H2'	1:0:2363:G:C8	2.51	0.46
26:X:25:ARG:HD2	39:X:3861:HOH:O	2.16	0.46
7:D:173:GLU:HG3	7:D:174:VAL:N	2.30	0.46
1:0:2415:A:O2'	16:N:29:SER:HB3	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:R:114:VAL:HA	20:R:144:GLU:O	2.15	0.46
1:0:2044:G:OP1	26:X:23:HIS:HE1	1.98	0.46
1:0:684:G:H2'	1:0:685:C:C6	2.51	0.46
27:Y:136:LYS:HE3	27:Y:138:ARG:NH1	2.30	0.46
6:C:129:HIS:HD2	6:C:165:ASP:OD2	1.98	0.46
1:0:1173:A:H4'	1:0:1174:A:C8	2.51	0.46
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.98	0.46
1:0:40:C:H6	1:0:40:C:O5'	1.99	0.46
1:0:2824:C:H5''	1:0:2825:C:H5'	1.98	0.46
1:0:271:C:H41	1:0:378:A:H2	1.64	0.46
1:0:2784:A:H1'	8:E:60:SER:OG	2.15	0.46
16:N:32:PRO:HD2	16:N:99:GLU:O	2.16	0.46
39:O:6254:HOH:O	13:K:87:ARG:CZ	2.64	0.46
4:A:94:LEU:HD12	4:A:98:GLU:CB	2.43	0.46
1:0:136:C:H2'	1:0:137:U:O4'	2.15	0.46
5:B:80:ARG:HB2	5:B:145:HIS:CE1	2.51	0.46
1:0:2911:C:O2'	1:0:2912:C:H5'	2.16	0.46
1:0:1786:C:OP1	18:P:74:GLN:HG2	2.16	0.46
19:Q:64:GLU:HG3	19:Q:74:ASP:OD2	2.16	0.46
1:0:2472:C:O2'	1:0:2634:G:H4'	2.15	0.46
1:0:899:C:H5'	39:O:3799:HOH:O	2.16	0.46
1:0:1342:C:O2'	1:0:1343:C:H5'	2.15	0.46
24:V:12:THR:HG23	24:V:14:ALA:N	2.31	0.46
24:V:1:THR:CG2	24:V:2:VAL:H	2.15	0.46
11:H:63:GLU:O	11:H:67:LEU:HB2	2.16	0.46
5:B:41:PHE:HA	5:B:79:MET:HE1	1.96	0.46
6:C:27:ARG:HG2	6:C:30:LEU:HG	1.97	0.46
1:0:710:G:H5'	17:O:25:VAL:CG1	2.46	0.46
16:N:86:LEU:O	16:N:90:LEU:HG	2.15	0.46
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.98	0.46
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.50	0.46
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.46	0.46
5:B:75:GLU:C	5:B:77:PRO:HD3	2.36	0.46
1:0:2348:C:H1'	7:D:131:THR:HG21	1.98	0.46
1:0:602:A:O2'	1:0:605:C:H4'	2.15	0.46
16:N:151:ASP:OD1	16:N:166:ALA:HA	2.16	0.46
15:M:49:ALA:C	15:M:54:TYR:HB3	2.36	0.46
8:E:85:GLU:HG3	8:E:169:THR:OG1	2.16	0.46
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.96	0.46
32:I:113:HIS:HE1	32:I:121:LEU:HD22	1.81	0.46
14:L:1:THR:HB	14:L:6:ARG:NH1	2.31	0.46
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:834:G:H3'	1:0:835:U:H4'	1.98	0.46
1:0:123:U:H1'	39:0:7856:HOH:O	2.16	0.46
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.51	0.46
8:E:81:GLU:HA	8:E:133:VAL:O	2.15	0.46
4:A:39:ALA:HB3	4:A:61:GLU:OE2	2.16	0.46
4:A:217:ARG:CG	4:A:217:ARG:HH11	2.29	0.46
29:1:56:GLU:HG2	29:1:56:GLU:OXT	2.16	0.46
1:0:1183:C:H5	1:0:1192:A:OP1	2.00	0.45
16:N:23:ARG:NH1	16:N:23:ARG:HG2	2.31	0.45
14:L:129:ALA:O	14:L:133:VAL:HG23	2.16	0.45
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.81	0.45
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.98	0.45
1:0:2064:U:H4'	1:0:2653:A:OP1	2.15	0.45
1:0:1200:A:H3'	39:0:6295:HOH:O	2.16	0.45
1:0:392:U:C5'	15:M:193:LYS:HB3	2.46	0.45
1:0:2679:G:H2'	1:0:2681:A:OP2	2.15	0.45
11:H:78:GLY:C	11:H:80:GLU:H	2.20	0.45
5:B:265:LEU:CD2	5:B:316:ARG:HD3	2.46	0.45
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.16	0.45
5:B:294:TYR:HE2	39:B:9647:HOH:O	1.99	0.45
1:0:288:A:H2'	1:0:289:G:C8	2.50	0.45
2:9:3050:G:H5''	16:N:159:TYR:HE1	1.81	0.45
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.51	0.45
1:0:121:U:O4	29:1:18:LYS:HG2	2.15	0.45
17:O:59:VAL:CG2	17:O:111:VAL:CG2	2.94	0.45
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.46	0.45
1:0:1025:C:H5'	25:W:23:MET:O	2.16	0.45
1:0:1503:U:H2'	1:0:1504:A:O4'	2.16	0.45
1:0:236:A:H8	1:0:236:A:OP1	1.99	0.45
20:R:84:ALA:O	20:R:88:PHE:HD1	1.99	0.45
20:R:132:ARG:CZ	39:R:9492:HOH:O	2.63	0.45
1:0:622:G:P	27:Y:148:GLY:HA3	2.56	0.45
9:F:52:GLU:OE1	9:F:78:GLU:OE1	2.34	0.45
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.63	0.45
32:I:72:VAL:HG13	32:I:73:PRO:HD2	1.98	0.45
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.98	0.45
25:W:11:VAL:O	25:W:12:ASN:HB2	2.16	0.45
12:J:63:ILE:HG22	12:J:64:GLY:N	2.30	0.45
1:0:968:G:H1'	11:H:32:LYS:HD2	1.98	0.45
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.32	0.45
1:0:2356:A:H5'	39:0:6178:HOH:O	2.16	0.45
15:M:74:LYS:HG3	15:M:75:ARG:N	2.31	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2748:G:H8	39:0:8049:HOH:O	2.00	0.45
1:0:2779:G:H21	8:E:143:GLN:HE22	1.64	0.45
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.31	0.45
7:D:10:PHE:CG	7:D:11:HIS:N	2.85	0.45
1:0:56:G:H5'	24:V:50:ARG:NH1	2.32	0.45
8:E:6:GLU:HA	8:E:46:THR:HG22	1.97	0.45
6:C:84:VAL:HG12	6:C:85:LYS:HG2	1.97	0.45
1:0:1335:C:OP2	27:Y:207:SER:HB3	2.16	0.45
1:0:259:G:H21	15:M:58:GLN:NE2	2.15	0.45
13:K:49:LEU:HD12	13:K:80:ILE:HD13	1.97	0.45
1:0:1603:A:H5'	1:0:1605:G:C4'	2.46	0.45
2:9:3042:C:O2	7:D:76:ARG:NH1	2.48	0.45
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.97	0.45
11:H:28:ILE:HG23	39:H:9544:HOH:O	2.16	0.45
30:2:35:ARG:HB2	39:2:2691:HOH:O	2.16	0.45
1:0:157:G:H4'	15:M:95:LYS:HE2	1.98	0.45
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.99	0.45
1:0:2015:A:H2'	1:0:2016:U:O4'	2.17	0.45
1:0:810:G:H1'	39:0:7740:HOH:O	2.17	0.45
2:9:3107:C:H5	39:9:3167:HOH:O	1.99	0.45
16:N:108:SER:HA	16:N:109:PRO:HD3	1.81	0.45
5:B:84:LEU:HB2	5:B:182:VAL:HG21	1.99	0.45
5:B:178:ALA:O	5:B:182:VAL:HG23	2.16	0.45
1:0:2421:G:H2'	39:0:4659:HOH:O	2.16	0.45
18:P:50:GLN:HG2	39:P:204:HOH:O	2.16	0.45
5:B:87:TYR:O	5:B:138:GLY:N	2.35	0.45
12:J:88:PRO:O	12:J:94:GLY:HA3	2.17	0.45
27:Y:212:ARG:HD2	39:Y:9402:HOH:O	2.16	0.45
8:E:15:GLN:NE2	8:E:40:VAL:O	2.50	0.45
7:D:40:ILE:HG13	7:D:41:LEU:N	2.32	0.45
16:N:143:ARG:HE	16:N:143:ARG:HB3	1.56	0.45
1:0:999:C:H2'	1:0:1000:C:O4'	2.17	0.45
4:A:123:GLY:HA2	4:A:159:VAL:O	2.17	0.45
23:U:4:ARG:NH1	23:U:4:ARG:HG2	2.31	0.45
5:B:243:ASN:HA	5:B:244:PRO:C	2.37	0.45
1:0:88:G:N7	30:2:28:LYS:HD2	2.31	0.45
21:S:11:THR:H	21:S:14:ALA:HB3	1.81	0.45
1:0:2398:A:H2'	1:0:2399:G:O4'	2.16	0.45
25:W:139:GLY:O	25:W:141:HIS:CD2	2.70	0.45
1:0:1592:G:H2'	1:0:1593:C:C6	2.52	0.45
1:0:1192:A:H3'	1:0:1193:A:H5'	1.99	0.45
27:Y:148:GLY:O	27:Y:154:ARG:HD3	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:1:18:LYS:HB2	30:2:49:GLU:CG	2.45	0.45
14:L:144:ASP:O	14:L:147:GLU:HB2	2.17	0.45
7:D:103:ASN:ND2	7:D:134:LEU:H	2.14	0.45
31:3:6:ARG:NH1	31:3:21:GLU:HG3	2.32	0.45
14:L:10:SER:O	14:L:11:ARG:HB3	2.17	0.45
1:0:328:U:O4'	6:C:202:THR:HG22	2.16	0.45
1:0:2809:G:H2'	1:0:2810:G:O4'	2.17	0.45
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.50	0.45
14:L:72:ASN:HB2	39:L:9478:HOH:O	2.16	0.45
1:0:812:A:H2'	1:0:813:C:C6	2.51	0.45
1:0:2857:C:H2'	1:0:2858:U:C6	2.52	0.45
22:T:20:HIS:HB3	22:T:41:ARG:HD2	1.98	0.45
39:0:7282:HOH:O	16:N:4:PRO:HD2	2.17	0.45
20:R:114:VAL:HG13	20:R:114:VAL:O	2.17	0.45
1:0:95:A:H5''	1:0:97:G:O4'	2.17	0.45
1:0:793:A:H5''	18:P:83:LYS:HG2	1.99	0.45
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.82	0.45
1:0:371:U:H2'	1:0:372:A:H8	1.82	0.45
24:V:51:LYS:O	24:V:55:ARG:HG3	2.17	0.45
32:I:99:ASP:O	32:I:100:LEU:HD23	2.17	0.45
1:0:1667:A:C8	1:0:1667:A:H5'	2.42	0.45
7:D:170:TYR:O	7:D:171:ASP:CB	2.65	0.45
1:0:1555:G:H4'	1:0:1630:A:C2	2.51	0.45
27:Y:115:ARG:NE	39:Y:9356:HOH:O	2.50	0.45
2:9:3054:A:O2'	2:9:3055:U:H5'	2.16	0.45
1:0:2699:A:H2'	1:0:2700:G:O4'	2.15	0.45
1:0:1994:A:P	13:K:66:ARG:HH22	2.40	0.45
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.18	0.44
25:W:122:ARG:HH22	25:W:154:ARG:HG2	1.79	0.44
7:D:60:GLU:O	7:D:60:GLU:HG3	2.17	0.44
1:0:1834:C:H2'	1:0:1840:A:N6	2.32	0.44
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.45	0.44
1:0:2866:U:C4	23:U:50:GLU:HB3	2.52	0.44
1:0:497:A:H2'	1:0:498:A:C5'	2.47	0.44
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.18	0.44
6:C:218:VAL:N	39:C:9229:HOH:O	2.50	0.44
21:S:81:ILE:HG23	39:S:9494:HOH:O	2.17	0.44
14:L:124:ASP:OD1	14:L:149:ARG:NH2	2.50	0.44
1:0:2568:A:H5''	1:0:2702:A:O2'	2.17	0.44
6:C:180:SER:HB2	39:C:9251:HOH:O	2.17	0.44
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.99	0.44
22:T:49:GLU:OE2	22:T:51:LEU:HD21	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:H:29:ALA:C	11:H:30:GLN:HG3	2.37	0.44
1:O:2545:U:OP2	5:B:2:GLN:NE2	2.50	0.44
1:O:2890:A:H1'	23:U:56:ARG:CZ	2.46	0.44
4:A:65:ARG:HH11	4:A:65:ARG:HG2	1.82	0.44
23:U:52:THR:CG2	23:U:54:THR:HB	2.47	0.44
18:P:16:VAL:HG13	18:P:20:ARG:CZ	2.47	0.44
15:M:22:GLU:HG2	15:M:26:GLN:NE2	2.32	0.44
6:C:168:ARG:NH2	6:C:190:ALA:O	2.50	0.44
9:F:60:VAL:O	9:F:60:VAL:CG1	2.64	0.44
20:R:39:THR:HG22	20:R:41:GLY:H	1.83	0.44
14:L:134:GLU:HA	14:L:138:GLY:O	2.17	0.44
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.81	0.44
39:O:6811:HOH:O	27:Y:158:LYS:HD3	2.18	0.44
1:O:415:A:O2'	1:O:416:G:H5'	2.18	0.44
18:P:135:ALA:HB1	18:P:139:ARG:HH12	1.82	0.44
1:O:629:A:H2'	1:O:630:A:O4'	2.17	0.44
1:O:366:U:H2'	1:O:367:G:O4'	2.17	0.44
32:I:87:THR:HG22	32:I:88:GLY:N	2.32	0.44
4:A:69:LEU:HD23	4:A:107:ASN:CG	2.37	0.44
5:B:71:VAL:CG1	5:B:296:LEU:HD22	2.48	0.44
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.18	0.44
13:K:65:ARG:NE	39:K:5358:HOH:O	2.46	0.44
1:O:1666:C:C2'	1:O:1667:A:H5''	2.47	0.44
1:O:1878:G:C1'	39:O:6649:HOH:O	2.60	0.44
1:O:338:C:H4'	6:C:174:ILE:HD11	1.99	0.44
15:M:187:LEU:HD22	15:M:194:ALA:HB3	1.99	0.44
1:O:40:C:H4'	39:O:7503:HOH:O	2.17	0.44
1:O:2101:A:OP2	6:C:66:GLY:HA2	2.18	0.44
22:T:52:ARG:O	22:T:53:GLY:O	2.35	0.44
1:O:2480:G:H3'	39:O:4764:HOH:O	2.16	0.44
1:O:2505:G:C2'	1:O:2506:A:H5'	2.48	0.44
13:K:109:LEU:HD13	13:K:113:ILE:CD1	2.45	0.44
2:9:3049:G:H2'	2:9:3050:G:O4'	2.18	0.44
4:A:207:GLN:O	4:A:208:HIS:HB3	2.17	0.44
25:W:5:VAL:O	25:W:52:VAL:CG2	2.65	0.44
5:B:5:ARG:HD2	5:B:8:LYS:NZ	2.33	0.44
1:O:1641:A:C2'	1:O:1642:A:H5'	2.46	0.44
22:T:48:VAL:CG1	22:T:96:VAL:HG21	2.47	0.44
16:N:152:GLU:HA	16:N:152:GLU:OE1	2.18	0.44
1:O:2907:C:H2'	1:O:2908:A:O4'	2.17	0.44
1:O:236:A:H4'	1:O:237:G:H5'	2.00	0.44
1:O:1086:A:C6	25:W:11:VAL:HG11	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.37	0.44
30:2:20:ARG:HG3	30:2:21:VAL:N	2.33	0.44
1:0:2506:A:O2'	1:0:2507:G:O5'	2.35	0.44
9:F:70:LYS:C	9:F:72:VAL:H	2.21	0.44
7:D:154:LYS:HD2	7:D:154:LYS:N	2.28	0.44
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.65	0.44
25:W:118:LEU:HD12	25:W:153:MET:HE3	1.99	0.44
14:L:149:ARG:O	14:L:150:GLN:HB2	2.17	0.44
1:0:12:U:H2'	1:0:13:G:H5'	2.00	0.44
31:3:69:TYR:CZ	31:3:80:ARG:HD2	2.53	0.44
1:0:2718:C:H5'	1:0:2718:C:C6	2.48	0.44
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.99	0.44
1:0:120:A:H5'	29:1:20:ARG:HH21	1.82	0.44
11:H:3:ALA:CB	11:H:58:ARG:HH12	2.30	0.44
8:E:23:GLU:HG2	8:E:28:SER:CB	2.47	0.44
6:C:107:ARG:NH1	39:C:9236:HOH:O	2.51	0.44
7:D:37:ALA:O	7:D:40:ILE:HG12	2.18	0.44
4:A:3:ARG:H	4:A:3:ARG:HG2	1.66	0.44
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.47	0.44
16:N:23:ARG:NH1	39:N:9346:HOH:O	2.51	0.44
5:B:56:ASP:HB3	5:B:322:ARG:HH21	1.83	0.44
10:G:64:ASN:N	10:G:64:ASN:ND2	2.66	0.44
5:B:171:VAL:HG23	5:B:172:SER:N	2.33	0.44
32:I:124:ALA:O	32:I:128:VAL:HG23	2.18	0.44
1:0:566:A:H2'	1:0:567:U:O4'	2.17	0.44
7:D:78:GLU:O	7:D:82:GLU:HG3	2.17	0.44
16:N:72:GLU:HG2	16:N:72:GLU:O	2.17	0.44
1:0:2541:U:O2'	3:4:76:DA:H4'	2.17	0.43
32:I:102:VAL:HG23	32:I:140:GLU:O	2.18	0.43
1:0:1298:U:H2'	1:0:1299:G:C8	2.52	0.43
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.64	0.43
5:B:138:GLY:O	5:B:139:ASP:O	2.36	0.43
16:N:89:GLY:O	16:N:92:ALA:HB3	2.18	0.43
1:0:1314:U:H2'	39:0:6410:HOH:O	2.18	0.43
28:Z:13:ARG:NH1	39:Z:9218:HOH:O	2.51	0.43
9:F:65:GLU:O	9:F:69:GLU:HG2	2.18	0.43
22:T:47:THR:HB	22:T:100:ASP:HB3	1.99	0.43
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.48	0.43
25:W:26:ILE:O	25:W:26:ILE:HG13	2.18	0.43
25:W:122:ARG:NH1	25:W:152:ALA:O	2.51	0.43
12:J:132:LEU:HA	12:J:132:LEU:HD23	1.85	0.43
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:N:167:ASP:O	16:N:168:LEU:HG	2.17	0.43
5:B:234:ARG:HH11	5:B:234:ARG:HB3	1.83	0.43
23:U:20:MET:CG	23:U:28:THR:HG23	2.48	0.43
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.53	0.43
1:O:2531:U:O2'	1:O:2532:A:H5'	2.17	0.43
1:O:2720:C:O2	13:K:87:ARG:NH2	2.51	0.43
1:O:1180:U:H1'	39:O:3831:HOH:O	2.18	0.43
14:L:145:LEU:C	14:L:145:LEU:HD23	2.38	0.43
5:B:41:PHE:HA	5:B:79:MET:CE	2.49	0.43
39:O:5535:HOH:O	11:H:58:ARG:HG3	2.18	0.43
28:Z:72:GLU:HB3	28:Z:77:LYS:HE3	2.00	0.43
22:T:79:LEU:HG	22:T:89:ARG:HB2	2.00	0.43
6:C:79:ARG:O	6:C:87:ARG:HG2	2.18	0.43
1:O:2415:A:H2'	1:O:2416:G:H5'	2.00	0.43
1:O:2036:C:O4'	13:K:44:LEU:HG	2.18	0.43
5:B:139:ASP:HB3	39:B:9547:HOH:O	2.17	0.43
20:R:34:GLU:HG2	20:R:46:TYR:OH	2.17	0.43
5:B:149:ASP:HB2	39:B:9577:HOH:O	2.18	0.43
1:O:2807:U:P	5:B:27:ASN:HD21	2.40	0.43
1:O:2372:A:H2'	1:O:2373:U:C6	2.53	0.43
9:F:110:ASP:O	9:F:114:LYS:HG3	2.18	0.43
16:N:116:PHE:HB3	16:N:136:LEU:HD23	2.00	0.43
25:W:122:ARG:HG2	25:W:152:ALA:O	2.17	0.43
7:D:25:MET:CE	7:D:41:LEU:HG	2.39	0.43
7:D:49:PRO:HB3	39:D:5828:HOH:O	2.19	0.43
32:I:88:GLY:C	32:I:97:VAL:HG21	2.38	0.43
1:O:2338:G:OP1	7:D:97:GLN:HG2	2.19	0.43
27:Y:184:GLU:HG2	27:Y:229:LEU:HD11	2.00	0.43
1:O:635:A:H2'	1:O:636:G:H5''	2.00	0.43
1:O:360:A:H2'	1:O:361:C:O4'	2.18	0.43
1:O:462:A:H2'	39:O:5450:HOH:O	2.17	0.43
1:O:450:C:OP1	6:C:184:ARG:NH2	2.38	0.43
7:D:25:MET:CE	7:D:40:ILE:HD11	2.49	0.43
7:D:25:MET:HE1	7:D:37:ALA:O	2.18	0.43
13:K:115:ARG:HG3	13:K:116:GLU:N	2.32	0.43
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.18	0.43
16:N:48:VAL:HG11	16:N:55:ASP:HB3	2.00	0.43
14:L:143:THR:CG2	14:L:144:ASP:H	2.31	0.43
5:B:73:VAL:HG22	5:B:296:LEU:CD2	2.48	0.43
5:B:305:ASP:O	5:B:306:LYS:CB	2.66	0.43
1:O:1741:U:O2'	1:O:2723:G:H4'	2.19	0.43
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2698:G:H2'	1:0:2699:A:C8	2.53	0.43
1:0:2898:G:H4'	5:B:288:GLY:HA2	1.99	0.43
1:0:2589:U:H2'	1:0:2590:U:C6	2.53	0.43
25:W:48:VAL:CG1	25:W:48:VAL:O	2.66	0.43
1:0:558:C:H2'	1:0:559:U:H5''	1.98	0.43
2:9:3014:G:H2'	2:9:3015:C:H5'	2.01	0.43
2:9:3029:C:C2'	2:9:3030:C:H5'	2.48	0.43
14:L:133:VAL:HB	39:L:9453:HOH:O	2.19	0.43
31:3:38:ARG:CB	31:3:42:ARG:HH12	2.31	0.43
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.84	0.43
1:0:2663:U:O2	39:0:8476:HOH:O	2.20	0.43
1:0:2820:A:H2'	1:0:2821:C:C6	2.53	0.43
5:B:91:PRO:O	12:J:144:THR:HG21	2.18	0.43
26:X:66:THR:HG22	26:X:67:PRO:O	2.18	0.43
14:L:150:GLN:HB3	39:L:9466:HOH:O	2.19	0.43
4:A:17:ARG:HD2	39:A:9527:HOH:O	2.18	0.43
13:K:49:LEU:HD12	13:K:80:ILE:HG21	2.00	0.43
24:V:8:ILE:CG2	24:V:59:ILE:HG13	2.48	0.43
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.39	0.43
32:I:139:ILE:CG2	32:I:140:GLU:N	2.82	0.43
30:2:48:ASP:O	30:2:49:GLU:HB2	2.18	0.43
1:0:969:G:H1	1:0:999:C:N4	2.16	0.43
7:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.66	0.43
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.47	0.43
18:P:37:ARG:HG2	18:P:37:ARG:HH11	1.84	0.43
1:0:249:G:O2'	1:0:250:C:H5'	2.19	0.43
1:0:2237:G:H1'	1:0:2238:A:C8	2.54	0.43
1:0:2353:A:H4'	1:0:2354:A:O5'	2.17	0.43
1:0:2011:A:H4'	1:0:2012:U:O5'	2.19	0.43
24:V:8:ILE:HA	24:V:11:MET:HE2	2.00	0.43
7:D:60:GLU:O	7:D:61:PHE:C	2.56	0.43
25:W:5:VAL:O	25:W:52:VAL:HG23	2.19	0.43
1:0:681:G:N7	39:0:7461:HOH:O	2.36	0.43
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.99	0.43
1:0:40:C:N3	1:0:441:A:H2	2.16	0.43
6:C:45:ASP:OD2	6:C:98:ARG:HD2	2.19	0.43
1:0:1992:U:OP2	13:K:66:ARG:HD2	2.18	0.43
1:0:2587:OMU:H2'	1:0:2589:U:H5''	2.00	0.43
1:0:941:G:C5	1:0:942:U:C4	3.07	0.43
1:0:2499:U:H2'	1:0:2500:C:H6	1.84	0.43
4:A:164:ARG:CZ	39:A:9571:HOH:O	2.66	0.43
1:0:644:G:N3	1:0:644:G:H5'	2.34	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
39:O:5842:HOH:O	25:W:119:HIS:CG	2.72	0.43
1:O:1174:A:C5	1:O:1201:C:H4'	2.54	0.43
25:W:3:ALA:O	25:W:54:PHE:HA	2.19	0.43
11:H:154:TYR:C	11:H:154:TYR:CD1	2.92	0.43
4:A:26:ASP:OD2	4:A:28:GLU:HG3	2.18	0.43
6:C:151:GLN:O	6:C:154:VAL:HB	2.18	0.43
1:O:204:A:H2'	1:O:205:U:H5'	1.99	0.43
1:O:1057:A:H2'	1:O:1058:A:C8	2.54	0.43
12:J:63:ILE:CG2	12:J:64:GLY:N	2.82	0.43
1:O:1470:A:OP1	15:M:93:ARG:HD2	2.18	0.43
5:B:119:HIS:O	5:B:121:PRO:HD3	2.19	0.43
11:H:83:TYR:C	11:H:83:TYR:CD1	2.91	0.43
1:O:802:G:H2'	1:O:803:C:C6	2.54	0.43
3:4:74:C:H2'	3:4:75:C:H5'	2.01	0.43
1:O:1160:G:HO2'	1:O:1190:G:H8	1.63	0.43
2:9:3050:G:H5''	16:N:159:TYR:CE1	2.54	0.43
17:O:25:VAL:HG23	17:O:26:TRP:N	2.33	0.43
12:J:131:THR:HG22	12:J:133:GLY:N	2.34	0.43
1:O:1477:C:H5'	1:O:1868:G:H5''	2.00	0.43
16:N:71:TRP:HB2	39:N:9338:HOH:O	2.18	0.43
1:O:1236:A:C8	12:J:63:ILE:HD11	2.54	0.43
1:O:2697:A:H2'	1:O:2698:G:O4'	2.19	0.43
26:X:45:GLU:HG3	39:X:6178:HOH:O	2.19	0.43
1:O:286:U:H2'	1:O:287:C:C6	2.54	0.43
13:K:49:LEU:HD22	13:K:117:VAL:CG2	2.49	0.42
1:O:364:C:H2'	1:O:365:G:O4'	2.19	0.42
1:O:1299:G:N2	39:O:5248:HOH:O	2.51	0.42
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.34	0.42
15:M:61:ILE:N	15:M:61:ILE:HD12	2.33	0.42
1:O:2452:G:H5'	39:3:9488:HOH:O	2.17	0.42
1:O:2416:G:O2'	16:N:25:ARG:HG2	2.19	0.42
20:R:132:ARG:NH2	39:R:9492:HOH:O	2.52	0.42
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.19	0.42
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.54	0.42
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.84	0.42
26:X:80:GLU:O	26:X:80:GLU:HG2	2.19	0.42
7:D:27:ILE:HG22	7:D:28:GLY:N	2.32	0.42
14:L:80:ASP:HB2	14:L:90:ARG:HB3	2.01	0.42
1:O:396:U:OP2	31:3:38:ARG:HD2	2.18	0.42
32:I:75:THR:HA	32:I:112:LYS:NZ	2.34	0.42
1:O:1351:G:OP1	6:C:96:LYS:NZ	2.41	0.42
1:O:92:G:H4'	24:V:44:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:2:18:ASN:HD21	30:2:40:ARG:H	1.66	0.42
11:H:119:LYS:HB2	11:H:119:LYS:HE3	1.81	0.42
1:0:669:G:O2'	1:0:670:G:H5'	2.19	0.42
1:0:526:U:H2'	1:0:527:U:C6	2.54	0.42
2:9:3059:C:O5'	2:9:3059:C:H6	2.02	0.42
16:N:103:ASP:OD1	16:N:103:ASP:C	2.58	0.42
32:I:129:VAL:HG13	32:I:139:ILE:HD11	2.01	0.42
5:B:42:ALA:H	5:B:79:MET:HE2	1.85	0.42
19:Q:11:ARG:HD3	39:Q:5620:HOH:O	2.18	0.42
1:0:2769:C:H2'	1:0:2770:G:C5'	2.48	0.42
16:N:152:GLU:C	16:N:154:LEU:N	2.72	0.42
24:V:42:ASN:O	24:V:44:GLY:N	2.52	0.42
1:0:1200:A:H4'	39:0:7822:HOH:O	2.19	0.42
6:C:157:LEU:CD1	6:C:166:ILE:HD11	2.49	0.42
30:2:20:ARG:HD2	30:2:39:ARG:NH2	2.34	0.42
1:0:2238:A:O2'	1:0:2239:C:H5'	2.18	0.42
1:0:200:U:H2'	39:0:4038:HOH:O	2.18	0.42
19:Q:77:ASP:HB3	19:Q:82:LYS:HE3	2.01	0.42
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.49	0.42
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.59	0.42
5:B:36:PRO:CA	5:B:168:GLY:HA3	2.44	0.42
14:L:77:ALA:C	14:L:79:ASP:H	2.23	0.42
27:Y:187:VAL:HB	27:Y:203:VAL:CG2	2.50	0.42
4:A:51:ARG:HH21	4:A:55:VAL:HG23	1.84	0.42
1:0:2421:G:H4'	39:0:5345:HOH:O	2.18	0.42
12:J:39:VAL:CG1	12:J:40:ASN:N	2.82	0.42
1:0:2036:C:C1'	13:K:44:LEU:HG	2.50	0.42
6:C:218:VAL:HG12	39:C:9229:HOH:O	2.18	0.42
2:9:3064:C:C2'	2:9:3065:A:H5'	2.49	0.42
1:0:2487:C:H5	39:0:5455:HOH:O	2.02	0.42
8:E:166:VAL:HG12	39:E:3134:HOH:O	2.18	0.42
24:V:8:ILE:HA	24:V:11:MET:CE	2.50	0.42
32:I:92:PRO:C	32:I:94:GLU:N	2.70	0.42
25:W:64:THR:O	25:W:68:THR:HG22	2.20	0.42
14:L:79:ASP:O	14:L:80:ASP:O	2.37	0.42
1:0:185:G:C4'	1:0:186:A:H4'	2.50	0.42
1:0:1477:C:C5'	1:0:1868:G:H5''	2.50	0.42
1:0:69:A:H5'	1:0:69:A:H8	1.85	0.42
6:C:98:ARG:NH1	39:C:9163:HOH:O	2.51	0.42
1:0:666:A:H2'	1:0:667:C:O4'	2.20	0.42
1:0:2900:G:H2'	1:0:2901:C:O4'	2.19	0.42
1:0:426:G:H2'	1:0:427:C:O4'	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:889:C:H2'	1:0:890:C:C6	2.55	0.42
20:R:69:LYS:HB2	20:R:72:VAL:HG23	2.00	0.42
1:0:1821:A:O2'	1:0:1822:A:H5'	2.20	0.42
9:F:79:GLN:HG3	9:F:82:ASP:OD2	2.18	0.42
13:K:115:ARG:HG2	13:K:116:GLU:OE1	2.19	0.42
9:F:30:LYS:HE2	9:F:99:THR:HG21	2.01	0.42
1:0:120:A:H2'	1:0:120:A:N3	2.35	0.42
1:0:1044:C:H5''	39:0:9648:HOH:O	2.19	0.42
17:O:77:ALA:HA	17:O:96:VAL:O	2.20	0.42
1:0:1099:G:H2'	1:0:1100:G:O4'	2.20	0.42
30:2:35:ARG:HG2	39:2:6391:HOH:O	2.19	0.42
1:0:2568:A:H2'	1:0:2569:A:O4'	2.20	0.42
13:K:27:ARG:HD2	39:K:4747:HOH:O	2.18	0.42
1:0:23:G:C6	1:0:24:G:N1	2.88	0.42
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.49	0.42
6:C:236:THR:HG22	6:C:239:ALA:HB2	2.01	0.42
25:W:125:HIS:HE1	39:W:3071:HOH:O	2.02	0.42
1:0:319:A:H4'	1:0:338:C:C5	2.54	0.42
16:N:24:LEU:HD22	39:Q:2847:HOH:O	2.19	0.42
1:0:960:G:N3	1:0:960:G:C2'	2.82	0.42
1:0:1328:A:C8	27:Y:169:ARG:HD3	2.54	0.42
15:M:82:ARG:O	15:M:84:LYS:N	2.52	0.42
1:0:440:C:H2'	1:0:441:A:C8	2.55	0.42
1:0:1236:A:H2'	1:0:1237:U:O4'	2.19	0.42
1:0:371:U:H2'	1:0:372:A:C8	2.55	0.42
32:I:80:LYS:HD3	32:I:86:GLU:O	2.20	0.42
1:0:27:U:H2'	1:0:28:G:O4'	2.20	0.42
1:0:697:G:H4'	1:0:730:G:O3'	2.19	0.42
26:X:54:ILE:HD11	26:X:85:VAL:HG12	2.02	0.42
39:0:3171:HOH:O	25:W:119:HIS:HE1	2.03	0.42
6:C:136:VAL:HG22	6:C:137:PRO:HA	2.01	0.42
27:Y:96:GLU:O	27:Y:235:GLU:HA	2.20	0.42
7:D:76:ARG:O	7:D:77:ASP:HB2	2.20	0.42
11:H:28:ILE:HG21	11:H:31:HIS:CE1	2.54	0.42
1:0:1168:C:H4'	39:I:5128:HOH:O	2.19	0.42
31:3:17:HIS:O	31:3:18:GLN:HG3	2.20	0.42
6:C:7:ASP:OD1	6:C:11:ASN:HB2	2.20	0.42
39:0:4983:HOH:O	4:A:11:ARG:CZ	2.68	0.42
12:J:143:LYS:HG3	12:J:145:TRP:CE2	2.55	0.42
1:0:1289:C:H3'	39:0:6930:HOH:O	2.20	0.42
1:0:2072:G:C6	1:0:2533:C:H1'	2.55	0.42
2:9:3014:G:C2'	16:N:1:ALA:HB2	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1878:G:O2'	1:0:1879:U:C5	2.66	0.42
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.55	0.42
1:0:2820:A:OP1	5:B:98:THR:HG22	2.20	0.42
1:0:1131:G:C6	1:0:1230:A:C4	3.08	0.42
19:Q:64:GLU:HG3	19:Q:74:ASP:CG	2.40	0.42
1:0:65:C:O2'	1:0:66:G:H5'	2.19	0.42
1:0:1081:A:H5''	39:0:3751:HOH:O	2.19	0.42
31:3:91:GLN:O	31:3:92:GLU:HB2	2.19	0.42
1:0:2133:U:H4'	1:0:2134:G:H5'	2.01	0.42
6:C:165:ASP:O	6:C:168:ARG:HB3	2.20	0.42
24:V:11:MET:HB3	24:V:15:GLU:HB2	2.00	0.42
1:0:1181:A:H2'	1:0:1182:C:H5'	2.02	0.42
12:J:19:MET:CE	12:J:132:LEU:HD21	2.48	0.42
4:A:34:ASP:OD1	4:A:35:GLY:N	2.38	0.42
4:A:36:ASP:HB2	4:A:83:GLY:HA3	2.02	0.42
14:L:69:ILE:HA	39:L:9478:HOH:O	2.20	0.42
1:0:2329:C:O2'	1:0:2330:U:H5'	2.20	0.42
25:W:41:TYR:CD2	25:W:44:MET:HE3	2.55	0.42
39:0:4845:HOH:O	19:Q:55:ARG:HD2	2.19	0.42
1:0:1714:C:O2'	1:0:1715:C:H5'	2.20	0.42
2:9:3006:C:H4'	16:N:35:VAL:HG11	2.02	0.42
6:C:123:LEU:HD23	6:C:123:LEU:HA	1.83	0.42
24:V:12:THR:HG23	24:V:14:ALA:H	1.84	0.41
25:W:122:ARG:CG	25:W:152:ALA:O	2.68	0.41
1:0:1180:U:O2'	32:I:92:PRO:HD2	2.20	0.41
29:1:10:LYS:N	39:1:9488:HOH:O	2.42	0.41
12:J:130:VAL:HG12	12:J:131:THR:N	2.35	0.41
7:D:173:GLU:O	7:D:174:VAL:C	2.59	0.41
1:0:2908:A:C2'	1:0:2909:G:H5'	2.49	0.41
1:0:2587:OMU:H6	1:0:2587:OMU:O5'	2.20	0.41
6:C:7:ASP:OD2	6:C:9:ASP:HB2	2.21	0.41
1:0:1495:C:H2'	1:0:1496:G:C8	2.54	0.41
4:A:76:VAL:HG23	28:Z:63:LYS:HB3	2.01	0.41
1:0:1311:G:O6	6:C:173:LYS:HE3	2.20	0.41
17:O:45:LEU:CD1	17:O:88:LYS:HD2	2.50	0.41
19:Q:53:HIS:HA	19:Q:54:PRO:HD3	1.95	0.41
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.78	0.41
1:0:2112:A:H2'	1:0:2113:G:C8	2.55	0.41
1:0:2672:C:O2'	1:0:2673:U:H5'	2.20	0.41
19:Q:30:VAL:O	19:Q:30:VAL:HG12	2.19	0.41
11:H:40:ALA:HB1	11:H:137:TYR:CD2	2.55	0.41
1:0:1202:A:H2'	1:0:1203:G:O4'	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:F:72:VAL:HA	9:F:73:PRO:HD3	1.90	0.41
11:H:26:SER:HA	11:H:59:HIS:CD2	2.55	0.41
22:T:21:LYS:HA	22:T:24:ARG:HG3	2.02	0.41
5:B:254:GLN:HG2	5:B:255:GLY:H	1.81	0.41
26:X:20:GLU:CD	26:X:21:PRO:HD2	2.40	0.41
8:E:91:PHE:HA	8:E:92:PRO:HD3	1.87	0.41
6:C:184:ARG:HB3	39:C:9169:HOH:O	2.19	0.41
11:H:70:ASN:O	11:H:74:ILE:HG13	2.20	0.41
13:K:75:ARG:HD3	13:K:112:PRO:O	2.21	0.41
2:9:3018:U:H2'	2:9:3019:G:H8	1.85	0.41
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.49	0.41
25:W:65:VAL:CG1	25:W:116:LEU:HD13	2.50	0.41
1:0:664:U:O4	1:0:681:G:H5''	2.20	0.41
9:F:49:PHE:CD1	9:F:49:PHE:N	2.88	0.41
1:0:2089:A:O2'	1:0:2090:G:H5'	2.19	0.41
12:J:71:TYR:CG	12:J:72:PRO:HD2	2.55	0.41
11:H:99:LYS:HD3	11:H:119:LYS:HD3	2.01	0.41
1:0:764:C:H2'	1:0:765:G:O4'	2.20	0.41
30:2:5:LYS:O	30:2:9:LYS:HG3	2.20	0.41
17:O:87:THR:O	17:O:91:GLN:HG3	2.19	0.41
1:0:517:U:H1'	39:0:8135:HOH:O	2.20	0.41
1:0:2388:C:H5'	19:Q:83:THR:O	2.20	0.41
1:0:2427:C:OP2	31:3:84:ARG:HD2	2.18	0.41
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.20	0.41
1:0:2715:G:N2	5:B:264:GLU:OE1	2.53	0.41
1:0:559:U:H5'	1:0:559:U:C6	2.41	0.41
20:R:25:PHE:CE2	20:R:29:LYS:CE	2.99	0.41
32:I:139:ILE:C	32:I:140:GLU:HG3	2.40	0.41
14:L:80:ASP:HB3	14:L:90:ARG:HB3	2.02	0.41
1:0:1838:U:H1'	1:0:2644:C:O4'	2.21	0.41
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.48	0.41
1:0:1164:U:OP1	32:I:74:PRO:HA	2.20	0.41
1:0:2326:U:H4'	1:0:2412:G:C4'	2.50	0.41
1:0:2067:A:H2'	1:0:2068:G:O4'	2.20	0.41
18:P:141:ILE:C	18:P:143:ALA:H	2.22	0.41
1:0:907:A:H2'	1:0:908:A:C8	2.55	0.41
13:K:80:ILE:O	13:K:87:ARG:HA	2.20	0.41
1:0:1119:G:H2'	12:J:52:GLN:NE2	2.35	0.41
16:N:37:ARG:CZ	16:N:105:GLY:HA3	2.51	0.41
6:C:30:LEU:HA	6:C:30:LEU:HD23	1.90	0.41
5:B:62:ARG:CB	5:B:65:MET:HE3	2.50	0.41
32:I:75:THR:HA	32:I:112:LYS:HZ3	1.86	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2032:U:H2'	1:0:2033:G:H5'	2.01	0.41
1:0:926:A:H5'	14:L:39:GLU:OE2	2.20	0.41
1:0:1342:C:C2'	1:0:1343:C:H5'	2.50	0.41
2:9:3052:A:O2'	2:9:3053:G:H5'	2.20	0.41
1:0:612:U:H2'	1:0:613:C:C6	2.56	0.41
1:0:1759:A:N3	1:0:1818:C:H2'	2.35	0.41
20:R:106:GLY:HA2	20:R:109:MET:CE	2.46	0.41
32:I:132:CYS:C	32:I:134:SER:N	2.74	0.41
1:0:1189:A:H1'	1:0:1209:C:H1'	2.02	0.41
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.21	0.41
29:1:18:LYS:CB	30:2:49:GLU:HG2	2.47	0.41
1:0:710:G:H5'	17:O:25:VAL:HG13	2.03	0.41
4:A:66:ARG:HH11	4:A:66:ARG:CB	2.30	0.41
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.48	0.41
4:A:135:VAL:HG21	4:A:147:ARG:HG2	2.02	0.41
17:O:97:SER:H	17:O:100:GLN:NE2	2.18	0.41
1:0:821:U:H2'	1:0:822:C:C6	2.56	0.41
9:F:31:LYS:HE3	39:F:2623:HOH:O	2.20	0.41
30:2:44:ARG:HA	30:2:44:ARG:HD3	1.78	0.41
5:B:146:THR:O	5:B:159:PRO:HB3	2.21	0.41
1:0:500:G:O2'	20:R:94:ASN:ND2	2.54	0.41
5:B:294:TYR:C	5:B:294:TYR:CD1	2.93	0.41
1:0:2326:U:H4'	1:0:2412:G:H4'	2.03	0.41
1:0:816:G:H5'	1:0:1598:A:H4'	2.02	0.41
25:W:146:ILE:HA	25:W:146:ILE:HD13	1.88	0.41
1:0:1603:A:C5'	1:0:1605:G:H5'	2.50	0.41
13:K:107:THR:HG22	13:K:108:GLU:CG	2.43	0.41
9:F:28:ALA:HB3	9:F:99:THR:O	2.20	0.41
27:Y:187:VAL:HB	27:Y:203:VAL:HG22	2.02	0.41
20:R:39:THR:CG2	20:R:107:GLU:O	2.68	0.41
4:A:66:ARG:CB	4:A:66:ARG:NH1	2.84	0.41
22:T:75:GLU:O	22:T:76:ASP:HB2	2.21	0.41
1:0:1573:A:H2'	1:0:1574:C:O4'	2.21	0.41
1:0:671:A:O2'	1:0:672:G:H2'	2.21	0.41
18:P:63:ARG:NH2	39:P:191:HOH:O	2.54	0.41
1:0:1226:G:H5'	39:O:5101:HOH:O	2.20	0.41
1:0:565:A:OP2	1:0:592:G:N1	2.48	0.41
5:B:150:ALA:O	5:B:152:PRO:HD3	2.21	0.41
1:0:2314:G:C2'	1:0:2315:C:H5'	2.51	0.41
1:0:2717:C:H5'	5:B:302:PRO:HA	2.02	0.41
7:D:44:ILE:HG23	7:D:45:THR:HG23	2.03	0.41
4:A:206:ARG:N	4:A:206:ARG:HD3	2.23	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1119:G:N2	1:0:1246:A:H2	2.09	0.41
1:0:1739:G:H1'	1:0:2726:U:O4	2.20	0.41
1:0:797:A:O4'	28:Z:10:ARG:N	2.54	0.41
1:0:2578:G:H5'	1:0:2578:G:C8	2.45	0.41
1:0:2361:A:H2'	1:0:2362:A:C8	2.55	0.41
1:0:2503:A:OP1	11:H:151:ARG:NH2	2.49	0.41
5:B:271:ASP:HB3	5:B:296:LEU:HD12	2.03	0.41
18:P:16:VAL:CG1	18:P:20:ARG:CZ	2.99	0.41
23:U:44:ARG:HB3	39:U:3805:HOH:O	2.20	0.41
5:B:260:HIS:HE1	39:B:9585:HOH:O	2.03	0.41
1:0:1940:C:H4'	39:0:7828:HOH:O	2.19	0.41
1:0:1132:A:H2'	1:0:1133:A:C8	2.56	0.41
5:B:49:THR:HG21	5:B:280:VAL:HG23	2.03	0.41
5:B:277:GLU:N	5:B:278:PRO:CD	2.84	0.41
14:L:89:PHE:N	39:L:9468:HOH:O	2.54	0.41
1:0:123:U:O2'	1:0:124:C:H5'	2.20	0.41
1:0:1849:G:H1'	1:0:2011:A:N1	2.35	0.41
17:O:45:LEU:HD12	17:O:88:LYS:HD2	2.02	0.41
1:0:1659:A:H2'	1:0:1660:G:O4'	2.19	0.41
1:0:1768:C:H2'	1:0:1769:C:O4'	2.20	0.41
4:A:43:VAL:HG21	4:A:59:GLU:HG3	2.03	0.41
1:0:177:A:H2'	1:0:178:U:O4'	2.21	0.41
1:0:2481:G:H5''	39:0:5116:HOH:O	2.20	0.41
1:0:2103:A:N3	1:0:2103:A:H2'	2.35	0.41
1:0:750:A:O3'	6:C:101:ASP:HB2	2.21	0.41
39:0:8066:HOH:O	15:M:91:ILE:HG12	2.21	0.41
1:0:2053:G:H4'	20:R:136:TRP:CE2	2.56	0.41
22:T:88:PRO:HB3	39:T:6320:HOH:O	2.20	0.41
1:0:2435:U:H1'	39:0:5981:HOH:O	2.21	0.41
1:0:887:G:H2'	1:0:888:U:C6	2.55	0.41
20:R:4:TYR:CZ	20:R:15:LYS:HB3	2.55	0.41
28:Z:39:CYS:SG	28:Z:41:ASN:HB3	2.60	0.41
4:A:6:GLY:HA3	39:A:9550:HOH:O	2.20	0.41
1:0:2506:A:O2'	1:0:2507:G:P	2.78	0.41
1:0:289:G:N1	1:0:363:A:C2	2.83	0.41
1:0:1166:A:H1'	1:0:1192:A:N3	2.36	0.41
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.21	0.41
27:Y:189:ASN:ND2	27:Y:189:ASN:C	2.73	0.41
15:M:73:ARG:HG3	39:M:9411:HOH:O	2.21	0.41
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.56	0.41
4:A:122:SER:O	4:A:124:VAL:HG13	2.21	0.41
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2061:C:C2'	1:0:2062:A:H5'	2.51	0.41
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.54	0.41
8:E:5:LEU:HD21	8:E:66:GLN:HG3	2.03	0.41
1:0:1065:G:H5'	39:0:4141:HOH:O	2.20	0.41
7:D:105:SER:HA	7:D:130:VAL:O	2.21	0.41
1:0:162:C:H2'	1:0:163:U:H5'	2.02	0.41
2:9:3095:C:O2'	2:9:3096:C:H5'	2.21	0.41
21:S:8:PRO:HD2	24:V:32:ALA:HA	2.04	0.41
17:O:23:GLY:C	39:O:3062:HOH:O	2.59	0.41
7:D:12:GLU:O	7:D:15:GLU:HG2	2.21	0.41
1:0:262:A:OP2	9:F:91:VAL:HG11	2.21	0.40
5:B:217:ARG:HG3	5:B:257:THR:CG2	2.51	0.40
9:F:32:GLY:N	39:F:3111:HOH:O	2.54	0.40
24:V:39:ALA:C	24:V:41:GLU:N	2.71	0.40
4:A:123:GLY:HA3	4:A:162:GLY:CA	2.49	0.40
17:O:98:LEU:O	17:O:102:ILE:HG13	2.21	0.40
1:0:1149:U:H5''	1:0:1151:G:O4'	2.21	0.40
4:A:164:ARG:HB2	28:Z:68:SER:OG	2.21	0.40
1:0:2791:U:H1'	1:0:2792:A:H5''	2.03	0.40
39:0:5961:HOH:O	14:L:34:GLY:HA2	2.20	0.40
7:D:88:LEU:N	7:D:89:PRO:CD	2.84	0.40
1:0:2856:A:OP1	26:X:15:ARG:NH2	2.52	0.40
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.21	0.40
28:Z:11:SER:O	28:Z:14:PHE:HB2	2.21	0.40
6:C:5:ILE:HG13	6:C:15:GLU:HA	2.03	0.40
5:B:174:ARG:HA	5:B:177:HIS:HB3	2.02	0.40
30:2:41:HIS:HD2	30:2:44:ARG:H	1.69	0.40
4:A:65:ARG:NH1	4:A:65:ARG:HG2	2.36	0.40
5:B:85:ARG:HB2	5:B:99:GLU:HG2	2.03	0.40
27:Y:112:GLU:OE1	27:Y:112:GLU:HA	2.21	0.40
18:P:16:VAL:CG1	18:P:17:GLY:N	2.83	0.40
11:H:47:ILE:HD12	11:H:146:VAL:HG13	2.03	0.40
1:0:920:C:H5'	1:0:921:G:C4	2.56	0.40
1:0:64:G:H2'	1:0:65:C:O4'	2.21	0.40
1:0:2793:A:H2'	1:0:2794:G:H5'	2.03	0.40
1:0:790:A:H1'	1:0:1710:A:H2'	2.03	0.40
12:J:12:VAL:HG21	12:J:116:LEU:HD11	2.03	0.40
27:Y:216:ARG:HD2	39:Y:9370:HOH:O	2.20	0.40
31:3:70:ARG:HG2	31:3:70:ARG:HH11	1.86	0.40
5:B:331:SER:OG	23:U:14:GLU:OE2	2.33	0.40
1:0:484:A:N1	1:0:506:G:H4'	2.36	0.40
1:0:797:A:H5'	28:Z:10:ARG:N	2.36	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:194:PHE:CD2	6:C:234:VAL:CG1	3.01	0.40
6:C:234:VAL:HG13	6:C:234:VAL:O	2.21	0.40
1:0:2361:A:H8	1:0:2361:A:H5'	1.86	0.40
15:M:183:THR:CG2	15:M:194:ALA:HB1	2.50	0.40
16:N:182:GLY:O	16:N:183:ASP:C	2.60	0.40
26:X:12:ILE:HD12	26:X:36:HIS:CG	2.56	0.40
1:0:2868:C:H2'	1:0:2869:G:O4'	2.22	0.40
1:0:1937:U:O2'	1:0:1938:G:H5'	2.21	0.40
1:0:2379:G:N3	1:0:2418:G:H2'	2.36	0.40
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.03	0.40
1:0:2401:A:H2'	1:0:2402:A:C8	2.57	0.40
1:0:2780:C:H1'	8:E:143:GLN:NE2	2.33	0.40
23:U:52:THR:HG21	23:U:54:THR:HB	2.03	0.40
7:D:36:ASN:HA	39:D:7500:HOH:O	2.22	0.40
1:0:2568:A:C2'	1:0:2569:A:H5'	2.51	0.40
30:2:20:ARG:HD2	30:2:39:ARG:HH21	1.85	0.40
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.57	0.40
9:F:79:GLN:HB2	9:F:82:ASP:OD2	2.22	0.40
27:Y:152:LYS:HB3	27:Y:160:LYS:HG3	2.03	0.40
1:0:2611:G:H5'	1:0:2613:G:C8	2.57	0.40
11:H:69:ALA:HB2	11:H:153:ALA:HB2	2.04	0.40
1:0:295:C:H2'	1:0:296:G:O4'	2.21	0.40
1:0:297:U:H1'	39:0:4518:HOH:O	2.21	0.40
5:B:274:GLU:HA	5:B:292:GLY:O	2.21	0.40
1:0:2754:G:H2'	1:0:2755:G:O4'	2.22	0.40
2:9:3012:C:H5'	2:9:3070:U:O4'	2.22	0.40
1:0:622:G:O2'	1:0:623:U:H5'	2.20	0.40
16:N:23:ARG:HD2	39:N:9357:HOH:O	2.20	0.40
1:0:1838:U:H1'	1:0:2644:C:H5'	2.04	0.40
1:0:2756:U:O2	1:0:2896:A:H2	2.05	0.40
5:B:10:SER:O	5:B:16:ARG:NH1	2.52	0.40
1:0:1819:G:H2'	1:0:1820:G:C4'	2.51	0.40
4:A:149:ASP:OD1	4:A:151:GLN:HB2	2.22	0.40
6:C:72:LYS:HG2	6:C:77:ALA:HA	2.03	0.40
1:0:1795:G:H2'	1:0:1796:A:O4'	2.22	0.40
1:0:1797:A:H2'	1:0:1799:G:O5'	2.21	0.40
1:0:1185:U:H2'	1:0:1186:C:C6	2.56	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%)	209 (89%)	23 (10%)	3 (1%)	18	17
5	B	335/338 (99%)	314 (94%)	17 (5%)	4 (1%)	19	19
6	C	244/246 (99%)	229 (94%)	15 (6%)	0	100	100
7	D	134/177 (76%)	105 (78%)	17 (13%)	12 (9%)	1	0
8	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
9	F	117/120 (98%)	100 (86%)	15 (13%)	2 (2%)	14	11
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	140 (90%)	14 (9%)	2 (1%)	18	17
12	J	140/145 (97%)	131 (94%)	6 (4%)	3 (2%)	11	8
13	K	130/132 (98%)	123 (95%)	7 (5%)	0	100	100
14	L	141/165 (86%)	118 (84%)	22 (16%)	1 (1%)	30	34
15	M	192/195 (98%)	182 (95%)	8 (4%)	2 (1%)	22	23
16	N	184/187 (98%)	163 (89%)	12 (6%)	9 (5%)	3	1
17	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
18	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
19	Q	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
21	S	79/85 (93%)	76 (96%)	2 (2%)	1 (1%)	18	17
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	25	26
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	59 (94%)	3 (5%)	1 (2%)	14	12
25	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
26	X	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
28	Z	71/83 (86%)	61 (86%)	7 (10%)	3 (4%)	4	2
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	88 (98%)	1 (1%)	1 (1%)	21	21
32	I	68/162 (42%)	55 (81%)	12 (18%)	1 (2%)	15	13
All	All	3705/4431 (84%)	3430 (93%)	229 (6%)	46 (1%)	19	19

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	27	LEU
4	A	37	VAL
5	B	139	ASP
7	D	137	PRO
9	F	101	ALA
11	H	166	SER
11	H	168	ALA
14	L	80	ASP
16	N	154	LEU
16	N	184	ILE
28	Z	81	ARG
4	A	34	ASP
7	D	27	ILE
7	D	60	GLU
7	D	171	ASP
12	J	143	LYS
15	M	83	SER
16	N	162	ASP
16	N	183	ASP
22	T	53	GLY
24	V	43	PRO
7	D	28	GLY
7	D	56	ARG
7	D	61	PHE
12	J	5	GLU
16	N	155	GLU
16	N	164	ASP
28	Z	20	ARG
31	3	56	PRO
5	B	185	GLY
7	D	97	GLN
7	D	164	ALA
9	F	71	GLY

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Mol	Chain	Res	Type
12	J	65	ASN
16	N	68	GLU
16	N	167	ASP
32	I	76	ALA
5	B	34	GLY
7	D	138	GLY
21	S	46	ASP
5	B	182	VAL
7	D	69	ILE
28	Z	21	VAL
16	N	161	GLY
7	D	16	PRO
15	M	88	VAL

### 5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/182 (98%)	169 (94%)	10 (6%)	30	38
5	B	282/283 (100%)	261 (93%)	21 (7%)	20	24
6	C	193/193 (100%)	178 (92%)	15 (8%)	18	22
7	D	117/148 (79%)	112 (96%)	5 (4%)	40	52
8	E	152/156 (97%)	145 (95%)	7 (5%)	37	48
9	F	93/94 (99%)	91 (98%)	2 (2%)	64	81
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	126 (96%)	6 (4%)	38	50
12	J	118/121 (98%)	109 (92%)	9 (8%)	19	22
13	K	106/106 (100%)	103 (97%)	3 (3%)	56	73
14	L	113/127 (89%)	109 (96%)	4 (4%)	48	63
15	M	158/159 (99%)	153 (97%)	5 (3%)	51	67
16	N	149/150 (99%)	144 (97%)	5 (3%)	49	64
17	O	93/94 (99%)	91 (98%)	2 (2%)	64	81
18	P	113/117 (97%)	112 (99%)	1 (1%)	87	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	Q	79/80 (99%)	75 (95%)	4 (5%)	33	43
20	R	117/122 (96%)	114 (97%)	3 (3%)	59	76
21	S	71/74 (96%)	69 (97%)	2 (3%)	56	73
22	T	105/106 (99%)	101 (96%)	4 (4%)	44	59
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	68	84
25	W	130/130 (100%)	126 (97%)	4 (3%)	52	68
26	X	66/74 (89%)	60 (91%)	6 (9%)	14	15
27	Y	120/196 (61%)	110 (92%)	10 (8%)	16	19
28	Z	60/68 (88%)	59 (98%)	1 (2%)	73	87
29	1	46/47 (98%)	45 (98%)	1 (2%)	64	81
30	2	42/46 (91%)	41 (98%)	1 (2%)	61	79
31	3	79/79 (100%)	78 (99%)	1 (1%)	80	91
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2960 (96%)	133 (4%)	40	52

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

Mol	Chain	Res	Type
4	A	3	ARG
4	A	33	GLU
4	A	36	ASP
4	A	94	LEU
4	A	131	HIS
4	A	153	ARG
4	A	165	THR
4	A	179	MET
4	A	206	ARG
4	A	217	ARG
5	B	11	LEU
5	B	27	ASN
5	B	51	VAL
5	B	53	LEU
5	B	71	VAL
5	B	82	VAL
5	B	98	THR
5	B	113	LEU

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Mol	Chain	Res	Type
5	B	149	ASP
5	B	162	MET
5	B	175	LEU
5	B	190	MET
5	B	234	ARG
5	B	251	VAL
5	B	254	GLN
5	B	257	THR
5	B	265	LEU
5	B	277	GLU
5	B	280	VAL
5	B	307	ARG
5	B	312	ARG
6	C	2	GLN
6	C	27	ARG
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	101	ASP
6	C	136	VAL
6	C	162	VAL
6	C	187	ARG
6	C	214	THR
6	C	222	ASP
6	C	223	LEU
6	C	236	THR
6	C	240	LEU
6	C	243	VAL
7	D	24	HIS
7	D	50	VAL
7	D	61	PHE
7	D	133	ASN
7	D	137	PRO
8	E	3	VAL
8	E	7	ILE
8	E	102	VAL
8	E	108	LEU
8	E	155	ASN
8	E	156	ASP
8	E	164	ASP
9	F	12	LEU
9	F	46	GLU

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Mol	Chain	Res	Type
11	H	1	LYS
11	H	18	GLU
11	H	84	LYS
11	H	88	ARG
11	H	154	TYR
11	H	170	ASN
12	J	45	VAL
12	J	52	GLN
12	J	70	PHE
12	J	74	ARG
12	J	79	PHE
12	J	107	ASN
12	J	117	ASP
12	J	127	ILE
12	J	131	THR
13	K	4	LEU
13	K	10	GLN
13	K	84	ASP
14	L	35	ARG
14	L	43	HIS
14	L	89	PHE
14	L	102	ASP
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
16	N	26	LEU
16	N	37	ARG
16	N	49	THR
16	N	65	ASP
16	N	139	TRP
17	O	3	THR
17	O	96	VAL
18	P	98	ILE
19	Q	16	ASN
19	Q	18	PRO
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR
20	R	82	GLU
20	R	132	ARG

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Mol	Chain	Res	Type
21	S	3	ASP
21	S	71	ASP
22	T	39	ASN
22	T	48	VAL
22	T	89	ARG
22	T	96	VAL
24	V	65	ASP
25	W	26	ILE
25	W	35	VAL
25	W	122	ARG
25	W	146	ILE
26	X	8	ARG
26	X	15	ARG
26	X	44	ASP
26	X	72	VAL
26	X	79	GLU
26	X	82	GLU
27	Y	103	THR
27	Y	141	THR
27	Y	144	ARG
27	Y	154	ARG
27	Y	163	THR
27	Y	189	ASN
27	Y	200	THR
27	Y	204	ARG
27	Y	220	GLU
27	Y	235	GLU
28	Z	44	GLU
29	1	47	ASP
30	2	18	ASN
31	3	56	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	199	HIS
5	B	2	GLN
5	B	27	ASN
5	B	145	HIS
5	B	191	ASN
5	B	221	GLN
5	B	238	ASN

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Mol	Chain	Res	Type
5	B	256	GLN
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	129	HIS
7	D	103	ASN
7	D	133	ASN
8	E	90	HIS
8	E	106	ASN
8	E	119	HIS
8	E	143	GLN
10	G	64	ASN
11	H	31	HIS
11	H	56	GLN
11	H	59	HIS
11	H	170	ASN
12	J	25	GLN
12	J	52	GLN
12	J	107	ASN
12	J	126	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
14	L	43	HIS
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	77	HIS
15	M	137	ASN
15	M	143	ASN
15	M	170	ASN
16	N	93	GLN
16	N	107	ASN
16	N	153	GLN
17	O	53	GLN
17	O	100	GLN
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS

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Mol	Chain	Res	Type
18	P	88	GLN
18	P	89	ASN
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
21	S	53	ASN
22	T	37	GLN
22	T	39	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	60	GLN
25	W	12	ASN
25	W	28	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	22	ASN
26	X	23	HIS
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	30	GLN
31	3	48	ASN
32	I	93	GLN
32	I	104	GLN
32	I	113	HIS

## 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	238 (8%)	33 (1%)
2	9	121/122 (99%)	16 (13%)	2 (1%)
3	4	1/5 (20%)	0	0
All	All	2867/3049 (94%)	254 (8%)	35 (1%)

All (254) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	219	G
1	0	237	G
1	0	249	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G

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Mol	Chain	Res	Type
1	0	397	A
1	0	417	G
1	0	457	U
1	0	461	C
1	0	473	A
1	0	487	G
1	0	498	A
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	735	C
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	875	A
1	0	877	G
1	0	878	G
1	0	905	C
1	0	920	C
1	0	921	G

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Mol	Chain	Res	Type
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1100	G
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1409	G

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Mol	Chain	Res	Type
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1562	C
1	0	1564	C
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1732	A
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1873	G
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1967	U
1	0	1971	G
1	0	1973	A
1	0	1979	G

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Mol	Chain	Res	Type
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2536	C
1	0	2537	G
1	0	2541	U

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Mol	Chain	Res	Type
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2611	G
1	0	2613	G
1	0	2634	G
1	0	2644	C
1	0	2645	U
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2783	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2852	A
1	0	2853	U
1	0	2867	G
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U

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Mol	Chain	Res	Type
2	9	3024	U
2	9	3025	G
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (35) 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	1232	A
1	0	1237	U
1	0	1246	A
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	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C

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Mol	Chain	Res	Type
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	3055	U
2	9	3065	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	OMU	0	2587	1	20,22,23	0.74	1 (5%)	24,31,34	0.78	0
1	OMG	0	2588	1,3	24,26,27	0.80	0	32,38,41	5.21	3 (9%)
1	UR3	0	2619	1	20,22,23	0.82	0	23,32,35	0.78	0
1	PSU	0	2621	1	19,21,22	1.19	2 (10%)	23,30,33	1.07	2 (8%)
1	1MA	0	628	1,35	23,25,26	0.80	0	32,37,40	0.96	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,35	-	1/8/25/26	0/1/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	3.23	1.43	1.37
1	0	2621	PSU	C6-N1	2.52	1.34	1.32
1	0	2587	OMU	P-OP1	2.31	1.49	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	C6-C5-N7	-28.90	130.25	134.14
1	0	2588	OMG	C6-N1-C2	3.18	125.08	119.51
1	0	628	1MA	C2-N3-C4	-3.16	110.83	116.23
1	0	2621	PSU	C5-C4-N3	-2.31	114.65	118.86
1	0	2588	OMG	C2-N3-C4	-2.22	111.98	115.09
1	0	2621	PSU	C5-C1'-C2'	-2.12	111.87	115.61

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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%)	-0.06	94 (3%) 43 53	22, 45, 89, 149	0
2	9	122/122 (100%)	0.21	5 (4%) 35 46	38, 63, 87, 149	0
3	4	5/5 (100%)	1.39	1 (20%) 2 3	61, 64, 72, 74	0
4	A	237/240 (98%)	0.50	20 (8%) 11 17	28, 50, 82, 104	0
5	B	337/338 (99%)	0.28	11 (3%) 44 54	28, 50, 75, 86	0
6	C	246/246 (100%)	0.10	4 (1%) 68 77	25, 46, 68, 80	0
7	D	140/177 (79%)	2.05	58 (41%) 1 1	58, 88, 120, 130	0
8	E	172/178 (96%)	0.96	30 (17%) 2 4	40, 62, 80, 86	0
9	F	119/120 (99%)	1.40	37 (31%) 1 1	44, 71, 100, 110	0
10	G	29/348 (8%)	2.51	18 (62%) 0 0	71, 89, 99, 100	0
11	H	160/171 (93%)	0.82	24 (15%) 3 5	43, 61, 93, 101	0
12	J	142/145 (97%)	0.17	4 (2%) 50 60	36, 47, 67, 89	0
13	K	132/132 (100%)	-0.08	1 (0%) 83 90	33, 46, 67, 72	0
14	L	145/165 (87%)	0.91	29 (20%) 2 3	27, 64, 110, 120	0
15	M	194/195 (99%)	0.58	22 (11%) 6 9	31, 44, 77, 87	0
16	N	186/187 (99%)	1.15	42 (22%) 1 2	43, 63, 108, 113	0
17	O	115/116 (99%)	0.19	3 (2%) 53 63	39, 53, 67, 75	0
18	P	143/149 (95%)	0.26	5 (3%) 42 52	38, 51, 65, 76	0
19	Q	95/96 (98%)	0.22	6 (6%) 19 28	38, 47, 61, 76	0
20	R	150/155 (96%)	0.02	3 (2%) 62 72	29, 43, 61, 71	0
21	S	81/85 (95%)	0.45	7 (8%) 11 17	42, 58, 80, 95	0
22	T	119/120 (99%)	0.68	10 (8%) 11 17	40, 54, 81, 110	0
23	U	53/66 (80%)	0.32	5 (9%) 9 14	40, 50, 68, 79	0
24	V	65/71 (91%)	2.01	20 (30%) 1 1	52, 76, 110, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	0.14	2 (1%) 74 82	37, 49, 69, 78	0
26	X	82/92 (89%)	0.73	8 (9%) 8 13	40, 53, 82, 101	0
27	Y	142/241 (58%)	0.26	11 (7%) 13 20	29, 42, 63, 85	0
28	Z	73/83 (87%)	0.91	13 (17%) 2 3	48, 70, 85, 92	0
29	1	56/57 (98%)	-0.36	0 100 100	26, 32, 39, 49	0
30	2	46/50 (92%)	0.63	6 (13%) 4 7	33, 51, 67, 80	0
31	3	92/92 (100%)	0.38	4 (4%) 34 44	33, 55, 70, 83	0
32	I	70/162 (43%)	5.95	65 (92%) 0 0	111, 123, 141, 143	0
All	All	6656/7480 (88%)	0.36	568 (8%) 11 17	22, 50, 95, 149	0

All (568) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	16.8
24	V	1	THR	15.1
24	V	39	ALA	14.7
24	V	40	PRO	14.6
7	D	63	ILE	13.9
32	I	133	THR	13.4
32	I	79	ILE	12.3
32	I	88	GLY	12.2
16	N	166	ALA	11.9
7	D	57	THR	11.1
32	I	118	SER	11.0
32	I	76	ALA	10.8
32	I	87	THR	10.6
32	I	116	LEU	10.3
32	I	96	PHE	10.1
32	I	75	THR	9.7
32	I	129	VAL	9.2
32	I	85	PHE	9.0
32	I	121	LEU	8.9
32	I	102	VAL	8.9
15	M	70	GLY	8.8
32	I	113	HIS	8.6
32	I	137	VAL	8.6
30	2	49	GLU	8.6
22	T	119	ALA	8.6
32	I	105	VAL	8.3

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Mol	Chain	Res	Type	RSRZ
32	I	109	ALA	8.2
32	I	132	CYS	8.0
7	D	61	PHE	8.0
7	D	90	LEU	7.9
32	I	125	ALA	7.9
2	9	3001	U	7.8
32	I	81	ASP	7.6
4	A	37	VAL	7.6
4	A	237	GLY	7.5
1	0	282	C	7.4
32	I	107	GLN	7.3
1	0	1951	G	7.3
24	V	38	GLY	7.2
32	I	77	GLU	7.1
1	0	1199	A	7.0
26	X	88	GLU	7.0
32	I	108	ILE	7.0
32	I	89	SER	6.7
32	I	93	GLN	6.7
32	I	111	GLN	6.6
32	I	117	LEU	6.6
15	M	79	ALA	6.4
32	I	104	GLN	6.4
1	0	960	G	6.3
32	I	78	LEU	6.2
32	I	74	PRO	6.2
28	Z	11	SER	6.2
1	0	2637	A	6.0
10	G	27	ILE	5.9
10	G	26	MET	5.8
32	I	124	ALA	5.7
1	0	1948	G	5.7
1	0	497	A	5.6
2	9	3024	U	5.6
32	I	126	LYS	5.6
32	I	86	GLU	5.6
2	9	3002	U	5.6
1	0	285	A	5.6
1	0	999	C	5.5
1	0	1173	A	5.5
32	I	91	GLU	5.5
32	I	97	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
32	I	122	THR	5.4
28	Z	22	SER	5.4
1	0	1172	G	5.4
15	M	71	SER	5.4
9	F	28	ALA	5.3
10	G	23	ILE	5.3
15	M	74	LYS	5.2
1	0	2748	G	5.2
7	D	69	ILE	5.2
7	D	170	TYR	5.2
1	0	2004	U	5.2
21	S	81	ILE	5.1
7	D	44	ILE	5.1
32	I	114	PRO	5.1
9	F	106	ALA	5.0
1	0	514	G	5.0
22	T	118	SER	5.0
22	T	116	ASP	4.9
12	J	70	PHE	4.9
32	I	120	ASP	4.9
1	0	1965	C	4.9
7	D	62	ASP	4.9
24	V	41	GLU	4.9
32	I	98	ALA	4.9
32	I	119	TYR	4.8
7	D	64	ARG	4.8
28	Z	20	ARG	4.8
28	Z	24	ARG	4.8
24	V	37	GLY	4.8
1	0	280	C	4.8
1	0	272	A	4.8
8	E	45	ASP	4.7
26	X	80	GLU	4.7
2	9	3023	U	4.7
11	H	171	ALA	4.7
14	L	106	VAL	4.7
1	0	1177	A	4.7
30	2	35	ARG	4.7
24	V	36	ALA	4.7
8	E	154	ILE	4.7
9	F	110	ASP	4.7
9	F	119	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
7	D	66	GLY	4.6
12	J	4	ALA	4.6
7	D	10	PHE	4.6
32	I	103	ASP	4.5
16	N	95	ALA	4.5
1	0	1200	A	4.5
32	I	123	ASN	4.4
8	E	87	PHE	4.4
7	D	172	VAL	4.4
7	D	92	GLU	4.4
1	0	2238	A	4.4
6	C	61	PHE	4.4
16	N	161	GLY	4.3
27	Y	108	ASP	4.3
7	D	93	LEU	4.3
4	A	35	GLY	4.3
32	I	138	THR	4.3
16	N	163	PHE	4.3
8	E	100	ASP	4.2
9	F	99	THR	4.2
9	F	118	LEU	4.2
1	0	2237	G	4.2
9	F	117	GLU	4.2
7	D	171	ASP	4.2
1	0	10	U	4.2
32	I	134	SER	4.2
1	0	1950	G	4.2
16	N	158	LEU	4.2
14	L	80	ASP	4.2
1	0	2769	C	4.1
1	0	1171	A	4.1
8	E	6	GLU	4.1
21	S	20	PHE	4.1
16	N	165	ALA	4.1
10	G	71	LEU	4.0
16	N	68	GLU	4.0
11	H	74	ILE	4.0
1	0	288	A	4.0
1	0	1525	G	4.0
16	N	147	ILE	4.0
32	I	106	LYS	4.0
7	D	73	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
9	F	108	VAL	4.0
7	D	166	ILE	4.0
23	U	47	ARG	4.0
24	V	43	PRO	4.0
9	F	100	ASP	4.0
16	N	175	LEU	4.0
9	F	16	ALA	3.9
14	L	97	VAL	3.9
11	H	73	LEU	3.9
14	L	75	LEU	3.9
14	L	60	GLU	3.9
16	N	155	GLU	3.9
7	D	18	ILE	3.9
1	0	970	U	3.9
4	A	236	GLY	3.9
7	D	91	ALA	3.9
19	Q	95	GLU	3.9
1	0	2508	C	3.8
9	F	107	ASP	3.8
14	L	82	ALA	3.8
7	D	11	HIS	3.8
7	D	88	LEU	3.8
7	D	27	ILE	3.8
32	I	83	ALA	3.7
8	E	10	ASP	3.7
7	D	173	GLU	3.7
4	A	38	ILE	3.7
27	Y	95	THR	3.7
1	0	1169	U	3.7
14	L	145	LEU	3.7
31	3	41	GLU	3.7
28	Z	21	VAL	3.7
3	4	77	PHE	3.7
28	Z	25	ARG	3.7
16	N	184	ILE	3.7
1	0	2747	C	3.7
27	Y	235	GLU	3.7
9	F	22	VAL	3.7
1	0	1198	U	3.7
2	9	3122	C	3.6
10	G	12	ILE	3.6
32	I	115	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
11	H	78	GLY	3.6
5	B	1	PRO	3.6
1	0	284	C	3.6
14	L	91	VAL	3.6
32	I	72	VAL	3.6
7	D	107	GLY	3.6
16	N	183	ASP	3.6
9	F	98	VAL	3.6
10	G	22	ALA	3.6
11	H	111	ASP	3.6
26	X	85	VAL	3.5
1	0	735	C	3.5
1	0	1192	A	3.5
22	T	115	GLU	3.5
14	L	105	TYR	3.5
16	N	154	LEU	3.5
11	H	83	TYR	3.5
10	G	69	ARG	3.5
15	M	86	GLN	3.5
11	H	143	ALA	3.5
7	D	51	ARG	3.5
8	E	86	VAL	3.5
13	K	132	VAL	3.5
7	D	26	GLY	3.5
6	C	132	ASP	3.5
16	N	181	ASP	3.5
4	A	133	ARG	3.5
8	E	4	GLU	3.5
1	0	969	G	3.4
10	G	24	VAL	3.4
32	I	128	VAL	3.4
14	L	99	GLU	3.4
16	N	185	GLU	3.4
1	0	138	U	3.4
1	0	2103	A	3.4
14	L	81	VAL	3.4
15	M	84	LYS	3.4
7	D	134	LEU	3.4
28	Z	36	ASP	3.4
1	0	2344	G	3.4
14	L	130	ARG	3.4
1	0	1000	C	3.4

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Mol	Chain	Res	Type	RSRZ
11	H	82	ASP	3.4
24	V	63	GLU	3.4
14	L	76	LEU	3.4
19	Q	18	PRO	3.3
4	A	97	ALA	3.3
17	O	22	GLY	3.3
10	G	66	LEU	3.3
24	V	8	ILE	3.3
1	0	716	G	3.3
7	D	23	VAL	3.3
25	W	86	GLU	3.3
1	0	2511	A	3.3
32	I	80	LYS	3.3
21	S	2	TRP	3.3
7	D	154	LYS	3.3
11	H	35	ARG	3.3
8	E	108	LEU	3.3
16	N	180	LEU	3.3
4	A	36	ASP	3.3
11	H	37	GLN	3.2
1	0	2645	U	3.2
7	D	35	ALA	3.2
9	F	49	PHE	3.2
25	W	76	ASP	3.2
15	M	78	LYS	3.2
28	Z	12	GLY	3.2
7	D	56	ARG	3.2
1	0	1202	A	3.2
16	N	159	TYR	3.2
1	0	1168	C	3.2
1	0	1163	G	3.2
7	D	85	GLN	3.2
32	I	112	LYS	3.2
1	0	1966	U	3.2
26	X	7	GLU	3.2
9	F	103	GLU	3.2
32	I	127	GLU	3.2
32	I	99	ASP	3.1
11	H	34	GLY	3.1
4	A	99	ILE	3.1
24	V	59	ILE	3.1
4	A	31	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
19	Q	76	VAL	3.1
1	0	283	U	3.1
1	0	1170	U	3.1
22	T	117	ASP	3.1
15	M	89	THR	3.1
9	F	15	ASP	3.1
26	X	71	ARG	3.1
18	P	108	LEU	3.1
16	N	137	ALA	3.1
32	I	110	GLU	3.1
8	E	128	GLY	3.1
32	I	139	ILE	3.1
15	M	80	GLY	3.0
32	I	84	GLY	3.0
7	D	89	PRO	3.0
9	F	17	LEU	3.0
1	0	1279	U	3.0
1	0	1947	G	3.0
7	D	65	GLU	3.0
7	D	167	GLU	3.0
31	3	92	GLU	3.0
24	V	14	ALA	2.9
1	0	362	G	2.9
22	T	112	LEU	2.9
1	0	281	U	2.9
4	A	82	VAL	2.9
15	M	88	VAL	2.9
24	V	32	ALA	2.9
15	M	75	ARG	2.9
32	I	135	LEU	2.9
1	0	1190	G	2.9
14	L	148	GLU	2.9
8	E	89	SER	2.9
9	F	72	VAL	2.9
27	Y	234	VAL	2.9
16	N	152	GLU	2.9
16	N	182	GLY	2.9
1	0	1189	A	2.9
26	X	10	VAL	2.9
10	G	67	LEU	2.9
16	N	72	GLU	2.8
15	M	83	SER	2.8

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Mol	Chain	Res	Type	RSRZ
27	Y	102	LEU	2.8
1	0	1165	G	2.8
4	A	85	SER	2.8
32	I	136	GLY	2.8
10	G	21	ASP	2.8
16	N	138	ASP	2.8
1	0	1164	U	2.8
1	0	289	G	2.8
28	Z	19	GLY	2.8
32	I	94	GLU	2.8
14	L	79	ASP	2.8
15	M	77	HIS	2.8
8	E	160	ARG	2.8
27	Y	236	VAL	2.8
1	0	1967	U	2.8
1	0	2345	A	2.8
7	D	52	THR	2.8
7	D	104	PHE	2.8
1	0	1929	G	2.8
28	Z	42	CYS	2.8
31	3	62	THR	2.8
7	D	79	MET	2.8
1	0	370	G	2.8
8	E	127	ASP	2.8
24	V	2	VAL	2.8
11	H	138	CYS	2.8
16	N	37	ARG	2.8
28	Z	23	ARG	2.8
8	E	162	PHE	2.7
1	0	1181	A	2.7
30	2	26	MET	2.7
14	L	61	ALA	2.7
16	N	94	GLU	2.7
8	E	99	GLY	2.7
7	D	17	ARG	2.7
24	V	33	VAL	2.7
8	E	5	LEU	2.7
4	A	65	ARG	2.7
14	L	100	ALA	2.7
15	M	81	ARG	2.7
16	N	145	ALA	2.7
27	Y	216	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
11	H	146	VAL	2.7
7	D	81	GLU	2.7
8	E	129	GLU	2.7
9	F	69	GLU	2.7
9	F	25	ASP	2.7
32	I	95	ASP	2.7
10	G	65	THR	2.7
22	T	82	THR	2.7
15	M	87	GLY	2.7
11	H	79	GLU	2.7
32	I	140	GLU	2.7
11	H	140	VAL	2.7
1	0	369	G	2.6
8	E	161	VAL	2.6
30	2	27	LEU	2.6
10	G	15	TRP	2.6
10	G	63	ARG	2.6
14	L	104	ASP	2.6
8	E	126	ILE	2.6
11	H	141	GLU	2.6
7	D	68	PRO	2.6
27	Y	98	GLN	2.6
1	0	1625	U	2.6
15	M	73	ARG	2.6
10	G	25	GLU	2.6
16	N	149	GLU	2.6
1	0	1197	G	2.6
8	E	118	ILE	2.6
10	G	70	ALA	2.6
32	I	82	GLU	2.6
7	D	130	VAL	2.6
8	E	88	TYR	2.6
8	E	98	GLU	2.6
5	B	119	HIS	2.6
14	L	120	LEU	2.6
1	0	1195	G	2.6
16	N	2	THR	2.6
11	H	47	ILE	2.5
1	0	358	G	2.5
7	D	84	LEU	2.5
9	F	115	VAL	2.5
24	V	5	VAL	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
8	E	94	GLN	2.5
1	0	1180	U	2.5
7	D	54	ALA	2.5
1	0	279	C	2.5
8	E	15	GLN	2.5
14	L	150	GLN	2.5
7	D	135	VAL	2.5
16	N	179	LEU	2.5
14	L	147	GLU	2.5
7	D	70	GLY	2.5
7	D	40	ILE	2.5
24	V	6	GLN	2.5
28	Z	18	TYR	2.5
11	H	24	PRO	2.5
1	0	1981	A	2.5
7	D	165	PHE	2.5
28	Z	45	ASP	2.5
32	I	90	GLY	2.5
1	0	372	A	2.5
1	0	1203	G	2.5
31	3	6	ARG	2.5
1	0	717	C	2.5
1	0	804	C	2.5
4	A	64	ASP	2.5
4	A	206	ARG	2.5
16	N	172	PHE	2.4
9	F	14	ASP	2.4
14	L	102	ASP	2.4
14	L	93	VAL	2.4
14	L	141	GLU	2.4
18	P	67	LYS	2.4
1	0	129	A	2.4
9	F	11	ASP	2.4
21	S	70	GLU	2.4
22	T	103	LEU	2.4
8	E	123	ASP	2.4
30	2	20	ARG	2.4
1	0	1949	G	2.4
5	B	57	GLU	2.4
27	Y	96	GLU	2.4
27	Y	106	THR	2.4
16	N	139	TRP	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
22	T	59	GLU	2.4
17	O	1	SER	2.4
32	I	92	PRO	2.4
9	F	21	GLU	2.4
16	N	156	GLU	2.4
1	0	295	C	2.3
14	L	62	ALA	2.3
15	M	194	ALA	2.3
9	F	109	GLU	2.3
15	M	68	ARG	2.3
1	0	805	G	2.3
16	N	134	ASP	2.3
16	N	178	THR	2.3
5	B	2	GLN	2.3
1	0	290	C	2.3
11	H	67	LEU	2.3
22	T	35	TYR	2.3
1	0	128	A	2.3
9	F	75	ILE	2.3
10	G	72	ASP	2.3
15	M	76	ARG	2.3
24	V	3	LEU	2.3
7	D	95	THR	2.3
1	0	1161	A	2.3
9	F	105	ASP	2.3
26	X	44	ASP	2.3
4	A	68	ILE	2.3
9	F	111	ILE	2.3
18	P	18	LYS	2.3
20	R	7	GLU	2.3
21	S	78	ALA	2.3
5	B	108	GLU	2.3
19	Q	81	GLU	2.3
11	H	168	ALA	2.3
16	N	67	ALA	2.3
1	0	1183	C	2.2
12	J	5	GLU	2.2
16	N	160	SER	2.2
24	V	10	ASP	2.2
4	A	209	PRO	2.2
7	D	41	LEU	2.2
9	F	101	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
15	M	164	THR	2.2
4	A	145	MET	2.2
17	O	31	GLU	2.2
9	F	70	LYS	2.2
7	D	106	PHE	2.2
11	H	139	ASN	2.2
19	Q	64	GLU	2.2
9	F	12	LEU	2.2
9	F	60	VAL	2.2
20	R	96	VAL	2.2
15	M	82	ARG	2.2
24	V	46	ILE	2.2
8	E	43	ASP	2.2
5	B	180	ASP	2.2
9	F	18	GLU	2.2
12	J	7	ASP	2.2
16	N	128	ASP	2.2
27	Y	187	VAL	2.2
18	P	141	ILE	2.2
16	N	71	TRP	2.2
30	2	39	ARG	2.2
16	N	167	ASP	2.2
7	D	157	LEU	2.2
9	F	48	VAL	2.2
1	0	809	G	2.2
5	B	133	GLU	2.1
4	A	34	ASP	2.1
16	N	164	ASP	2.1
9	F	44	SER	2.1
14	L	101	ASP	2.1
1	0	1178	G	2.1
5	B	104	GLU	2.1
19	Q	17	LYS	2.1
11	H	166	SER	2.1
7	D	74	THR	2.1
5	B	134	ALA	2.1
9	F	19	ALA	2.1
10	G	64	ASN	2.1
11	H	149	ALA	2.1
15	M	72	ALA	2.1
1	0	1174	A	2.1
8	E	1	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
21	S	72	ASP	2.1
1	0	1523	G	2.1
14	L	142	LEU	2.1
1	0	31	C	2.1
1	0	368	C	2.1
8	E	11	VAL	2.1
8	E	159	VAL	2.1
11	H	70	ASN	2.1
1	0	1964	U	2.1
7	D	45	THR	2.1
23	U	54	THR	2.1
4	A	59	GLU	2.1
8	E	121	ASP	2.1
14	L	123	ASP	2.1
1	0	1878	G	2.1
7	D	77	ASP	2.1
18	P	110	ASP	2.1
7	D	94	ALA	2.1
7	D	75	LEU	2.0
9	F	47	LEU	2.0
26	X	65	ASN	2.0
5	B	117	GLU	2.0
6	C	16	VAL	2.0
1	0	1196	C	2.0
1	0	2644	C	2.0
1	0	373	G	2.0
21	S	1	SER	2.0
14	L	121	ILE	2.0
23	U	4	ARG	2.0
16	N	92	ALA	2.0
16	N	148	ALA	2.0
6	C	135	GLU	2.0
23	U	53	ASP	2.0
23	U	52	THR	2.0
5	B	123	ALA	2.0
20	R	104	PHE	2.0
7	D	67	ASP	2.0
16	N	168	LEU	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	OMU	0	2587	21/22	0.11	-0.02	35,37,38,39	0
1	1MA	0	628	23/24	0.12	-0.64	31,33,36,39	0
1	UR3	0	2619	21/22	0.14	-0.66	42,46,49,51	0
1	PSU	0	2621	20/21	0.11	-1.01	33,36,44,45	0
1	OMG	0	2588	24/25	0.11	-1.24	32,34,38,40	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	1.05	373.00	200,200,200,200	0
37	SR	0	9501	1/1	0.31	77.00	200,200,200,200	0
33	MG	0	8047	1/1	0.47	74.60	94,94,94,94	0
33	MG	0	8092	1/1	1.40	68.87	83,83,83,83	0
35	NA	0	9179	1/1	0.99	66.42	84,84,84,84	0
37	SR	0	9500	1/1	1.60	64.81	200,200,200,200	0
33	MG	0	8085	1/1	0.39	63.89	102,102,102,102	0
33	MG	0	8094	1/1	0.34	62.81	82,82,82,82	0
35	NA	0	9125	1/1	0.90	55.04	106,106,106,106	0
37	SR	0	9539	1/1	0.46	54.19	167,167,167,167	0
35	NA	0	9164	1/1	0.49	53.98	67,67,67,67	0
33	MG	0	8059	1/1	0.32	52.14	60,60,60,60	0
35	NA	0	9106	1/1	0.28	47.88	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
35	NA	0	9111	1/1	0.20	42.21	57,57,57,57	0
35	NA	0	9129	1/1	0.39	41.76	88,88,88,88	0
35	NA	0	9184	1/1	0.46	40.47	86,86,86,86	0
33	MG	0	8025	1/1	0.31	35.75	23,23,23,23	0
35	NA	0	9161	1/1	0.41	32.88	57,57,57,57	0
33	MG	0	8026	1/1	0.16	32.83	26,26,26,26	0
35	NA	0	9122	1/1	0.54	32.34	98,98,98,98	0
35	NA	0	9152	1/1	0.32	26.93	67,67,67,67	0
33	MG	0	8024	1/1	1.07	25.31	90,90,90,90	0
33	MG	0	8082	1/1	0.39	24.74	103,103,103,103	0
37	SR	B	9521	1/1	0.73	23.37	200,200,200,200	0
33	MG	0	8084	1/1	0.42	22.58	109,109,109,109	0
35	NA	0	9107	1/1	0.32	21.71	58,58,58,58	0
35	NA	0	9185	1/1	0.47	21.69	54,54,54,54	0
35	NA	0	9168	1/1	0.23	19.84	72,72,72,72	0
35	NA	0	9162	1/1	0.32	19.80	51,51,51,51	0
35	NA	0	9150	1/1	0.24	18.27	54,54,54,54	0
37	SR	0	9547	1/1	0.41	17.97	200,200,200,200	0
35	NA	0	9116	1/1	0.31	17.46	45,45,45,45	0
33	MG	0	8108	1/1	0.24	17.45	115,115,115,115	0
33	MG	0	8072	1/1	0.20	17.21	74,74,74,74	0
35	NA	0	9154	1/1	0.25	16.87	51,51,51,51	0
35	NA	0	9115	1/1	0.26	15.45	43,43,43,43	0
33	MG	0	8052	1/1	0.32	15.30	72,72,72,72	0
35	NA	0	9177	1/1	0.34	14.33	70,70,70,70	0
35	NA	9	9183	1/1	0.30	14.05	72,72,72,72	0
37	SR	0	9484	1/1	0.15	14.00	150,150,150,150	0
35	NA	0	9173	1/1	0.31	12.94	66,66,66,66	0
33	MG	0	8038	1/1	0.24	12.93	13,13,13,13	0
35	NA	0	9132	1/1	0.31	12.42	61,61,61,61	0
33	MG	0	8022	1/1	0.54	12.30	113,113,113,113	0
33	MG	0	8051	1/1	0.26	11.67	22,22,22,22	0
33	MG	0	8013	1/1	0.35	11.51	16,16,16,16	0
33	MG	0	8021	1/1	0.22	11.47	51,51,51,51	0
33	MG	0	8057	1/1	0.55	11.43	79,79,79,79	0
35	NA	0	9157	1/1	0.17	11.27	41,41,41,41	0
35	NA	0	9156	1/1	0.25	11.15	55,55,55,55	0
35	NA	0	9120	1/1	0.23	10.88	61,61,61,61	0
33	MG	0	8103	1/1	0.23	10.74	79,79,79,79	0
35	NA	0	9172	1/1	0.34	10.71	68,68,68,68	0
33	MG	0	8058	1/1	0.48	10.49	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	9163	1/1	0.30	10.18	77,77,77,77	0
37	SR	0	9626	1/1	0.26	9.98	140,140,140,140	0
33	MG	0	8012	1/1	0.25	9.29	37,37,37,37	0
35	NA	0	9149	1/1	0.20	9.11	41,41,41,41	0
35	NA	0	9171	1/1	0.21	8.99	63,63,63,63	0
37	SR	0	9482	1/1	0.20	8.94	118,118,118,118	0
34	K	0	9001	1/1	0.44	8.81	95,95,95,95	0
35	NA	0	9170	1/1	0.27	8.42	75,75,75,75	0
33	MG	0	8114	1/1	0.17	8.42	83,83,83,83	0
35	NA	0	9174	1/1	0.19	8.41	67,67,67,67	0
33	MG	B	8055	1/1	0.26	8.41	104,104,104,104	0
35	NA	3	9169	1/1	0.45	7.74	102,102,102,102	0
33	MG	0	8001	1/1	0.20	7.35	17,17,17,17	0
36	CL	0	9322	1/1	0.18	7.06	54,54,54,54	0
33	MG	0	8008	1/1	0.20	6.82	14,14,14,14	0
33	MG	0	8050	1/1	0.21	6.43	94,94,94,94	0
35	NA	0	9140	1/1	0.25	6.39	61,61,61,61	0
35	NA	0	9160	1/1	0.17	6.32	42,42,42,42	0
35	NA	0	9118	1/1	0.19	6.14	41,41,41,41	0
33	MG	9	8095	1/1	0.21	5.36	44,44,44,44	0
37	SR	0	9405	1/1	0.14	5.20	54,54,54,54	0
33	MG	K	8069	1/1	0.18	5.18	23,23,23,23	0
33	MG	0	8070	1/1	0.15	5.03	21,21,21,21	0
37	SR	0	9406	1/1	0.15	4.95	33,33,33,33	0
35	NA	0	9135	1/1	0.16	4.53	46,46,46,46	0
33	MG	0	8029	1/1	0.21	4.36	27,27,27,27	0
33	MG	0	8089	1/1	0.15	4.35	61,61,61,61	0
33	MG	0	8040	1/1	0.36	4.23	94,94,94,94	0
37	SR	0	9434	1/1	0.14	4.19	58,58,58,58	0
35	NA	0	9102	1/1	0.14	4.07	58,58,58,58	0
33	MG	0	8102	1/1	0.14	3.98	70,70,70,70	0
35	NA	0	9165	1/1	0.32	3.76	41,41,41,41	0
36	CL	0	9316	1/1	0.22	3.64	74,74,74,74	0
35	NA	0	9178	1/1	0.18	3.64	54,54,54,54	0
33	MG	0	8076	1/1	0.14	3.50	55,55,55,55	0
35	NA	0	9175	1/1	0.16	3.48	52,52,52,52	0
37	SR	0	9452	1/1	0.16	3.39	114,114,114,114	0
33	MG	0	8017	1/1	0.15	3.38	20,20,20,20	0
35	NA	0	9110	1/1	0.17	3.17	49,49,49,49	0
35	NA	R	9186	1/1	0.19	3.07	64,64,64,64	0
33	MG	0	8099	1/1	0.15	2.97	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	9127	1/1	0.16	2.90	65,65,65,65	0
33	MG	0	8061	1/1	0.13	2.88	81,81,81,81	0
37	SR	0	9432	1/1	0.11	2.79	63,63,63,63	0
37	SR	0	9515	1/1	0.18	2.67	100,100,100,100	0
33	MG	0	8107	1/1	0.20	2.47	68,68,68,68	0
33	MG	0	8065	1/1	0.27	2.37	92,92,92,92	0
37	SR	0	9408	1/1	0.14	2.34	38,38,38,38	0
33	MG	0	8080	1/1	0.20	2.29	48,48,48,48	0
33	MG	0	8020	1/1	0.18	2.17	30,30,30,30	0
37	SR	0	9477	1/1	0.12	2.14	82,82,82,82	0
33	MG	0	8027	1/1	0.16	1.95	30,30,30,30	0
37	SR	9	9588	1/1	0.15	1.86	122,122,122,122	0
37	SR	0	9411	1/1	0.14	1.82	42,42,42,42	0
33	MG	0	8056	1/1	0.19	1.81	47,47,47,47	0
33	MG	A	8066	1/1	0.18	1.75	53,53,53,53	0
35	NA	0	9181	1/1	0.13	1.74	48,48,48,48	0
37	SR	0	9407	1/1	0.12	1.71	42,42,42,42	0
35	NA	0	9159	1/1	0.15	1.68	56,56,56,56	0
33	MG	0	8104	1/1	0.28	1.53	83,83,83,83	0
33	MG	0	8014	1/1	0.27	1.52	78,78,78,78	0
37	SR	0	9475	1/1	0.12	1.48	77,77,77,77	0
37	SR	S	9470	1/1	0.13	1.33	95,95,95,95	0
33	MG	0	8054	1/1	0.12	1.28	58,58,58,58	0
33	MG	0	8045	1/1	0.17	1.28	75,75,75,75	0
33	MG	0	8079	1/1	0.12	1.20	30,30,30,30	0
37	SR	H	9486	1/1	0.17	1.19	121,121,121,121	0
33	MG	0	8090	1/1	0.27	1.18	81,81,81,81	0
35	NA	0	9126	1/1	0.13	1.15	55,55,55,55	0
34	K	0	9002	1/1	0.23	1.14	86,86,86,86	0
33	MG	0	8003	1/1	0.17	1.10	29,29,29,29	0
35	NA	0	9155	1/1	0.21	1.05	54,54,54,54	0
37	SR	0	9420	1/1	0.14	1.01	60,60,60,60	0
33	MG	0	8074	1/1	0.19	1.00	20,20,20,20	0
33	MG	0	8043	1/1	0.11	0.88	47,47,47,47	0
35	NA	S	9112	1/1	0.17	0.64	74,74,74,74	0
36	CL	R	9306	1/1	0.12	0.60	46,46,46,46	0
36	CL	B	9319	1/1	0.13	0.48	59,59,59,59	0
33	MG	0	8097	1/1	0.12	0.31	55,55,55,55	0
33	MG	0	8031	1/1	0.12	0.24	48,48,48,48	0
37	SR	0	9410	1/1	0.13	0.20	34,34,34,34	0
36	CL	A	9309	1/1	0.17	0.19	64,64,64,64	0
33	MG	0	8096	1/1	0.13	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	9141	1/1	0.10	0.09	61,61,61,61	0
37	SR	0	9415	1/1	0.10	0.08	50,50,50,50	0
35	NA	0	9124	1/1	0.12	0.05	51,51,51,51	0
35	NA	0	9139	1/1	0.17	0.04	57,57,57,57	0
37	SR	0	9433	1/1	0.10	0.02	73,73,73,73	0
35	NA	0	9114	1/1	0.14	0.01	51,51,51,51	0
35	NA	C	9104	1/1	0.14	-0.10	27,27,27,27	0
37	SR	0	9537	1/1	0.14	-0.11	152,152,152,152	0
37	SR	F	9595	1/1	0.15	-0.12	95,95,95,95	0
33	MG	0	8002	1/1	0.12	-0.12	22,22,22,22	0
37	SR	0	9474	1/1	0.09	-0.14	96,96,96,96	0
36	CL	0	9303	1/1	0.13	-0.14	49,49,49,49	0
35	NA	0	9128	1/1	0.10	-0.18	40,40,40,40	0
35	NA	0	9182	1/1	0.11	-0.20	84,84,84,84	0
37	SR	R	9418	1/1	0.13	-0.25	53,53,53,53	0
33	MG	0	8041	1/1	0.12	-0.30	47,47,47,47	0
37	SR	0	9417	1/1	0.12	-0.32	53,53,53,53	0
37	SR	A	9437	1/1	0.12	-0.37	64,64,64,64	0
35	NA	0	9131	1/1	0.12	-0.38	47,47,47,47	0
37	SR	0	9505	1/1	0.12	-0.43	104,104,104,104	0
35	NA	0	9117	1/1	0.11	-0.44	32,32,32,32	0
37	SR	0	9509	1/1	0.12	-0.61	83,83,83,83	0
37	SR	0	9488	1/1	0.10	-0.65	78,78,78,78	0
37	SR	A	9497	1/1	0.10	-0.76	85,85,85,85	0
37	SR	1	9419	1/1	0.10	-0.80	38,38,38,38	0
33	MG	0	8093	1/1	0.13	-0.80	42,42,42,42	0
37	SR	0	9534	1/1	0.11	-0.81	106,106,106,106	0
37	SR	0	9414	1/1	0.11	-0.82	53,53,53,53	0
36	CL	J	9302	1/1	0.08	-0.87	55,55,55,55	0
37	SR	0	9421	1/1	0.09	-0.89	65,65,65,65	0
35	NA	J	9146	1/1	0.10	-0.90	62,62,62,62	0
37	SR	0	9413	1/1	0.10	-0.92	44,44,44,44	0
33	MG	0	8004	1/1	0.10	-0.92	27,27,27,27	0
37	SR	0	9430	1/1	0.12	-0.93	41,41,41,41	0
36	CL	M	9318	1/1	0.13	-0.95	37,37,37,37	0
33	MG	0	8015	1/1	0.10	-0.96	29,29,29,29	0
37	SR	0	9424	1/1	0.14	-0.97	43,43,43,43	0
37	SR	0	9504	1/1	0.10	-1.00	92,92,92,92	0
38	CD	U	9201	1/1	0.09	-1.00	56,56,56,56	0
37	SR	0	9462	1/1	0.12	-1.00	66,66,66,66	0
35	NA	0	9158	1/1	0.11	-1.04	62,62,62,62	0
33	MG	0	8068	1/1	0.13	-1.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	D	9151	1/1	0.19	-1.18	63,63,63,63	0
37	SR	0	9447	1/1	0.10	-1.20	66,66,66,66	0
36	CL	J	9321	1/1	0.07	-1.20	58,58,58,58	0
37	SR	0	9490	1/1	0.10	-1.22	105,105,105,105	0
35	NA	R	9137	1/1	0.09	-1.28	32,32,32,32	0
38	CD	Z	9203	1/1	0.07	-1.33	75,75,75,75	0
37	SR	0	9530	1/1	0.12	-1.37	94,94,94,94	0
33	MG	0	8088	1/1	0.06	-1.37	43,43,43,43	0
35	NA	0	9166	1/1	0.09	-1.38	65,65,65,65	0
33	MG	T	8073	1/1	0.13	-1.45	42,42,42,42	0
35	NA	Q	9148	1/1	0.10	-1.51	50,50,50,50	0
37	SR	0	9545	1/1	0.04	-1.55	67,67,67,67	0
35	NA	0	9134	1/1	0.07	-1.56	47,47,47,47	0
36	CL	J	9301	1/1	0.08	-1.57	55,55,55,55	0
35	NA	0	9108	1/1	0.08	-1.63	34,34,34,34	0
37	SR	0	9590	1/1	0.07	-1.64	142,142,142,142	0
37	SR	0	9450	1/1	0.06	-1.65	64,64,64,64	0
35	NA	R	9138	1/1	0.06	-1.65	52,52,52,52	0
35	NA	M	9147	1/1	0.07	-1.65	38,38,38,38	0
33	MG	0	8046	1/1	0.07	-1.66	40,40,40,40	0
37	SR	0	9423	1/1	0.09	-1.66	51,51,51,51	0
38	CD	3	9204	1/1	0.05	-1.67	58,58,58,58	0
37	SR	0	9451	1/1	0.07	-1.69	63,63,63,63	0
36	CL	0	9311	1/1	0.08	-1.71	56,56,56,56	0
35	NA	0	9113	1/1	0.11	-1.73	64,64,64,64	0
37	SR	0	9566	1/1	0.05	-1.76	75,75,75,75	0
36	CL	O	9308	1/1	0.08	-1.84	67,67,67,67	0
37	SR	1	9460	1/1	0.10	-1.84	49,49,49,49	0
35	NA	0	9136	1/1	0.10	-1.84	31,31,31,31	0
35	NA	0	9105	1/1	0.10	-1.91	41,41,41,41	0
33	MG	0	8117	1/1	0.09	-1.92	39,39,39,39	0
33	MG	0	8060	1/1	0.09	-1.93	81,81,81,81	0
33	MG	0	8101	1/1	0.10	-2.02	51,51,51,51	0
37	SR	0	9431	1/1	0.12	-2.04	55,55,55,55	0
37	SR	0	9425	1/1	0.07	-2.14	71,71,71,71	0
33	MG	0	8067	1/1	0.11	-2.15	36,36,36,36	0
37	SR	3	9439	1/1	0.05	-2.18	63,63,63,63	0
37	SR	0	9422	1/1	0.10	-2.32	53,53,53,53	0
36	CL	N	9307	1/1	0.08	-2.38	54,54,54,54	0
33	MG	Y	8109	1/1	0.10	-2.39	38,38,38,38	0
37	SR	0	9568	1/1	0.08	-2.40	75,75,75,75	0
37	SR	0	9446	1/1	0.08	-2.41	80,80,80,80	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	0.05	-2.42	115,115,115,115	0
36	CL	0	9317	1/1	0.09	-2.47	49,49,49,49	0
33	MG	0	8115	1/1	0.10	-2.50	53,53,53,53	0
35	NA	0	9130	1/1	0.07	-2.60	45,45,45,45	0
37	SR	0	9427	1/1	0.10	-2.66	53,53,53,53	0
37	SR	0	9467	1/1	0.09	-2.66	74,74,74,74	0
37	SR	0	9444	1/1	0.07	-2.67	47,47,47,47	0
37	SR	0	9517	1/1	0.05	-2.67	96,96,96,96	0
37	SR	0	9506	1/1	0.07	-2.68	86,86,86,86	0
37	SR	L	9409	1/1	0.09	-2.69	36,36,36,36	0
36	CL	L	9310	1/1	0.09	-2.72	56,56,56,56	0
37	SR	A	9436	1/1	0.05	-2.74	57,57,57,57	0
37	SR	0	9429	1/1	0.10	-2.75	63,63,63,63	0
37	SR	0	9473	1/1	0.04	-2.85	69,69,69,69	0
37	SR	0	9459	1/1	0.07	-2.86	96,96,96,96	0
36	CL	0	9312	1/1	0.06	-2.88	45,45,45,45	0
36	CL	0	9313	1/1	0.08	-2.89	51,51,51,51	0
35	NA	0	9123	1/1	0.09	-2.89	37,37,37,37	0
36	CL	Y	9320	1/1	0.07	-2.91	42,42,42,42	0
37	SR	0	9455	1/1	0.08	-2.94	61,61,61,61	0
37	SR	0	9443	1/1	0.09	-2.96	59,59,59,59	0
37	SR	0	9461	1/1	0.03	-3.00	73,73,73,73	0
33	MG	0	8042	1/1	0.06	-3.05	53,53,53,53	0
33	MG	0	8098	1/1	0.07	-3.08	43,43,43,43	0
37	SR	0	9426	1/1	0.07	-3.09	66,66,66,66	0
37	SR	0	9457	1/1	0.08	-3.11	47,47,47,47	0
37	SR	0	9508	1/1	0.08	-3.12	83,83,83,83	0
36	CL	0	9314	1/1	0.06	-3.13	47,47,47,47	0
37	SR	0	9581	1/1	0.07	-3.16	134,134,134,134	0
33	MG	0	8032	1/1	0.08	-3.18	36,36,36,36	0
35	NA	0	9143	1/1	0.07	-3.19	38,38,38,38	0
37	SR	0	9442	1/1	0.09	-3.31	59,59,59,59	0
33	MG	0	8110	1/1	0.10	-3.63	46,46,46,46	0
37	SR	9	9481	1/1	0.05	-3.63	83,83,83,83	0
33	MG	0	8036	1/1	0.08	-3.64	63,63,63,63	0
37	SR	0	9412	1/1	0.10	-3.64	43,43,43,43	0
33	MG	0	8028	1/1	0.10	-3.65	34,34,34,34	0
37	SR	0	9438	1/1	0.07	-3.67	63,63,63,63	0
38	CD	1	9202	1/1	0.03	-3.71	51,51,51,51	0
35	NA	0	9101	1/1	0.12	-3.76	43,43,43,43	0
33	MG	0	8005	1/1	0.08	-3.80	29,29,29,29	0
33	MG	0	8113	1/1	0.08	-3.81	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8116	1/1	0.06	-3.86	51,51,51,51	0
37	SR	0	9560	1/1	0.07	-3.95	97,97,97,97	0
37	SR	0	9465	1/1	0.07	-3.95	96,96,96,96	0
33	MG	0	8106	1/1	0.04	-3.97	37,37,37,37	0
37	SR	0	9445	1/1	0.08	-4.02	62,62,62,62	0
37	SR	0	9478	1/1	0.07	-4.13	70,70,70,70	0
33	MG	0	8063	1/1	0.07	-4.23	74,74,74,74	0
37	SR	0	9469	1/1	0.03	-4.27	85,85,85,85	0
36	CL	3	9304	1/1	0.08	-4.31	59,59,59,59	0
37	SR	0	9529	1/1	0.09	-4.41	116,116,116,116	0
37	SR	0	9448	1/1	0.06	-4.42	62,62,62,62	0
37	SR	0	9480	1/1	0.04	-4.58	86,86,86,86	0
37	SR	0	9466	1/1	0.03	-4.70	87,87,87,87	0
37	SR	0	9489	1/1	0.05	-4.74	87,87,87,87	0
37	SR	0	9435	1/1	0.07	-4.87	68,68,68,68	0
33	MG	0	8044	1/1	0.04	-4.92	42,42,42,42	0
38	CD	O	9205	1/1	0.04	-4.94	85,85,85,85	0
37	SR	0	9449	1/1	0.07	-4.98	59,59,59,59	0
37	SR	0	9441	1/1	0.07	-5.02	54,54,54,54	0
37	SR	0	9428	1/1	0.05	-5.21	43,43,43,43	0
37	SR	0	9483	1/1	0.06	-5.50	67,67,67,67	0
37	SR	0	9532	1/1	0.05	-5.55	100,100,100,100	0
33	MG	0	8091	1/1	0.06	-5.58	56,56,56,56	0
37	SR	0	9498	1/1	0.04	-5.60	63,63,63,63	0
37	SR	0	9629	1/1	0.07	-5.85	69,69,69,69	0
37	SR	0	9453	1/1	0.07	-5.93	68,68,68,68	0
36	CL	0	9305	1/1	0.05	-6.09	52,52,52,52	0
33	MG	0	8075	1/1	0.04	-6.12	37,37,37,37	0
33	MG	0	8037	1/1	0.06	-6.18	40,40,40,40	0
36	CL	0	9315	1/1	0.08	-6.21	54,54,54,54	0
33	MG	0	8009	1/1	0.06	-6.27	31,31,31,31	0
33	MG	0	8112	1/1	0.03	-6.36	44,44,44,44	0
33	MG	0	8019	1/1	0.04	-6.46	53,53,53,53	0
37	SR	0	9416	1/1	0.07	-6.61	45,45,45,45	0
37	SR	0	9495	1/1	0.10	-6.72	88,88,88,88	0
37	SR	0	9454	1/1	0.06	-6.86	73,73,73,73	0
37	SR	0	9464	1/1	0.04	-7.30	80,80,80,80	0
37	SR	B	9458	1/1	0.06	-8.05	73,73,73,73	0
37	SR	0	9456	1/1	0.06	-8.13	67,67,67,67	0
33	MG	0	8039	1/1	0.05	-8.37	56,56,56,56	0
37	SR	0	9585	1/1	0.07	-9.31	86,86,86,86	0
35	NA	0	9167	1/1	0.06	-9.43	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8030	1/1	0.04	-10.22	34,34,34,34	0
37	SR	0	9440	1/1	0.04	-10.40	63,63,63,63	0
37	SR	9	9503	1/1	0.03	-12.62	109,109,109,109	0
33	MG	0	8083	1/1	0.06	-14.21	51,51,51,51	0
37	SR	0	9570	1/1	0.05	-35.36	96,96,96,96	0
37	SR	0	9522	1/1	0.06	-69.49	104,104,104,104	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.