



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:23 AM GMT

PDB ID : 1VQ4
Title : The structure of the transition state analogue "DAA" bound to the large ribosomal subunit of Haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.70 Å(reported)

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

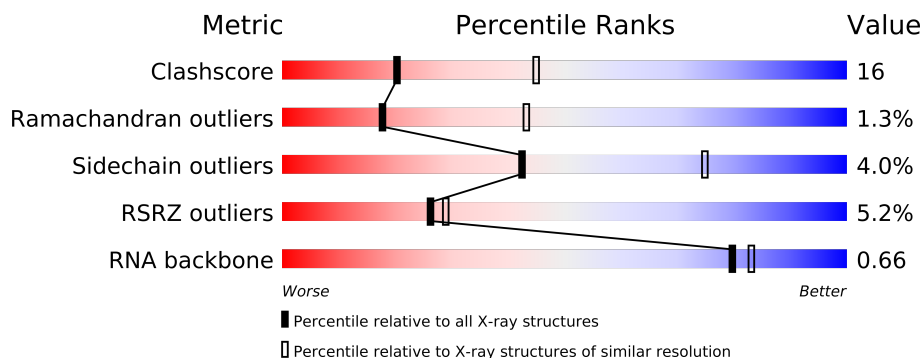
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	8	
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	194	
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	8011	-	X
33	MG	0	8016	-	X
33	MG	0	8021	-	X
33	MG	0	8023	-	X
33	MG	0	8024	-	X
33	MG	0	8041	-	X
33	MG	0	8047	-	X
33	MG	0	8049	-	X
33	MG	0	8053	-	X
33	MG	0	8060	-	X
33	MG	0	8072	-	X
33	MG	0	8081	-	X
33	MG	0	8082	-	X
33	MG	0	8085	-	X
33	MG	0	8087	-	X
33	MG	0	8090	-	X
33	MG	0	8092	-	X
33	MG	0	8098	-	X
33	MG	0	8100	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
33	MG	0	8114	-	X
34	K	0	9001	-	X
35	NA	0	9101	-	X
35	NA	0	9102	-	X
35	NA	0	9106	-	X
35	NA	0	9107	-	X
35	NA	0	9110	-	X
35	NA	0	9113	-	X
35	NA	0	9118	-	X
35	NA	0	9121	-	X
35	NA	0	9125	-	X
35	NA	0	9126	-	X
35	NA	0	9129	-	X
35	NA	0	9135	-	X
35	NA	0	9142	-	X
35	NA	0	9150	-	X
35	NA	0	9152	-	X
35	NA	0	9154	-	X
35	NA	0	9155	-	X
35	NA	0	9156	-	X
35	NA	0	9158	-	X
35	NA	0	9159	-	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	9169	-	X
35	NA	0	9170	-	X
35	NA	0	9171	-	X
35	NA	0	9172	-	X
35	NA	0	9173	-	X
35	NA	0	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	9182	-	X
35	NA	0	9184	-	X
35	NA	0	9185	-	X
35	NA	L	9180	-	X
35	NA	M	9147	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	NA	Q	9148	-	X
35	NA	R	9186	-	X
35	NA	S	9112	-	X
36	CL	0	9305	-	X
36	CL	0	9315	-	X
36	CL	0	9316	-	X
36	CL	0	9322	-	X
37	CD	O	9205	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 98999 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

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

There are 5 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*(5AA)P*(2OP)P*(PO2)P*(DA)P*C*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	8	Total	C	N	O	P	0	0	0
			127	61	23	38	5			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	108	Total	Mg	0	0
			108	108		
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	2	Total	Mg	0	0
			2	2		
33	T	1	Total	Mg	0	0
			1	1		
33	9	2	Total	Mg	0	0
			2	2		
33	3	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	3	Total	K	0	0
			3	3		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	72	Total Na 72 72	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	2	Total Na 2 2	0	0
35	C	1	Total Na 1 1	0	0
35	A	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	9	2	Total Na 2 2	0	0
35	L	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

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

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

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

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5764	Total 5764	O 5764	0	0
38	9	133	Total 133	O 133	0	0
38	4	3	Total 3	O 3	0	0
38	A	116	Total 116	O 116	0	0
38	B	143	Total 143	O 143	0	0
38	C	173	Total 173	O 173	0	0
38	D	44	Total 44	O 44	0	0
38	E	43	Total 43	O 43	0	0
38	F	24	Total 24	O 24	0	0
38	G	17	Total 17	O 17	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	H	66	Total 66	O 66	0	0
38	J	52	Total 52	O 52	0	0
38	K	57	Total 57	O 57	0	0
38	L	81	Total 81	O 81	0	0
38	M	115	Total 115	O 115	0	0
38	N	61	Total 61	O 61	0	0
38	O	45	Total 45	O 45	0	0
38	P	63	Total 63	O 63	0	0
38	Q	52	Total 52	O 52	0	0
38	R	89	Total 89	O 89	0	0
38	S	31	Total 31	O 31	0	0
38	T	36	Total 36	O 36	0	0
38	U	26	Total 26	O 26	0	0
38	V	13	Total 13	O 13	0	0
38	W	70	Total 70	O 70	0	0
38	X	31	Total 31	O 31	0	0
38	Y	93	Total 93	O 93	0	0
38	Z	31	Total 31	O 31	0	0
38	1	61	Total 61	O 61	0	0
38	2	42	Total 42	O 42	0	0
38	3	71	Total 71	O 71	0	0

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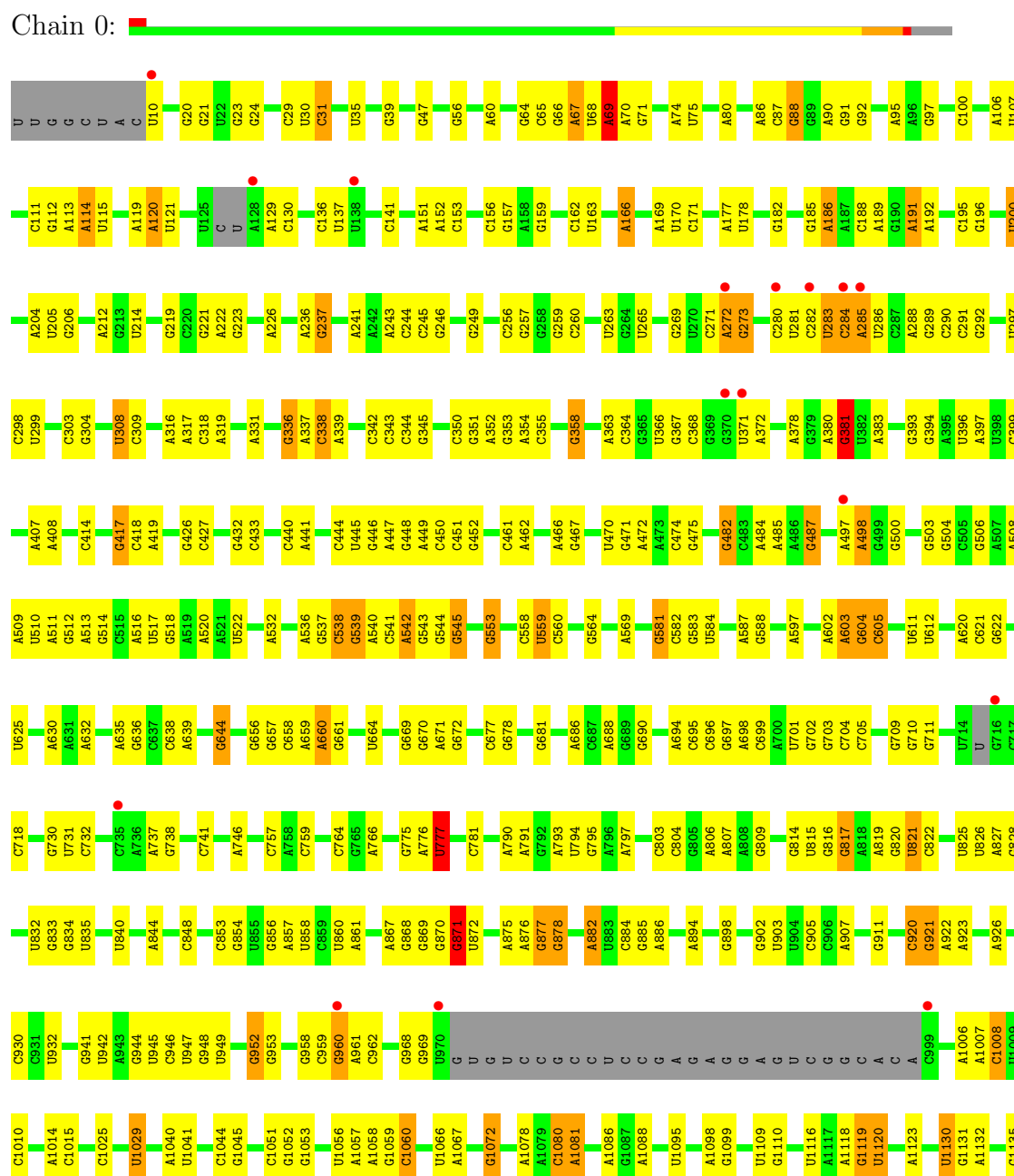
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	I	9	Total	O	0	0
			9	9		

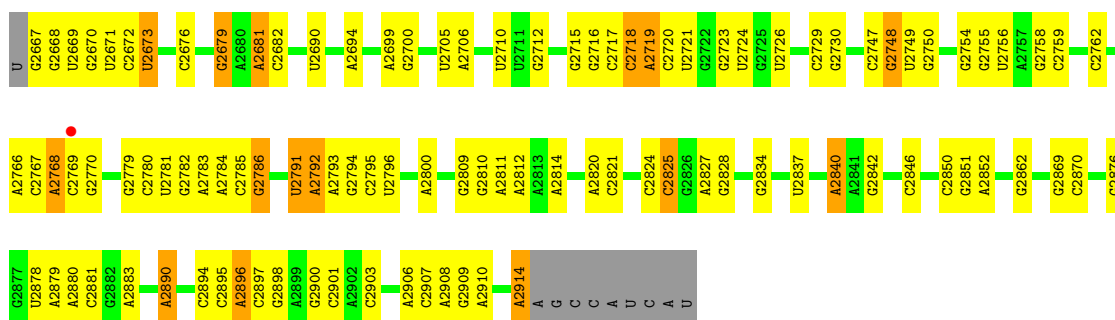
3 Residue-property plots

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

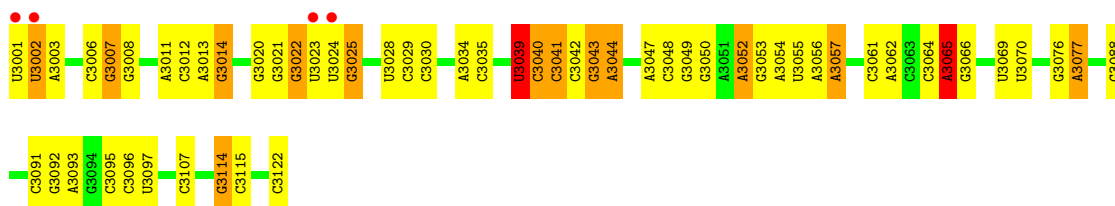


U2545	G2453	A	A2081	C	A	A2345	G2463	U2546	U1336
C2547	G2462	C	A2089	U	C	G2344	G2466	C2548	G1337
C2548	A2465	A	G2090	G	U	A2345	G2467	G1511	G1515
C2552	G2466	A	G2091	C	C	G2346	G2468	G1516	G1557
A2553	G2467	A	G2092	C	C	G2347	G2469	G1558	G1559
C2561	G2468	A	G2093	A	A	G2348	G2470	G1560	G1561
C2562	A2469	A	G2094	G	G	G2349	G2471	G1562	G1563
U2563	A2470	A	A2095	U	U	G2350	G2472	G1564	G1565
C2564	A2471	A	A2096	A	A	G2351	G2473	G1566	G1567
C2565	A2472	A	A2097	C	C	G2352	G2474	G1568	G1569
G2570	A2473	A	A2101	C	C	G2353	G2475	G1570	G1571
U2578	G2474	A	G2102	G	G	G2354	G2476	G1572	G1573
C2587	A2475	A	A2103	C	C	G2355	G2477	G1574	G1575
U2588	G2476	A	G2104	G	G	G2356	G2478	G1576	G1577
C2589	G2477	A	C2105	C	C	G2357	G2479	G1578	G1579
U2591	A2478	A	G2106	G	G	G2358	G2480	G1580	G1581
G2592	A2479	A	G2110	U	U	G2359	G2481	G1582	G1583
U2597	G2480	A	G2111	C	C	G2360	G2482	G1584	G1585
C2598	A2483	A	G2112	G	G	G2361	G2483	G1586	G1587
U2599	G2484	A	G2113	C	C	G2362	G2484	G1588	G1589
A2601	C2485	A	A2135	G	G	G2363	G2485	G1590	G1591
G2602	G2486	A	G2136	C	C	G2364	G2486	G1592	G1593
U2607	A2487	A	A	C	C	G2365	G2487	G1594	G1595
C2608	G2488	A	C	C	C	G2366	G2488	G1596	G1597
G2613	C2489	A	G	A	A	G2367	G2489	G1598	G1599
C2614	A2490	A	U	U	U	G2368	G2490	G1600	G1601
U2619	G2491	A	G	G	G	G2369	G2491	G1602	G1603
C2626	U2492	A	G	G	G	G2370	G2492	G1604	G1605
G2627	C2493	A	A	C	C	G2371	G2493	G1606	G1607
U2630	G2494	A	A	C	C	G2372	G2494	G1608	G1609
G2634	A2495	A	A	C	C	G2373	G2495	G1610	G1611
U2637	G2496	A	A	C	C	G2374	G2496	G1612	G1613
G2638	A2497	A	A	C	C	G2375	G2497	G1614	G1615
G2642	U2498	A	A	C	C	G2376	G2498	G1616	G1617
C2643	G2499	A	A	C	C	G2377	G2499	G1618	G1619
G2644	A2499	A	A	C	C	G2378	G2500	G1620	G1621
A2649	U2500	A	A	C	C	G2379	G2501	G1622	G1623
U2652	C2501	A	A	C	C	G2380	G2502	G1624	G1625
A2664	G2502	A	A	C	C	G2381	G2503	G1626	G1627
A	C2503	A	A	C	C	G2382	G2504	G1628	G1629
	U2504	A	A	C	C	G2383	G2505	G1630	G1631
	G2505	A	A	C	C	G2384	G2506	G1632	G1633
	C2506	A	A	C	C	G2385	G2507	G1634	G1635
	U2507	A	A	C	C	G2386	G2508	G1636	G1637
	G2508	A	A	C	C	G2387	G2509	G1638	G1639
	C2509	A	A	C	C	G2388	G2510	G1640	G1641
	U2510	A	A	C	C	G2389	G2511	G1642	G1643
	G2511	A	A	C	C	G2390	G2512	G1644	G1645
	C2512	A	A	C	C	G2391	G2513	G1646	G1647
	U2513	A	A	C	C	G2392	G2514	G1648	G1649
	G2514	A	A	C	C	G2393	G2515	G1650	G1651
	C2515	A	A	C	C	G2394	G2516	G1652	G1653
	U2516	A	A	C	C	G2395	G2517	G1654	G1655
	G2517	A	A	C	C	G2396	G2518	G1656	G1657
	C2518	A	A	C	C	G2397	G2519	G1658	G1659
	U2519	A	A	C	C	G2398	G2520	G1660	G1661
	G2520	A	A	C	C	G2399	G2521	G1662	G1663
	C2521	A	A	C	C	G2400	G2522	G1664	G1665
	U2522	A	A	C	C	G2401	G2523	G1666	G1667
	G2523	A	A	C	C	G2402	G2524	G1668	G1669
	C2524	A	A	C	C	G2403	G2525	G1670	G1671
	U2525	A	A	C	C	G2404	G2526	G1672	G1673
	G2526	A	A	C	C	G2405	G2527	G1674	G1675
	C2527	A	A	C	C	G2406	G2528	G1676	G1677
	U2528	A	A	C	C	G2407	G2529	G1678	G1679
	G2529	A	A	C	C	G2408	G2530	G1680	G1681
	C2530	A	A	C	C	G2409	G2531	G1682	G1683
	U2531	A	A	C	C	G2410	G2532	G1684	G1685
	G2532	A	A	C	C	G2411	G2533	G1686	G1687
	C2533	A	A	C	C	G2412	G2534	G1688	G1689
	U2534	A	A	C	C	G2413	G2535	G1690	G1691
	G2535	A	A	C	C	G2414	G2536	G1692	G1693
	C2536	A	A	C	C	G2415	G2537	G1694	G1695
	U2537	A	A	C	C	G2416	G2538	G1696	G1697
	G2538	A	A	C	C	G2417	G2539	G1698	G1699
	C2539	A	A	C	C	G2418	G2540	G1700	G1701
	U2540	A	A	C	C	G2419	G2541	G1702	G1703
	G2541	A	A	C	C	G2420	G2542	G1704	G1705
	C2542	A	A	C	C	G2421	G2543	G1706	G1707
	U2543	A	A	C	C	G2422	G2544	G1708	G1709
	G2544	A	A	C	C	G2423	G2545	G1710	G1711
	C2545	A	A	C	C	G2424	G2546	G1712	G1713
	U2546	A	A	C	C	G2425	G2547	G1714	G1715
	G2547	A	A	C	C	G2426	G2548	G1716	G1717
	C2548	A	A	C	C	G2427	G2549	G1718	G1719
	U2549	A	A	C	C	G2428	G2550	G1720	G1721
	G2550	A	A	C	C	G2429	G2551	G1722	G1723
	C2551	A	A	C	C	G2430	G2552	G1724	G1725
	U2552	A	A	C	C	G2431	G2553	G1726	G1727
	G2553	A	A	C	C	G2432	G2554	G1728	G1729
	C2554	A	A	C	C	G2433	G2555	G1730	G1731
	U2555	A	A	C	C	G2434	G2556	G1732	G1733
	G2556	A	A	C	C	G2435	G2557	G1734	G1735
	C2557	A	A	C	C	G2436	G2558	G1736	G1737
	U2558	A	A	C	C	G2437	G2559	G1738	G1739
	G2559	A	A	C	C	G2438	G2560	G1740	G1741
	C2560	A	A	C	C	G2439	G2561	G1742	G1743
	U2561	A	A	C	C	G2440	G2562	G1744	G1745
	G2562	A	A	C	C	G2441	G2563	G1746	G1747
	C2563	A	A	C	C	G2442	G2564	G1748	G1749
	U2564	A	A	C	C	G2443	G2565	G1750	G1751
	G2565	A	A	C	C	G2444	G2566	G1752	G1753
	C2566	A	A	C	C	G2445	G2567	G1754	G1755
	U2567	A	A	C	C	G2446	G2568	G1756	G1757
	G2568	A	A	C	C	G2447	G2569	G1758	G1759
	C2569	A	A	C	C	G2448	G2570	G1760	G1761
	U2570	A	A	C	C	G2449	G2571	G1762	G1763
	G2571	A	A	C	C	G2450	G2572	G1764	G1765
	C2572	A	A	C	C	G2451	G2573	G1766	G1767
	U2573	A	A	C	C	G2452	G2574	G1768	G1769
	G2574	A	A	C	C	G2453	G2575	G1770	G1771
	C2575	A	A	C	C	G2454	G2576	G1772	G1773
	U2576	A	A	C	C	G2455	G2577	G1774	G1775
	G2577	A	A	C	C	G2456	G2578	G1776	G1777
	C2578	A	A	C	C	G2457	G2579	G1778	G1779
	U2579	A	A	C	C	G2458	G2580	G1780	G1781
	G2580	A	A	C	C	G2459	G2581	G1782	G1783
	C2581	A	A	C	C	G2460	G2582	G1784	G1785
	U2582	A	A	C	C	G2461	G2583	G1786	G1787
	G2583	A	A	C	C	G2462	G2584	G1788	G1789
	C2584	A	A	C	C	G2463	G2585	G1790	G1791
	U2585	A	A	C	C	G2464	G2586	G1792	G1793
	G2586	A	A	C	C	G2465	G2587	G1794	G1795
	C2587	A	A	C	C	G2466	G2588	G1796	G1797
	U2588	A	A	C	C	G2467	G2589	G1798	G1799
	G2589	A	A	C	C	G2468	G2590	G1800	G1801
	C2590	A	A	C	C	G2469	G2591	G1802	G1803
	U2591	A	A	C	C	G2470	G2592	G1804	G1805
	G2592	A	A	C	C	G2471	G2593	G1806	G1807
	C2593	A	A	C	C	G2472	G2594	G1808	G1809
	U2594	A	A	C	C	G2473	G2595	G1810	G1811
	G2595	A	A	C	C	G2474	G2596	G1812	G1813
	C2596	A	A	C	C	G2475	G2597	G1814	G1815
	U2597	A	A	C	C	G2476	G2598	G1816	G1817
	G2598	A	A	C	C	G2477	G2599	G1818	G1819
	C2599	A	A	C	C	G2478	G2600	G1820	G1821
	U2600	A	A	C	C	G2479	G2601	G1822	G1823
	G2601	A	A	C	C	G2480	G2602	G1824	G1825
	C2602	A	A	C	C	G2481	G2603	G1826	G1827
	U2603	A	A	C	C	G2482	G2604	G1828	G1829
	G2604	A	A	C	C	G2483	G2605	G1830	G1831
	C2605	A	A	C	C	G2484	G2606	G1832	G1833
	U2606	A	A	C	C	G2485	G2607	G1834	G1835
	G2607	A	A	C	C	G2486	G2608	G1836	G1837
	C2608	A	A	C	C	G2487	G2609	G1838	G1839
	U2609	A	A	C	C	G2488	G2610	G1840	G1841
	G2610	A	A	C	C	G2489	G2611	G1842	G1843
	C2611	A	A	C	C	G2490	G2612	G1844	G1845
	U2612	A	A	C	C	G2491	G2613	G1846	G1847
	G2613	A	A	C	C	G2492	G2614	G1848	G1849
	C2614	A	A	C	C	G2493	G2615	G1850	G1851
	U2615	A	A	C	C	G2494	G2616	G1852	G1853
	G2616	A	A	C	C	G2495	G2617	G1854	G1855
	C2617	A	A	C	C	G2496	G2618	G1856	G1857
	U2618	A	A	C	C	G2497	G2619	G1858	G1859
	G2619	A	A	C	C	G2498	G2620	G1860	G1861
	C2620	A	A	C	C	G2499	G2621	G1862	G1863
	U2621	A	A	C	C	G2500	G2622	G1864	G1865
	G2622	A	A	C	C	G2501	G262		



• Molecule 2: 5S ribosomal RNA

Chain 9:



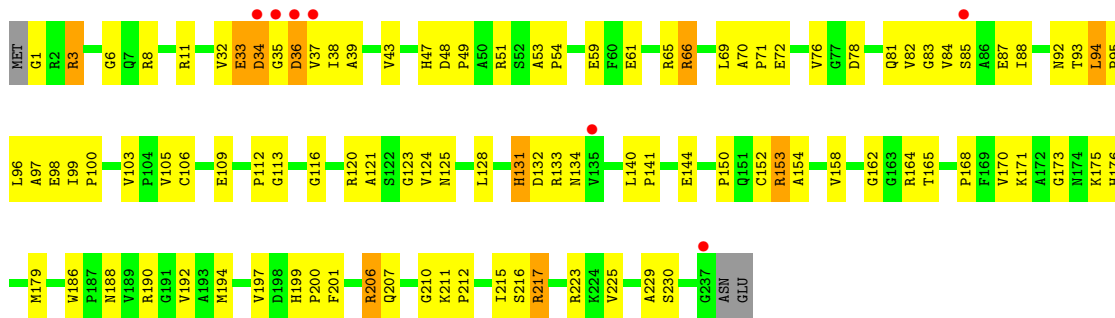
• Molecule 3: 5'-R(*CP*CP*(5AA)P*(2OP)P*(PO2)P*(DA)P*C*C)-3'

Chain 4:



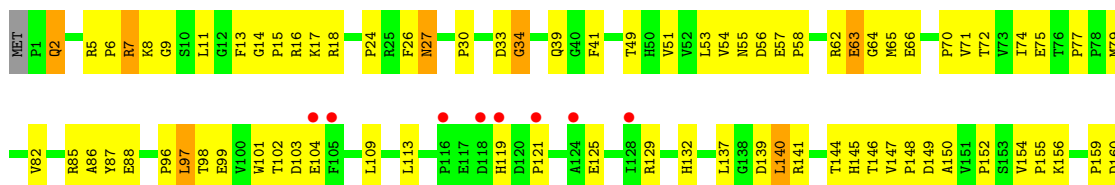
• Molecule 4: 50S ribosomal protein L2P

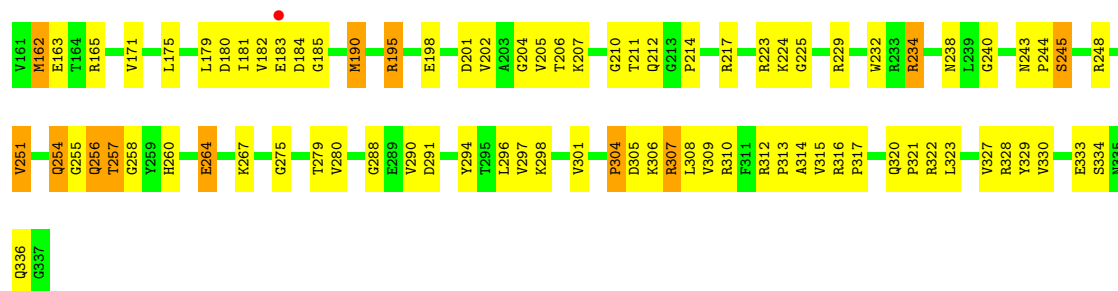
Chain A:



• Molecule 5: 50S ribosomal protein L3P

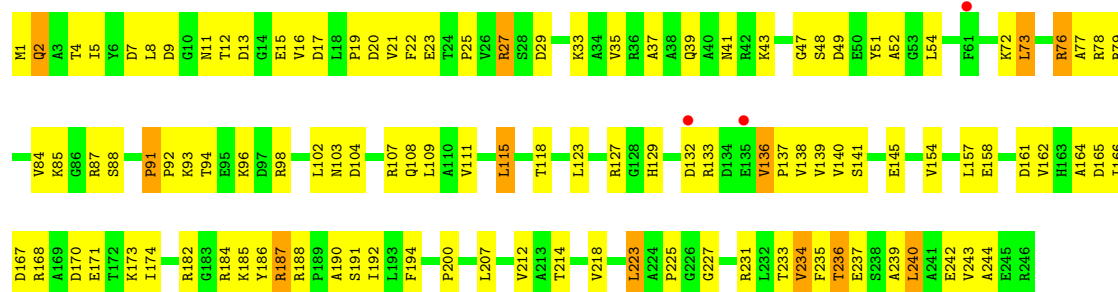
Chain B:





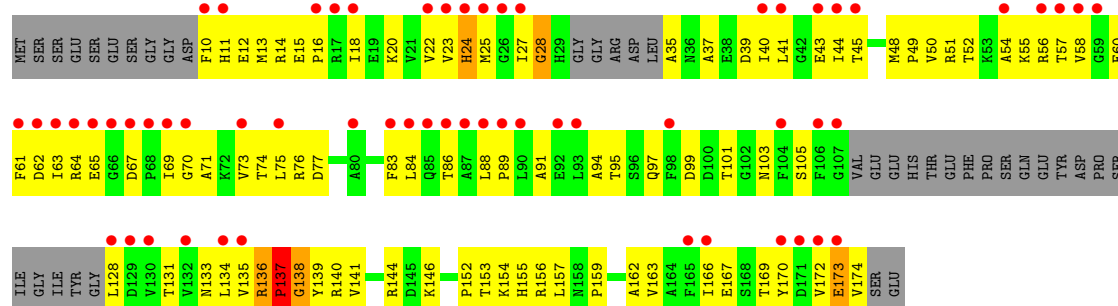
- Molecule 6: 50S ribosomal protein L4E

Chain C:



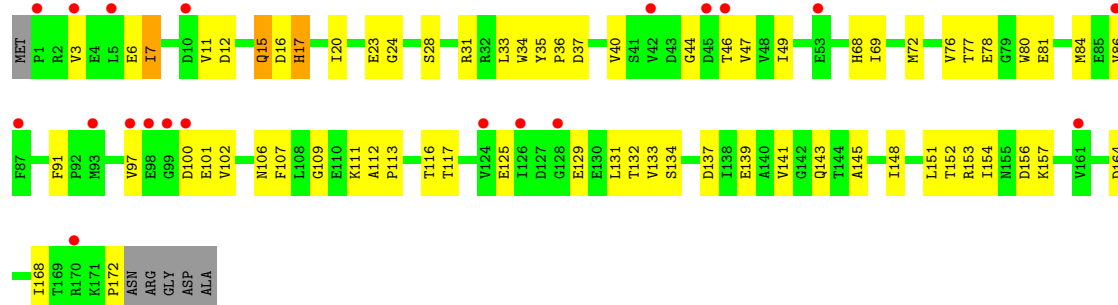
- Molecule 7: 50S ribosomal protein L5P

Chain D:



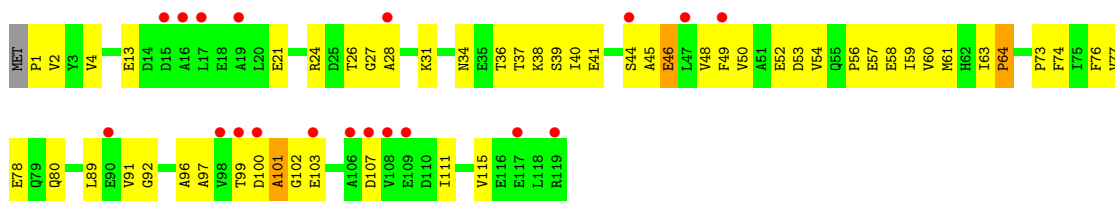
- Molecule 8: 50S ribosomal protein L6P

Chain E:



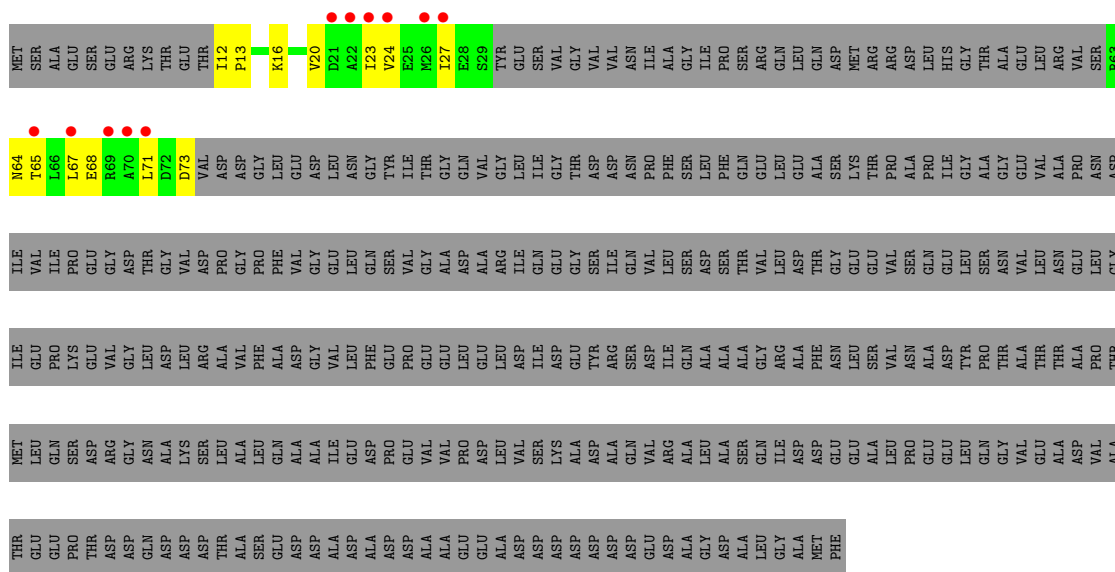
- Molecule 9: 50S ribosomal protein L7AE

Chain E:



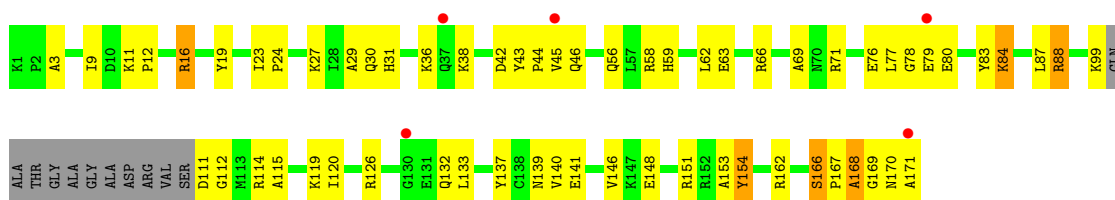
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

Chain G:



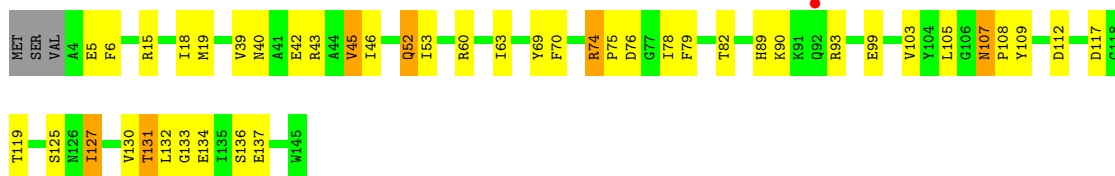
• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

Chain H:



• Molecule 12: 50S ribosomal protein L13P

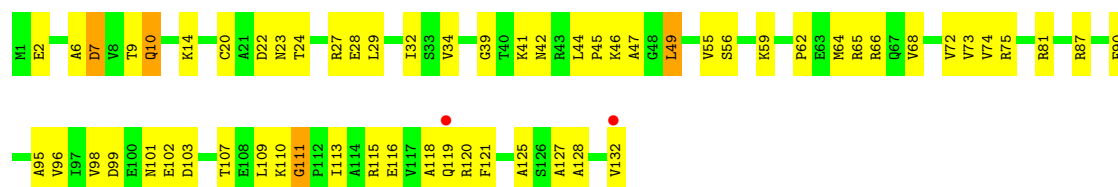
Chain J:



• Molecule 13: 50S ribosomal protein L14P

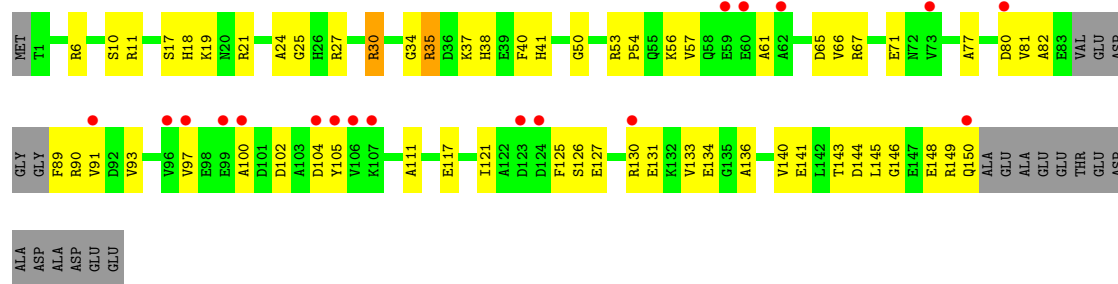
Chain K:





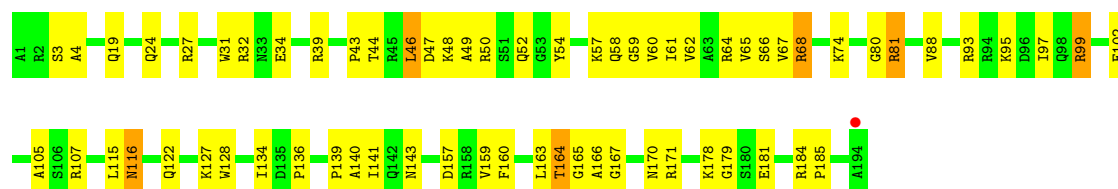
• Molecule 14: 50S ribosomal protein L15P

Chain L:



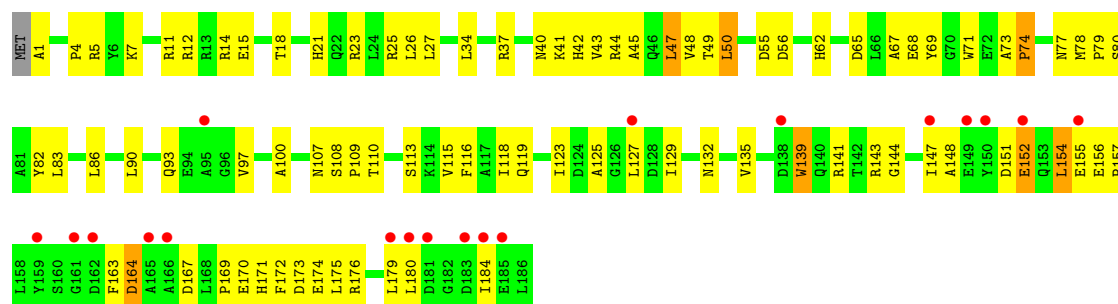
• Molecule 15: 50S Ribosomal Protein L15E

Chain M:



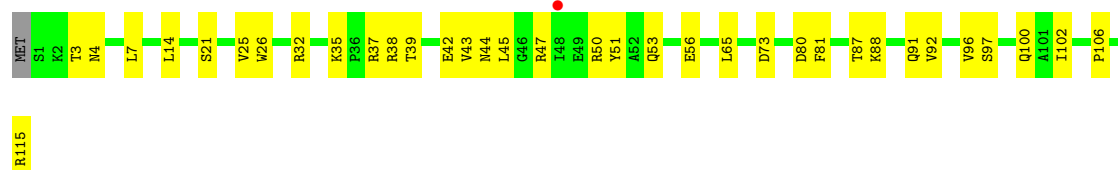
• Molecule 16: 50S ribosomal protein L18P

Chain N:



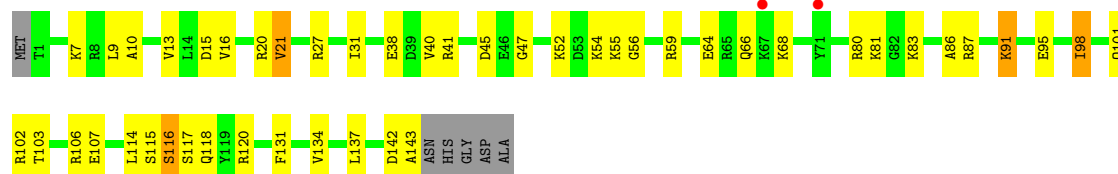
• Molecule 17: 50S ribosomal protein L18e

Chain O:



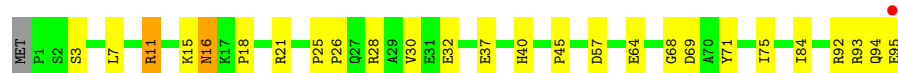
- Molecule 18: 50S ribosomal protein L19E

Chain P:



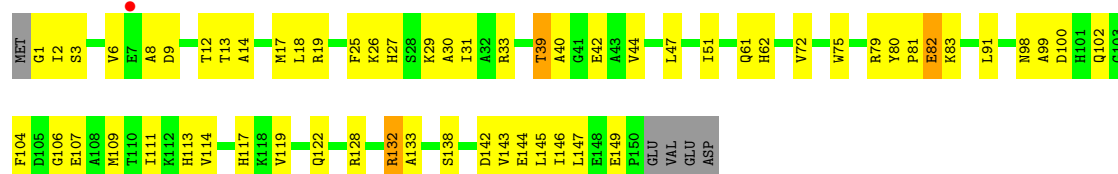
- Molecule 19: 50S ribosomal protein L21e

Chain Q:



- Molecule 20: 50S ribosomal protein L22P

Chain R:



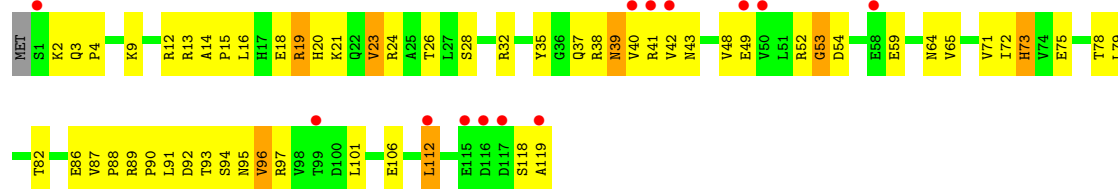
- Molecule 21: 50S ribosomal protein L23P

Chain S:



- Molecule 22: 50S ribosomal protein L24P

Chain T:



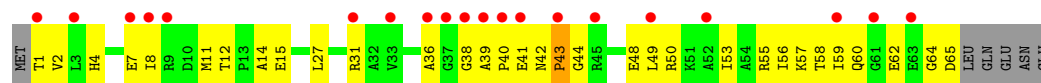
- Molecule 23: 50S ribosomal protein L24E

Chain U:



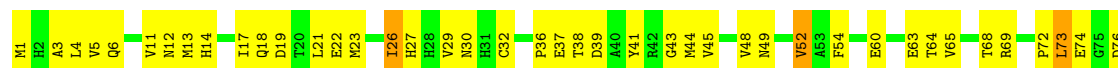
- Molecule 24: 50S ribosomal protein L29P

Chain V:



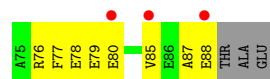
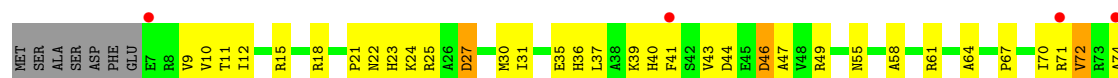
- Molecule 25: 50S ribosomal protein L30P

Chain W:



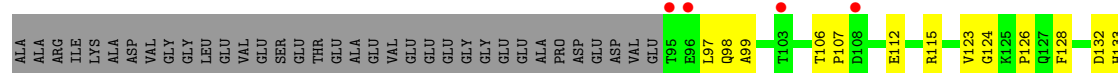
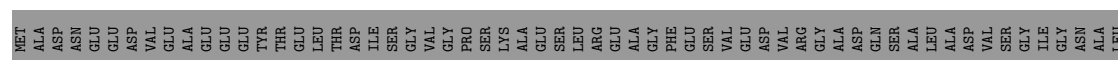
- Molecule 26: 50S ribosomal protein L31e

Chain X:



- Molecule 27: 50S ribosomal protein L32E

Chain Y:



- Molecule 28: 50S ribosomal protein L37Ae

Chain Z:



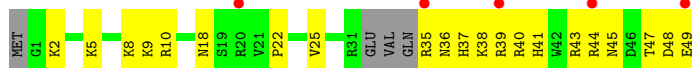
- Molecule 29: 50S ribosomal protein L37e

Chain 1:



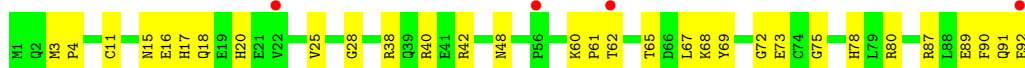
- Molecule 30: 50S ribosomal protein L39e

Chain 2:



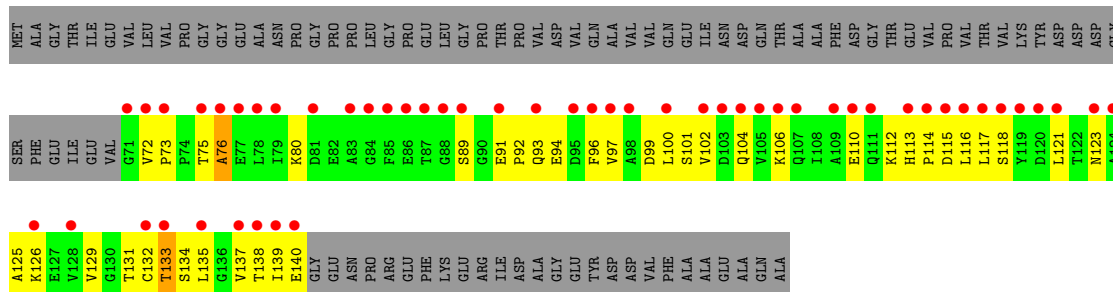
- Molecule 31: 50S ribosomal protein L44E

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, α , β , γ	213.00Å 301.03Å 575.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 49.83 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.70) 94.8 (49.83-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.190 , 0.230 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.4	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 505940 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	98999	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, NA, K, PO2, CD, 5AA, OMU, UR3, 2OP, 1MA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.38	0/65959	0.69	20/102870 (0.0%)
2	9	0.35	0/2905	0.71	2/4528 (0.0%)
3	4	0.46	0/102	0.73	0/149
4	A	0.31	0/1786	0.65	0/2408
5	B	0.34	0/2690	0.65	0/3652
6	C	0.37	0/1884	0.65	1/2551 (0.0%)
7	D	0.30	0/1111	0.53	0/1498
8	E	0.33	0/1382	0.58	0/1880
9	F	0.30	0/901	0.54	0/1224
10	G	0.30	0/241	0.49	0/324
11	H	0.35	0/1287	0.67	0/1725
12	J	0.37	0/1136	0.63	0/1530
13	K	0.36	0/1001	0.69	0/1347
14	L	0.33	0/1130	0.64	0/1509
15	M	0.33	0/1584	0.61	0/2119
16	N	0.30	0/1474	0.63	0/1999
17	O	0.31	0/874	0.56	0/1181
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.36	0/749	0.72	0/1005
20	R	0.36	0/1172	0.65	0/1578
21	S	0.32	0/648	0.57	0/875
22	T	0.32	0/958	0.61	0/1289
23	U	0.34	0/417	0.58	0/562
24	V	0.27	0/502	0.54	0/675
25	W	0.36	0/1219	0.63	0/1655
26	X	0.36	0/664	0.58	0/895
27	Y	0.37	0/1146	0.64	0/1536
28	Z	0.36	0/589	0.67	0/787
29	1	0.36	0/438	0.62	0/578
30	2	0.33	0/401	0.52	0/529
31	3	0.38	0/771	0.58	0/1024
32	I	0.30	0/526	0.54	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.37	0/98794	0.67	23/147726 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	47
2	9	0	2
3	4	0	1
25	W	0	1
All	All	0	51

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	8.54	128.28	109.50
1	0	1942	A	C5'-C4'-C3'	8.16	129.06	116.00
1	0	1979	G	C2'-C3'-O3'	6.72	124.45	113.70
1	0	871	G	C5'-C4'-O4'	-6.61	101.17	109.10
2	9	3039	U	N1-C1'-C2'	6.29	122.18	114.00
1	0	2313	C	C5'-C4'-O4'	6.29	116.65	109.10
1	0	2291	A	N9-C1'-C2'	6.28	122.16	114.00
2	9	3065	A	N9-C1'-C2'	6.26	122.14	114.00
1	0	1504	A	C1'-O4'-C4'	-6.11	105.01	109.90
1	0	2467	A	C1'-O4'-C4'	-5.87	105.21	109.90
1	0	2541	U	C2'-C3'-O3'	5.70	122.83	113.70
1	0	206	G	C5'-C4'-C3'	-5.49	107.22	116.00
1	0	1504	A	N9-C1'-C2'	5.34	120.94	114.00
1	0	1979	G	N9-C1'-C2'	5.28	120.87	114.00
1	0	2526	C	N1-C1'-C2'	5.21	120.77	114.00
1	0	777	U	O4'-C1'-N1	5.16	112.33	108.20
1	0	2313	C	C1'-O4'-C4'	-5.14	105.79	109.90
1	0	2313	C	C5'-C4'-C3'	5.10	124.15	116.00
6	C	73	LEU	CA-CB-CG	-5.09	103.58	115.30
1	0	2607	U	N1-C1'-C2'	5.09	120.62	114.00
1	0	1942	A	C5'-C4'-O4'	5.07	115.19	109.10
1	0	381	G	N9-C1'-C2'	5.07	120.59	114.00
1	0	69	A	C5'-C4'-O4'	-5.07	103.02	109.10

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1351	G	Sidechain
1	0	1377	C	Sidechain
1	0	1417	G	Sidechain
1	0	1614	G	Sidechain
1	0	1681	G	Sidechain
1	0	1744	G	Sidechain
1	0	1829	A	Sidechain
1	0	1835	U	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	191	A	Sidechain
1	0	1970	G	Sidechain
1	0	221	G	Sidechain
1	0	2312	G	Sidechain
1	0	2316	G	Sidechain
1	0	2395	A	Sidechain
1	0	24	G	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2526	C	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2673	U	Sidechain
1	0	2679	G	Sidechain
1	0	2840	A	Sidechain
1	0	2842	G	Sidechain
1	0	417	G	Sidechain
1	0	471	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	781	C	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	882	A	Sidechain
1	0	952	G	Sidechain
3	4	176	DA	Sidechain
2	9	3039	U	Sidechain
2	9	3065	A	Sidechain
25	W	90	TYR	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	849	0
2	9	2600	0	1326	65	0
3	4	127	0	75	4	0
4	A	1753	0	1766	119	0
5	B	2625	0	2533	159	0
6	C	1859	0	1816	127	0
7	D	1094	0	1085	91	0
8	E	1357	0	1266	64	0
9	F	890	0	843	56	0
10	G	240	0	231	13	0
11	H	1266	0	1268	70	0
12	J	1120	0	1098	55	0
13	K	992	0	1031	65	0
14	L	1118	0	1076	55	0
15	M	1560	0	1568	70	0
16	N	1445	0	1401	107	0
17	O	865	0	873	39	0
18	P	1136	0	1123	44	0
19	Q	735	0	729	23	0
20	R	1149	0	1122	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	S	641	0	605	21	0
22	T	950	0	923	61	0
23	U	410	0	364	24	0
24	V	499	0	511	33	0
25	W	1196	0	1137	95	0
26	X	654	0	653	50	0
27	Y	1130	0	1133	55	0
28	Z	578	0	539	27	0
29	1	431	0	426	30	0
30	2	396	0	413	27	0
31	3	755	0	728	31	0
32	I	519	0	500	54	0
33	0	108	0	0	0	0
33	3	1	0	0	0	0
33	9	2	0	0	0	0
33	A	2	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	3	0	0	0	0
35	0	72	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	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	1	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	K	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	1	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	R	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5764	0	0	97	0
38	1	61	0	0	3	0
38	2	42	0	0	3	0
38	3	71	0	0	5	0
38	4	3	0	0	0	0
38	9	133	0	0	4	0
38	A	116	0	0	18	0
38	B	143	0	0	23	0
38	C	173	0	0	21	0
38	D	44	0	0	8	0
38	E	43	0	0	5	0
38	F	24	0	0	4	0
38	G	17	0	0	0	0
38	H	66	0	0	9	0
38	I	9	0	0	2	0
38	J	52	0	0	3	0
38	K	57	0	0	8	0
38	L	81	0	0	11	0
38	M	115	0	0	4	0
38	N	61	0	0	10	0
38	O	45	0	0	6	0
38	P	63	0	0	3	0
38	Q	52	0	0	1	0
38	R	89	0	0	5	0
38	S	31	0	0	2	0
38	T	36	0	0	2	0
38	U	26	0	0	0	0
38	V	13	0	0	1	0
38	W	70	0	0	5	0
38	X	31	0	0	5	0
38	Y	93	0	0	7	0
38	Z	31	0	0	1	0
All	All	98999	0	59974	2378	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 16.

All (2378) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:9:3006:C:H5"	16:N:37:ARG:NH1	1.64	1.13
6:C:236:THR:HG22	6:C:239:ALA:H	1.11	1.13
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.32	1.11
2:9:3006:C:H5"	16:N:37:ARG:HH12	1.08	1.07
1:0:1160:G:H5'	1:0:1161:A:H5'	1.34	1.04
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.71	1.04
1:0:156:C:H5"	15:M:171:ARG:HD3	1.38	1.03
12:J:19:MET:HE3	12:J:132:LEU:HD21	1.37	1.03
1:0:1242:A:H5'	12:J:82:THR:HG23	1.40	1.03
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.39	1.02
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.02	1.01
28:Z:10:ARG:HA	38:Z:9216:HOH:O	1.57	1.01
5:B:238:ASN:HD22	5:B:240:GLY:H	1.06	1.00
13:K:10:GLN:H	13:K:10:GLN:HE21	1.05	1.00
4:A:211:LYS:HB3	4:A:212:PRO:HD2	1.43	0.99
1:0:2364:A:H5"	19:Q:15:LYS:HD3	1.45	0.98
1:0:871:G:H8	1:0:871:G:H5'	1.27	0.97
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.44	0.97
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.45	0.96
1:0:871:G:C8	1:0:871:G:H5'	1.99	0.96
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.46	0.96
1:0:56:G:H5"	24:V:50:ARG:HH12	1.31	0.95
1:0:1751:G:H2'	1:0:1752:G:H5"	1.46	0.95
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.47	0.95
1:0:870:G:H2'	1:0:871:G:H5"	1.45	0.94
2:9:3056:A:H2'	2:9:3057:A:H5"	1.48	0.94
18:P:115:SER:H	18:P:118:GLN:HE21	0.96	0.94
9:F:91:VAL:HG12	9:F:92:GLY:H	1.32	0.92
7:D:154:LYS:HD2	7:D:154:LYS:H	1.31	0.92
1:0:1187:U:HO2'	1:0:1189:A:H2	1.10	0.91
20:R:39:THR:HG22	20:R:42:GLU:H	1.35	0.91
1:0:1474:C:H6	1:0:1474:C:H5'	1.36	0.91
13:K:39:GLY:HA2	38:K:4183:HOH:O	1.71	0.91
1:0:1835:U:H5	1:0:1840:A:N7	1.69	0.90
2:9:3076:G:H3'	2:9:3077:A:H5"	1.52	0.90
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.33	0.90
21:S:57:THR:HG22	21:S:59:ASP:H	1.37	0.90
1:0:2717:C:H2'	1:0:2718:C:H5"	1.53	0.90
15:M:164:THR:HG22	15:M:167:GLY:H	1.36	0.89
13:K:10:GLN:H	13:K:10:GLN:NE2	1.70	0.89
1:0:2717:C:C2'	1:0:2718:C:H5"	2.03	0.88
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.56	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1116:U:HO2'	1:0:1118:A:H2	0.89	0.88
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.55	0.88
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.89	0.88
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.15	0.88
1:0:2812:A:H2	1:0:2814:A:H62	1.22	0.88
1:0:2506:A:HO2'	1:0:2507:G:H8	0.89	0.87
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.53	0.87
24:V:1:THR:HG23	24:V:2:VAL:H	1.36	0.87
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.56	0.87
6:C:1:MET:HG2	6:C:2:GLN:H	1.38	0.87
1:0:506:G:H22	1:0:509:A:H5'	1.40	0.87
1:0:56:G:H5''	24:V:50:ARG:NH1	1.90	0.87
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.56	0.86
18:P:115:SER:N	18:P:118:GLN:HE21	1.74	0.85
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.56	0.85
7:D:25:MET:HE3	7:D:37:ALA:HB1	1.59	0.85
5:B:179:LEU:O	5:B:183:GLU:HG2	1.75	0.85
1:0:282:C:H1'	1:0:368:C:N4	1.91	0.85
16:N:144:GLY:O	16:N:147:ILE:HG22	1.76	0.85
1:0:2533:C:H6	1:0:2533:C:H5'	1.42	0.84
1:0:1162:G:H1'	32:I:117:LEU:HD11	1.59	0.84
25:W:88:THR:HG22	25:W:89:ASP:H	1.41	0.84
6:C:236:THR:HG22	6:C:239:ALA:N	1.90	0.84
1:0:1667:A:H8	1:0:1667:A:H5'	1.42	0.84
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.59	0.83
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.42	0.83
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.44	0.83
1:0:1160:G:C5'	1:0:1161:A:H5'	2.08	0.83
32:I:99:ASP:OD1	32:I:138:THR:HB	1.77	0.83
1:0:21:G:H5'	20:R:2:ILE:HA	1.61	0.83
1:0:545:G:H8	1:0:545:G:H5'	1.44	0.83
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.59	0.82
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.61	0.82
30:2:41:HIS:H	30:2:45:ASN:HD22	1.23	0.82
6:C:78:ARG:HG3	6:C:78:ARG:HH11	1.44	0.82
1:0:2506:A:O2'	1:0:2507:G:H8	1.61	0.82
1:0:2890:A:H1'	23:U:56:ARG:NH2	1.94	0.82
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.60	0.82
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.62	0.82
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.62	0.82
18:P:115:SER:H	18:P:118:GLN:NE2	1.76	0.81
25:W:88:THR:HB	38:W:6679:HOH:O	1.80	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.79	0.81
13:K:10:GLN:N	13:K:10:GLN:HE21	1.79	0.81
24:V:57:LYS:HA	24:V:60:GLN:HE21	1.46	0.81
1:0:1372:A:H3'	38:0:7376:HOH:O	1.81	0.80
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.44	0.80
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.81	0.80
4:A:36:ASP:OD2	4:A:85:SER:HB2	1.79	0.80
2:9:3006:C:C5'	16:N:37:ARG:NH1	2.45	0.80
1:0:1593:C:H5'	18:P:116:SER:O	1.81	0.80
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.46	0.79
1:0:559:U:H5'	1:0:559:U:H6	1.47	0.79
1:0:870:G:C2'	1:0:871:G:H5''	2.11	0.79
5:B:62:ARG:HA	5:B:65:MET:HE3	1.62	0.79
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.48	0.79
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.64	0.79
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.63	0.79
9:F:46:GLU:O	9:F:73:PRO:HD2	1.83	0.79
1:0:1116:U:O2'	1:0:1118:A:H2	1.66	0.79
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.64	0.79
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.81	0.78
1:0:506:G:H22	1:0:509:A:C5'	1.95	0.78
16:N:176:ARG:HE	16:N:180:LEU:HD21	1.48	0.78
1:0:542:A:H5'	1:0:542:A:H8	1.48	0.78
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.65	0.78
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.13	0.78
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.49	0.78
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.66	0.78
7:D:99:ASP:HB3	7:D:103:ASN:H	1.47	0.78
1:0:21:G:C5'	20:R:2:ILE:HA	2.14	0.77
1:0:1116:U:H3	1:0:1246:A:H62	1.32	0.77
1:0:1180:U:H4'	32:I:91:GLU:HG2	1.64	0.77
1:0:1450:C:H4'	1:0:1451:C:OP2	1.82	0.77
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.65	0.77
8:E:6:GLU:HA	8:E:46:THR:HG22	1.67	0.77
5:B:238:ASN:HD22	5:B:240:GLY:N	1.83	0.77
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.66	0.77
1:0:541:C:H2'	1:0:542:A:H5''	1.65	0.77
22:T:48:VAL:HG11	22:T:96:VAL:HG13	1.66	0.77
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.66	0.76
1:0:541:C:C2'	1:0:542:A:H5''	2.16	0.76
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.67	0.76
28:Z:26:VAL:O	28:Z:30:GLU:HG3	1.85	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:182:ARG:HB2	6:C:184:ARG:NH1	1.99	0.76
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.68	0.76
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.66	0.76
1:0:2908:A:H2'	1:0:2909:G:O4'	1.86	0.76
2:9:3014:G:H8	2:9:3014:G:H5'	1.50	0.76
29:1:21:ARG:HD2	29:1:39:PHE:HB2	1.68	0.76
1:0:1603:A:H5'	1:0:1605:G:O4'	1.86	0.76
1:0:188:C:H5''	15:M:163:LEU:HD21	1.68	0.76
2:9:3039:U:H1'	2:9:3044:A:H61	1.50	0.76
1:0:871:G:H8	1:0:871:G:C5'	1.99	0.76
1:0:1118:A:H3'	1:0:1118:A:C8	2.21	0.76
1:0:1120:U:H6	1:0:1120:U:H5'	1.51	0.75
1:0:2716:G:H5''	5:B:206:THR:HG21	1.66	0.75
1:0:2291:A:C8	1:0:2309:C:H5'	2.21	0.75
1:0:1474:C:C6	1:0:1474:C:H5'	2.21	0.75
16:N:113:SER:HB2	38:N:9357:HOH:O	1.86	0.75
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.69	0.75
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.52	0.75
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.66	0.75
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.16	0.74
32:I:75:THR:HA	32:I:112:LYS:HZ1	1.51	0.74
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.69	0.74
1:0:236:A:H4'	1:0:237:G:H5'	1.69	0.74
1:0:1118:A:H3'	1:0:1118:A:H8	1.51	0.74
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.04	0.74
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.17	0.74
1:0:111:C:O2'	29:1:20:ARG:HG2	1.87	0.74
1:0:1181:A:H5'	32:I:94:GLU:OE2	1.88	0.74
20:R:17:MET:HE1	20:R:19:ARG:NH2	2.02	0.74
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.69	0.74
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.52	0.74
5:B:320:GLN:HE21	5:B:321:PRO:HD2	1.53	0.74
5:B:320:GLN:NE2	5:B:321:PRO:HD2	2.03	0.74
6:C:236:THR:H	6:C:239:ALA:HB3	1.53	0.73
2:9:3056:A:C2'	2:9:3057:A:H5''	2.18	0.73
1:0:1189:A:H1'	1:0:1209:C:O4'	1.89	0.73
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.18	0.73
1:0:1160:G:H5'	1:0:1161:A:C5'	2.15	0.73
31:3:17:HIS:O	31:3:18:GLN:HG3	1.88	0.73
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.03	0.73
16:N:164:ASP:CG	16:N:167:ASP:HA	2.09	0.73
5:B:238:ASN:ND2	5:B:240:GLY:H	1.86	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:657:G:OP1	6:C:27:ARG:NH2	2.21	0.73
5:B:98:THR:HG22	5:B:99:GLU:H	1.53	0.73
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.89	0.73
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.22	0.73
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.04	0.72
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.88	0.72
1:0:1234:U:N3	5:B:244:PRO:HB3	2.03	0.72
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.54	0.72
1:0:396:U:H1'	38:0:7793:HOH:O	1.90	0.72
1:0:289:G:H22	1:0:363:A:H2	1.38	0.72
10:G:16:LYS:O	10:G:20:VAL:HG23	1.90	0.72
1:0:1206:U:H6	1:0:1206:U:H5'	1.55	0.72
16:N:132:ASN:O	16:N:135:VAL:HG12	1.89	0.72
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.72	0.72
1:0:877:G:H5'	1:0:878:G:OP1	1.89	0.72
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.36	0.72
1:0:272:A:H5'	1:0:273:G:OP2	1.90	0.72
4:A:36:ASP:HB2	4:A:83:GLY:HA3	1.72	0.72
1:0:2524:G:H21	1:0:2526:C:N4	1.88	0.72
21:S:57:THR:HG22	21:S:59:ASP:N	2.04	0.72
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.71	0.72
9:F:38:LYS:NZ	15:M:3:SER:HA	2.04	0.72
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.20	0.72
15:M:164:THR:CG2	15:M:167:GLY:H	2.02	0.71
5:B:125:GLU:O	5:B:129:ARG:HG3	1.90	0.71
26:X:78:GLU:HG2	26:X:79:GLU:H	1.55	0.71
1:0:541:C:H2'	1:0:542:A:C5'	2.19	0.71
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.18	0.71
1:0:2426:G:H1'	38:0:6331:HOH:O	1.89	0.71
8:E:100:ASP:HB2	38:E:2789:HOH:O	1.89	0.71
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.91	0.71
1:0:1167:G:H4'	32:I:135:LEU:HD22	1.72	0.71
1:0:2769:C:H2'	1:0:2770:G:O4'	1.90	0.71
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.90	0.71
1:0:1165:G:H4'	1:0:1174:A:O2'	1.89	0.71
1:0:1119:G:N2	1:0:1246:A:C2	2.58	0.71
4:A:43:VAL:HG21	4:A:59:GLU:HG3	1.71	0.71
1:0:2524:G:H21	1:0:2526:C:H41	1.37	0.71
1:0:962:C:H1'	16:N:5:ARG:NH1	2.06	0.71
20:R:14:ALA:HB3	20:R:147:LEU:HB2	1.70	0.71
14:L:133:VAL:HA	38:L:9372:HOH:O	1.91	0.71
20:R:39:THR:HG23	20:R:107:GLU:O	1.90	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:O:73:ASP:HA	17:O:92:VAL:O	1.91	0.71
11:H:169:GLY:HA3	38:H:9187:HOH:O	1.91	0.70
6:C:139:VAL:HG13	38:C:9249:HOH:O	1.89	0.70
1:O:2533:C:C6	1:O:2533:C:H5'	2.25	0.70
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.38	0.70
1:O:1058:A:H2'	1:O:1060:C:H5''	1.71	0.70
7:D:136:ARG:HD2	7:D:155:HIS:O	1.91	0.70
1:O:1751:G:C2'	1:O:1752:G:H5''	2.20	0.70
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.71	0.70
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.72	0.70
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.74	0.70
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.22	0.70
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.72	0.70
11:H:9:ILE:HG23	11:H:126:ARG:CZ	2.21	0.70
24:V:56:ILE:O	24:V:60:GLN:HG3	1.90	0.70
15:M:164:THR:HG22	15:M:167:GLY:N	2.07	0.70
1:O:2587:OMU:H2'	1:O:2589:U:H5''	1.74	0.70
7:D:146:LYS:NZ	16:N:107:ASN:HD21	1.90	0.70
1:O:1119:G:H2'	12:J:52:GLN:NE2	2.06	0.70
30:2:39:ARG:HG2	38:2:3143:HOH:O	1.92	0.70
1:O:2586:U:H3	1:O:2592:G:H22	1.38	0.69
1:O:553:G:P	27:Y:204:ARG:HH22	2.16	0.69
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.73	0.69
1:O:1118:A:H62	1:O:1244:U:H3	1.39	0.69
1:O:1201:C:H2'	1:O:1202:A:H5'	1.74	0.69
18:P:103:THR:HA	18:P:106:ARG:NH1	2.06	0.69
13:K:81:ARG:HB2	13:K:87:ARG:NH1	2.07	0.69
11:H:166:SER:HB2	11:H:167:PRO:CD	2.22	0.69
1:O:544:G:H2'	1:O:545:G:H5''	1.73	0.69
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.74	0.69
23:U:52:THR:CG2	23:U:54:THR:HB	2.23	0.69
24:V:12:THR:HG22	24:V:15:GLU:CG	2.23	0.69
13:K:14:LYS:CB	13:K:45:PRO:HG2	2.23	0.69
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.91	0.69
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.93	0.69
1:O:1205:U:H2'	1:O:1206:U:C5'	2.23	0.68
27:Y:144:ARG:CZ	38:Y:8197:HOH:O	2.40	0.68
24:V:44:GLY:O	24:V:48:GLU:HG2	1.94	0.68
6:C:115:LEU:HD21	6:C:243:VAL:HG13	1.75	0.68
1:O:1351:G:OP1	6:C:96:LYS:NZ	2.25	0.68
1:O:797:A:H4'	28:Z:10:ARG:N	2.08	0.68
12:J:76:ASP:HA	38:J:9361:HOH:O	1.92	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.57	0.68
20:R:99:ALA:HB1	20:R:109:MET:CE	2.22	0.68
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.09	0.68
1:O:1205:U:H2'	1:O:1206:U:H5''	1.75	0.68
1:O:2768:A:H5''	38:O:4707:HOH:O	1.94	0.68
1:O:2768:A:H2'	1:O:2769:C:O4'	1.93	0.68
12:J:131:THR:HG22	12:J:134:GLU:H	1.57	0.68
16:N:154:LEU:HD11	16:N:157:PRO:HA	1.75	0.68
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.06	0.68
32:I:138:THR:HG22	32:I:139:ILE:H	1.58	0.68
24:V:39:ALA:N	24:V:40:PRO:HD2	2.09	0.68
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.31	0.68
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.58	0.68
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.57	0.68
2:9:3039:U:H1'	2:9:3044:A:N6	2.08	0.68
17:O:32:ARG:HD3	17:O:32:ARG:O	1.94	0.68
14:L:37:LYS:HG2	38:L:9334:HOH:O	1.92	0.68
7:D:37:ALA:O	7:D:40:ILE:HG12	1.94	0.68
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.76	0.68
2:9:3064:C:H2'	2:9:3065:A:H5'	1.76	0.68
30:2:41:HIS:HD2	30:2:44:ARG:H	1.41	0.68
1:O:656:G:OP2	17:O:37:ARG:HD2	1.94	0.68
9:F:58:GLU:HA	9:F:61:MET:HG3	1.75	0.67
30:2:36:ASN:O	30:2:39:ARG:HG3	1.93	0.67
5:B:202:VAL:HG11	5:B:301:VAL:HG13	1.77	0.67
1:O:2468:A:H61	31:3:48:ASN:HD21	1.41	0.67
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.57	0.67
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.76	0.67
7:D:50:VAL:O	7:D:71:ALA:HA	1.95	0.67
1:O:157:G:H4'	15:M:95:LYS:HE2	1.77	0.67
24:V:64:GLY:O	24:V:65:ASP:HB2	1.94	0.67
5:B:304:PRO:HD2	5:B:307:ARG:HD2	1.76	0.67
1:O:2252:A:C5	1:O:2253:G:H1'	2.30	0.67
21:S:33:SER:O	21:S:37:VAL:HG23	1.93	0.67
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.95	0.67
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.76	0.67
1:O:1119:G:H2'	12:J:52:GLN:HE22	1.58	0.67
1:O:871:G:C5'	1:O:871:G:C8	2.76	0.67
1:O:1666:C:O2'	1:O:1667:A:H5''	1.95	0.67
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.75	0.67
1:O:1819:G:H5'	38:O:4985:HOH:O	1.93	0.67
1:O:2054:A:N3	20:R:128:ARG:NH2	2.42	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.29	0.67
9:F:46:GLU:OE1	9:F:100:ASP:HA	1.95	0.67
1:0:1701:A:H5'	38:0:6518:HOH:O	1.93	0.67
1:0:1080:C:H4'	1:0:1081:A:OP1	1.94	0.67
6:C:16:VAL:HG12	6:C:17:ASP:H	1.59	0.66
6:C:236:THR:CG2	6:C:239:ALA:H	1.99	0.66
10:G:20:VAL:O	10:G:24:VAL:HG23	1.96	0.66
6:C:7:ASP:OD2	6:C:9:ASP:HB2	1.95	0.66
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.95	0.66
32:I:129:VAL:HG13	32:I:139:ILE:HD11	1.75	0.66
15:M:59:GLY:HA3	15:M:141:ILE:HD11	1.77	0.66
29:1:25:LYS:HD2	30:2:49:GLU:H	1.59	0.66
25:W:88:THR:HG22	25:W:89:ASP:N	2.10	0.66
5:B:5:ARG:HD2	5:B:8:LYS:NZ	2.10	0.66
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.59	0.66
22:T:101:LEU:HD13	22:T:112:LEU:HD11	1.77	0.66
38:0:5785:HOH:O	15:M:58:GLN:HG3	1.95	0.66
1:0:2649:A:H5'	1:0:2649:A:H8	1.60	0.66
1:0:1641:A:H2'	1:0:1642:A:H5'	1.76	0.66
1:0:1666:C:H2'	1:0:1667:A:H5'	1.77	0.66
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.78	0.66
25:W:4:LEU:CD2	25:W:54:PHE:HB3	2.26	0.66
25:W:65:VAL:HA	25:W:68:THR:HG22	1.78	0.66
20:R:6:VAL:HG21	20:R:113:HIS:CD2	2.31	0.66
38:0:7598:HOH:O	22:T:9:LYS:HB2	1.93	0.66
9:F:52:GLU:HG3	9:F:77:VAL:O	1.96	0.66
1:0:2851:G:O2'	1:0:2852:A:H5'	1.96	0.66
32:I:110:GLU:HA	32:I:113:HIS:CD2	2.31	0.65
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.31	0.65
32:I:125:ALA:O	32:I:129:VAL:HG23	1.96	0.65
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.78	0.65
1:0:1130:U:H2'	1:0:1131:G:O4'	1.97	0.65
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.78	0.65
2:9:3029:C:O3'	7:D:138:GLY:HA2	1.97	0.65
1:0:470:U:O2'	29:1:16:HIS:HD2	1.80	0.65
1:0:1189:A:H1'	1:0:1209:C:C1'	2.27	0.65
1:0:870:G:OP2	4:A:3:ARG:HD3	1.97	0.65
1:0:558:C:O2'	1:0:559:U:H5''	1.96	0.65
2:9:3029:C:H2'	2:9:3030:C:H5'	1.78	0.65
11:H:166:SER:CB	11:H:167:PRO:HD3	2.26	0.65
1:0:560:C:H42	1:0:597:A:H61	1.43	0.65
10:G:27:ILE:HD13	10:G:71:LEU:HD23	1.78	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:162:MET:CE	5:B:308:LEU:HD21	2.27	0.65
1:O:820:G:C6	4:A:171:LYS:HB2	2.32	0.65
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.26	0.65
1:O:1681:G:H5''	1:O:1682:A:H5'	1.78	0.65
14:L:67:ARG:O	14:L:71:GLU:HG3	1.96	0.65
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.95	0.65
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.62	0.65
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.78	0.65
12:J:52:GLN:HG3	12:J:53:ILE:N	2.11	0.64
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.12	0.64
1:O:777:U:O2'	29:1:11:LYS:HG2	1.97	0.64
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.32	0.64
1:O:1701:A:H4'	1:O:1702:U:H5''	1.78	0.64
10:G:64:ASN:N	10:G:64:ASN:HD22	1.95	0.64
22:T:48:VAL:HG11	22:T:96:VAL:CG1	2.27	0.64
13:K:98:VAL:HG11	13:K:102:GLU:HA	1.78	0.64
19:Q:18:PRO:O	19:Q:21:ARG:HB2	1.97	0.64
16:N:119:GLN:O	16:N:123:ILE:HG13	1.97	0.64
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.79	0.64
1:O:2827:A:H2'	1:O:2828:G:O4'	1.98	0.64
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.79	0.64
1:O:545:G:C8	1:O:545:G:H5'	2.31	0.64
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.78	0.64
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.12	0.64
8:E:69:ILE:HA	8:E:72:MET:HE3	1.79	0.64
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.80	0.64
1:O:538:C:OP2	27:Y:134:HIS:HE1	1.81	0.64
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.78	0.64
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.78	0.64
12:J:93:ARG:NH1	12:J:93:ARG:HB3	2.12	0.64
2:9:3014:G:C8	2:9:3014:G:H5'	2.32	0.64
1:O:2690:U:O2'	8:E:111:LYS:HE3	1.98	0.64
1:O:380:A:H2'	38:O:7412:HOH:O	1.97	0.64
1:O:2491:G:H1'	38:O:7076:HOH:O	1.98	0.64
1:O:1667:A:C8	1:O:1667:A:H5'	2.31	0.64
1:O:558:C:H2'	1:O:559:U:H5'	1.79	0.64
8:E:69:ILE:HA	8:E:72:MET:CE	2.28	0.63
1:O:1060:C:H6	1:O:1060:C:H5'	1.63	0.63
1:O:1819:G:H2'	1:O:1820:G:H4'	1.79	0.63
7:D:57:THR:HG23	7:D:63:ILE:HA	1.79	0.63
7:D:105:SER:HB2	7:D:131:THR:HG23	1.80	0.63
11:H:27:LYS:H	11:H:59:HIS:HD2	1.46	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:281:U:H2'	1:0:282:C:O4'	1.98	0.63
18:P:134:VAL:O	18:P:137:LEU:HB3	1.98	0.63
16:N:169:PRO:O	16:N:172:PHE:HB3	1.99	0.63
1:0:2896:A:H5''	38:0:6338:HOH:O	1.98	0.63
1:0:285:A:H2'	1:0:286:U:O4'	1.98	0.63
14:L:143:THR:HG22	14:L:144:ASP:N	2.14	0.63
14:L:149:ARG:O	14:L:150:GLN:HB2	1.98	0.63
1:0:2570:G:H5''	38:0:5188:HOH:O	1.99	0.63
7:D:99:ASP:HA	38:D:5675:HOH:O	1.97	0.63
18:P:91:LYS:O	18:P:95:GLU:HG3	1.99	0.63
8:E:145:ALA:HB1	8:E:168:ILE:HD11	1.81	0.63
1:0:447:A:OP1	22:T:2:LYS:HG2	1.98	0.63
25:W:125:HIS:HD2	25:W:127:GLY:H	1.46	0.63
38:0:7629:HOH:O	6:C:188:ARG:HD2	1.96	0.63
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.28	0.63
7:D:57:THR:HG23	7:D:63:ILE:HG22	1.80	0.63
1:0:2414:A:H2'	1:0:2415:A:C8	2.34	0.63
32:I:75:THR:HA	32:I:112:LYS:NZ	2.14	0.63
5:B:41:PHE:CD2	5:B:190:MET:HE3	2.34	0.63
16:N:170:GLU:HA	16:N:173:ASP:OD2	1.98	0.63
1:0:1377:C:H6	1:0:1377:C:H5'	1.64	0.63
38:0:4132:HOH:O	11:H:11:LYS:HE2	1.99	0.63
1:0:1741:U:H5'	1:0:1742:A:OP1	1.98	0.63
21:S:11:THR:H	21:S:14:ALA:HB3	1.64	0.63
1:0:1184:C:H1'	38:0:7636:HOH:O	1.99	0.63
1:0:1130:U:H5'	38:0:7834:HOH:O	1.98	0.62
1:0:1299:G:O6	14:L:6:ARG:HD3	1.98	0.62
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.81	0.62
4:A:65:ARG:C	4:A:66:ARG:HG3	2.19	0.62
1:0:1159:G:H21	1:0:1189:A:H8	1.45	0.62
1:0:1834:C:H2'	1:0:1840:A:N6	2.14	0.62
16:N:47:LEU:HD11	16:N:127:LEU:HD21	1.81	0.62
26:X:41:PHE:O	26:X:43:VAL:HG23	1.98	0.62
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.81	0.62
1:0:2756:U:H3	1:0:2896:A:H2	1.47	0.62
1:0:564:G:H1'	38:0:6543:HOH:O	1.99	0.62
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.61	0.62
2:9:3114:G:O6	16:N:11:ARG:HD3	1.98	0.62
1:0:2320:U:H4'	1:0:2321:A:O4'	1.98	0.62
6:C:145:GLU:HG3	38:C:9175:HOH:O	1.99	0.62
1:0:1187:U:O2'	1:0:1189:A:H2	1.80	0.62
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.82	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:797:A:C4'	28:Z:10:ARG:N	2.62	0.62
26:X:30:MET:HE1	26:X:55:ASN:HA	1.81	0.62
4:A:200:PRO:HG2	4:A:225:VAL:HG21	1.82	0.62
38:O:7228:HOH:O	4:A:211:LYS:HG2	2.00	0.62
1:O:2251:G:H2'	1:O:2252:A:C8	2.34	0.62
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.28	0.62
16:N:154:LEU:O	16:N:155:GLU:HB3	2.00	0.62
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.97	0.62
1:O:2004:U:H4'	38:O:5568:HOH:O	1.99	0.62
7:D:95:THR:OG1	7:D:174:VAL:HG22	1.99	0.62
20:R:9:ASP:O	20:R:13:THR:HB	1.99	0.62
22:T:48:VAL:CG1	22:T:96:VAL:HG13	2.30	0.62
2:9:3002:U:OP2	2:9:3003:A:H5'	1.99	0.62
32:I:134:SER:O	32:I:135:LEU:HD23	2.00	0.62
16:N:110:THR:HB	16:N:113:SER:OG	2.00	0.62
5:B:254:GLN:HG2	5:B:255:GLY:N	2.15	0.62
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.82	0.62
6:C:127:ARG:HH21	6:C:225:PRO:HG2	1.61	0.61
1:O:544:G:C2'	1:O:545:G:H5''	2.30	0.61
16:N:23:ARG:HD3	38:N:9346:HOH:O	1.99	0.61
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.68	0.61
15:M:24:GLN:NE2	15:M:27:ARG:HH11	1.98	0.61
14:L:143:THR:HG21	38:L:9336:HOH:O	1.99	0.61
1:O:926:A:O2'	14:L:41:HIS:HD2	1.81	0.61
9:F:21:GLU:O	9:F:24:ARG:HG3	2.00	0.61
1:O:1086:A:C6	25:W:11:VAL:HG11	2.35	0.61
1:O:2840:A:OP1	5:B:211:THR:HG23	2.00	0.61
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.03	0.61
26:X:25:ARG:HD2	38:X:3861:HOH:O	1.99	0.61
31:3:62:THR:HB	38:3:9349:HOH:O	2.00	0.61
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.16	0.61
1:O:399:C:H5'	15:M:179:GLY:O	2.01	0.61
8:E:11:VAL:HG12	8:E:12:ASP:N	2.16	0.61
2:9:3055:U:H4'	2:9:3056:A:C8	2.36	0.61
25:W:149:LEU:HG	25:W:153:MET:HE2	1.81	0.61
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.82	0.61
22:T:48:VAL:HG13	22:T:97:ARG:O	2.00	0.61
1:O:2256:G:C2'	1:O:2257:G:H5'	2.31	0.61
38:O:7081:HOH:O	15:M:178:LYS:HB2	2.00	0.61
1:O:1625:U:H4'	38:O:4940:HOH:O	2.00	0.61
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.24	0.61
13:K:74:VAL:HG12	13:K:75:ARG:HG3	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:88:ILE:HG22	4:A:88:ILE:O	1.99	0.61
32:I:131:THR:O	32:I:135:LEU:HG	2.01	0.61
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.36	0.61
25:W:125:HIS:CD2	25:W:127:GLY:H	2.19	0.61
1:O:902:G:N7	14:L:18:HIS:HD2	1.98	0.61
15:M:60:VAL:C	15:M:61:ILE:HD12	2.20	0.61
5:B:297:VAL:HB	38:B:9406:HOH:O	2.00	0.61
8:E:137:ASP:O	8:E:141:VAL:HG23	2.01	0.61
1:O:1166:A:H1'	1:O:1192:A:C2	2.36	0.61
27:Y:235:GLU:H	27:Y:235:GLU:CD	2.03	0.61
12:J:6:PHE:HB3	12:J:109:TYR:OH	2.01	0.61
6:C:16:VAL:HG12	6:C:17:ASP:N	2.16	0.60
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.66	0.60
38:O:7626:HOH:O	5:B:211:THR:HG21	2.01	0.60
1:O:848:C:H5'	38:O:7455:HOH:O	1.99	0.60
5:B:140:LEU:HD23	38:B:9378:HOH:O	1.99	0.60
1:O:2346:C:O5'	1:O:2346:C:H6	1.84	0.60
15:M:64:ARG:HD2	38:M:9378:HOH:O	2.00	0.60
1:O:1189:A:O2'	1:O:1208:C:H2'	2.00	0.60
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.17	0.60
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.65	0.60
25:W:38:THR:HG22	25:W:39:ASP:H	1.67	0.60
11:H:166:SER:CB	11:H:167:PRO:CD	2.78	0.60
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.83	0.60
12:J:99:GLU:HA	38:J:9371:HOH:O	2.01	0.60
1:O:1266:U:H4'	27:Y:115:ARG:HH21	1.65	0.60
1:O:282:C:O2'	1:O:283:U:H5'	2.01	0.60
16:N:152:GLU:C	16:N:154:LEU:H	2.03	0.60
1:O:2256:G:H2'	1:O:2257:G:H5'	1.83	0.60
11:H:23:ILE:HA	11:H:120:ILE:HG21	1.82	0.60
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.84	0.60
11:H:63:GLU:HA	38:H:9177:HOH:O	2.00	0.60
1:O:2502:C:C2'	1:O:2503:A:H5'	2.32	0.60
1:O:449:A:N7	6:C:43:LYS:HG2	2.16	0.60
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.16	0.60
1:O:2504:A:H4'	11:H:71:ARG:HH11	1.67	0.60
1:O:793:A:H5''	18:P:83:LYS:HG2	1.83	0.60
7:D:13:MET:HA	7:D:137:PRO:HG2	1.83	0.60
11:H:45:VAL:HA	11:H:167:PRO:O	2.01	0.60
9:F:91:VAL:HG12	9:F:92:GLY:N	2.09	0.60
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.32	0.60
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:210:GLY:HA3	38:A:9380:HOH:O	2.02	0.60
4:A:194:MET:CE	4:A:199:HIS:HB2	2.31	0.60
6:C:33:LYS:HE2	38:C:9160:HOH:O	2.01	0.60
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.83	0.60
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.42	0.60
1:O:1119:G:H8	12:J:52:GLN:HE22	1.48	0.60
1:O:2837:U:H1'	5:B:307:ARG:HH12	1.67	0.60
6:C:233:THR:HG22	6:C:234:VAL:N	2.17	0.60
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.32	0.60
1:O:338:C:H4'	6:C:174:ILE:CD1	2.32	0.60
16:N:27:LEU:HD13	16:N:50:LEU:HD21	1.82	0.59
14:L:136:ALA:HB3	38:L:9372:HOH:O	2.01	0.59
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.84	0.59
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.32	0.59
4:A:211:LYS:HB3	4:A:212:PRO:CD	2.25	0.59
10:G:64:ASN:O	10:G:68:GLU:HG3	2.02	0.59
5:B:150:ALA:O	5:B:152:PRO:HD3	2.02	0.59
2:9:3055:U:H4'	2:9:3056:A:H8	1.67	0.59
15:M:164:THR:HG23	15:M:165:GLY:N	2.17	0.59
1:O:485:A:N3	1:O:487:G:H5''	2.17	0.59
29:1:10:LYS:HG3	38:1:9236:HOH:O	2.01	0.59
1:O:120:A:H5'	29:1:20:ARG:HH21	1.68	0.59
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.36	0.59
1:O:1926:G:H2'	1:O:1927:A:C8	2.36	0.59
14:L:61:ALA:HA	38:L:9363:HOH:O	2.03	0.59
1:O:1441:G:O2'	1:O:1442:A:H5'	2.02	0.59
26:X:43:VAL:HG12	26:X:44:ASP:N	2.17	0.59
1:O:1118:A:H2'	1:O:1120:U:H5''	1.84	0.59
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.84	0.59
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.84	0.59
7:D:22:VAL:HG22	7:D:74:THR:HG22	1.84	0.59
1:O:2748:G:H5'	38:O:7705:HOH:O	2.02	0.59
2:9:3064:C:C2'	2:9:3065:A:H5'	2.33	0.59
1:O:121:U:OP2	30:2:10:ARG:NH2	2.32	0.59
1:O:1299:G:N7	14:L:6:ARG:NH1	2.50	0.59
25:W:38:THR:HG22	25:W:39:ASP:N	2.18	0.59
21:S:52:VAL:C	21:S:53:ASN:HD22	2.06	0.59
4:A:94:LEU:HG	4:A:99:ILE:CD1	2.31	0.59
4:A:94:LEU:N	4:A:94:LEU:HD23	2.18	0.59
4:A:194:MET:HE2	4:A:199:HIS:HB2	1.85	0.59
1:O:65:C:O2'	1:O:66:G:H5'	2.02	0.59
1:O:625:U:H5''	1:O:1044:C:N4	2.17	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2668:G:H2'	1:0:2669:U:C6	2.38	0.59
7:D:10:PHE:CG	7:D:11:HIS:N	2.71	0.59
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.84	0.59
7:D:166:ILE:HB	38:D:6326:HOH:O	2.03	0.59
12:J:74:ARG:CB	12:J:74:ARG:HH11	2.13	0.59
2:9:3028:U:H5''	16:N:40:ASN:HD21	1.67	0.59
32:I:76:ALA:O	32:I:80:LYS:HG3	2.01	0.59
30:2:5:LYS:O	30:2:9:LYS:HG3	2.03	0.59
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.33	0.59
1:0:1733:A:H4'	5:B:212:GLN:HA	1.84	0.59
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.38	0.59
14:L:143:THR:HG22	14:L:145:LEU:H	1.66	0.59
1:0:1213:C:O2'	1:0:1214:G:H5'	2.03	0.59
1:0:1813:U:O2'	18:P:81:LYS:HE3	2.03	0.59
4:A:39:ALA:HB3	4:A:61:GLU:OE2	2.02	0.59
27:Y:212:ARG:HD2	38:Y:8187:HOH:O	2.02	0.59
1:0:88:G:H5'	1:0:88:G:H8	1.68	0.59
5:B:16:ARG:NH1	38:B:9416:HOH:O	2.36	0.59
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.33	0.59
31:3:73:GLU:HB3	38:3:9360:HOH:O	2.02	0.59
26:X:25:ARG:HD3	26:X:64:ALA:O	2.01	0.59
5:B:16:ARG:HB3	5:B:217:ARG:NH2	2.18	0.58
38:0:7333:HOH:O	29:1:1:THR:HB	2.01	0.58
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.38	0.58
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.76	0.58
1:0:2649:A:H5'	1:0:2649:A:C8	2.38	0.58
1:0:2779:G:H21	8:E:143:GLN:NE2	2.01	0.58
1:0:2502:C:H2'	1:0:2503:A:H5'	1.84	0.58
1:0:381:G:H5''	38:0:4603:HOH:O	2.02	0.58
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.84	0.58
4:A:217:ARG:HH11	4:A:217:ARG:HG3	1.67	0.58
2:9:3092:G:H2'	2:9:3093:A:C8	2.38	0.58
4:A:8:ARG:HG2	38:A:9349:HOH:O	2.03	0.58
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.03	0.58
11:H:167:PRO:O	11:H:168:ALA:HB2	2.02	0.58
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.32	0.58
20:R:40:ALA:O	20:R:44:VAL:HG23	2.03	0.58
1:0:2717:C:H2'	1:0:2718:C:C5'	2.31	0.58
1:0:1450:C:O2'	1:0:1494:A:H5'	2.03	0.58
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.84	0.58
5:B:307:ARG:HB2	5:B:307:ARG:HH11	1.68	0.58
5:B:41:PHE:HB3	5:B:190:MET:HE3	1.84	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.38	0.58
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.67	0.58
1:0:2546:U:H5	5:B:2:GLN:HE22	1.50	0.58
20:R:132:ARG:HG2	20:R:133:ALA:N	2.17	0.58
1:0:1730:G:H5'	1:0:1731:C:C5	2.38	0.58
7:D:25:MET:HE3	7:D:37:ALA:CB	2.31	0.58
1:0:2524:G:N2	1:0:2526:C:H41	2.01	0.58
1:0:2094:G:H4'	5:B:245:SER:HB3	1.84	0.58
1:0:2365:G:H4'	19:Q:45:PRO:O	2.03	0.58
6:C:154:VAL:O	6:C:158:GLU:HG3	2.03	0.58
1:0:31:C:H4'	38:0:7598:HOH:O	2.03	0.58
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.51	0.58
1:0:1741:U:O2'	1:0:2723:G:H4'	2.04	0.58
32:I:139:ILE:HG22	32:I:140:GLU:N	2.19	0.58
22:T:48:VAL:HG12	22:T:49:GLU:N	2.18	0.58
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.37	0.58
25:W:13:MET:HE1	25:W:18:GLN:HA	1.86	0.58
1:0:2578:G:H5'	1:0:2578:G:H8	1.69	0.58
1:0:2241:C:H2'	1:0:2242:U:C6	2.39	0.58
32:I:72:VAL:HG13	32:I:73:PRO:HD2	1.85	0.58
26:X:31:ILE:O	26:X:35:GLU:HG3	2.03	0.58
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.34	0.58
13:K:62:PRO:CG	13:K:65:ARG:HH21	2.16	0.58
6:C:182:ARG:HB2	6:C:184:ARG:HH12	1.68	0.58
1:0:1527:A:H1'	1:0:1528:A:C8	2.38	0.58
25:W:4:LEU:O	25:W:32:CYS:HA	2.04	0.58
20:R:145:LEU:HD12	20:R:146:ILE:N	2.19	0.58
1:0:447:A:O2'	1:0:448:G:H5'	2.04	0.58
11:H:120:ILE:N	11:H:120:ILE:HD12	2.19	0.58
1:0:1180:U:H1'	38:0:3528:HOH:O	2.03	0.58
8:E:31:ARG:HH12	8:E:68:HIS:CD2	2.22	0.58
1:0:962:C:H1'	16:N:5:ARG:HH12	1.68	0.58
17:O:37:ARG:HG3	38:O:3002:HOH:O	2.03	0.58
1:0:1790:C:H2'	1:0:1791:U:H6	1.69	0.58
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.84	0.58
1:0:182:G:H5'	38:0:5426:HOH:O	2.03	0.58
1:0:1835:U:C5	1:0:1840:A:N7	2.61	0.57
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.86	0.57
6:C:168:ARG:NH2	6:C:190:ALA:O	2.37	0.57
12:J:19:MET:HE2	12:J:132:LEU:HD11	1.85	0.57
25:W:84:VAL:HG12	38:W:6679:HOH:O	2.03	0.57
32:I:138:THR:HG22	32:I:139:ILE:N	2.19	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:U:17:THR:HG22	23:U:18:GLY:N	2.19	0.57
1:0:644:G:N3	1:0:644:G:H5'	2.18	0.57
25:W:108:ARG:HE	25:W:114:PRO:CG	2.17	0.57
1:0:2256:G:H2'	1:0:2257:G:C5'	2.35	0.57
20:R:47:LEU:O	20:R:51:ILE:HG13	2.04	0.57
5:B:55:ASN:HB3	5:B:63:GLU:HA	1.86	0.57
18:P:9:LEU:O	18:P:13:VAL:HG12	2.03	0.57
7:D:39:ASP:O	7:D:43:GLU:HG3	2.03	0.57
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.70	0.57
4:A:121:ALA:O	4:A:124:VAL:HG22	2.04	0.57
4:A:109:GLU:HG2	4:A:116:GLY:N	2.18	0.57
15:M:61:ILE:N	15:M:61:ILE:HD12	2.19	0.57
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.87	0.57
1:0:1008:C:H5''	11:H:16:ARG:HH12	1.70	0.57
27:Y:200:THR:HG22	27:Y:201:GLU:HG2	1.86	0.57
1:0:2878:U:H2'	1:0:2879:A:O4'	2.04	0.57
25:W:88:THR:CG2	25:W:110:GLN:NE2	2.68	0.57
13:K:55:VAL:HG12	13:K:56:SER:N	2.20	0.57
1:0:1182:C:H1'	1:0:1192:A:H8	1.68	0.57
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.19	0.57
1:0:2508:C:H2'	38:0:6966:HOH:O	2.04	0.57
18:P:64:GLU:HG2	38:P:170:HOH:O	2.05	0.57
1:0:2679:G:H2'	1:0:2681:A:OP2	2.05	0.57
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.18	0.57
16:N:80:SER:HB2	38:N:9336:HOH:O	2.04	0.57
1:0:703:G:O2'	1:0:704:C:H5'	2.05	0.57
5:B:275:GLY:O	5:B:291:ASP:HA	2.05	0.57
8:E:80:TRP:O	8:E:134:SER:HA	2.05	0.57
30:2:36:ASN:HB3	30:2:39:ARG:HE	1.70	0.57
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.87	0.57
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.34	0.57
1:0:1163:G:H5'	32:I:115:ASP:O	2.05	0.57
17:O:87:THR:O	17:O:91:GLN:HG3	2.04	0.57
1:0:1118:A:C8	1:0:1118:A:C3'	2.85	0.57
1:0:1926:G:H2'	1:0:1927:A:H8	1.70	0.57
1:0:960:G:H2'	1:0:960:G:N3	2.20	0.57
21:S:17:ASP:HB3	21:S:23:LYS:HB2	1.87	0.57
6:C:35:VAL:HG21	6:C:227:GLY:HA2	1.86	0.57
5:B:280:VAL:CG1	5:B:334:SER:HA	2.35	0.57
20:R:145:LEU:HD12	20:R:146:ILE:H	1.70	0.56
1:0:256:C:H2'	1:0:257:G:O4'	2.05	0.56
14:L:77:ALA:HB3	38:L:9329:HOH:O	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1189:A:H3'	38:0:7842:HOH:O	2.04	0.56
4:A:82:VAL:HG13	4:A:93:THR:HB	1.87	0.56
9:F:38:LYS:HZ1	15:M:3:SER:HA	1.68	0.56
29:1:25:LYS:O	29:1:25:LYS:HG2	2.05	0.56
1:0:2346:C:O2'	7:D:52:THR:HG21	2.04	0.56
9:F:96:ALA:HA	38:F:3111:HOH:O	2.04	0.56
2:9:3041:C:H4'	7:D:48:MET:HB2	1.87	0.56
1:0:2265:U:H2'	1:0:2266:A:C8	2.40	0.56
1:0:1462:C:H2'	1:0:1463:A:C8	2.41	0.56
1:0:280:C:H2'	1:0:281:U:O4'	2.05	0.56
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.34	0.56
7:D:135:VAL:HG22	7:D:136:ARG:N	2.20	0.56
24:V:39:ALA:N	24:V:40:PRO:CD	2.69	0.56
1:0:2256:G:O2'	1:0:2257:G:H5'	2.05	0.56
1:0:1657:A:H2'	1:0:1658:A:C8	2.40	0.56
2:9:3054:A:O2'	2:9:3055:U:H5'	2.06	0.56
23:U:9:CYS:HA	23:U:52:THR:HG23	1.87	0.56
21:S:33:SER:OG	21:S:36:GLU:HG3	2.06	0.56
1:0:2415:A:C2	16:N:25:ARG:HB3	2.41	0.56
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.35	0.56
5:B:305:ASP:O	5:B:306:LYS:HB2	2.06	0.56
1:0:2563:U:H2'	1:0:2565:C:O5'	2.05	0.56
38:0:4274:HOH:O	22:T:82:THR:HA	2.06	0.56
1:0:1314:U:H2'	38:0:6124:HOH:O	2.03	0.56
22:T:35:TYR:CD2	22:T:112:LEU:HD22	2.40	0.56
1:0:1682:A:H5''	38:0:9763:HOH:O	2.06	0.56
1:0:602:A:O2'	1:0:605:C:H4'	2.04	0.56
1:0:1535:G:H2'	1:0:1536:C:C6	2.41	0.56
32:I:75:THR:CA	32:I:112:LYS:HZ1	2.19	0.56
1:0:119:A:H2'	1:0:120:A:H5''	1.88	0.56
23:U:14:GLU:O	23:U:17:THR:HB	2.05	0.56
22:T:24:ARG:HH21	22:T:39:ASN:ND2	2.04	0.56
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.88	0.56
1:0:820:G:OP2	4:A:171:LYS:NZ	2.37	0.56
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.52	0.56
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.40	0.56
18:P:7:LYS:HD3	18:P:21:VAL:CG2	2.36	0.56
1:0:709:G:O2'	17:O:25:VAL:HG12	2.05	0.56
31:3:87:ARG:HD2	31:3:89:GLU:OE2	2.06	0.56
23:U:52:THR:HG21	23:U:54:THR:HB	1.87	0.56
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.41	0.56
2:9:3049:G:O2'	2:9:3050:G:H5'	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:136:C:H2'	1:0:137:U:O4'	2.06	0.56
1:0:2271:G:H5'	38:0:5025:HOH:O	2.06	0.56
24:V:1:THR:HG23	24:V:2:VAL:N	2.15	0.55
23:U:52:THR:HG22	23:U:54:THR:N	2.21	0.55
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.39	0.55
1:0:1778:A:H2'	1:0:1779:A:H5'	1.88	0.55
7:D:51:ARG:HD3	38:D:7636:HOH:O	2.06	0.55
20:R:3:SER:HA	38:R:9348:HOH:O	2.06	0.55
18:P:115:SER:O	18:P:117:SER:N	2.36	0.55
2:9:3013:A:O2'	2:9:3014:G:H5''	2.05	0.55
1:0:2769:C:C2'	1:0:2770:G:H5'	2.36	0.55
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.06	0.55
8:E:23:GLU:HG2	8:E:28:SER:CB	2.35	0.55
6:C:109:LEU:O	6:C:109:LEU:HD12	2.05	0.55
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.88	0.55
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.06	0.55
1:0:426:G:H2'	1:0:427:C:O4'	2.07	0.55
2:9:3006:C:OP1	16:N:37:ARG:NH1	2.39	0.55
1:0:2718:C:H6	1:0:2718:C:H5'	1.71	0.55
4:A:35:GLY:O	4:A:36:ASP:HB3	2.06	0.55
5:B:198:GLU:HA	38:B:9454:HOH:O	2.06	0.55
1:0:290:C:H1'	38:0:6342:HOH:O	2.05	0.55
4:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.87	0.55
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.88	0.55
1:0:1766:U:O2	1:0:1778:A:H5'	2.07	0.55
1:0:660:A:H4'	1:0:661:G:O5'	2.07	0.55
3:4:176:DA:O4'	3:4:175:C:H2'	2.06	0.55
13:K:115:ARG:HG3	13:K:116:GLU:N	2.20	0.55
1:0:2755:G:H1'	38:0:4956:HOH:O	2.06	0.55
1:0:1909:A:H2'	1:0:1910:A:C8	2.40	0.55
7:D:86:THR:C	7:D:89:PRO:HD2	2.27	0.55
25:W:73:LEU:O	25:W:74:GLU:HG3	2.06	0.55
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.20	0.55
6:C:111:VAL:HB	38:C:9123:HOH:O	2.07	0.55
1:0:968:G:O2'	1:0:969:G:H5'	2.07	0.55
25:W:119:HIS:HD2	25:W:120:PRO:O	1.89	0.55
1:0:1506:U:H6	1:0:1506:U:H5'	1.72	0.55
20:R:39:THR:HB	20:R:42:GLU:HG3	1.89	0.55
1:0:2505:G:O2'	1:0:2506:A:H5'	2.07	0.55
20:R:104:PHE:HB2	20:R:109:MET:HE1	1.88	0.55
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.88	0.55
5:B:88:GLU:HB3	5:B:97:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1687:C:O2	29:1:9:GLY:HA2	2.06	0.55
1:0:1972:U:H2'	1:0:1973:A:H5'	1.88	0.55
12:J:19:MET:HE1	12:J:78:ILE:HG22	1.89	0.55
1:0:1242:A:C5'	12:J:82:THR:HG23	2.25	0.55
1:0:2768:A:O2'	1:0:2769:C:H5'	2.07	0.55
21:S:37:VAL:O	21:S:41:VAL:HG23	2.06	0.55
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.88	0.55
1:0:681:G:N3	1:0:681:G:H5'	2.22	0.55
1:0:1505:U:H6	1:0:1505:U:H5'	1.70	0.55
11:H:9:ILE:O	11:H:9:ILE:HG22	2.07	0.55
25:W:80:ASP:O	25:W:84:VAL:HG23	2.06	0.55
17:O:21:SER:OG	17:O:106:PRO:HB2	2.07	0.55
1:0:2613:G:O2'	1:0:2614:C:H5'	2.07	0.55
28:Z:13:ARG:NH1	28:Z:14:PHE:CZ	2.75	0.55
28:Z:25:ARG:O	28:Z:29:ILE:HG13	2.06	0.55
18:P:143:ALA:HA	38:P:190:HOH:O	2.07	0.55
9:F:107:ASP:O	9:F:111:ILE:HG13	2.07	0.55
11:H:166:SER:HB2	11:H:167:PRO:HD3	1.86	0.54
26:X:78:GLU:HG2	26:X:79:GLU:N	2.20	0.54
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.22	0.54
32:I:89:SER:HB3	32:I:97:VAL:CG2	2.37	0.54
1:0:2630:G:O6	4:A:206:ARG:NH2	2.41	0.54
38:O:4897:HOH:O	4:A:6:GLY:HA3	2.07	0.54
25:W:139:GLY:O	25:W:141:HIS:CD2	2.59	0.54
1:0:2526:C:O2'	1:0:2527:U:H5'	2.07	0.54
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.36	0.54
1:0:2783:A:H3'	38:O:5494:HOH:O	2.07	0.54
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.72	0.54
1:0:2509:A:H2'	1:0:2510:C:O4'	2.08	0.54
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.88	0.54
1:0:1234:U:C4	5:B:244:PRO:HB3	2.43	0.54
26:X:22:ASN:O	26:X:25:ARG:HG3	2.07	0.54
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.42	0.54
1:0:1289:C:H3'	38:O:6638:HOH:O	2.06	0.54
7:D:25:MET:SD	7:D:40:ILE:HD11	2.48	0.54
1:0:282:C:H1'	1:0:368:C:H42	1.68	0.54
32:I:139:ILE:HG22	32:I:140:GLU:H	1.71	0.54
1:0:21:G:H4'	20:R:2:ILE:HG22	1.87	0.54
6:C:77:ALA:O	6:C:78:ARG:HG3	2.07	0.54
1:0:92:G:H4'	24:V:44:GLY:HA3	1.89	0.54
2:9:3028:U:H5''	16:N:40:ASN:ND2	2.22	0.54
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.42	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:G:64:ASN:N	10:G:64:ASN:ND2	2.54	0.54
8:E:84:MET:HB2	8:E:131:LEU:HB2	1.90	0.54
2:9:3001:U:H5''	2:9:3003:A:OP1	2.08	0.54
5:B:51:VAL:HG13	5:B:53:LEU:HD13	1.89	0.54
4:A:217:ARG:CG	4:A:217:ARG:HH11	2.20	0.54
2:9:3091:C:H2'	2:9:3092:G:O4'	2.07	0.54
5:B:119:HIS:O	5:B:121:PRO:HD3	2.08	0.54
1:0:2862:G:H4'	5:B:336:GLN:O	2.07	0.54
26:X:80:GLU:HB3	38:X:5564:HOH:O	2.07	0.54
1:0:2717:C:O2'	1:0:2718:C:H5''	2.06	0.54
12:J:103:VAL:HG12	38:J:9361:HOH:O	2.07	0.54
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.39	0.54
6:C:1:MET:HG2	6:C:2:GLN:N	2.15	0.54
1:0:776:A:OP1	29:1:28:HIS:HE1	1.91	0.54
20:R:17:MET:CE	20:R:19:ARG:CZ	2.85	0.54
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.05	0.54
6:C:235:PHE:HE2	6:C:243:VAL:HG21	1.72	0.54
16:N:151:ASP:OD1	16:N:154:LEU:HD13	2.08	0.54
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.37	0.54
27:Y:112:GLU:OE1	27:Y:112:GLU:HA	2.07	0.54
13:K:27:ARG:HD2	38:K:4747:HOH:O	2.07	0.54
1:0:583:G:H2'	1:0:584:U:C6	2.42	0.54
9:F:27:GLY:HA3	9:F:101:ALA:O	2.08	0.54
6:C:140:VAL:HB	38:C:9252:HOH:O	2.07	0.54
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.72	0.54
24:V:38:GLY:C	24:V:40:PRO:HD2	2.27	0.54
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.08	0.54
5:B:146:THR:O	5:B:159:PRO:HB3	2.08	0.54
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.07	0.54
32:I:92:PRO:C	32:I:94:GLU:H	2.10	0.54
23:U:52:THR:HG22	23:U:54:THR:HB	1.90	0.54
25:W:122:ARG:HG3	25:W:152:ALA:O	2.07	0.54
27:Y:133:HIS:HD2	38:Y:8168:HOH:O	1.90	0.54
1:0:1342:C:O2'	1:0:1343:C:H5'	2.08	0.54
1:0:1278:A:H4'	1:0:1279:U:C4	2.43	0.54
1:0:1116:U:O2'	1:0:1118:A:C2	2.51	0.54
5:B:162:MET:HG3	5:B:310:ARG:CZ	2.38	0.54
2:9:3003:A:N6	2:9:3022:G:H1'	2.23	0.54
14:L:104:ASP:O	14:L:105:TYR:HB3	2.06	0.54
19:Q:28:ARG:HD2	19:Q:92:ARG:NH1	2.23	0.54
1:0:371:U:H2'	1:0:372:A:H8	1.73	0.54
1:0:56:G:C5'	24:V:50:ARG:HH12	2.12	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:2:GLN:HB3	38:C:9186:HOH:O	2.07	0.53
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.08	0.53
1:O:2720:C:O2	13:K:87:ARG:NH2	2.41	0.53
16:N:100:ALA:O	16:N:129:ILE:HG23	2.08	0.53
22:T:16:LEU:HA	22:T:19:ARG:HG3	1.90	0.53
1:O:2300:A:H4'	1:O:2301:A:O5'	2.09	0.53
32:I:75:THR:CA	32:I:112:LYS:NZ	2.71	0.53
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.90	0.53
16:N:37:ARG:NE	38:N:9334:HOH:O	2.41	0.53
1:O:1942:A:O2'	1:O:1943:C:H5'	2.09	0.53
7:D:25:MET:HE1	7:D:41:LEU:HG	1.91	0.53
27:Y:144:ARG:NH1	38:Y:8163:HOH:O	2.41	0.53
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.73	0.53
6:C:127:ARG:HG2	6:C:127:ARG:NH1	2.24	0.53
4:A:36:ASP:HB2	4:A:83:GLY:CA	2.39	0.53
12:J:45:VAL:HG22	12:J:130:VAL:O	2.09	0.53
2:9:3042:C:H5'	2:9:3043:G:OP2	2.08	0.53
16:N:23:ARG:O	16:N:27:LEU:HG	2.08	0.53
1:O:1164:U:H3	1:O:1192:A:H2	1.56	0.53
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.37	0.53
1:O:657:G:H2'	1:O:658:C:C6	2.43	0.53
38:C:9168:HOH:O	22:T:2:LYS:HE2	2.06	0.53
38:O:9668:HOH:O	29:1:1:THR:HA	2.07	0.53
1:O:407:A:H2'	1:O:408:A:C8	2.43	0.53
1:O:2064:U:H5'	1:O:2652:U:H4'	1.90	0.53
5:B:294:TYR:HE2	38:B:9446:HOH:O	1.90	0.53
1:O:1014:A:H2'	1:O:1015:C:H5'	1.91	0.53
1:O:2597:U:H2'	1:O:2598:U:H5'	1.90	0.53
25:W:63:GLU:HG2	25:W:93:ILE:HG22	1.89	0.53
1:O:1667:A:H2'	1:O:1668:U:C6	2.44	0.53
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.91	0.53
32:I:102:VAL:CG1	32:I:106:LYS:HE3	2.37	0.53
27:Y:186:ARG:HG2	27:Y:186:ARG:NH1	2.23	0.53
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.39	0.53
7:D:153:THR:HA	7:D:156:ARG:HG3	1.91	0.53
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.34	0.53
9:F:38:LYS:HZ2	15:M:3:SER:HA	1.70	0.53
1:O:2769:C:O2'	1:O:2770:G:H5'	2.09	0.53
1:O:1377:C:H5'	1:O:1377:C:C6	2.44	0.53
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.23	0.53
1:O:90:A:H2'	1:O:91:G:O4'	2.09	0.53
1:O:539:G:H2'	1:O:540:A:C8	2.43	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:289:G:N2	1:0:363:A:H2	2.04	0.53
5:B:41:PHE:CZ	5:B:79:MET:HG3	2.44	0.53
11:H:76:GLU:C	11:H:77:LEU:HD23	2.29	0.53
9:F:101:ALA:HA	38:F:5413:HOH:O	2.09	0.53
38:9:4707:HOH:O	16:N:147:ILE:HB	2.08	0.53
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.39	0.53
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.35	0.53
2:9:3044:A:O4'	7:D:76:ARG:NE	2.42	0.53
15:M:46:LEU:HG	38:M:9411:HOH:O	2.09	0.53
5:B:27:ASN:H	5:B:27:ASN:HD22	1.57	0.53
12:J:19:MET:CE	12:J:132:LEU:HD11	2.38	0.52
6:C:184:ARG:CZ	38:C:9216:HOH:O	2.57	0.52
26:X:30:MET:CE	26:X:58:ALA:HB3	2.39	0.52
25:W:122:ARG:CZ	38:W:5817:HOH:O	2.57	0.52
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.91	0.52
12:J:39:VAL:HG12	12:J:40:ASN:ND2	2.25	0.52
22:T:78:THR:OG1	22:T:86:GLU:HG2	2.08	0.52
1:0:2324:G:H4'	1:0:2418:G:O2'	2.09	0.52
5:B:17:LYS:O	5:B:260:HIS:HD2	1.92	0.52
1:0:1175:G:H1'	1:0:1193:A:H2'	1.91	0.52
16:N:37:ARG:HD3	36:N:9307:CL:CL	2.47	0.52
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.10	0.52
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.38	0.52
20:R:114:VAL:HG13	20:R:114:VAL:O	2.09	0.52
1:0:338:C:H4'	6:C:174:ILE:HD11	1.91	0.52
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.90	0.52
6:C:139:VAL:HG21	6:C:240:LEU:HD12	1.92	0.52
18:P:114:LEU:HA	18:P:118:GLN:NE2	2.25	0.52
20:R:106:GLY:HA2	20:R:109:MET:CE	2.35	0.52
16:N:176:ARG:O	16:N:180:LEU:HD13	2.09	0.52
1:0:2909:G:H2'	1:0:2910:A:H8	1.74	0.52
25:W:139:GLY:O	25:W:141:HIS:HD2	1.92	0.52
22:T:28:SER:O	22:T:32:ARG:HG3	2.08	0.52
11:H:24:PRO:HD3	11:H:120:ILE:HG22	1.90	0.52
18:P:83:LYS:O	18:P:86:ALA:HB3	2.09	0.52
17:O:4:ASN:HB3	17:O:7:LEU:HB3	1.92	0.52
11:H:31:HIS:HD2	11:H:87:LEU:O	1.93	0.52
1:0:814:G:H4'	38:0:3429:HOH:O	2.09	0.52
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.20	0.52
1:0:120:A:H2'	1:0:120:A:N3	2.25	0.52
25:W:13:MET:CE	25:W:17:ILE:HG22	2.39	0.52
1:0:1342:C:C2'	1:0:1343:C:H5'	2.40	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
38:0:4516:HOH:O	30:2:38:LYS:HE3	2.10	0.52
1:0:475:G:H5'	6:C:73:LEU:HD23	1.91	0.52
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.10	0.52
1:0:553:G:O4'	1:0:1325:G:H5'	2.09	0.52
8:E:11:VAL:CG1	8:E:12:ASP:N	2.72	0.52
12:J:107:ASN:HD22	12:J:107:ASN:C	2.13	0.52
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.40	0.52
1:0:1634:G:H3'	38:0:4181:HOH:O	2.09	0.52
1:0:2758:G:H2'	1:0:2759:C:C6	2.45	0.52
6:C:127:ARG:HG2	6:C:127:ARG:HH11	1.75	0.52
25:W:5:VAL:HG11	25:W:153:MET:CE	2.40	0.52
6:C:132:ASP:HB3	38:C:9162:HOH:O	2.09	0.52
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.10	0.52
1:0:2364:A:OP1	19:Q:11:ARG:NH1	2.42	0.52
1:0:1119:G:H8	12:J:52:GLN:NE2	2.08	0.52
26:X:21:PRO:HD3	38:X:6179:HOH:O	2.09	0.52
1:0:503:G:H2'	1:0:504:G:H8	1.75	0.52
1:0:1423:C:O2'	1:0:1424:A:H5'	2.10	0.52
22:T:71:VAL:HG13	22:T:91:LEU:O	2.10	0.52
38:0:7598:HOH:O	22:T:9:LYS:HD2	2.10	0.52
1:0:542:A:H2'	1:0:543:G:O4'	2.10	0.52
2:9:3003:A:OP2	2:9:3025:G:N2	2.42	0.52
25:W:11:VAL:O	25:W:12:ASN:HB2	2.10	0.52
1:0:816:G:H5'	1:0:1598:A:H4'	1.91	0.52
1:0:1654:U:H2'	4:A:47:HIS:HD2	1.75	0.52
5:B:54:VAL:HB	38:B:9412:HOH:O	2.09	0.52
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.90	0.52
1:0:259:G:O2'	1:0:260:C:H5'	2.10	0.52
4:A:66:ARG:HH11	4:A:66:ARG:CB	2.22	0.52
26:X:25:ARG:HG2	38:X:5356:HOH:O	2.10	0.52
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.45	0.52
1:0:69:A:H5'	1:0:69:A:C8	2.45	0.52
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.40	0.52
1:0:1874:U:OP1	4:A:51:ARG:HD2	2.10	0.52
8:E:34:TRP:O	12:J:127:ILE:HD11	2.10	0.52
7:D:146:LYS:NZ	16:N:107:ASN:ND2	2.56	0.52
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.92	0.52
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.45	0.52
1:0:960:G:H4'	38:0:7605:HOH:O	2.10	0.51
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.40	0.51
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.09	0.51
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.91	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:J:15:ARG:NH1	12:J:43:ARG:NH1	2.57	0.51
1:0:1855:G:H8	4:A:144:GLU:OE2	1.93	0.51
5:B:214:PRO:HD2	38:B:9321:HOH:O	2.09	0.51
31:3:69:TYR:CZ	31:3:80:ARG:HD2	2.45	0.51
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.35	0.51
16:N:11:ARG:O	16:N:15:GLU:HG3	2.10	0.51
1:0:1205:U:C2'	1:0:1206:U:H5''	2.40	0.51
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.22	0.51
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.25	0.51
5:B:162:MET:HG3	5:B:310:ARG:HD3	1.92	0.51
14:L:145:LEU:O	14:L:148:GLU:HG3	2.10	0.51
5:B:258:GLY:H	5:B:260:HIS:CE1	2.27	0.51
1:0:67:A:H5''	1:0:69:A:C8	2.46	0.51
15:M:107:ARG:HD2	38:M:9370:HOH:O	2.09	0.51
15:M:65:VAL:HG21	15:M:105:ALA:HB2	1.90	0.51
5:B:62:ARG:CA	5:B:65:MET:HE3	2.35	0.51
29:1:8:GLN:NE2	29:1:11:LYS:NZ	2.55	0.51
28:Z:46:ARG:HD3	28:Z:58:SER:OG	2.11	0.51
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.45	0.51
1:0:1850:U:H2'	1:0:1851:G:H8	1.74	0.51
1:0:2894:C:O2'	1:0:2895:C:H5'	2.10	0.51
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.45	0.51
1:0:512:G:O3'	1:0:513:A:H8	1.94	0.51
4:A:36:ASP:CB	4:A:83:GLY:HA3	2.41	0.51
22:T:35:TYR:CG	22:T:112:LEU:HD22	2.46	0.51
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.40	0.51
5:B:310:ARG:HD2	38:B:9444:HOH:O	2.08	0.51
4:A:199:HIS:CD2	4:A:201:PHE:H	2.28	0.51
24:V:27:LEU:HA	24:V:49:LEU:HD13	1.92	0.51
30:2:48:ASP:O	30:2:49:GLU:HB2	2.10	0.51
1:0:159:G:OP1	15:M:74:LYS:HE3	2.10	0.51
5:B:141:ARG:HD2	5:B:163:GLU:OE2	2.11	0.51
11:H:148:GLU:HA	11:H:148:GLU:OE1	2.10	0.51
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.26	0.51
1:0:1180:U:H2'	1:0:1181:A:C8	2.46	0.51
1:0:775:G:OP1	29:1:16:HIS:HE1	1.94	0.51
10:G:23:ILE:O	10:G:27:ILE:HG13	2.10	0.51
1:0:2897:C:H2'	1:0:2898:G:H8	1.74	0.51
31:3:40:ARG:HD2	38:3:9357:HOH:O	2.10	0.51
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.93	0.51
20:R:132:ARG:CZ	38:R:9385:HOH:O	2.59	0.51
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
32:I:101:SER:OG	32:I:104:GLN:HG3	2.11	0.51
26:X:10:VAL:HG11	26:X:36:HIS:HE1	1.75	0.51
17:O:42:GLU:HB2	38:O:2176:HOH:O	2.09	0.51
4:A:179:MET:HG3	4:A:186:TRP:CG	2.46	0.51
21:S:43:GLU:HB3	38:S:9141:HOH:O	2.10	0.51
1:O:1500:U:P	18:P:41:ARG:HH22	2.33	0.51
1:O:638:C:H2'	1:O:639:A:C8	2.46	0.51
15:M:59:GLY:CA	15:M:141:ILE:HD11	2.41	0.51
23:U:39:ASN:HD22	23:U:44:ARG:HH11	1.57	0.51
1:O:474:C:O3'	6:C:73:LEU:CD2	2.59	0.51
1:O:2036:C:O4'	13:K:44:LEU:HG	2.11	0.51
15:M:157:ASP:HB3	15:M:160:PHE:HD1	1.75	0.51
1:O:419:A:H1'	1:O:1921:A:C2	2.45	0.51
1:O:1252:A:H2'	1:O:1253:C:O4'	2.11	0.51
25:W:5:VAL:HG11	25:W:153:MET:HE3	1.93	0.51
1:O:1167:G:H2'	1:O:1168:C:O4'	2.11	0.51
32:I:91:GLU:HB3	32:I:94:GLU:OE2	2.11	0.51
16:N:151:ASP:O	16:N:154:LEU:HB2	2.10	0.51
6:C:233:THR:HG22	6:C:234:VAL:H	1.76	0.51
1:O:702:G:O2'	1:O:703:G:H5'	2.11	0.51
18:P:7:LYS:HD3	18:P:21:VAL:HG21	1.92	0.51
38:O:9863:HOH:O	25:W:119:HIS:HE1	1.93	0.51
1:O:583:G:H2'	1:O:584:U:H6	1.76	0.51
1:O:1422:U:H2'	1:O:1423:C:C6	2.46	0.51
11:H:36:LYS:HA	11:H:84:LYS:NZ	2.26	0.51
1:O:694:A:H2'	1:O:695:C:H5'	1.93	0.51
1:O:790:A:H2'	1:O:791:A:O4'	2.10	0.51
25:W:130:HIS:O	25:W:136:GLY:HA3	2.10	0.51
1:O:263:U:C4	9:F:54:VAL:HG13	2.45	0.51
4:A:105:VAL:HG12	4:A:106:CYS:N	2.26	0.51
24:V:42:ASN:O	24:V:44:GLY:N	2.43	0.51
21:S:53:ASN:N	21:S:53:ASN:HD22	2.09	0.51
4:A:217:ARG:HG2	4:A:229:ALA:HB2	1.93	0.51
1:O:1528:A:H2'	1:O:1529:G:O4'	2.11	0.51
6:C:13:ASP:OD1	6:C:13:ASP:O	2.27	0.51
25:W:36:PRO:HD2	25:W:41:TYR:CE1	2.46	0.51
1:O:1555:G:H4'	1:O:1630:A:H2	1.75	0.51
1:O:2361:A:H5'	1:O:2361:A:H8	1.76	0.51
4:A:211:LYS:HB2	38:A:9412:HOH:O	2.10	0.50
1:O:2533:C:H6	1:O:2533:C:C5'	2.20	0.50
1:O:1730:G:H5''	1:O:1731:C:H6	1.76	0.50
13:K:6:ALA:CB	13:K:116:GLU:HG2	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:945:U:H2'	1:0:946:C:C6	2.46	0.50
18:P:55:LYS:HG2	18:P:56:GLY:N	2.25	0.50
1:0:1189:A:H1'	1:0:1209:C:H1'	1.92	0.50
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.94	0.50
32:I:106:LYS:O	32:I:110:GLU:HG3	2.12	0.50
1:0:289:G:O2'	1:0:290:C:H5'	2.11	0.50
16:N:170:GLU:O	16:N:174:GLU:HG3	2.10	0.50
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.12	0.50
6:C:242:GLU:HG3	38:C:9183:HOH:O	2.11	0.50
9:F:56:PRO:HG2	15:M:43:PRO:O	2.11	0.50
1:0:243:A:H61	1:0:269:G:H1'	1.76	0.50
1:0:366:U:H2'	1:0:367:G:O4'	2.11	0.50
5:B:315:VAL:HG23	5:B:316:ARG:HG2	1.94	0.50
38:O:3252:HOH:O	26:X:23:HIS:HD2	1.93	0.50
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.92	0.50
1:0:2453:G:H4'	14:L:50:GLY:C	2.31	0.50
1:0:1904:A:H2'	1:0:1905:U:O4'	2.12	0.50
1:0:451:C:O2'	1:0:452:G:H5'	2.11	0.50
23:U:13:ILE:HG12	23:U:32:CYS:HB3	1.93	0.50
4:A:164:ARG:CZ	38:A:9383:HOH:O	2.59	0.50
5:B:7:ARG:HG2	5:B:7:ARG:HH11	1.76	0.50
1:0:559:U:H2'	1:0:560:C:O4'	2.11	0.50
1:0:657:G:H2'	1:0:658:C:H6	1.75	0.50
11:H:170:ASN:N	11:H:170:ASN:HD22	2.08	0.50
5:B:304:PRO:CG	5:B:307:ARG:NH1	2.74	0.50
14:L:148:GLU:HA	38:L:9371:HOH:O	2.10	0.50
13:K:22:ASP:HB2	38:K:5264:HOH:O	2.10	0.50
1:0:2419:U:H5''	1:0:2420:G:H5'	1.94	0.50
7:D:23:VAL:HG11	7:D:83:PHE:CZ	2.46	0.50
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.11	0.50
1:0:1236:A:H2'	1:0:1237:U:O4'	2.11	0.50
1:0:241:A:C2	1:0:378:A:H4'	2.46	0.50
14:L:54:PRO:HG2	14:L:57:VAL:CG2	2.41	0.50
1:0:2507:G:H2'	1:0:2510:C:H42	1.77	0.50
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.42	0.50
5:B:145:HIS:HD2	5:B:146:THR:O	1.94	0.50
1:0:263:U:O4'	9:F:59:ILE:HD13	2.11	0.50
4:A:33:GLU:O	4:A:34:ASP:HB2	2.11	0.50
6:C:237:GLU:HB2	38:C:9234:HOH:O	2.11	0.50
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.12	0.50
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.92	0.50
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.27	0.50
1:0:113:A:OP2	1:0:114:A:H2'	2.11	0.50
9:F:99:THR:HA	38:F:3461:HOH:O	2.11	0.50
17:O:38:ARG:HD3	38:O:7674:HOH:O	2.10	0.50
1:0:1641:A:C2'	1:0:1642:A:H5'	2.42	0.50
1:0:1289:C:O2'	1:0:1290:G:H5'	2.11	0.50
14:L:54:PRO:HG2	14:L:57:VAL:HG21	1.93	0.50
26:X:18:ARG:NH1	38:X:4132:HOH:O	2.41	0.50
8:E:24:GLY:HA3	8:E:76:VAL:HB	1.93	0.50
1:0:1304:U:H2'	1:0:1305:C:C6	2.47	0.50
1:0:1563:G:O2'	1:0:1564:C:OP2	2.25	0.50
12:J:117:ASP:O	12:J:119:THR:HG23	2.12	0.50
1:0:189:A:OP1	15:M:171:ARG:NH2	2.45	0.50
6:C:72:LYS:HG2	6:C:77:ALA:HA	1.94	0.50
1:0:1205:U:H2'	1:0:1206:U:H5'	1.92	0.50
1:0:2851:G:C2'	1:0:2852:A:H5'	2.41	0.50
6:C:104:ASP:O	6:C:108:GLN:HG3	2.11	0.50
16:N:77:ASN:OD1	16:N:79:PRO:HD2	2.12	0.50
16:N:73:ALA:HB1	16:N:74:PRO:HD2	1.93	0.50
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.11	0.50
1:0:2353:A:H4'	1:0:2354:A:O5'	2.12	0.50
38:K:7438:HOH:O	23:U:20:MET:HE1	2.12	0.50
3:4:74:C:H2'	3:4:75:C:H5'	1.93	0.50
15:M:99:ARG:HD2	15:M:167:GLY:CA	2.39	0.50
1:0:2509:A:OP2	1:0:2510:C:H5	1.94	0.50
29:1:25:LYS:HD2	30:2:49:GLU:N	2.26	0.50
7:D:84:LEU:C	7:D:86:THR:H	2.16	0.50
1:0:1183:C:N4	1:0:1184:C:H41	2.09	0.50
7:D:52:THR:N	7:D:70:GLY:O	2.45	0.50
25:W:41:TYR:HA	25:W:44:MET:HE3	1.94	0.50
4:A:97:ALA:HB2	4:A:150:PRO:HB2	1.94	0.50
13:K:72:VAL:HG11	13:K:121:PHE:CD1	2.46	0.50
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.94	0.50
22:T:65:VAL:HG22	22:T:72:ILE:HG22	1.94	0.49
24:V:64:GLY:O	24:V:65:ASP:CB	2.60	0.49
5:B:147:VAL:HG12	5:B:150:ALA:H	1.76	0.49
6:C:129:HIS:HD2	6:C:165:ASP:OD2	1.95	0.49
1:0:475:G:OP1	6:C:73:LEU:HD22	2.12	0.49
9:F:31:LYS:HD3	9:F:89:LEU:HG	1.94	0.49
22:T:106:GLU:HG3	38:T:4913:HOH:O	2.12	0.49
12:J:75:PRO:HB3	12:J:132:LEU:HB3	1.95	0.49
1:0:1593:C:OP1	18:P:117:SER:HB3	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1180:U:H2'	1:0:1181:A:O4'	2.12	0.49
20:R:17:MET:HE1	20:R:19:ARG:CZ	2.42	0.49
1:0:396:U:O2'	1:0:418:C:H4'	2.12	0.49
5:B:79:MET:HE3	5:B:144:THR:HG21	1.93	0.49
1:0:1730:G:C5'	1:0:1731:C:C6	2.95	0.49
1:0:69:A:H5'	1:0:69:A:H8	1.77	0.49
1:0:944:G:H21	25:W:44:MET:CE	2.25	0.49
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.42	0.49
22:T:53:GLY:HA3	38:T:6384:HOH:O	2.11	0.49
6:C:139:VAL:CG2	6:C:240:LEU:HD12	2.43	0.49
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.94	0.49
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.13	0.49
16:N:154:LEU:O	16:N:155:GLU:CB	2.60	0.49
18:P:38:GLU:HA	18:P:41:ARG:NH1	2.27	0.49
22:T:79:LEU:HG	22:T:89:ARG:HB2	1.94	0.49
5:B:75:GLU:C	5:B:77:PRO:HD3	2.33	0.49
1:0:1406:A:H4'	1:0:1407:A:H5''	1.93	0.49
1:0:316:A:H5'	22:T:54:ASP:OD2	2.12	0.49
1:0:2506:A:O2'	1:0:2507:G:O5'	2.30	0.49
22:T:48:VAL:CG1	22:T:49:GLU:N	2.74	0.49
4:A:99:ILE:O	4:A:131:HIS:HE1	1.95	0.49
38:0:5245:HOH:O	11:H:58:ARG:HG3	2.12	0.49
1:0:1701:A:H4'	1:0:1702:U:C5'	2.42	0.49
16:N:47:LEU:CD1	16:N:97:VAL:HG11	2.42	0.49
26:X:30:MET:CE	26:X:55:ASN:HA	2.41	0.49
1:0:2241:C:O2'	1:0:2242:U:H5'	2.12	0.49
17:O:25:VAL:HG23	17:O:26:TRP:N	2.26	0.49
16:N:67:ALA:C	16:N:69:TYR:H	2.14	0.49
19:Q:3:SER:HB3	38:Q:5998:HOH:O	2.13	0.49
15:M:80:GLY:O	15:M:81:ARG:HD3	2.12	0.49
1:0:1735:C:OP2	5:B:234:ARG:HG3	2.12	0.49
1:0:500:G:H21	20:R:98:ASN:HD21	1.58	0.49
1:0:317:A:OP1	22:T:52:ARG:O	2.30	0.49
18:P:55:LYS:CG	18:P:56:GLY:N	2.75	0.49
15:M:57:LYS:HE2	15:M:140:ALA:O	2.12	0.49
1:0:1537:C:H1'	38:0:6807:HOH:O	2.12	0.49
8:E:125:GLU:HB2	8:E:132:THR:CG2	2.43	0.49
6:C:170:ASP:O	6:C:171:GLU:HG3	2.12	0.49
27:Y:123:VAL:HG12	27:Y:124:GLY:O	2.12	0.49
7:D:159:PRO:O	7:D:163:VAL:HG23	2.13	0.49
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.94	0.49
1:0:1166:A:H61	1:0:1180:U:H3	1.61	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:9:3008:G:O6	16:N:11:ARG:NH1	2.46	0.49
13:K:101:ASN:HB2	13:K:103:ASP:OD2	2.13	0.49
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.48	0.49
32:I:123:ASN:HA	32:I:126:LYS:HD2	1.94	0.49
12:J:107:ASN:ND2	12:J:109:TYR:H	2.11	0.49
25:W:60:GLU:O	25:W:63:GLU:HB2	2.13	0.49
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.94	0.49
4:A:132:ASP:OD1	4:A:133:ARG:N	2.45	0.49
1:0:2793:A:H2'	1:0:2794:G:H5'	1.94	0.49
1:0:80:A:H3'	22:T:43:ASN:OD1	2.11	0.49
8:E:106:ASN:ND2	8:E:109:GLY:HA2	2.27	0.49
31:3:65:THR:HG23	31:3:67:LEU:HG	1.94	0.49
1:0:1804:A:H2'	1:0:1805:G:C8	2.48	0.49
1:0:542:A:H5'	1:0:542:A:C8	2.37	0.49
15:M:134:ILE:O	15:M:136:PRO:HD3	2.13	0.49
1:0:1086:A:N6	25:W:11:VAL:HG11	2.28	0.49
2:9:3034:A:H2'	2:9:3035:C:O4'	2.12	0.49
1:0:2834:G:OP1	26:X:39:LYS:HE2	2.12	0.49
17:O:96:VAL:CG1	17:O:100:GLN:HB2	2.43	0.49
5:B:248:ARG:O	5:B:251:VAL:HG13	2.13	0.49
25:W:126:ASP:HB3	25:W:135:GLY:O	2.12	0.49
1:0:2587:OMU:H6	1:0:2587:OMU:O5'	2.13	0.49
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.95	0.49
23:U:17:THR:CG2	23:U:18:GLY:N	2.75	0.49
27:Y:200:THR:HG22	27:Y:201:GLU:CG	2.42	0.49
1:0:371:U:H2'	1:0:372:A:C8	2.48	0.49
1:0:894:A:C2	6:C:87:ARG:NH2	2.80	0.49
1:0:1787:C:H4'	1:0:2883:A:O4'	2.12	0.49
1:0:1311:G:O6	6:C:173:LYS:HE3	2.13	0.49
1:0:569:A:H5''	1:0:587:A:N1	2.27	0.49
38:0:9527:HOH:O	4:A:11:ARG:HD3	2.13	0.49
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.94	0.49
20:R:72:VAL:CG1	20:R:75:TRP:HB3	2.43	0.49
6:C:25:PRO:HG2	38:C:9124:HOH:O	2.11	0.49
29:1:22:CYS:SG	29:1:24:GLU:HB2	2.53	0.49
6:C:39:GLN:O	6:C:43:LYS:HD3	2.13	0.49
7:D:23:VAL:HG23	7:D:23:VAL:O	2.13	0.49
1:0:1393:A:H2'	1:0:1394:C:C6	2.48	0.49
1:0:603:A:H5''	1:0:604:G:OP1	2.12	0.49
1:0:432:G:O2'	1:0:433:C:H5'	2.12	0.49
1:0:2073:G:OP2	1:0:2490:A:H5'	2.13	0.49
1:0:2619:UR3:H6	1:0:2619:UR3:O5'	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:541:C:H2'	1:0:542:A:H5'	1.95	0.49
6:C:118:THR:O	6:C:136:VAL:HG13	2.13	0.49
1:0:1878:G:H1'	38:0:6359:HOH:O	2.13	0.49
4:A:168:PRO:O	4:A:170:VAL:HG23	2.12	0.49
14:L:81:VAL:HG12	14:L:82:ALA:N	2.28	0.49
11:H:46:GLN:CB	11:H:167:PRO:HD2	2.22	0.48
20:R:39:THR:HG22	20:R:42:GLU:N	2.16	0.48
1:0:506:G:N2	1:0:509:A:H5'	2.20	0.48
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.48	0.48
9:F:111:ILE:O	9:F:115:VAL:HG23	2.12	0.48
11:H:80:GLU:HA	38:H:9182:HOH:O	2.13	0.48
38:0:6921:HOH:O	27:Y:165:GLU:HB3	2.11	0.48
1:0:482:G:H4'	1:0:508:A:N1	2.28	0.48
1:0:383:A:H4'	38:0:5588:HOH:O	2.13	0.48
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.94	0.48
8:E:101:GLU:HB2	8:E:116:THR:O	2.13	0.48
4:A:211:LYS:CB	4:A:212:PRO:HD2	2.28	0.48
30:2:41:HIS:CD2	30:2:44:ARG:H	2.27	0.48
1:0:2890:A:C1'	23:U:56:ARG:NH2	2.72	0.48
1:0:2269:C:H2'	1:0:2270:G:H5'	1.94	0.48
1:0:1206:U:H2'	1:0:1207:A:O4'	2.13	0.48
11:H:120:ILE:CD1	11:H:120:ILE:N	2.76	0.48
20:R:29:LYS:NZ	38:R:9341:HOH:O	2.47	0.48
5:B:85:ARG:NH1	38:B:9431:HOH:O	2.45	0.48
1:0:1636:G:O2'	1:0:1637:A:H5'	2.12	0.48
32:I:135:LEU:HB2	32:I:137:VAL:HG23	1.95	0.48
27:Y:184:GLU:OE2	27:Y:204:ARG:HD2	2.13	0.48
17:O:32:ARG:HH21	17:O:35:LYS:NZ	2.11	0.48
1:0:926:A:O2'	14:L:41:HIS:CD2	2.65	0.48
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.95	0.48
1:0:214:U:H5'	38:0:6378:HOH:O	2.13	0.48
1:0:1507:C:H4'	38:0:3891:HOH:O	2.14	0.48
1:0:440:C:H2'	1:0:441:A:C8	2.48	0.48
18:P:115:SER:OG	18:P:118:GLN:HG3	2.13	0.48
7:D:39:ASP:HB2	38:D:5583:HOH:O	2.14	0.48
8:E:31:ARG:NH1	38:E:5919:HOH:O	2.46	0.48
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.77	0.48
25:W:14:HIS:HB2	25:W:17:ILE:HG13	1.95	0.48
22:T:26:THR:HA	22:T:39:ASN:HB3	1.94	0.48
4:A:164:ARG:HA	28:Z:69:TYR:CE1	2.48	0.48
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.12	0.48
13:K:75:ARG:CZ	38:K:4172:HOH:O	2.61	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2428:G:N7	31:3:60:LYS:HE2	2.29	0.48
20:R:17:MET:HE3	20:R:19:ARG:CZ	2.43	0.48
5:B:98:THR:HG22	5:B:99:GLU:N	2.26	0.48
5:B:132:HIS:HB2	5:B:137:LEU:HD22	1.95	0.48
4:A:194:MET:HE2	4:A:199:HIS:CB	2.44	0.48
4:A:53:ALA:HB3	38:A:9401:HOH:O	2.12	0.48
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.94	0.48
1:0:920:C:H5'	1:0:921:G:O5'	2.13	0.48
24:V:55:ARG:O	24:V:59:ILE:HG12	2.14	0.48
4:A:72:GLU:OE1	28:Z:72:GLU:HA	2.13	0.48
22:T:41:ARG:HH11	22:T:41:ARG:HG2	1.79	0.48
1:0:1029:U:O2'	1:0:1273:C:OP1	2.29	0.48
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.49	0.48
6:C:236:THR:HG21	38:C:9175:HOH:O	2.13	0.48
4:A:32:VAL:HG22	4:A:38:ILE:HG13	1.95	0.48
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.43	0.48
5:B:5:ARG:HD2	5:B:8:LYS:HZ1	1.79	0.48
9:F:58:GLU:CD	15:M:27:ARG:HH22	2.17	0.48
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.42	0.48
24:V:58:THR:O	24:V:62:GLU:HG3	2.13	0.48
1:0:1132:A:N6	1:0:1229:C:H2'	2.29	0.48
1:0:1333:U:H2'	1:0:1334:C:C6	2.49	0.48
1:0:152:A:O2'	1:0:153:C:H5'	2.13	0.48
1:0:2561:C:OP1	8:E:153:ARG:NH2	2.46	0.48
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.47	0.48
1:0:2362:A:H2'	1:0:2363:G:C8	2.48	0.48
7:D:163:VAL:HA	38:D:6326:HOH:O	2.13	0.48
1:0:558:C:H2'	1:0:559:U:C5'	2.41	0.48
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.92	0.48
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.44	0.48
9:F:99:THR:O	9:F:99:THR:HG23	2.13	0.48
1:0:1878:G:O2'	1:0:1879:U:C6	2.64	0.48
27:Y:155:ARG:NH1	38:Y:8147:HOH:O	2.47	0.48
1:0:1168:C:H4'	38:I:5128:HOH:O	2.13	0.48
14:L:133:VAL:HB	38:L:9357:HOH:O	2.13	0.48
1:0:319:A:H4'	1:0:338:C:C5	2.49	0.48
22:T:24:ARG:NH2	22:T:39:ASN:HD22	2.12	0.48
1:0:2898:G:H4'	5:B:288:GLY:HA2	1.95	0.48
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.43	0.48
6:C:102:LEU:HD12	38:C:9117:HOH:O	2.14	0.48
1:0:2541:U:H4'	1:0:2542:C:OP1	2.13	0.48
1:0:2015:A:H2'	1:0:2016:U:O4'	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:9:3012:C:H5'	2:9:3070:U:O4'	2.12	0.48
19:Q:30:VAL:HG12	19:Q:30:VAL:O	2.13	0.48
6:C:236:THR:O	6:C:237:GLU:C	2.52	0.48
11:H:9:ILE:HG12	11:H:56:GLN:CG	2.44	0.48
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.94	0.48
12:J:52:GLN:HG3	12:J:53:ILE:H	1.77	0.48
1:0:2783:A:H2'	1:0:2784:A:C8	2.49	0.48
26:X:12:ILE:HB	26:X:70:ILE:HG22	1.95	0.48
1:0:2478:U:O2'	1:0:2479:A:H5'	2.14	0.48
1:0:1352:A:N1	6:C:48:SER:HB3	2.28	0.48
8:E:16:ASP:O	8:E:17:HIS:HB2	2.13	0.48
25:W:3:ALA:O	25:W:54:PHE:HA	2.14	0.48
1:0:2269:C:C2'	1:0:2270:G:H5'	2.43	0.48
1:0:1849:G:H1'	1:0:2011:A:N1	2.28	0.48
1:0:1942:A:H3'	38:0:7527:HOH:O	2.15	0.47
7:D:159:PRO:O	7:D:162:ALA:HB3	2.14	0.47
31:3:16:GLU:HG3	31:3:18:GLN:HE21	1.79	0.47
1:0:396:U:OP2	31:3:38:ARG:HD2	2.13	0.47
1:0:157:G:H4'	15:M:95:LYS:CE	2.43	0.47
5:B:72:THR:HB	38:B:9406:HOH:O	2.13	0.47
7:D:153:THR:HA	7:D:156:ARG:CG	2.43	0.47
1:0:832:U:H2'	1:0:833:G:C8	2.49	0.47
1:0:1568:G:O2'	1:0:1569:U:H5'	2.14	0.47
17:O:45:LEU:HD12	17:O:88:LYS:HD2	1.95	0.47
1:0:2472:C:O2'	1:0:2634:G:H4'	2.13	0.47
1:0:2846:C:H4'	5:B:156:LYS:HB3	1.96	0.47
27:Y:151:SER:HB3	27:Y:154:ARG:CB	2.44	0.47
1:0:1634:G:H2'	1:0:1635:U:C6	2.49	0.47
8:E:132:THR:HB	38:E:2227:HOH:O	2.15	0.47
7:D:128:LEU:C	7:D:128:LEU:HD23	2.35	0.47
18:P:20:ARG:NH1	18:P:54:LYS:HD3	2.28	0.47
1:0:1940:C:H4'	38:0:7527:HOH:O	2.13	0.47
22:T:71:VAL:HG12	22:T:72:ILE:N	2.28	0.47
1:0:558:C:C2'	1:0:559:U:C5'	2.92	0.47
20:R:119:VAL:HG12	20:R:119:VAL:O	2.14	0.47
1:0:1307:A:H2'	1:0:1308:A:C8	2.49	0.47
1:0:1120:U:H5'	1:0:1120:U:C6	2.40	0.47
7:D:135:VAL:HG22	7:D:136:ARG:H	1.79	0.47
2:9:3028:U:H2'	2:9:3029:C:C6	2.48	0.47
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.48	0.47
32:I:133:THR:N	38:I:5371:HOH:O	2.47	0.47
1:0:1613:C:H2'	1:0:1614:G:O4'	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:343:C:O2'	1:0:344:C:H5'	2.14	0.47
15:M:48:LYS:HE3	15:M:52:GLN:NE2	2.29	0.47
32:I:129:VAL:HG13	32:I:139:ILE:CD1	2.41	0.47
2:9:3114:G:H2'	2:9:3115:C:C6	2.50	0.47
24:V:39:ALA:O	24:V:41:GLU:N	2.42	0.47
7:D:138:GLY:N	38:D:7597:HOH:O	2.47	0.47
25:W:125:HIS:HE1	38:W:3071:HOH:O	1.97	0.47
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.97	0.47
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.15	0.47
9:F:26:THR:HG21	9:F:102:GLY:C	2.34	0.47
1:0:1825:U:O2'	1:0:1826:C:H5'	2.14	0.47
7:D:25:MET:CE	7:D:41:LEU:HG	2.44	0.47
7:D:28:GLY:CA	7:D:69:ILE:HG23	2.42	0.47
18:P:103:THR:O	18:P:106:ARG:HB3	2.15	0.47
24:V:39:ALA:C	24:V:41:GLU:H	2.18	0.47
14:L:145:LEU:O	14:L:145:LEU:HD23	2.15	0.47
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.96	0.47
1:0:1925:G:O2'	1:0:1926:G:H5'	2.15	0.47
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.15	0.47
8:E:37:ASP:OD1	12:J:125:SER:HB3	2.14	0.47
5:B:14:GLY:HA2	5:B:15:PRO:C	2.35	0.47
1:0:2379:G:H5'	1:0:2381:C:O4'	2.14	0.47
13:K:132:VAL:HG11	23:U:22:VAL:HG22	1.96	0.47
1:0:731:U:H2'	1:0:732:C:C6	2.50	0.47
16:N:37:ARG:CZ	38:N:9334:HOH:O	2.62	0.47
12:J:19:MET:HE3	12:J:132:LEU:CD2	2.27	0.47
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.49	0.47
30:2:40:ARG:HD2	30:2:47:THR:HG22	1.95	0.47
32:I:132:CYS:O	32:I:135:LEU:N	2.47	0.47
32:I:92:PRO:O	32:I:94:GLU:HG3	2.14	0.47
1:0:2547:C:OP2	5:B:5:ARG:NH1	2.47	0.47
4:A:192:VAL:HG13	38:A:9354:HOH:O	2.15	0.47
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.45	0.47
1:0:1010:C:H4'	16:N:4:PRO:HB2	1.97	0.47
38:0:4353:HOH:O	5:B:27:ASN:HB2	2.14	0.47
31:3:69:TYR:HB2	31:3:78:HIS:CE1	2.49	0.47
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.80	0.47
21:S:42:GLU:HG2	21:S:49:VAL:HG23	1.95	0.47
28:Z:33:MET:SD	28:Z:49:ARG:HD2	2.54	0.47
1:0:1427:A:H61	1:0:1440:U:C1'	2.27	0.47
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.45	0.47
1:0:1118:A:H8	1:0:1119:G:H5''	1.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:36:ASP:HB2	4:A:84:VAL:N	2.30	0.47
32:I:112:LYS:C	32:I:114:PRO:HD2	2.35	0.47
13:K:99:ASP:OD1	13:K:101:ASN:N	2.43	0.47
4:A:217:ARG:NH1	4:A:217:ARG:CG	2.77	0.47
1:O:1730:G:H5'	1:O:1731:C:H5	1.78	0.47
1:O:1462:C:H2'	1:O:1463:A:H8	1.78	0.47
1:O:705:C:H2'	1:O:705:C:O2	2.15	0.47
1:O:1503:U:H2'	1:O:1504:A:O4'	2.15	0.47
1:O:1890:U:H4'	1:O:2010:A:C6	2.50	0.47
6:C:76:ARG:HH11	6:C:76:ARG:CG	2.28	0.47
2:9:3076:G:C3'	2:9:3077:A:H5''	2.36	0.47
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.76	0.47
25:W:76:ASP:O	25:W:77:ALA:C	2.52	0.47
1:O:1701:A:H5''	1:O:1702:U:H3'	1.97	0.47
2:9:3029:C:C2'	2:9:3030:C:H5'	2.44	0.47
5:B:162:MET:HE3	5:B:308:LEU:HD21	1.96	0.47
2:9:3001:U:O3'	2:9:3003:A:H5'	2.14	0.47
1:O:945:U:O2'	25:W:43:GLY:HA3	2.14	0.47
9:F:56:PRO:HG2	15:M:44:THR:HA	1.95	0.47
5:B:279:THR:OG1	5:B:290:VAL:HB	2.14	0.47
6:C:20:ASP:O	6:C:23:GLU:HB2	2.15	0.47
8:E:97:VAL:HG12	38:E:4191:HOH:O	2.15	0.47
1:O:2869:G:H2'	1:O:2870:C:C6	2.50	0.47
4:A:211:LYS:NZ	38:A:9413:HOH:O	2.46	0.47
2:9:3056:A:H1'	7:D:14:ARG:HG2	1.97	0.47
1:O:284:C:H4'	1:O:285:A:O5'	2.15	0.47
5:B:210:GLY:HA2	5:B:256:GLN:HE22	1.80	0.47
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.45	0.47
9:F:61:MET:HB3	15:M:19:GLN:OE1	2.14	0.47
16:N:5:ARG:HG3	19:Q:18:PRO:CB	2.44	0.47
8:E:84:MET:HG2	8:E:168:ILE:HD13	1.97	0.47
1:O:2748:G:H2'	38:O:7705:HOH:O	2.15	0.47
1:O:2668:G:H2'	1:O:2669:U:H6	1.77	0.47
1:O:952:G:N3	1:O:2302:A:H2'	2.30	0.47
4:A:48:ASP:HB3	38:A:9401:HOH:O	2.15	0.47
1:O:659:A:N1	17:O:42:GLU:OE2	2.48	0.47
7:D:91:ALA:HB1	38:D:5198:HOH:O	2.15	0.47
2:9:3107:C:H5	38:9:3167:HOH:O	1.97	0.47
11:H:154:TYR:C	11:H:154:TYR:CD1	2.87	0.47
21:S:57:THR:CG2	21:S:58:MET:N	2.78	0.46
2:9:3013:A:N3	16:N:14:ARG:NH2	2.57	0.46
5:B:5:ARG:HD2	5:B:8:LYS:HZ3	1.79	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:41:PHE:HB3	5:B:190:MET:CE	2.45	0.46
15:M:59:GLY:C	15:M:141:ILE:HD11	2.35	0.46
30:2:10:ARG:HD2	30:2:49:GLU:OE2	2.15	0.46
20:R:113:HIS:O	20:R:145:LEU:HD12	2.15	0.46
1:O:2545:U:OP2	5:B:2:GLN:HG2	2.14	0.46
17:O:47:ARG:HA	17:O:50:ARG:NH1	2.30	0.46
1:O:100:C:H4'	22:T:16:LEU:HB2	1.98	0.46
1:O:1787:C:OP1	18:P:68:LYS:HE2	2.15	0.46
1:O:947:U:H2'	1:O:948:G:C8	2.50	0.46
9:F:37:THR:O	9:F:41:GLU:HG3	2.14	0.46
1:O:1419:U:H2'	1:O:1685:A:C2	2.51	0.46
9:F:4:VAL:HG13	9:F:76:PHE:CE1	2.50	0.46
1:O:1162:G:H1'	32:I:117:LEU:CD1	2.37	0.46
11:H:66:ARG:HD3	38:H:9177:HOH:O	2.14	0.46
20:R:19:ARG:HA	20:R:142:ASP:OD1	2.15	0.46
13:K:81:ARG:HD3	13:K:87:ARG:CZ	2.45	0.46
1:O:1285:U:H4'	25:W:74:GLU:OE1	2.15	0.46
11:H:162:ARG:HD3	38:H:9180:HOH:O	2.14	0.46
1:O:352:A:H2'	1:O:353:G:C8	2.49	0.46
15:M:164:THR:HG23	15:M:166:ALA:N	2.30	0.46
7:D:18:ILE:HD13	7:D:84:LEU:CD1	2.45	0.46
14:L:146:GLY:C	14:L:148:GLU:H	2.18	0.46
1:O:2840:A:H3'	38:O:7810:HOH:O	2.14	0.46
16:N:69:TYR:CE2	16:N:184:ILE:HD11	2.51	0.46
26:X:10:VAL:HG12	26:X:11:THR:N	2.29	0.46
4:A:164:ARG:NE	38:A:9383:HOH:O	2.47	0.46
6:C:76:ARG:HH11	6:C:76:ARG:HG2	1.81	0.46
1:O:669:G:O2'	1:O:670:G:H5'	2.16	0.46
1:O:2534:C:H1'	38:O:3787:HOH:O	2.14	0.46
1:O:1434:A:H2'	1:O:1436:C:C5	2.50	0.46
6:C:4:THR:HA	6:C:15:GLU:HB3	1.96	0.46
1:O:1187:U:H2'	38:O:7102:HOH:O	2.16	0.46
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.15	0.46
1:O:2591:C:H2'	1:O:2592:G:O4'	2.15	0.46
13:K:87:ARG:NH1	38:K:4066:HOH:O	2.48	0.46
17:O:96:VAL:HG12	17:O:97:SER:N	2.30	0.46
18:P:101:GLN:HG3	38:P:164:HOH:O	2.16	0.46
20:R:30:ALA:HA	20:R:33:ARG:HH12	1.81	0.46
14:L:35:ARG:O	14:L:40:PHE:HA	2.15	0.46
1:O:2820:A:H2'	1:O:2821:C:C6	2.51	0.46
5:B:24:PRO:HG2	5:B:204:GLY:HA2	1.98	0.46
31:3:72:GLY:HA2	38:3:9373:HOH:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:166:ILE:CD1	6:C:207:LEU:HD13	2.45	0.46
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.29	0.46
1:0:1759:A:N3	1:0:1818:C:H2'	2.31	0.46
5:B:66:GLU:OE1	5:B:328:ARG:HD2	2.15	0.46
17:O:39:THR:O	17:O:115:ARG:NH2	2.48	0.46
1:0:466:A:H2'	1:0:467:G:O4'	2.15	0.46
1:0:506:G:H22	1:0:509:A:H5''	1.79	0.46
32:I:132:CYS:O	32:I:134:SER:N	2.49	0.46
1:0:308:U:C4	1:0:342:C:H1'	2.51	0.46
23:U:53:ASP:O	23:U:54:THR:C	2.54	0.46
1:0:259:G:H21	15:M:58:GLN:NE2	2.14	0.46
10:G:67:LEU:O	10:G:71:LEU:HG	2.16	0.46
1:0:945:U:H2'	1:0:946:C:H6	1.80	0.46
23:U:6:CYS:HB2	23:U:32:CYS:HB3	1.97	0.46
15:M:139:PRO:O	15:M:143:ASN:ND2	2.49	0.46
1:0:1521:C:H2'	1:0:1522:A:H8	1.80	0.46
1:0:20:G:H21	20:R:117:HIS:HD2	1.62	0.46
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.45	0.46
2:9:3014:G:O2'	16:N:1:ALA:HB2	2.15	0.46
1:0:1603:A:H5'	1:0:1605:G:C4'	2.45	0.46
1:0:1058:A:H2'	1:0:1060:C:C5'	2.43	0.46
1:0:1185:U:H5'	38:0:7636:HOH:O	2.16	0.46
16:N:34:LEU:HD22	16:N:129:ILE:HD13	1.97	0.46
15:M:61:ILE:HG22	15:M:62:VAL:N	2.31	0.46
29:1:28:HIS:HD2	29:1:30:LYS:H	1.62	0.46
15:M:159:VAL:HG13	15:M:160:PHE:N	2.30	0.46
1:0:2421:G:H4'	38:0:5056:HOH:O	2.15	0.46
27:Y:97:LEU:C	27:Y:98:GLN:HG2	2.36	0.46
1:0:853:C:H2'	1:0:854:G:O4'	2.15	0.46
1:0:226:A:H1'	1:0:393:G:C5	2.50	0.46
1:0:1329:A:N1	36:0:9313:CL:CL	2.85	0.46
1:0:166:A:N7	14:L:25:GLY:HA2	2.30	0.46
15:M:49:ALA:C	15:M:54:TYR:HB3	2.35	0.46
1:0:1545:C:H2'	1:0:1546:G:O4'	2.16	0.46
1:0:1919:A:H5'	38:0:6245:HOH:O	2.16	0.46
1:0:2715:G:N2	5:B:264:GLU:OE1	2.45	0.46
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.15	0.46
1:0:820:G:H5'	1:0:821:U:H5'	1.96	0.46
1:0:821:U:H2'	1:0:822:C:H6	1.80	0.46
32:I:123:ASN:HA	32:I:126:LYS:CD	2.46	0.46
9:F:56:PRO:CG	15:M:44:THR:HA	2.45	0.46
1:0:1804:A:H2'	1:0:1805:G:H8	1.80	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:74:A:H2'	1:0:75:U:C6	2.51	0.46
6:C:88:SER:O	6:C:91:PRO:HD3	2.15	0.46
1:0:2900:G:H2'	1:0:2901:C:O4'	2.16	0.46
1:0:522:U:O2'	1:0:1366:C:H5'	2.15	0.46
38:9:3472:HOH:O	16:N:41:LYS:HD3	2.15	0.46
25:W:149:LEU:HG	25:W:153:MET:CE	2.46	0.46
6:C:182:ARG:HD2	6:C:184:ARG:HH12	1.81	0.46
7:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.63	0.46
12:J:131:THR:HB	12:J:134:GLU:OE1	2.15	0.46
13:K:23:ASN:HD21	13:K:107:THR:HB	1.81	0.46
1:0:1517:U:C2	1:0:1670:G:N2	2.84	0.46
1:0:1385:G:O3'	26:X:49:ARG:NH1	2.49	0.46
6:C:12:THR:HB	38:C:9244:HOH:O	2.15	0.46
1:0:911:G:H5'	1:0:932:U:OP1	2.16	0.46
7:D:67:ASP:O	7:D:69:ILE:HG13	2.16	0.46
16:N:34:LEU:HD13	16:N:47:LEU:HD21	1.97	0.46
12:J:108:PRO:HG2	12:J:109:TYR:CD1	2.51	0.46
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.50	0.46
2:9:3049:G:H2'	2:9:3050:G:O4'	2.15	0.46
1:0:497:A:H2'	1:0:498:A:C5'	2.46	0.46
14:L:17:SER:C	14:L:19:LYS:H	2.18	0.46
6:C:93:LYS:O	6:C:98:ARG:NH2	2.49	0.46
4:A:188:ASN:HA	38:A:9363:HOH:O	2.16	0.46
8:E:77:THR:OG1	8:E:78:GLU:N	2.48	0.46
18:P:15:ASP:O	18:P:16:VAL:HG23	2.16	0.46
26:X:27:ASP:OD2	26:X:27:ASP:N	2.48	0.46
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.80	0.46
22:T:88:PRO:O	22:T:90:PRO:HD3	2.16	0.46
25:W:64:THR:O	25:W:68:THR:HG22	2.16	0.46
5:B:195:ARG:N	5:B:198:GLU:OE1	2.50	0.46
7:D:64:ARG:CD	7:D:67:ASP:HB3	2.46	0.46
13:K:7:ASP:OD2	13:K:81:ARG:NH2	2.49	0.46
29:1:25:LYS:HD2	30:2:48:ASP:CA	2.45	0.46
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.97	0.46
1:0:1072:G:P	27:Y:154:ARG:HH22	2.39	0.46
1:0:960:G:N3	1:0:960:G:C2'	2.79	0.46
11:H:84:LYS:NZ	11:H:84:LYS:HB2	2.31	0.46
14:L:35:ARG:HD3	14:L:35:ARG:C	2.36	0.46
25:W:154:ARG:HE	25:W:154:ARG:HB3	1.53	0.46
1:0:671:A:O2'	1:0:672:G:H2'	2.16	0.46
12:J:133:GLY:O	12:J:137:GLU:HG3	2.16	0.46
1:0:2338:G:OP1	7:D:97:GLN:HG2	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:W:131:PRO:HD2	25:W:134:GLU:OE1	2.15	0.46
4:A:96:LEU:HD22	4:A:128:LEU:HD13	1.97	0.46
5:B:56:ASP:OD1	5:B:322:ARG:HB3	2.15	0.46
11:H:9:ILE:HG12	11:H:56:GLN:HG3	1.98	0.45
7:D:35:ALA:C	7:D:37:ALA:H	2.18	0.45
1:O:1184:C:O2'	1:O:1185:U:OP2	2.24	0.45
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.51	0.45
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.17	0.45
1:O:2420:G:O2'	1:O:2421:G:H5'	2.17	0.45
17:O:45:LEU:CD1	17:O:88:LYS:HD2	2.45	0.45
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.80	0.45
29:1:45:ARG:NH2	38:1:9232:HOH:O	2.43	0.45
14:L:10:SER:O	14:L:11:ARG:HB3	2.16	0.45
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.98	0.45
9:F:1:PRO:HB2	38:F:5897:HOH:O	2.16	0.45
6:C:19:PRO:CB	6:C:244:ALA:HB2	2.45	0.45
1:O:1666:C:C2'	1:O:1667:A:C5'	2.94	0.45
1:O:553:G:O2'	27:Y:179:PRO:HG3	2.16	0.45
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.27	0.45
14:L:143:THR:CG2	14:L:144:ASP:N	2.79	0.45
25:W:38:THR:HG22	38:W:3580:HOH:O	2.16	0.45
16:N:67:ALA:C	16:N:69:TYR:N	2.69	0.45
15:M:122:GLN:HG3	15:M:122:GLN:O	2.15	0.45
1:O:316:A:N3	1:O:336:G:O2'	2.45	0.45
13:K:66:ARG:HD3	38:K:2777:HOH:O	2.16	0.45
11:H:171:ALA:HA	38:H:9168:HOH:O	2.17	0.45
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.97	0.45
1:O:2506:A:H1'	38:O:4035:HOH:O	2.15	0.45
13:K:6:ALA:HB2	13:K:116:GLU:HG2	1.98	0.45
19:Q:94:GLN:HG2	19:Q:95:GLU:OE1	2.17	0.45
19:Q:94:GLN:O	19:Q:95:GLU:HB2	2.16	0.45
1:O:285:A:C2	1:O:368:C:H4'	2.51	0.45
16:N:43:VAL:CG1	16:N:118:ILE:HD11	2.44	0.45
1:O:86:A:C2	30:2:25:VAL:HG13	2.51	0.45
31:3:3:MET:O	31:3:90:PHE:HA	2.16	0.45
6:C:136:VAL:HA	6:C:137:PRO:C	2.37	0.45
1:O:1406:A:H4'	1:O:1407:A:C5'	2.46	0.45
22:T:20:HIS:ND1	22:T:41:ARG:NE	2.60	0.45
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.83	0.45
7:D:101:THR:O	7:D:157:LEU:HB3	2.16	0.45
6:C:200:PRO:HB3	6:C:212:VAL:HG23	1.97	0.45
5:B:149:ASP:HB2	38:B:9379:HOH:O	2.15	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:236:THR:O	6:C:239:ALA:N	2.50	0.45
2:9:3052:A:H2'	2:9:3053:G:O4'	2.17	0.45
25:W:65:VAL:HA	25:W:68:THR:CG2	2.46	0.45
1:0:2589:U:H2'	1:0:2590:U:C6	2.51	0.45
17:O:32:ARG:HH21	17:O:35:LYS:HD2	1.81	0.45
1:0:1641:A:H2'	1:0:1642:A:C5'	2.45	0.45
2:9:3020:G:O2'	2:9:3021:G:H5'	2.16	0.45
4:A:109:GLU:CD	4:A:113:GLY:H	2.20	0.45
16:N:67:ALA:O	16:N:69:TYR:N	2.50	0.45
5:B:7:ARG:HD3	5:B:9:GLY:O	2.16	0.45
1:0:35:U:H5'	6:C:47:GLY:O	2.17	0.45
20:R:30:ALA:HA	20:R:33:ARG:NH1	2.31	0.45
14:L:34:GLY:HA3	14:L:38:HIS:CE1	2.51	0.45
1:0:2404:G:OP1	19:Q:68:GLY:HA3	2.16	0.45
1:0:1155:G:H2'	1:0:1156:C:C6	2.52	0.45
16:N:44:ARG:HG3	16:N:45:ALA:N	2.32	0.45
5:B:320:GLN:NE2	5:B:321:PRO:CD	2.79	0.45
32:I:93:GLN:HA	32:I:96:PHE:CE2	2.45	0.45
5:B:145:HIS:HA	5:B:160:ASP:O	2.17	0.45
26:X:36:HIS:CE1	26:X:40:HIS:CD2	3.05	0.45
5:B:82:VAL:HG12	5:B:101:TRP:CE3	2.51	0.45
15:M:32:ARG:NH2	38:M:9391:HOH:O	2.49	0.45
1:0:710:G:O2'	1:0:711:G:H5'	2.16	0.45
2:9:3056:A:C3'	2:9:3057:A:H5''	2.45	0.45
25:W:4:LEU:HD23	25:W:4:LEU:HA	1.75	0.45
4:A:103:VAL:O	4:A:105:VAL:HG23	2.16	0.45
17:O:32:ARG:HG2	38:O:2336:HOH:O	2.16	0.45
1:0:1185:U:O2'	1:0:1186:C:H5'	2.17	0.45
1:0:1298:U:H2'	1:0:1299:G:C8	2.51	0.45
6:C:138:VAL:O	6:C:234:VAL:HA	2.16	0.45
4:A:8:ARG:NH1	38:A:9349:HOH:O	2.45	0.45
1:0:1279:U:O2	1:0:1279:U:H2'	2.17	0.45
17:O:44:ASN:OD1	17:O:65:LEU:HB2	2.17	0.45
1:0:2050:G:H5''	20:R:80:TYR:O	2.17	0.45
19:Q:64:GLU:HA	19:Q:64:GLU:OE1	2.17	0.45
12:J:75:PRO:HD3	12:J:136:SER:OG	2.16	0.45
1:0:2812:A:C2	1:0:2814:A:N6	2.72	0.45
16:N:152:GLU:C	16:N:154:LEU:N	2.70	0.45
1:0:2781:U:H1'	8:E:139:GLU:OE2	2.16	0.45
1:0:1874:U:P	4:A:51:ARG:HD2	2.57	0.45
11:H:36:LYS:HA	11:H:84:LYS:HZ1	1.82	0.45
23:U:6:CYS:C	23:U:8:TYR:H	2.20	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:2039:A:OP2	5:B:234:ARG:NH2	2.50	0.45
5:B:248:ARG:NH2	38:B:9325:HOH:O	2.49	0.45
14:L:89:PHE:CD1	14:L:89:PHE:N	2.84	0.45
14:L:97:VAL:O	14:L:100:ALA:HB2	2.16	0.45
1:O:1573:A:H2'	1:O:1574:C:O4'	2.16	0.45
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.17	0.45
1:O:2424:U:H1'	19:Q:7:LEU:HD12	1.99	0.45
1:O:2045:G:H2'	1:O:2046:G:O4'	2.17	0.45
26:X:43:VAL:CG1	26:X:44:ASP:N	2.79	0.45
1:O:1666:C:H2'	1:O:1667:A:C5'	2.46	0.45
32:I:113:HIS:NE2	32:I:121:LEU:HD22	2.32	0.45
16:N:163:PHE:O	16:N:164:ASP:OD1	2.35	0.45
7:D:167:GLU:OE2	7:D:173:GLU:HG2	2.17	0.45
15:M:61:ILE:CG2	15:M:62:VAL:N	2.80	0.45
21:S:52:VAL:HG22	21:S:66:VAL:HG13	1.98	0.45
1:O:1730:G:C5'	1:O:1731:C:H6	2.30	0.45
1:O:1790:C:H2'	1:O:1791:U:C6	2.50	0.45
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.99	0.45
1:O:1855:G:H4'	1:O:1856:C:O5'	2.16	0.45
20:R:33:ARG:NH1	38:R:9344:HOH:O	2.49	0.45
6:C:218:VAL:HG12	38:C:9228:HOH:O	2.16	0.45
7:D:15:GLU:HA	7:D:16:PRO:HD3	1.83	0.45
22:T:64:ASN:HB3	22:T:73:HIS:HB2	1.98	0.45
1:O:21:G:H5''	20:R:1:GLY:O	2.17	0.45
5:B:62:ARG:HG2	5:B:65:MET:CE	2.47	0.45
10:G:64:ASN:H	10:G:64:ASN:ND2	2.15	0.45
1:O:1185:U:H2'	1:O:1186:C:C6	2.51	0.45
1:O:902:G:N7	14:L:18:HIS:CD2	2.83	0.45
4:A:53:ALA:HB1	4:A:54:PRO:HD2	1.99	0.45
1:O:746:A:C6	17:O:65:LEU:HD13	2.52	0.45
1:O:222:A:H2'	1:O:223:G:O4'	2.17	0.45
1:O:1293:U:O2'	27:Y:149:GLN:NE2	2.46	0.45
1:O:1425:G:O2'	1:O:1426:C:H5'	2.17	0.45
7:D:170:TYR:CD1	7:D:170:TYR:N	2.85	0.45
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.32	0.44
5:B:243:ASN:HA	5:B:244:PRO:C	2.37	0.44
38:O:6984:HOH:O	16:N:5:ARG:HB2	2.17	0.44
6:C:115:LEU:CD2	6:C:243:VAL:HG13	2.45	0.44
5:B:137:LEU:HD21	5:B:140:LEU:HD21	1.98	0.44
6:C:132:ASP:HB2	6:C:161:ASP:HB3	1.98	0.44
9:F:28:ALA:CB	9:F:99:THR:HG23	2.47	0.44
2:9:3035:C:H5''	38:9:4078:HOH:O	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2404:G:OP1	19:Q:69:ASP:N	2.46	0.44
19:Q:37:GLU:OE1	19:Q:93:ARG:NE	2.49	0.44
13:K:110:LYS:O	13:K:111:GLY:O	2.34	0.44
1:0:1098:A:H2'	1:0:1099:G:O4'	2.17	0.44
1:0:1209:C:H2'	1:0:1210:G:H8	1.82	0.44
1:0:558:C:C2'	1:0:559:U:H5''	2.46	0.44
1:0:877:G:H1'	38:0:9479:HOH:O	2.17	0.44
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.47	0.44
31:3:69:TYR:CE1	31:3:80:ARG:HD2	2.52	0.44
1:0:694:A:H4'	1:0:2441:U:OP1	2.18	0.44
13:K:68:VAL:O	13:K:68:VAL:HG12	2.17	0.44
1:0:2699:A:H2'	1:0:2700:G:O4'	2.16	0.44
1:0:303:C:H2'	1:0:304:G:O4'	2.17	0.44
1:0:949:U:O2'	19:Q:40:HIS:HE1	2.00	0.44
1:0:1486:A:C5	30:2:2:LYS:HG3	2.52	0.44
22:T:18:GLU:O	22:T:21:LYS:HE2	2.17	0.44
1:0:170:U:H2'	1:0:171:C:H5'	1.99	0.44
1:0:1589:G:N2	1:0:1605:G:H1'	2.33	0.44
1:0:1205:U:C2'	1:0:1206:U:C5'	2.95	0.44
11:H:170:ASN:N	11:H:170:ASN:ND2	2.66	0.44
12:J:42:GLU:O	12:J:131:THR:HG23	2.18	0.44
5:B:207:LYS:HG2	5:B:304:PRO:HB3	1.99	0.44
2:9:3002:U:P	2:9:3003:A:H5'	2.58	0.44
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.53	0.44
18:P:142:ASP:O	18:P:143:ALA:O	2.35	0.44
1:0:2301:A:H5''	1:0:2302:A:H5'	1.98	0.44
1:0:2044:G:OP1	26:X:23:HIS:HE1	2.00	0.44
4:A:33:GLU:OE1	4:A:33:GLU:N	2.47	0.44
1:0:1803:C:H2'	1:0:1804:A:C8	2.52	0.44
1:0:1496:G:H5'	1:0:1572:A:H1'	1.98	0.44
38:0:4497:HOH:O	13:K:2:GLU:HA	2.17	0.44
16:N:115:VAL:HG23	16:N:116:PHE:N	2.31	0.44
13:K:96:VAL:HG21	13:K:109:LEU:HD22	1.99	0.44
1:0:2781:U:C2'	1:0:2782:G:H5'	2.47	0.44
32:I:89:SER:HB3	32:I:97:VAL:HG23	1.98	0.44
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.99	0.44
1:0:604:G:H2'	38:0:7912:HOH:O	2.17	0.44
1:0:920:C:H5'	1:0:921:G:C4	2.53	0.44
22:T:41:ARG:NH1	22:T:42:VAL:O	2.51	0.44
1:0:1398:G:O2'	1:0:1399:A:H5'	2.18	0.44
6:C:103:ASN:HB3	38:C:9109:HOH:O	2.18	0.44
1:0:2795:C:O2'	1:0:2796:U:H5'	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1477:C:H5'	1:0:1868:G:H5''	2.00	0.44
22:T:14:ALA:HA	22:T:15:PRO:HD3	1.87	0.44
1:0:162:C:H2'	1:0:163:U:H5'	2.00	0.44
1:0:299:U:H5'	38:0:7516:HOH:O	2.16	0.44
1:0:827:A:H2'	1:0:828:G:O4'	2.17	0.44
4:A:212:PRO:HB2	38:A:9357:HOH:O	2.17	0.44
1:0:290:C:O2'	1:0:291:C:H5'	2.17	0.44
31:3:25:VAL:HG13	31:3:68:LYS:HE3	2.00	0.44
5:B:125:GLU:OE2	5:B:129:ARG:NH1	2.51	0.44
17:O:32:ARG:HH21	17:O:35:LYS:CD	2.31	0.44
1:0:1131:G:C6	1:0:1230:A:C4	3.05	0.44
4:A:194:MET:HE3	4:A:199:HIS:HB2	1.99	0.44
4:A:199:HIS:HD2	4:A:201:PHE:H	1.65	0.44
18:P:38:GLU:HA	18:P:41:ARG:HH11	1.82	0.44
1:0:958:G:H2'	1:0:959:C:C6	2.53	0.44
1:0:794:U:H3	1:0:819:A:H61	1.66	0.44
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.48	0.44
6:C:19:PRO:HB3	6:C:244:ALA:HB2	2.00	0.44
1:0:1119:G:C8	12:J:52:GLN:NE2	2.85	0.44
1:0:484:A:N1	1:0:506:G:H4'	2.33	0.44
32:I:99:ASP:O	32:I:100:LEU:HG	2.18	0.44
25:W:6:GLN:HA	25:W:52:VAL:HG23	1.99	0.44
13:K:125:ALA:C	13:K:127:ALA:H	2.21	0.44
8:E:7:ILE:HD11	8:E:11:VAL:C	2.37	0.44
1:0:2271:G:N3	1:0:2271:G:H2'	2.33	0.44
1:0:2092:G:H2'	1:0:2613:G:OP1	2.18	0.44
5:B:175:LEU:HD23	5:B:175:LEU:O	2.18	0.44
4:A:87:GLU:HB3	38:A:9415:HOH:O	2.16	0.44
24:V:31:ARG:NE	38:V:2682:HOH:O	2.51	0.44
1:0:825:U:H5''	1:0:826:U:OP1	2.18	0.44
16:N:37:ARG:NH2	38:N:9334:HOH:O	2.51	0.44
24:V:12:THR:HG23	24:V:14:ALA:H	1.83	0.44
2:9:3053:G:O2'	2:9:3054:A:H5'	2.18	0.44
4:A:36:ASP:O	4:A:38:ILE:N	2.50	0.44
5:B:62:ARG:HA	5:B:65:MET:CE	2.40	0.44
29:1:8:GLN:NE2	29:1:11:LYS:HZ2	2.11	0.44
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.60	0.44
1:0:2769:C:H2'	1:0:2770:G:C5'	2.48	0.44
5:B:310:ARG:HB3	38:B:9444:HOH:O	2.16	0.44
22:T:78:THR:HB	22:T:87:VAL:O	2.18	0.44
15:M:159:VAL:HG12	36:M:9318:CL:CL	2.54	0.44
15:M:47:ASP:CG	15:M:48:LYS:N	2.71	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:106:A:H2'	1:0:107:U:O4'	2.18	0.44
1:0:1525:G:H5'	1:0:1526:A:OP2	2.17	0.44
38:0:5004:HOH:O	16:N:21:HIS:HD2	2.01	0.44
5:B:180:ASP:O	5:B:181:ILE:C	2.55	0.44
20:R:82:GLU:HG3	20:R:83:LYS:N	2.32	0.44
1:0:2670:G:O2'	1:0:2671:U:H5'	2.17	0.44
6:C:19:PRO:HG2	6:C:22:PHE:CE1	2.53	0.44
13:K:113:ILE:HD12	13:K:128:ALA:HB2	2.00	0.44
7:D:35:ALA:C	7:D:37:ALA:N	2.71	0.44
16:N:147:ILE:HG23	16:N:148:ALA:N	2.33	0.44
1:0:2451:G:O2'	31:3:38:ARG:NH2	2.51	0.44
1:0:64:G:H2'	1:0:65:C:O4'	2.18	0.44
6:C:54:LEU:HD23	6:C:79:ARG:HG3	1.98	0.44
19:Q:32:GLU:O	19:Q:93:ARG:NH2	2.51	0.44
1:0:1135:G:H5'	38:0:6173:HOH:O	2.18	0.44
1:0:2312:G:H2'	1:0:2313:C:H5'	1.99	0.44
1:0:2314:G:C2'	1:0:2315:C:H5'	2.47	0.44
1:0:2112:A:H2'	1:0:2113:G:C8	2.53	0.44
1:0:2467:A:O2'	1:0:2468:A:H2'	2.17	0.44
4:A:192:VAL:HB	38:A:9387:HOH:O	2.18	0.44
1:0:820:G:C5	4:A:171:LYS:HB2	2.53	0.44
11:H:83:TYR:C	11:H:83:TYR:CD1	2.91	0.44
1:0:1596:U:H2'	1:0:1598:A:OP2	2.17	0.44
1:0:1334:C:H2'	1:0:1335:C:H6	1.83	0.44
1:0:1711:A:O2'	1:0:1712:A:H5'	2.18	0.44
14:L:91:VAL:HB	38:L:9358:HOH:O	2.17	0.44
4:A:165:THR:O	4:A:165:THR:HG22	2.17	0.44
26:X:76:ARG:NH1	26:X:76:ARG:CG	2.74	0.43
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.48	0.43
16:N:86:LEU:O	16:N:90:LEU:HG	2.18	0.43
32:I:132:CYS:C	32:I:134:SER:H	2.21	0.43
14:L:134:GLU:HG3	38:L:9357:HOH:O	2.18	0.43
38:0:4890:HOH:O	17:O:35:LYS:HD3	2.18	0.43
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.47	0.43
16:N:127:LEU:HB2	38:N:9356:HOH:O	2.17	0.43
23:U:14:GLU:OE1	23:U:15:PRO:HD2	2.17	0.43
1:0:816:G:C6	1:0:817:G:N1	2.86	0.43
17:O:38:ARG:NH1	38:O:7674:HOH:O	2.51	0.43
1:0:794:U:H2'	1:0:795:G:H5'	2.00	0.43
15:M:68:ARG:O	15:M:68:ARG:HD3	2.17	0.43
1:0:2326:U:H4'	1:0:2412:G:H4'	2.00	0.43
1:0:941:G:C5	1:0:942:U:C4	3.06	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.36	0.43
16:N:62:HIS:O	16:N:65:ASP:OD1	2.35	0.43
6:C:84:VAL:O	6:C:85:LYS:HB2	2.17	0.43
22:T:23:VAL:C	22:T:93:THR:HG21	2.38	0.43
1:O:445:U:H2'	1:O:446:G:H8	1.82	0.43
8:E:107:PHE:CE1	8:E:152:THR:HB	2.52	0.43
6:C:236:THR:HA	38:C:9252:HOH:O	2.18	0.43
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.99	0.43
7:D:76:ARG:O	7:D:77:ASP:HB2	2.18	0.43
16:N:71:TRP:HE3	16:N:175:LEU:HD22	1.82	0.43
18:P:59:ARG:NH2	18:P:66:GLN:NE2	2.62	0.43
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.99	0.43
1:O:474:C:O3'	6:C:73:LEU:HD21	2.17	0.43
1:O:2050:G:OP1	20:R:79:ARG:HB3	2.18	0.43
14:L:93:VAL:HG12	14:L:97:VAL:HG23	2.00	0.43
1:O:757:C:OP1	14:L:27:ARG:HD2	2.16	0.43
26:X:43:VAL:HG12	26:X:47:ALA:HB3	2.00	0.43
11:H:9:ILE:HG23	11:H:126:ARG:NE	2.33	0.43
14:L:121:ILE:HA	14:L:141:GLU:O	2.18	0.43
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.34	0.43
27:Y:187:VAL:HG12	27:Y:205:ILE:HA	2.00	0.43
11:H:59:HIS:HA	11:H:62:LEU:HD23	1.98	0.43
8:E:20:ILE:HD12	8:E:33:LEU:HD12	2.00	0.43
1:O:1850:U:H2'	1:O:1851:G:C8	2.53	0.43
11:H:154:TYR:C	11:H:154:TYR:HD1	2.22	0.43
4:A:128:LEU:HG	38:A:9366:HOH:O	2.18	0.43
5:B:109:LEU:CG	5:B:113:LEU:HD12	2.49	0.43
30:2:35:ARG:HB2	38:2:2691:HOH:O	2.18	0.43
14:L:21:ARG:N	38:L:9330:HOH:O	2.51	0.43
11:H:146:VAL:HG22	38:H:9174:HOH:O	2.19	0.43
6:C:49:ASP:HB3	6:C:52:ALA:HB2	1.99	0.43
18:P:27:ARG:O	18:P:31:ILE:HG13	2.18	0.43
6:C:5:ILE:HG23	38:C:9234:HOH:O	2.18	0.43
24:V:7:GLU:O	24:V:11:MET:HG3	2.18	0.43
1:O:541:C:O2'	1:O:542:A:H5''	2.19	0.43
6:C:184:ARG:NE	38:C:9216:HOH:O	2.51	0.43
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.99	0.43
7:D:49:PRO:HA	7:D:73:VAL:HG22	2.00	0.43
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.82	0.43
1:O:136:C:P	15:M:39:ARG:HH22	2.42	0.43
31:3:65:THR:CG2	31:3:67:LEU:HG	2.48	0.43
6:C:79:ARG:O	6:C:87:ARG:HG2	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:690:G:H4'	1:0:741:C:O2	2.19	0.43
1:0:1768:C:H2'	1:0:1769:C:H5'	2.00	0.43
9:F:36:THR:O	9:F:40:ILE:HG13	2.19	0.43
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.76	0.43
1:0:1375:A:C2'	1:0:1376:G:H5'	2.48	0.43
6:C:19:PRO:HD2	6:C:240:LEU:CD2	2.49	0.43
5:B:13:PHE:N	38:B:9416:HOH:O	2.47	0.43
25:W:88:THR:CG2	25:W:89:ASP:H	2.22	0.43
30:2:40:ARG:HG3	30:2:45:ASN:CB	2.48	0.43
8:E:47:VAL:HG11	8:E:69:ILE:HD13	2.01	0.43
5:B:147:VAL:O	5:B:147:VAL:HG12	2.19	0.43
1:0:2719:A:C2	5:B:70:PRO:HG3	2.53	0.43
9:F:34:ASN:HA	15:M:4:ALA:HB2	2.01	0.43
1:0:922:A:N7	1:0:2281:C:H5'	2.33	0.43
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.42	0.43
1:0:2909:G:H2'	1:0:2910:A:C8	2.52	0.43
16:N:163:PHE:O	16:N:164:ASP:CG	2.56	0.43
1:0:244:C:OP2	9:F:38:LYS:HE3	2.19	0.43
1:0:2781:U:H2'	1:0:2782:G:H5'	1.99	0.43
1:0:661:G:C5	1:0:686:A:C2	3.07	0.43
1:0:2754:G:H2'	1:0:2755:G:O4'	2.18	0.43
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.99	0.43
5:B:148:PRO:HD2	38:B:9379:HOH:O	2.18	0.43
1:0:1398:G:H2'	1:0:1399:A:C8	2.53	0.43
1:0:1772:C:H5'	1:0:1773:G:C5	2.53	0.43
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.01	0.43
13:K:49:LEU:HA	13:K:73:VAL:HG12	2.00	0.43
1:0:737:A:H2'	1:0:738:G:O4'	2.18	0.43
14:L:130:ARG:O	14:L:131:GLU:C	2.57	0.43
13:K:9:THR:O	13:K:10:GLN:C	2.57	0.43
8:E:81:GLU:O	8:E:172:PRO:HD3	2.18	0.43
8:E:3:VAL:CG2	8:E:49:ILE:HB	2.44	0.43
1:0:363:A:O2'	1:0:364:C:H5'	2.18	0.43
25:W:146:ILE:HG23	25:W:150:LEU:HD12	2.00	0.43
5:B:26:PHE:HE1	38:B:9444:HOH:O	2.00	0.43
26:X:12:ILE:HB	26:X:70:ILE:CG2	2.48	0.43
11:H:84:LYS:HB2	11:H:84:LYS:HZ2	1.84	0.43
1:0:1151:G:OP2	10:G:65:THR:HG21	2.19	0.43
4:A:35:GLY:O	4:A:36:ASP:CB	2.67	0.43
1:0:1174:A:C5	1:0:1201:C:H4'	2.53	0.43
12:J:130:VAL:HG12	12:J:131:THR:H	1.84	0.43
5:B:41:PHE:CB	5:B:190:MET:HE3	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:7:ASP:C	6:C:9:ASP:H	2.22	0.43
1:0:470:U:O2'	29:1:16:HIS:CD2	2.68	0.43
7:D:58:VAL:HB	7:D:62:ASP:HB3	2.01	0.43
1:0:2241:C:H2'	1:0:2242:U:H6	1.81	0.43
1:0:2264:A:H2'	1:0:2265:U:C6	2.54	0.43
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.49	0.43
1:0:1594:C:O2'	1:0:1607:A:H4'	2.19	0.43
13:K:72:VAL:O	13:K:95:ALA:HA	2.18	0.43
8:E:132:THR:O	8:E:132:THR:HG23	2.19	0.43
1:0:204:A:C2'	1:0:205:U:H5'	2.49	0.43
1:0:766:A:H5'	38:0:4926:HOH:O	2.18	0.43
1:0:1852:A:H4'	4:A:230:SER:HB2	2.00	0.43
25:W:1:MET:N	25:W:103:GLU:OE2	2.47	0.43
1:0:2531:U:O2'	1:0:2532:A:H5'	2.19	0.43
6:C:162:VAL:CG1	6:C:192:ILE:HD11	2.49	0.43
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.54	0.43
1:0:2382:A:H5'	38:0:5017:HOH:O	2.18	0.43
1:0:635:A:H2'	1:0:636:G:H5''	2.01	0.43
11:H:112:GLY:N	38:H:9185:HOH:O	2.52	0.43
1:0:1943:C:O4'	4:A:212:PRO:HA	2.18	0.43
38:0:3098:HOH:O	13:K:39:GLY:HA3	2.18	0.43
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.54	0.43
32:I:113:HIS:N	32:I:114:PRO:HD2	2.33	0.43
27:Y:144:ARG:HG3	27:Y:144:ARG:HH11	1.84	0.43
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.32	0.43
7:D:169:THR:C	7:D:170:TYR:HD1	2.22	0.43
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.19	0.43
28:Z:81:ARG:O	28:Z:82:SER:C	2.56	0.43
1:0:677:C:O2'	1:0:678:G:H5'	2.18	0.43
4:A:140:LEU:HB3	4:A:141:PRO:HD2	2.00	0.43
7:D:140:ARG:O	7:D:144:ARG:HG2	2.19	0.43
5:B:217:ARG:CD	5:B:257:THR:HG22	2.49	0.43
1:0:2070:G:H2'	1:0:2072:G:OP1	2.18	0.43
1:0:553:G:P	27:Y:204:ARG:NH2	2.89	0.43
1:0:1080:C:H6	1:0:1080:C:O5'	2.01	0.43
6:C:107:ARG:CZ	6:C:107:ARG:HB3	2.49	0.43
25:W:73:LEU:HA	25:W:73:LEU:HD12	1.76	0.43
28:Z:56:GLN:HG3	28:Z:62:TYR:O	2.19	0.43
1:0:2785:C:H4'	1:0:2786:G:OP2	2.18	0.43
5:B:103:ASP:HB2	38:B:9395:HOH:O	2.19	0.43
1:0:1123:A:C6	1:0:1238:C:H5'	2.54	0.43
1:0:10:U:O4	1:0:532:A:OP2	2.37	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:E:156:ASP:OD2	8:E:157:LYS:NZ	2.46	0.43
6:C:5:ILE:HA	6:C:139:VAL:HG12	2.01	0.42
1:0:1603:A:H5''	1:0:1605:G:H5'	2.00	0.42
1:0:288:A:H61	1:0:364:C:H42	1.67	0.42
20:R:114:VAL:HA	20:R:144:GLU:O	2.19	0.42
7:D:11:HIS:CG	7:D:12:GLU:N	2.87	0.42
1:0:1675:C:H5''	30:2:5:LYS:HD2	2.01	0.42
1:0:2265:U:H2'	1:0:2266:A:H8	1.84	0.42
1:0:1095:U:O2	25:W:120:PRO:HG2	2.19	0.42
5:B:66:GLU:HG2	38:B:9443:HOH:O	2.18	0.42
1:0:2791:U:H1'	1:0:2792:A:H5''	2.00	0.42
6:C:37:ALA:O	6:C:41:ASN:ND2	2.51	0.42
1:0:1617:C:C4	1:0:1643:C:H4'	2.54	0.42
4:A:123:GLY:HA3	4:A:162:GLY:HA2	2.01	0.42
31:3:75:GLY:HA2	38:3:9358:HOH:O	2.18	0.42
1:0:177:A:H2'	1:0:178:U:O4'	2.18	0.42
13:K:14:LYS:HD2	13:K:45:PRO:HG3	2.01	0.42
32:I:132:CYS:C	32:I:134:SER:N	2.72	0.42
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.32	0.42
8:E:84:MET:HE1	8:E:148:ILE:HD12	2.00	0.42
28:Z:60:CYS:SG	28:Z:62:TYR:HB2	2.59	0.42
1:0:451:C:C2'	1:0:452:G:H5'	2.49	0.42
1:0:1236:A:C8	12:J:63:ILE:HD11	2.53	0.42
5:B:154:VAL:HA	5:B:155:PRO:HD3	1.84	0.42
1:0:2489:G:H1'	38:0:7457:HOH:O	2.19	0.42
1:0:1829:A:H5''	38:0:3377:HOH:O	2.18	0.42
20:R:39:THR:HB	20:R:42:GLU:CG	2.48	0.42
1:0:1306:U:OP1	6:C:184:ARG:HD2	2.19	0.42
1:0:907:A:H4'	1:0:1328:A:C2	2.54	0.42
17:O:26:TRP:HB2	38:O:3062:HOH:O	2.18	0.42
1:0:1903:U:O2'	1:0:1904:A:N7	2.50	0.42
1:0:2869:G:H2'	1:0:2870:C:H6	1.84	0.42
1:0:2326:U:H4'	1:0:2412:G:C4'	2.49	0.42
13:K:28:GLU:HB3	13:K:59:LYS:HB2	2.02	0.42
1:0:1051:C:H2'	1:0:1052:G:O4'	2.20	0.42
1:0:23:G:H1'	1:0:520:A:N6	2.35	0.42
1:0:1158:G:O2'	1:0:1159:G:H5'	2.20	0.42
21:S:58:MET:SD	30:2:8:LYS:HE3	2.59	0.42
7:D:40:ILE:HG23	38:D:5583:HOH:O	2.18	0.42
1:0:1603:A:C5'	1:0:1605:G:H5'	2.50	0.42
16:N:151:ASP:HB3	38:N:9328:HOH:O	2.19	0.42
1:0:1299:G:H5'	38:0:4362:HOH:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:65:ARG:O	4:A:66:ARG:HG3	2.18	0.42
4:A:199:HIS:HD2	4:A:201:PHE:HB2	1.85	0.42
2:9:3047:A:C2	2:9:3048:C:C2	3.07	0.42
14:L:57:VAL:O	14:L:57:VAL:HG12	2.19	0.42
1:0:2664:A:H8	1:0:2664:A:OP1	2.02	0.42
25:W:19:ASP:O	25:W:23:MET:HG3	2.19	0.42
1:0:2434:A:O3'	31:3:28:GLY:HA3	2.19	0.42
1:0:2809:G:H2'	1:0:2810:G:O4'	2.19	0.42
1:0:297:U:H2'	1:0:298:C:H6	1.84	0.42
21:S:76:GLU:HB3	38:S:9143:HOH:O	2.19	0.42
21:S:57:THR:C	21:S:59:ASP:H	2.22	0.42
1:0:2269:C:H2'	1:0:2270:G:C5'	2.48	0.42
2:9:3007:G:H5'	38:N:9346:HOH:O	2.18	0.42
11:H:169:GLY:C	11:H:170:ASN:HD22	2.23	0.42
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.33	0.42
9:F:28:ALA:HB3	9:F:99:THR:O	2.19	0.42
3:4:74:C:C2'	3:4:75:C:H5'	2.49	0.42
1:0:95:A:H5''	1:0:97:G:O4'	2.19	0.42
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.20	0.42
1:0:292:G:H2'	1:0:358:G:N2	2.34	0.42
8:E:112:ALA:HA	8:E:113:PRO:HD3	1.88	0.42
8:E:86:VAL:CG1	8:E:129:GLU:HA	2.48	0.42
1:0:2672:C:O2'	1:0:2673:U:H5'	2.20	0.42
1:0:156:C:H5''	15:M:171:ARG:CD	2.27	0.42
7:D:41:LEU:HA	7:D:44:ILE:CG2	2.48	0.42
25:W:29:VAL:O	25:W:30:ASN:HB2	2.19	0.42
5:B:62:ARG:HG2	5:B:65:MET:HE3	2.02	0.42
5:B:195:ARG:HG2	5:B:323:LEU:HD22	2.02	0.42
1:0:1201:C:C2'	1:0:1202:A:H5'	2.46	0.42
7:D:173:GLU:O	7:D:174:VAL:C	2.58	0.42
13:K:34:VAL:HG21	13:K:46:LYS:O	2.20	0.42
20:R:25:PHE:CZ	20:R:29:LYS:HE2	2.55	0.42
1:0:2323:G:H5'	38:0:7221:HOH:O	2.19	0.42
7:D:20:LYS:HA	7:D:75:LEU:O	2.20	0.42
1:0:1676:G:O2'	1:0:1677:U:H5'	2.20	0.42
11:H:139:ASN:O	11:H:141:GLU:N	2.52	0.42
7:D:55:LYS:O	7:D:56:ARG:HB2	2.19	0.42
1:0:245:C:H2'	1:0:246:G:H5'	2.02	0.42
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.20	0.42
6:C:164:ALA:O	6:C:167:ASP:HB2	2.20	0.42
5:B:238:ASN:ND2	5:B:240:GLY:N	2.56	0.42
24:V:60:GLN:O	24:V:65:ASP:N	2.47	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1166:A:N3	1:0:1166:A:H2'	2.35	0.42
32:I:112:LYS:HB3	32:I:116:LEU:HG	2.02	0.42
1:0:111:C:H2'	1:0:112:G:O4'	2.20	0.42
5:B:195:ARG:CG	5:B:323:LEU:HD22	2.50	0.42
7:D:64:ARG:HG2	7:D:67:ASP:HB3	2.02	0.42
24:V:42:ASN:N	24:V:43:PRO:HD3	2.34	0.42
20:R:61:GLN:CD	38:R:9341:HOH:O	2.58	0.42
1:0:1314:U:H5''	1:0:1316:G:O4'	2.19	0.42
1:0:2064:U:H5'	1:0:2652:U:O3'	2.20	0.42
5:B:17:LYS:O	5:B:260:HIS:CD2	2.73	0.42
26:X:70:ILE:O	26:X:70:ILE:HG23	2.20	0.42
1:0:2541:U:H3'	1:0:2541:U:H6	1.84	0.42
1:0:794:U:C2'	1:0:795:G:H5'	2.50	0.42
1:0:1025:C:H5'	25:W:23:MET:O	2.20	0.42
1:0:394:G:H1	15:M:181:GLU:CD	2.23	0.42
10:G:12:ILE:N	10:G:13:PRO:HD3	2.34	0.42
1:0:1979:G:H2'	38:0:3589:HOH:O	2.19	0.42
1:0:2638:G:H1'	38:0:4856:HOH:O	2.19	0.42
1:0:517:U:H1'	38:0:7742:HOH:O	2.17	0.42
1:0:2824:C:H5''	1:0:2825:C:H5'	2.00	0.42
21:S:6:LYS:O	21:S:7:HIS:HB3	2.20	0.42
1:0:1631:A:H2'	1:0:1632:A:C8	2.54	0.42
6:C:187:ARG:NH2	38:C:9164:HOH:O	2.51	0.42
18:P:115:SER:OG	18:P:118:GLN:CG	2.68	0.42
1:0:2506:A:O2'	1:0:2507:G:P	2.78	0.42
27:Y:187:VAL:HB	38:Y:8158:HOH:O	2.19	0.42
1:0:656:G:H3'	17:O:37:ARG:HH12	1.84	0.42
5:B:86:ALA:HA	38:B:9378:HOH:O	2.19	0.42
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.50	0.42
4:A:51:ARG:HB2	38:A:9401:HOH:O	2.19	0.42
1:0:947:U:O2'	1:0:948:G:H5'	2.19	0.42
38:0:6519:HOH:O	27:Y:158:LYS:HD3	2.19	0.42
1:0:472:A:H5'	29:1:35:SER:OG	2.19	0.42
19:Q:75:ILE:CD1	19:Q:84:ILE:HD11	2.50	0.42
11:H:69:ALA:HB2	11:H:153:ALA:HB2	2.02	0.42
1:0:39:G:N2	1:0:444:C:C2	2.88	0.42
15:M:115:LEU:HD13	15:M:116:ASN:HB2	2.02	0.42
1:0:2425:A:H5'	1:0:2426:G:OP2	2.20	0.42
30:2:49:GLU:HB2	38:2:719:HOH:O	2.20	0.42
1:0:1878:G:O2'	1:0:1879:U:OP2	2.37	0.42
5:B:104:GLU:HG3	38:B:9395:HOH:O	2.20	0.42
14:L:24:ALA:HB2	14:L:30:ARG:HD2	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:115:LEU:HA	6:C:115:LEU:HD12	1.92	0.42
10:G:71:LEU:C	10:G:73:ASP:N	2.73	0.42
21:S:39:ASP:HB3	21:S:43:GLU:OE2	2.20	0.42
1:0:790:A:H1'	1:0:1710:A:H2'	2.02	0.42
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.35	0.42
1:0:1878:G:O2'	1:0:1879:U:P	2.78	0.42
8:E:101:GLU:HB3	8:E:117:THR:HA	2.01	0.42
1:0:462:A:C8	30:2:37:HIS:CE1	3.08	0.42
4:A:95:PRO:HG2	4:A:98:GLU:HG2	2.02	0.42
1:0:1562:C:N4	38:0:6115:HOH:O	2.51	0.42
38:0:9421:HOH:O	5:B:229:ARG:HD2	2.20	0.42
1:0:611:U:H2'	1:0:612:U:C6	2.55	0.42
22:T:37:GLN:OE1	22:T:118:SER:HA	2.19	0.42
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.88	0.42
1:0:195:C:H2'	1:0:196:G:H5'	2.02	0.42
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.49	0.41
22:T:49:GLU:HB3	22:T:59:GLU:HG3	2.02	0.41
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.19	0.41
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.55	0.41
25:W:141:HIS:HB2	25:W:146:ILE:HG12	2.02	0.41
4:A:99:ILE:O	4:A:131:HIS:CE1	2.72	0.41
14:L:143:THR:HG22	14:L:144:ASP:H	1.83	0.41
22:T:12:ARG:O	22:T:19:ARG:NH2	2.53	0.41
1:0:1921:A:C6	1:0:1922:A:C2	3.08	0.41
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.55	0.41
1:0:2642:G:H2'	1:0:2643:G:O4'	2.20	0.41
1:0:249:G:H1'	1:0:265:U:O2	2.20	0.41
9:F:91:VAL:CG1	9:F:92:GLY:H	2.15	0.41
16:N:50:LEU:HD12	16:N:55:ASP:OD1	2.20	0.41
1:0:1192:A:N6	32:I:134:SER:CB	2.82	0.41
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.59	0.41
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.56	0.41
1:0:2003:U:H4'	1:0:2004:U:H5	1.85	0.41
1:0:2780:C:H2'	1:0:2781:U:C6	2.56	0.41
7:D:22:VAL:HA	7:D:73:VAL:O	2.19	0.41
1:0:1163:G:H5''	32:I:115:ASP:HB3	2.03	0.41
11:H:76:GLU:O	11:H:77:LEU:HD23	2.20	0.41
24:V:49:LEU:O	24:V:53:ILE:HG13	2.20	0.41
5:B:82:VAL:O	5:B:82:VAL:HG12	2.19	0.41
1:0:711:G:C2	1:0:718:C:C2	3.08	0.41
7:D:169:THR:HG22	7:D:169:THR:O	2.19	0.41
1:0:886:A:OP2	1:0:2113:G:H5'	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:51:TYR:CE2	29:1:53:LYS:HB3	2.55	0.41
1:0:2515:C:H2'	1:0:2516:G:O4'	2.20	0.41
13:K:24:THR:HB	13:K:64:MET:HE2	2.01	0.41
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.53	0.41
1:0:806:A:H2'	1:0:807:A:O4'	2.20	0.41
2:9:3096:C:O2'	2:9:3097:U:H5'	2.21	0.41
28:Z:67:GLY:N	28:Z:70:LYS:O	2.52	0.41
26:X:44:ASP:HB3	26:X:46:ASP:OD2	2.20	0.41
26:X:72:VAL:HG22	26:X:85:VAL:CG1	2.45	0.41
1:0:1474:C:C5'	1:0:1474:C:H6	2.20	0.41
4:A:36:ASP:HA	4:A:83:GLY:HA3	2.01	0.41
8:E:68:HIS:O	8:E:72:MET:HG3	2.19	0.41
9:F:58:GLU:HG3	9:F:61:MET:HE1	2.02	0.41
5:B:205:VAL:O	5:B:307:ARG:NE	2.53	0.41
20:R:114:VAL:HB	20:R:145:LEU:HD13	2.01	0.41
14:L:66:VAL:HG23	14:L:67:ARG:N	2.35	0.41
5:B:51:VAL:HG23	5:B:330:VAL:HG22	2.01	0.41
6:C:165:ASP:O	6:C:168:ARG:HB3	2.19	0.41
5:B:280:VAL:HG13	5:B:333:GLU:O	2.19	0.41
1:0:664:U:O4	1:0:681:G:H5''	2.19	0.41
1:0:2676:C:H4'	12:J:70:PHE:HE1	1.85	0.41
7:D:153:THR:O	7:D:156:ARG:HB2	2.20	0.41
2:9:3095:C:O2'	2:9:3096:C:H5'	2.20	0.41
1:0:1481:G:H2'	1:0:1482:A:O4'	2.21	0.41
13:K:41:LYS:O	13:K:42:ASN:HB2	2.20	0.41
1:0:2363:G:O2'	19:Q:11:ARG:HG3	2.20	0.41
25:W:6:GLN:HG2	25:W:29:VAL:HA	2.01	0.41
1:0:559:U:O2'	1:0:560:C:H5'	2.20	0.41
4:A:93:THR:HG23	4:A:154:ALA:O	2.21	0.41
22:T:48:VAL:O	22:T:59:GLU:HG2	2.20	0.41
9:F:58:GLU:HA	9:F:61:MET:HE2	2.00	0.41
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.67	0.41
1:0:1730:G:H5''	1:0:1731:C:C6	2.54	0.41
2:9:3049:G:C2'	2:9:3050:G:H5'	2.51	0.41
1:0:1343:C:H2'	1:0:1344:G:O5'	2.20	0.41
1:0:815:U:O2'	1:0:1598:A:H4'	2.20	0.41
2:9:3088:G:OP1	25:W:130:HIS:NE2	2.49	0.41
1:0:200:U:H2'	38:O:3736:HOH:O	2.20	0.41
1:0:1945:G:O2'	1:0:1946:C:H5'	2.20	0.41
1:0:1764:C:H2'	1:0:1765:G:O4'	2.20	0.41
1:0:1414:A:H2'	1:0:1415:G:O4'	2.20	0.41
1:0:1041:U:H4'	1:0:1295:G:H5'	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:33:ASP:O	5:B:34:GLY:O	2.38	0.41
6:C:123:LEU:HA	6:C:123:LEU:HD23	1.94	0.41
6:C:140:VAL:HG12	6:C:141:SER:N	2.34	0.41
1:0:2712:G:H5'	38:K:4183:HOH:O	2.21	0.41
13:K:109:LEU:HD13	13:K:113:ILE:CD1	2.51	0.41
1:0:656:G:H5'	17:O:3:THR:HB	2.02	0.41
1:0:2252:A:H2'	1:0:2253:G:H5'	2.02	0.41
6:C:7:ASP:OD1	6:C:11:ASN:O	2.37	0.41
1:0:88:G:C8	1:0:88:G:H5'	2.53	0.41
1:0:2474:A:N6	3:4:176:DA:OP2	2.53	0.41
12:J:70:PHE:CD2	12:J:70:PHE:O	2.74	0.41
4:A:134:ASN:O	4:A:150:PRO:HD3	2.20	0.41
15:M:50:ARG:N	15:M:54:TYR:HB3	2.34	0.41
14:L:17:SER:C	14:L:19:LYS:N	2.74	0.41
1:0:1477:C:H4'	1:0:1868:G:H5''	2.01	0.41
1:0:1056:U:H2'	1:0:1057:A:O4'	2.20	0.41
20:R:122:GLN:HB3	20:R:138:SER:HB2	2.03	0.41
1:0:2766:A:O2'	1:0:2767:C:H5'	2.20	0.41
38:0:5775:HOH:O	5:B:298:LYS:HD3	2.19	0.41
16:N:82:TYR:C	16:N:82:TYR:CD2	2.94	0.41
1:0:870:G:C3'	1:0:871:G:H5''	2.50	0.41
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.48	0.41
1:0:1188:A:C6	1:0:1189:A:C6	3.09	0.41
7:D:41:LEU:CA	7:D:44:ILE:HG22	2.48	0.41
9:F:63:ILE:HB	9:F:64:PRO:CD	2.47	0.41
5:B:5:ARG:HA	5:B:6:PRO:HD3	1.97	0.41
1:0:2436:U:H5'	31:3:68:LYS:HE2	2.01	0.41
26:X:78:GLU:CG	26:X:79:GLU:H	2.27	0.41
16:N:154:LEU:C	16:N:156:GLU:H	2.22	0.41
1:0:2781:U:H2'	1:0:2782:G:C5'	2.51	0.41
5:B:280:VAL:HG13	5:B:334:SER:HA	2.03	0.41
4:A:76:VAL:CG2	28:Z:63:LYS:HB3	2.49	0.41
5:B:27:ASN:HB3	38:B:9425:HOH:O	2.20	0.41
11:H:78:GLY:C	11:H:80:GLU:H	2.24	0.41
1:0:947:U:H2'	1:0:948:G:H8	1.83	0.41
1:0:711:G:H1'	38:0:7290:HOH:O	2.20	0.41
1:0:1773:G:N2	1:0:1774:G:C8	2.88	0.41
1:0:1755:A:H2'	1:0:1756:G:O4'	2.20	0.41
18:P:45:ASP:C	18:P:47:GLY:H	2.24	0.41
1:0:1838:U:O2'	1:0:2644:C:H5'	2.21	0.41
5:B:224:LYS:HD3	5:B:224:LYS:HA	1.93	0.41
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:9:3057:A:C8	7:D:141:VAL:HG21	2.56	0.41
1:0:1328:A:C8	27:Y:169:ARG:HD3	2.56	0.41
1:0:820:G:O2'	1:0:856:G:H4'	2.21	0.41
11:H:27:LYS:H	11:H:59:HIS:CD2	2.32	0.41
4:A:66:ARG:NH1	4:A:66:ARG:CB	2.84	0.41
1:0:695:C:H2'	1:0:696:C:C6	2.56	0.41
23:U:20:MET:CG	23:U:28:THR:HG23	2.51	0.41
1:0:212:A:O4'	1:0:214:U:C6	2.74	0.41
2:9:3011:A:O2'	2:9:3012:C:H3'	2.21	0.41
1:0:1717:A:H5''	18:P:54:LYS:HB2	2.03	0.41
28:Z:80:ARG:O	28:Z:81:ARG:O	2.39	0.41
1:0:1937:U:O2'	1:0:1938:G:H5'	2.20	0.41
1:0:844:A:C6	1:0:882:A:C5	3.09	0.41
4:A:173:GLY:O	4:A:176:HIS:HB3	2.21	0.41
1:0:2090:G:H2'	1:0:2091:G:C8	2.55	0.41
20:R:26:LYS:HB3	20:R:62:HIS:CD2	2.56	0.41
1:0:1915:U:O2'	1:0:1916:C:H5'	2.20	0.41
11:H:114:ARG:O	11:H:115:ALA:C	2.59	0.41
1:0:876:A:H2'	1:0:876:A:N3	2.36	0.41
6:C:140:VAL:CG1	6:C:141:SER:N	2.84	0.41
7:D:44:ILE:HG23	7:D:45:THR:HG23	2.02	0.41
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.21	0.41
4:A:200:PRO:HD3	38:A:9319:HOH:O	2.21	0.41
1:0:903:U:O4	14:L:18:HIS:HB2	2.21	0.41
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.51	0.41
1:0:47:G:N3	1:0:114:A:C2	2.89	0.41
1:0:1333:U:H2'	1:0:1334:C:H6	1.86	0.41
6:C:76:ARG:NH1	6:C:76:ARG:CG	2.81	0.41
1:0:1439:C:H6	1:0:1439:C:O5'	2.04	0.41
1:0:1659:A:H2'	1:0:1660:G:O4'	2.20	0.41
26:X:61:ARG:HH12	26:X:67:PRO:HD3	1.84	0.41
1:0:350:C:O2'	1:0:351:G:H5'	2.21	0.41
22:T:40:VAL:HG23	22:T:119:ALA:C	2.41	0.41
8:E:81:GLU:HA	8:E:133:VAL:O	2.21	0.41
24:V:4:HIS:O	24:V:8:ILE:HG13	2.20	0.41
24:V:1:THR:O	24:V:4:HIS:CE1	2.74	0.41
22:T:48:VAL:CG1	22:T:96:VAL:HG22	2.50	0.41
2:9:3039:U:H3'	2:9:3040:C:H5''	2.02	0.41
23:U:9:CYS:O	23:U:52:THR:HG23	2.20	0.41
1:0:1820:G:C6	1:0:2030:A:C2	3.09	0.41
29:1:25:LYS:HE2	38:1:9262:HOH:O	2.20	0.41
1:0:1543:G:N1	1:0:1641:A:OP2	2.39	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:N:47:LEU:HD13	16:N:97:VAL:HG11	2.02	0.41
16:N:93:GLN:HG2	38:N:9356:HOH:O	2.21	0.41
7:D:172:VAL:HG12	7:D:173:GLU:N	2.35	0.41
2:9:3003:A:H2	2:9:3021:G:N3	2.19	0.41
8:E:12:ASP:HA	38:E:1750:HOH:O	2.19	0.41
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.20	0.41
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.54	0.41
1:0:638:C:H2'	1:0:639:A:H8	1.85	0.41
1:0:1747:A:C8	13:K:44:LEU:HD13	2.56	0.41
5:B:7:ARG:CG	5:B:7:ARG:HH11	2.33	0.41
1:0:1406:A:H5'	1:0:1407:A:C8	2.56	0.41
1:0:764:C:OP1	6:C:87:ARG:NH1	2.54	0.41
1:0:2403:C:H2'	1:0:2404:G:O5'	2.20	0.41
1:0:1477:C:O2'	1:0:1478:U:H5'	2.21	0.41
1:0:2435:U:OP1	31:3:28:GLY:HA3	2.20	0.41
1:0:1839:A:H5'	1:0:2643:G:H4'	2.02	0.41
5:B:33:ASP:HB3	5:B:34:GLY:H	1.76	0.41
26:X:61:ARG:NH1	26:X:67:PRO:HD3	2.36	0.41
13:K:90:PHE:N	13:K:90:PHE:CD1	2.89	0.41
5:B:225:GLY:HA3	38:B:9367:HOH:O	2.21	0.41
1:0:318:C:H5'	1:0:339:A:C4	2.55	0.41
1:0:2626:C:H2'	1:0:2627:G:C8	2.56	0.41
1:0:697:G:H4'	1:0:730:G:O3'	2.21	0.41
20:R:12:THR:HG22	20:R:149:GLU:OE1	2.21	0.41
11:H:88:ARG:HG2	11:H:133:LEU:O	2.20	0.41
20:R:27:HIS:O	20:R:31:ILE:HG13	2.21	0.41
1:0:1313:A:H5'	27:Y:208:LYS:O	2.21	0.41
1:0:930:C:N3	1:0:1040:A:N6	2.68	0.41
1:0:1321:A:H2'	1:0:1322:G:C8	2.56	0.41
1:0:1811:A:H2'	1:0:1812:G:H5'	2.01	0.41
1:0:2724:U:O5'	1:0:2724:U:H6	2.03	0.41
6:C:19:PRO:HD2	6:C:240:LEU:HD21	2.03	0.41
7:D:154:LYS:H	7:D:154:LYS:CD	2.09	0.41
20:R:39:THR:O	20:R:40:ALA:C	2.59	0.41
26:X:76:ARG:O	26:X:77:PHE:HB3	2.20	0.41
15:M:99:ARG:HE	15:M:170:ASN:ND2	2.19	0.41
1:0:396:U:P	31:3:38:ARG:HH11	2.44	0.41
1:0:1173:A:H4'	1:0:1174:A:C8	2.56	0.41
7:D:24:HIS:HB2	7:D:71:ALA:O	2.21	0.41
25:W:92:ASP:OD1	25:W:92:ASP:N	2.54	0.41
1:0:1130:U:H4'	38:0:6364:HOH:O	2.20	0.41
5:B:55:ASN:HB3	5:B:64:GLY:H	1.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:O:50:ARG:HD2	17:O:51:TYR:CE1	2.56	0.41
25:W:1:MET:N	25:W:37:GLU:HG3	2.36	0.41
9:F:49:PHE:CD1	9:F:49:PHE:N	2.89	0.41
1:O:2880:A:H2'	1:O:2881:C:H5'	2.03	0.41
1:O:1471:A:H2'	1:O:1472:C:C6	2.55	0.41
1:O:2705:U:O2'	1:O:2706:A:H5'	2.20	0.41
2:9:3061:C:H2'	2:9:3062:A:H8	1.85	0.41
1:O:414:C:H5'	38:O:9961:HOH:O	2.20	0.41
4:A:215:ILE:HG13	4:A:216:SER:N	2.36	0.41
1:O:185:G:H4'	1:O:186:A:H4'	2.03	0.41
1:O:29:C:O2'	1:O:30:U:H5'	2.21	0.41
6:C:21:VAL:HG23	6:C:22:PHE:CD1	2.56	0.40
4:A:211:LYS:CB	38:A:9412:HOH:O	2.68	0.40
4:A:36:ASP:HB2	4:A:83:GLY:C	2.41	0.40
1:O:1705:C:C5'	18:P:59:ARG:HH12	2.34	0.40
9:F:102:GLY:O	9:F:103:GLU:HB2	2.21	0.40
1:O:1969:A:N7	1:O:1970:G:C6	2.89	0.40
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.41	0.40
1:O:2408:A:H4'	31:3:15:ASN:O	2.21	0.40
4:A:1:GLY:HA2	4:A:197:VAL:HG23	2.02	0.40
5:B:57:GLU:HA	5:B:58:PRO:HD2	1.96	0.40
19:Q:16:ASN:HD22	19:Q:16:ASN:HA	1.70	0.40
11:H:167:PRO:O	11:H:168:ALA:CB	2.67	0.40
1:O:1160:G:O2'	1:O:1190:G:H1'	2.21	0.40
24:V:12:THR:H	24:V:15:GLU:HB2	1.86	0.40
15:M:99:ARG:HE	15:M:170:ASN:HD22	1.69	0.40
1:O:2072:G:N2	38:O:7076:HOH:O	2.46	0.40
1:O:2072:G:C6	1:O:2533:C:H1'	2.57	0.40
11:H:66:ARG:HB3	38:H:9177:HOH:O	2.21	0.40
32:I:92:PRO:C	32:I:94:GLU:N	2.74	0.40
1:O:450:C:OP1	6:C:184:ARG:NH2	2.55	0.40
25:W:69:ARG:HD2	25:W:117:ARG:O	2.21	0.40
5:B:321:PRO:HA	38:B:9454:HOH:O	2.21	0.40
1:O:1268:C:O2'	27:Y:169:ARG:HB2	2.22	0.40
7:D:146:LYS:HZ1	16:N:107:ASN:ND2	2.19	0.40
18:P:103:THR:O	18:P:107:GLU:HG3	2.21	0.40
27:Y:234:VAL:HG12	27:Y:235:GLU:N	2.37	0.40
5:B:132:HIS:CE1	5:B:171:VAL:CG2	3.05	0.40
1:O:2503:A:OP1	11:H:151:ARG:NH2	2.50	0.40
5:B:51:VAL:HG23	5:B:329:TYR:O	2.21	0.40
1:O:1634:G:H2'	1:O:1635:U:H6	1.86	0.40
7:D:94:ALA:HB3	7:D:97:GLN:NE2	2.35	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1477:C:H5'	1:0:1868:G:C5'	2.51	0.40
6:C:191:SER:OG	6:C:192:ILE:N	2.54	0.40
8:E:154:ILE:HD11	8:E:157:LYS:HE2	2.03	0.40
21:S:29:ASP:OD1	21:S:31:ARG:HG3	2.21	0.40
27:Y:141:THR:HG23	38:Y:8175:HOH:O	2.19	0.40
1:0:803:C:O2'	1:0:804:C:H5'	2.21	0.40
1:0:354:A:H2'	1:0:355:C:C6	2.56	0.40
9:F:13:GLU:OE2	9:F:78:GLU:HG2	2.21	0.40
4:A:112:PRO:HD3	4:A:152:CYS:SG	2.61	0.40
1:0:2047:C:H5'	38:0:3119:HOH:O	2.20	0.40
26:X:41:PHE:CZ	26:X:74:ALA:HB3	2.57	0.40
1:0:1118:A:C8	1:0:1119:G:H5'	2.56	0.40
1:0:308:U:H5'	22:T:97:ARG:NH2	2.37	0.40
8:E:69:ILE:HA	8:E:72:MET:HE2	2.00	0.40
13:K:98:VAL:CG1	13:K:99:ASP:N	2.85	0.40
1:0:1819:G:H2'	1:0:1820:G:C4'	2.48	0.40
13:K:118:ALA:O	13:K:120:ARG:N	2.54	0.40
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.51	0.40
4:A:48:ASP:HA	4:A:49:PRO:HD3	1.82	0.40
1:0:2281:C:C2'	1:0:2282:U:H5'	2.50	0.40
1:0:622:G:P	27:Y:148:GLY:HA3	2.60	0.40
1:0:860:U:H2'	1:0:861:A:C8	2.56	0.40
17:O:80:ASP:OD1	17:O:81:PHE:N	2.54	0.40
1:0:2710:U:H1'	38:0:7786:HOH:O	2.21	0.40
1:0:2906:A:H5'	1:0:2907:C:O4'	2.21	0.40
1:0:2105:C:H2'	1:0:2106:C:C6	2.56	0.40
14:L:126:SER:O	14:L:127:GLU:C	2.57	0.40
15:M:67:VAL:HB	15:M:97:ILE:HG23	2.04	0.40
31:3:91:GLN:O	31:3:92:GLU:HB2	2.21	0.40
16:N:108:SER:HA	16:N:109:PRO:HD3	1.79	0.40
15:M:164:THR:HG23	15:M:166:ALA:H	1.85	0.40
12:J:74:ARG:HH12	12:J:76:ASP:CB	2.34	0.40
9:F:57:GLU:O	9:F:61:MET:HG3	2.22	0.40
11:H:27:LYS:N	11:H:59:HIS:HD2	2.14	0.40
7:D:13:MET:CA	7:D:137:PRO:HG2	2.51	0.40
1:0:475:G:C5'	6:C:73:LEU:HD23	2.52	0.40
1:0:694:A:C2'	1:0:695:C:H5'	2.51	0.40
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.51	0.40
5:B:313:PRO:O	5:B:314:ALA:C	2.59	0.40
1:0:1375:A:H2'	1:0:1376:G:H5'	2.03	0.40
8:E:154:ILE:HG13	8:E:156:ASP:OD1	2.21	0.40
1:0:2089:A:O2'	1:0:2090:G:H5'	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:318:C:H5'	1:0:339:A:C2	2.57	0.40
1:0:581:G:O2'	1:0:582:C:H5'	2.21	0.40
5:B:87:TYR:CE2	5:B:96:PRO:HG3	2.56	0.40
1:0:1783:A:O2'	1:0:1784:U:H5'	2.20	0.40
5:B:223:ARG:HG3	5:B:232:TRP:O	2.22	0.40
1:0:2729:C:O2'	1:0:2730:G:H5'	2.22	0.40
9:F:39:SER:HB3	9:F:45:ALA:HB2	2.04	0.40
1:0:536:A:H3'	38:0:5321:HOH:O	2.21	0.40
1:0:1556:G:O2'	1:0:1557:G:H5'	2.21	0.40
16:N:139:TRP:CZ2	16:N:176:ARG:NH1	2.90	0.40
15:M:24:GLN:HE22	15:M:27:ARG:HH11	1.67	0.40
5:B:162:MET:HE1	5:B:308:LEU:HD21	2.03	0.40
7:D:57:THR:CG2	7:D:63:ILE:HG22	2.49	0.40
4:A:109:GLU:HG2	4:A:116:GLY:H	1.85	0.40
1:0:68:U:O2'	1:0:69:A:H5''	2.22	0.40
26:X:12:ILE:HD13	26:X:36:HIS:CE1	2.56	0.40
1:0:1311:G:C2	1:0:1312:G:C8	3.09	0.40
9:F:26:THR:CG2	9:F:102:GLY:HA3	2.52	0.40
1:0:1391:G:H2'	1:0:1392:A:H5'	2.03	0.40
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.37	0.40
4:A:125:ASN:HB3	4:A:158:VAL:HG12	2.03	0.40
1:0:1388:U:H2'	1:0:1389:G:O4'	2.22	0.40
1:0:1066:U:H2'	1:0:1067:A:C8	2.57	0.40
1:0:2667:G:H1'	1:0:2914:A:N3	2.36	0.40
20:R:100:ASP:C	20:R:102:GLN:N	2.74	0.40
6:C:157:LEU:HD11	6:C:194:PHE:HZ	1.85	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%)	205 (87%)	28 (12%)	2 (1%)	25 55
5	B	335/338 (99%)	303 (90%)	27 (8%)	5 (2%)	15 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	244/246 (99%)	223 (91%)	20 (8%)	1 (0%)	43	76
7	D	134/177 (76%)	94 (70%)	34 (25%)	6 (4%)	4	7
8	E	170/178 (96%)	161 (95%)	7 (4%)	2 (1%)	19	45
9	F	117/120 (98%)	101 (86%)	13 (11%)	3 (3%)	8	20
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	144 (92%)	7 (4%)	5 (3%)	6	14
12	J	140/145 (97%)	128 (91%)	10 (7%)	2 (1%)	16	41
13	K	130/132 (98%)	116 (89%)	12 (9%)	2 (2%)	15	38
14	L	141/165 (86%)	118 (84%)	23 (16%)	0	100	100
15	M	192/194 (99%)	178 (93%)	13 (7%)	1 (0%)	38	70
16	N	184/187 (98%)	167 (91%)	12 (6%)	5 (3%)	8	19
17	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
18	P	141/149 (95%)	131 (93%)	9 (6%)	1 (1%)	30	62
19	Q	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	R	148/155 (96%)	133 (90%)	14 (10%)	1 (1%)	30	62
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	108 (92%)	8 (7%)	1 (1%)	25	55
23	U	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	11	28
24	V	63/71 (89%)	55 (87%)	7 (11%)	1 (2%)	14	35
25	W	152/154 (99%)	144 (95%)	6 (4%)	2 (1%)	18	43
26	X	80/92 (87%)	72 (90%)	7 (9%)	1 (1%)	18	43
27	Y	140/241 (58%)	134 (96%)	6 (4%)	0	100	100
28	Z	71/83 (86%)	57 (80%)	9 (13%)	5 (7%)	2	2
29	1	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
30	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
31	3	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
32	I	68/162 (42%)	55 (81%)	11 (16%)	2 (3%)	7	16
All	All	3705/4430 (84%)	3348 (90%)	308 (8%)	49 (1%)	18	43

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	D	27	ILE

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Mol	Chain	Res	Type
7	D	137	PRO
7	D	173	GLU
9	F	101	ALA
11	H	140	VAL
11	H	166	SER
11	H	168	ALA
16	N	154	LEU
28	Z	42	CYS
28	Z	81	ARG
5	B	34	GLY
6	C	8	LEU
7	D	65	GLU
7	D	138	GLY
12	J	5	GLU
13	K	111	GLY
16	N	139	TRP
24	V	43	PRO
4	A	34	ASP
5	B	139	ASP
5	B	184	ASP
11	H	16	ARG
12	J	89	HIS
16	N	68	GLU
16	N	164	ASP
18	P	116	SER
25	W	49	ASN
25	W	77	ALA
26	X	87	ALA
28	Z	41	ASN
32	I	76	ALA
32	I	133	THR
5	B	185	GLY
8	E	17	HIS
9	F	44	SER
13	K	119	GLN
28	Z	43	GLY
4	A	37	VAL
7	D	28	GLY
23	U	7	ASP
28	Z	28	GLU
8	E	44	GLY
9	F	64	PRO

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Mol	Chain	Res	Type
11	H	79	GLU
22	T	53	GLY
5	B	2	GLN
15	M	88	VAL
20	R	81	PRO
16	N	74	PRO

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%)	167 (93%)	12 (7%)	23	49
5	B	282/283 (100%)	263 (93%)	19 (7%)	23	49
6	C	193/193 (100%)	180 (93%)	13 (7%)	23	49
7	D	117/148 (79%)	112 (96%)	5 (4%)	40	72
8	E	152/156 (97%)	148 (97%)	4 (3%)	59	88
9	F	93/94 (99%)	92 (99%)	1 (1%)	84	96
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	126 (96%)	6 (4%)	38	70
12	J	118/121 (98%)	109 (92%)	9 (8%)	19	41
13	K	106/106 (100%)	103 (97%)	3 (3%)	56	86
14	L	113/127 (89%)	108 (96%)	5 (4%)	39	71
15	M	158/158 (100%)	151 (96%)	7 (4%)	39	71
16	N	149/150 (99%)	145 (97%)	4 (3%)	57	87
17	O	93/94 (99%)	92 (99%)	1 (1%)	84	96
18	P	113/117 (97%)	109 (96%)	4 (4%)	48	80
19	Q	79/80 (99%)	76 (96%)	3 (4%)	44	76
20	R	117/122 (96%)	114 (97%)	3 (3%)	59	88
21	S	71/74 (96%)	69 (97%)	2 (3%)	56	86
22	T	105/106 (99%)	98 (93%)	7 (7%)	23	49
23	U	44/52 (85%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	V	51/57 (90%)	51 (100%)	0	100	100
25	W	130/130 (100%)	123 (95%)	7 (5%)	31	61
26	X	66/74 (89%)	62 (94%)	4 (6%)	26	54
27	Y	120/196 (61%)	116 (97%)	4 (3%)	50	81
28	Z	60/68 (88%)	59 (98%)	1 (2%)	73	94
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	61	89
31	3	79/79 (100%)	79 (100%)	0	100	100
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2968 (96%)	125 (4%)	42	75

All (125) 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	66	ARG
4	A	69	LEU
4	A	78	ASP
4	A	94	LEU
4	A	120	ARG
4	A	131	HIS
4	A	153	ARG
4	A	206	ARG
4	A	217	ARG
5	B	7	ARG
5	B	11	LEU
5	B	27	ASN
5	B	49	THR
5	B	63	GLU
5	B	97	LEU
5	B	140	LEU
5	B	162	MET
5	B	190	MET
5	B	195	ARG
5	B	234	ARG
5	B	245	SER
5	B	251	VAL

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Mol	Chain	Res	Type
5	B	254	GLN
5	B	256	GLN
5	B	257	THR
5	B	264	GLU
5	B	304	PRO
5	B	307	ARG
6	C	2	GLN
6	C	27	ARG
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	115	LEU
6	C	136	VAL
6	C	187	ARG
6	C	214	THR
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	240	LEU
7	D	24	HIS
7	D	61	PHE
7	D	133	ASN
7	D	136	ARG
7	D	137	PRO
8	E	7	ILE
8	E	15	GLN
8	E	102	VAL
8	E	164	ASP
9	F	46	GLU
11	H	30	GLN
11	H	84	LYS
11	H	88	ARG
11	H	111	ASP
11	H	132	GLN
11	H	154	TYR
12	J	45	VAL
12	J	46	ILE
12	J	52	GLN
12	J	74	ARG
12	J	79	PHE
12	J	107	ASN
12	J	112	ASP

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Mol	Chain	Res	Type
12	J	127	ILE
12	J	131	THR
13	K	7	ASP
13	K	10	GLN
13	K	49	LEU
14	L	30	ARG
14	L	35	ARG
14	L	80	ASP
14	L	102	ASP
14	L	117	GLU
15	M	46	LEU
15	M	68	ARG
15	M	81	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
15	M	164	THR
16	N	26	LEU
16	N	47	LEU
16	N	50	LEU
16	N	152	GLU
17	O	43	VAL
18	P	21	VAL
18	P	52	LYS
18	P	91	LYS
18	P	98	ILE
19	Q	11	ARG
19	Q	16	ASN
19	Q	57	ASP
20	R	39	THR
20	R	82	GLU
20	R	132	ARG
21	S	71	ASP
21	S	80	ARG
22	T	19	ARG
22	T	23	VAL
22	T	39	ASN
22	T	73	HIS
22	T	75	GLU
22	T	96	VAL
22	T	112	LEU
25	W	26	ILE

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Mol	Chain	Res	Type
25	W	45	VAL
25	W	52	VAL
25	W	73	LEU
25	W	142	ASP
25	W	146	ILE
25	W	154	ARG
26	X	15	ARG
26	X	27	ASP
26	X	46	ASP
26	X	72	VAL
27	Y	154	ARG
27	Y	163	THR
27	Y	189	ASN
27	Y	203	VAL
28	Z	13	ARG
30	2	18	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	29	HIS
4	A	47	HIS
4	A	92	ASN
4	A	125	ASN
4	A	127	GLN
4	A	199	HIS
5	B	27	ASN
5	B	145	HIS
5	B	238	ASN
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
6	C	163	HIS
7	D	47	GLN
7	D	97	GLN
7	D	103	ASN
7	D	133	ASN
8	E	74	HIS

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Mol	Chain	Res	Type
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	70	ASN
11	H	132	GLN
12	J	52	GLN
12	J	107	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	58	GLN
15	M	24	GLN
15	M	58	GLN
15	M	137	ASN
15	M	143	ASN
15	M	170	ASN
16	N	40	ASN
16	N	107	ASN
18	P	50	GLN
18	P	66	GLN
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
20	R	123	GLN
21	S	25	GLN
21	S	53	ASN
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	27	HIS

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Mol	Chain	Res	Type
25	W	28	HIS
25	W	87	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	23	HIS
26	X	36	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	15	ASN
31	3	30	GLN
31	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	237 (8%)	34 (1%)
2	9	121/122 (99%)	17 (14%)	1 (0%)
3	4	1/8 (12%)	0	0
All	All	2867/3052 (93%)	254 (8%)	35 (1%)

All (254) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C

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Mol	Chain	Res	Type
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	200	U
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	331	A
1	0	336	G
1	0	337	A
1	0	345	G
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	516	A
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G

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Mol	Chain	Res	Type
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	605	C
1	0	620	A
1	0	630	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	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U

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Mol	Chain	Res	Type
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	1109	U
1	0	1110	G
1	0	1119	G
1	0	1120	U
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	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	1407	A
1	0	1451	C
1	0	1474	C
1	0	1485	A
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	1563	G

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Mol	Chain	Res	Type
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	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1980	U
1	0	1996	U
1	0	2004	U
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

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Mol	Chain	Res	Type
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2332	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2467	A
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2542	C
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2637	A
1	0	2649	A
1	0	2664	A
1	0	2681	A

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Mol	Chain	Res	Type
1	0	2682	C
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2850	C
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
2	9	3024	U
2	9	3025	G
2	9	3040	C
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A

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Mol	Chain	Res	Type
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	604	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	869	G
1	0	871	G
1	0	877	G
1	0	898	G
1	0	1080	C
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1506	U
1	0	1563	G
1	0	1692	C
1	0	1730	G
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2536	C
1	0	2541	U
1	0	2649	A
1	0	2718	C
1	0	2791	U
2	9	3065	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OMU	0	2587	1	20,22,23	0.72	1 (5%)	24,31,34	0.66	0
1	OMG	0	2588	1,3	24,26,27	0.90	1 (4%)	32,38,41	5.38	4 (12%)
1	UR3	0	2619	1	20,22,23	0.82	0	23,32,35	0.81	0
1	PSU	0	2621	1	19,21,22	1.28	3 (15%)	23,30,33	1.06	1 (4%)
1	1MA	0	628	1	23,25,26	0.81	0	32,37,40	1.03	2 (6%)
3	5AA	4	76	1,3	24,26,27	0.82	0	35,38,41	0.96	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/8/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/10/27/28	0/1/3/3
1	UR3	0	2619	1	-	0/6/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/8/25/26	0/2/2/2
1	1MA	0	628	1	-	1/8/25/26	0/1/3/3
3	5AA	4	76	1,3	-	0/12/29/30	0/1/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	3.24	1.43	1.37
1	0	2621	PSU	C6-N1	2.68	1.34	1.32
1	0	2588	OMG	P-OP1	2.61	1.49	1.46
1	0	2621	PSU	P-OP1	2.48	1.49	1.46
1	0	2587	OMU	P-OP1	2.20	1.49	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	C6-C5-N7	-29.85	130.12	134.14
3	4	76	5AA	C2-N1-C6	3.46	119.04	111.53
1	0	628	1MA	C2-N3-C4	-3.18	110.80	116.23
1	0	2588	OMG	C6-N1-C2	3.17	125.05	119.51
1	0	2621	PSU	C5-C4-N3	-2.34	114.60	118.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	C2-N3-C4	-2.30	111.85	115.09
1	0	628	1MA	CM1-N1-C6	2.19	123.60	120.56
1	0	2588	OMG	N2-C2-N1	-2.05	115.60	117.86
3	4	76	5AA	C9-N6-C6	2.04	126.20	119.88

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 233 ligands modelled in this entry, 233 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2754/2922 (94%)	-0.24	46 (1%) 67 73	29, 51, 94, 161	0
2	9	122/122 (100%)	-0.25	4 (3%) 44 49	39, 62, 91, 152	0
3	4	8/8 (100%)	-0.48	0 100 100	41, 46, 47, 49	0
4	A	237/240 (98%)	0.11	7 (2%) 48 54	33, 57, 95, 119	0
5	B	337/338 (99%)	0.02	9 (2%) 52 57	29, 57, 80, 94	0
6	C	246/246 (100%)	-0.09	3 (1%) 75 81	27, 53, 75, 84	0
7	D	140/177 (79%)	1.98	60 (42%) 1 0	58, 101, 127, 137	0
8	E	172/178 (96%)	0.66	20 (11%) 5 6	47, 67, 87, 93	0
9	F	119/120 (99%)	0.88	19 (15%) 3 3	60, 82, 104, 119	0
10	G	29/348 (8%)	1.77	11 (37%) 1 1	65, 90, 102, 105	0
11	H	160/171 (93%)	0.26	5 (3%) 47 52	41, 59, 90, 99	0
12	J	142/145 (97%)	-0.02	1 (0%) 84 89	37, 52, 72, 90	0
13	K	132/132 (100%)	-0.08	2 (1%) 70 75	34, 56, 77, 87	0
14	L	145/165 (87%)	0.57	18 (12%) 5 5	30, 72, 118, 132	0
15	M	194/194 (100%)	-0.11	1 (0%) 88 92	34, 50, 67, 74	0
16	N	186/187 (99%)	0.53	19 (10%) 7 7	38, 66, 115, 121	0
17	O	115/116 (99%)	0.21	1 (0%) 81 85	45, 61, 77, 85	0
18	P	143/149 (95%)	0.29	2 (1%) 72 77	45, 60, 77, 85	0
19	Q	95/96 (98%)	-0.03	1 (1%) 77 82	40, 48, 60, 75	0
20	R	150/155 (96%)	-0.17	1 (0%) 84 89	37, 48, 68, 75	0
21	S	81/85 (95%)	0.24	2 (2%) 54 61	49, 67, 85, 94	0
22	T	119/120 (99%)	0.70	13 (10%) 6 6	46, 63, 91, 110	0
23	U	53/66 (80%)	0.13	2 (3%) 38 43	43, 57, 74, 85	0
24	V	65/71 (91%)	1.53	20 (30%) 1 1	63, 86, 117, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	-0.10	1 (0%) 86 90	39, 50, 67, 76	0
26	X	82/92 (89%)	0.43	7 (8%) 11 11	45, 59, 77, 95	0
27	Y	142/241 (58%)	0.04	6 (4%) 35 39	30, 49, 71, 86	0
28	Z	73/83 (87%)	0.18	4 (5%) 24 26	44, 63, 77, 97	0
29	1	56/57 (98%)	-0.40	0 100 100	33, 40, 46, 54	0
30	2	46/50 (92%)	0.60	5 (10%) 6 6	41, 65, 97, 109	0
31	3	92/92 (100%)	0.24	4 (4%) 34 38	37, 59, 73, 84	0
32	I	70/162 (43%)	3.40	52 (74%) 0 0	99, 121, 143, 145	0
All	All	6659/7482 (89%)	0.09	346 (5%) 26 29	27, 56, 102, 161	0

All (346) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	11.7
24	V	1	THR	10.0
32	I	133	THR	9.8
7	D	63	ILE	9.6
32	I	93	GLN	8.8
32	I	96	PHE	8.4
24	V	39	ALA	7.1
32	I	113	HIS	6.9
7	D	88	LEU	6.8
32	I	88	GLY	6.7
30	2	49	GLU	6.7
24	V	40	PRO	6.5
1	0	1173	A	6.5
1	0	2237	G	6.5
7	D	57	THR	6.4
22	T	119	ALA	6.2
32	I	137	VAL	6.1
7	D	90	LEU	6.1
7	D	66	GLY	6.1
32	I	117	LEU	6.1
16	N	183	ASP	5.9
7	D	128	LEU	5.8
7	D	69	ILE	5.8
32	I	102	VAL	5.7
32	I	79	ILE	5.7
16	N	166	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
32	I	76	ALA	5.6
14	L	60	GLU	5.5
24	V	43	PRO	5.5
24	V	38	GLY	5.4
1	0	1171	A	5.3
32	I	97	VAL	5.3
32	I	109	ALA	5.2
2	9	3023	U	5.2
7	D	65	GLU	5.2
14	L	105	TYR	5.2
1	0	1199	A	5.2
7	D	130	VAL	5.1
32	I	116	LEU	5.1
7	D	64	ARG	5.1
7	D	18	ILE	5.0
32	I	91	GLU	5.0
7	D	106	PHE	5.0
2	9	3001	U	5.0
7	D	93	LEU	4.9
2	9	3024	U	4.9
32	I	111	GLN	4.8
30	2	35	ARG	4.8
32	I	118	SER	4.8
1	0	2238	A	4.8
32	I	98	ALA	4.8
32	I	85	PHE	4.7
21	S	81	ILE	4.7
4	A	37	VAL	4.7
7	D	44	ILE	4.6
1	0	1172	G	4.6
14	L	80	ASP	4.6
22	T	112	LEU	4.5
1	0	282	C	4.5
10	G	27	ILE	4.5
7	D	56	ARG	4.5
7	D	170	TYR	4.4
7	D	68	PRO	4.3
1	0	960	G	4.3
1	0	1177	A	4.3
7	D	85	GLN	4.3
7	D	87	ALA	4.2
14	L	104	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
24	V	41	GLU	4.2
8	E	45	ASP	4.1
27	Y	235	GLU	4.1
32	I	139	ILE	4.1
7	D	84	LEU	4.1
7	D	25	MET	4.1
9	F	119	ARG	4.0
7	D	41	LEU	4.0
7	D	26	GLY	4.0
1	0	735	C	4.0
32	I	87	THR	4.0
9	F	28	ALA	4.0
26	X	88	GLU	3.9
22	T	42	VAL	3.9
14	L	100	ALA	3.9
1	0	1198	U	3.9
7	D	89	PRO	3.8
32	I	77	GLU	3.8
32	I	110	GLU	3.8
1	0	1951	G	3.8
7	D	58	VAL	3.8
10	G	23	ILE	3.8
16	N	147	ILE	3.8
27	Y	108	ASP	3.8
1	0	284	C	3.8
1	0	1279	U	3.7
32	I	95	ASP	3.6
5	B	119	HIS	3.6
1	0	2239	C	3.6
32	I	121	LEU	3.6
24	V	8	ILE	3.6
9	F	47	LEU	3.6
7	D	62	ASP	3.6
7	D	165	PHE	3.6
14	L	106	VAL	3.6
7	D	10	PHE	3.5
7	D	61	PHE	3.5
16	N	179	LEU	3.5
4	A	237	GLY	3.4
9	F	107	ASP	3.4
32	I	114	PRO	3.4
31	3	22	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	0	1202	A	3.4
32	I	107	GLN	3.3
9	F	100	ASP	3.3
32	I	81	ASP	3.3
8	E	100	ASP	3.3
7	D	23	VAL	3.3
16	N	138	ASP	3.3
23	U	47	ARG	3.2
7	D	104	PHE	3.2
7	D	172	VAL	3.2
2	9	3002	U	3.2
6	C	135	GLU	3.2
19	Q	95	GLU	3.2
9	F	17	LEU	3.2
9	F	108	VAL	3.2
6	C	132	ASP	3.2
8	E	170	ARG	3.2
7	D	27	ILE	3.1
7	D	45	THR	3.1
22	T	40	VAL	3.1
30	2	39	ARG	3.1
9	F	106	ALA	3.1
7	D	92	GLU	3.1
7	D	83	PHE	3.1
14	L	96	VAL	3.1
5	B	104	GLU	3.1
7	D	129	ASP	3.1
26	X	85	VAL	3.1
24	V	37	GLY	3.1
26	X	41	PHE	3.0
32	I	103	ASP	3.0
32	I	89	SER	3.0
31	3	62	THR	3.0
4	A	35	GLY	3.0
7	D	171	ASP	3.0
32	I	128	VAL	3.0
16	N	127	LEU	3.0
16	N	165	ALA	3.0
7	D	86	THR	3.0
32	I	106	LYS	3.0
14	L	150	GLN	2.9
24	V	52	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
16	N	185	GLU	2.9
32	I	138	THR	2.9
1	O	970	U	2.9
14	L	99	GLU	2.9
28	Z	20	ARG	2.9
7	D	75	LEU	2.9
9	F	103	GLU	2.9
22	T	1	SER	2.9
32	I	135	LEU	2.9
32	I	119	TYR	2.9
32	I	140	GLU	2.9
8	E	5	LEU	2.9
5	B	105	PHE	2.9
9	F	90	GLU	2.9
7	D	166	ILE	2.8
9	F	98	VAL	2.8
11	H	45	VAL	2.8
10	G	24	VAL	2.8
15	M	194	ALA	2.8
8	E	42	VAL	2.8
7	D	17	ARG	2.8
14	L	59	GLU	2.8
16	N	149	GLU	2.8
9	F	99	THR	2.8
32	I	75	THR	2.8
10	G	71	LEU	2.8
24	V	63	GLU	2.8
9	F	16	ALA	2.7
1	O	716	G	2.7
7	D	40	ILE	2.7
9	F	49	PHE	2.7
22	T	116	ASP	2.7
11	H	171	ALA	2.7
24	V	59	ILE	2.7
1	O	2769	C	2.7
24	V	3	LEU	2.7
1	O	2664	A	2.7
4	A	36	ASP	2.7
9	F	117	GLU	2.7
22	T	49	GLU	2.7
28	Z	24	ARG	2.6
1	O	1950	G	2.6

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Mol	Chain	Res	Type	RSRZ
16	N	159	TYR	2.6
1	0	272	A	2.6
9	F	109	GLU	2.6
32	I	124	ALA	2.6
1	0	999	C	2.6
24	V	49	LEU	2.6
8	E	126	ILE	2.6
7	D	80	ALA	2.6
1	0	1200	A	2.6
7	D	134	LEU	2.6
14	L	124	ASP	2.6
10	G	65	THR	2.6
7	D	43	GLU	2.5
24	V	36	ALA	2.5
30	2	44	ARG	2.5
11	H	79	GLU	2.5
8	E	124	VAL	2.5
5	B	116	PRO	2.5
7	D	98	PHE	2.5
7	D	11	HIS	2.5
32	I	104	GLN	2.5
21	S	20	PHE	2.5
5	B	118	ASP	2.5
16	N	155	GLU	2.5
32	I	83	ALA	2.5
32	I	123	ASN	2.5
7	D	70	GLY	2.5
16	N	161	GLY	2.5
8	E	3	VAL	2.5
1	0	1170	U	2.5
5	B	128	ILE	2.5
32	I	72	VAL	2.5
32	I	78	LEU	2.4
32	I	73	PRO	2.4
16	N	150	TYR	2.4
9	F	44	SER	2.4
1	0	1525	G	2.4
27	Y	95	THR	2.4
4	A	135	VAL	2.4
17	O	48	ILE	2.4
16	N	152	GLU	2.4
13	K	119	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
28	Z	80	ARG	2.4
1	0	1181	A	2.4
8	E	99	GLY	2.4
1	0	2344	G	2.4
1	0	280	C	2.4
30	2	20	ARG	2.4
16	N	181	ASP	2.4
7	D	24	HIS	2.4
20	R	7	GLU	2.4
1	0	138	U	2.4
24	V	9	ARG	2.4
1	0	1180	U	2.3
7	D	132	VAL	2.3
8	E	86	VAL	2.3
8	E	97	VAL	2.3
1	0	2250	G	2.3
11	H	37	GLN	2.3
26	X	71	ARG	2.3
27	Y	96	GLU	2.3
23	U	55	ALA	2.3
24	V	31	ARG	2.3
1	0	1913	C	2.3
13	K	132	VAL	2.3
14	L	62	ALA	2.3
9	F	15	ASP	2.3
7	D	107	GLY	2.3
7	D	22	VAL	2.3
14	L	130	ARG	2.3
1	0	497	A	2.3
32	I	84	GLY	2.3
8	E	87	PHE	2.3
32	I	86	GLU	2.2
1	0	370	G	2.2
11	H	130	GLY	2.2
22	T	58	GLU	2.2
32	I	100	LEU	2.2
22	T	99	THR	2.2
27	Y	236	VAL	2.2
32	I	105	VAL	2.2
8	E	53	GLU	2.2
24	V	45	ARG	2.2
1	0	1948	G	2.2

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Mol	Chain	Res	Type	RSRZ
16	N	162	ASP	2.2
32	I	132	CYS	2.2
26	X	80	GLU	2.2
10	G	21	ASP	2.2
16	N	180	LEU	2.2
31	3	56	PRO	2.2
10	G	67	LEU	2.2
32	I	120	ASP	2.2
7	D	135	VAL	2.1
7	D	67	ASP	2.1
18	P	67	LYS	2.1
22	T	117	ASP	2.1
12	J	92	GLN	2.1
26	X	74	ALA	2.1
5	B	121	PRO	2.1
14	L	91	VAL	2.1
24	V	33	VAL	2.1
1	0	2508	C	2.1
14	L	123	ASP	2.1
1	0	1197	G	2.1
10	G	69	ARG	2.1
25	W	79	VAL	2.1
1	0	2103	A	2.1
9	F	19	ALA	2.1
27	Y	103	THR	2.1
7	D	54	ALA	2.1
1	0	285	A	2.1
8	E	93	MET	2.1
10	G	26	MET	2.1
14	L	107	LYS	2.1
5	B	183	GLU	2.1
8	E	46	THR	2.1
10	G	70	ALA	2.1
14	L	73	VAL	2.1
32	I	115	ASP	2.1
1	0	128	A	2.1
26	X	7	GLU	2.1
16	N	95	ALA	2.1
4	A	34	ASP	2.1
16	N	184	ILE	2.1
18	P	71	TYR	2.1
1	0	1203	G	2.1

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Mol	Chain	Res	Type	RSRZ
1	0	1929	G	2.1
8	E	128	GLY	2.1
24	V	61	GLY	2.1
4	A	85	SER	2.0
7	D	16	PRO	2.0
8	E	98	GLU	2.0
24	V	7	GLU	2.0
28	Z	25	ARG	2.0
31	3	92	GLU	2.0
6	C	61	PHE	2.0
1	0	10	U	2.0
1	0	371	U	2.0
8	E	10	ASP	2.0
22	T	115	GLU	2.0
8	E	161	VAL	2.0
32	I	126	LYS	2.0
5	B	124	ALA	2.0
7	D	73	VAL	2.0
8	E	1	PRO	2.0
14	L	97	VAL	2.0
22	T	50	VAL	2.0
7	D	59	GLY	2.0
1	0	2135	A	2.0
7	D	173	GLU	2.0
22	T	41	ARG	2.0
10	G	22	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	UR3	0	2619	21/22	0.15	1.06	32,39,41,42	0
1	1MA	0	628	23/24	0.14	-0.10	29,32,34,36	0
3	5AA	4	76	24/25	0.13	-0.48	38,44,48,48	0
1	OMG	0	2588	24/25	0.13	-0.69	32,36,39,40	0
1	OMU	0	2587	21/22	0.12	-0.70	35,37,39,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	PSU	0	2621	20/21	0.12	-1.36	30,33,37,38	0

6.3 Carbohydrates i

There are no carbohydrates in this entry.

6.4 Ligands i

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	9106	1/1	0.68	238.34	51,51,51,51	0
35	NA	0	9185	1/1	0.61	76.55	54,54,54,54	0
35	NA	0	9170	1/1	0.45	69.00	97,97,97,97	0
33	MG	0	8024	1/1	0.78	63.21	83,83,83,83	0
33	MG	0	8092	1/1	0.71	58.31	115,115,115,115	0
36	CL	0	9315	1/1	0.39	58.30	84,84,84,84	0
35	NA	0	9175	1/1	0.39	52.30	56,56,56,56	0
36	CL	0	9322	1/1	0.49	36.77	92,92,92,92	0
35	NA	0	9152	1/1	0.37	36.05	65,65,65,65	0
35	NA	0	9171	1/1	0.40	35.93	64,64,64,64	0
35	NA	0	9174	1/1	0.74	34.30	64,64,64,64	0
35	NA	0	9158	1/1	0.59	31.65	84,84,84,84	0
35	NA	0	9156	1/1	0.49	25.90	51,51,51,51	0
35	NA	0	9160	1/1	0.47	24.15	49,49,49,49	0
35	NA	R	9186	1/1	0.71	21.40	84,84,84,84	0
35	NA	0	9163	1/1	0.41	19.43	63,63,63,63	0
35	NA	L	9180	1/1	0.52	18.41	72,72,72,72	0
35	NA	S	9112	1/1	0.56	18.22	75,75,75,75	0
35	NA	0	9169	1/1	0.39	17.74	79,79,79,79	0
35	NA	0	9177	1/1	0.40	17.71	73,73,73,73	0
35	NA	0	9182	1/1	0.38	16.13	84,84,84,84	0
35	NA	0	9135	1/1	0.29	15.84	50,50,50,50	0
35	NA	0	9150	1/1	0.28	14.54	48,48,48,48	0
35	NA	0	9107	1/1	0.18	14.49	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	9125	1/1	0.23	11.37	69,69,69,69	0
35	NA	0	9172	1/1	0.35	11.09	61,61,61,61	0
35	NA	0	9162	1/1	0.26	10.69	72,72,72,72	0
33	MG	0	8060	1/1	0.29	10.31	49,49,49,49	0
35	NA	0	9155	1/1	0.47	10.11	78,78,78,78	0
33	MG	0	8072	1/1	0.22	10.06	55,55,55,55	0
33	MG	0	8114	1/1	0.22	9.99	56,56,56,56	0
33	MG	0	8082	1/1	0.20	9.67	65,65,65,65	0
35	NA	0	9161	1/1	0.32	9.53	56,56,56,56	0
35	NA	0	9113	1/1	0.17	9.35	66,66,66,66	0
35	NA	0	9121	1/1	0.33	9.25	58,58,58,58	0
33	MG	0	8085	1/1	0.21	8.58	74,74,74,74	0
35	NA	0	9118	1/1	0.18	8.57	47,47,47,47	0
35	NA	0	9184	1/1	0.62	8.23	96,96,96,96	0
33	MG	0	8047	1/1	0.16	8.20	78,78,78,78	0
33	MG	0	8041	1/1	0.28	7.99	72,72,72,72	0
35	NA	0	9164	1/1	0.21	7.39	55,55,55,55	0
35	NA	0	9129	1/1	0.17	7.36	65,65,65,65	0
33	MG	0	8011	1/1	0.16	7.22	23,23,23,23	0
33	MG	0	8090	1/1	0.57	6.86	69,69,69,69	0
35	NA	0	9179	1/1	0.17	6.80	57,57,57,57	0
33	MG	0	8087	1/1	0.14	6.16	54,54,54,54	0
35	NA	0	9102	1/1	0.18	6.01	44,44,44,44	0
35	NA	0	9159	1/1	0.20	6.01	56,56,56,56	0
34	K	0	9001	1/1	0.22	5.43	74,74,74,74	0
35	NA	0	9154	1/1	0.21	5.31	38,38,38,38	0
35	NA	0	9142	1/1	0.16	4.92	53,53,53,53	0
33	MG	0	8049	1/1	0.26	4.84	80,80,80,80	0
33	MG	0	8098	1/1	0.23	4.15	40,40,40,40	0
33	MG	0	8021	1/1	0.16	4.07	30,30,30,30	0
33	MG	0	8016	1/1	0.21	3.95	44,44,44,44	0
35	NA	0	9126	1/1	0.19	3.88	44,44,44,44	0
36	CL	0	9316	1/1	0.26	3.64	61,61,61,61	0
35	NA	0	9110	1/1	0.17	3.55	38,38,38,38	0
33	MG	0	8053	1/1	0.17	3.43	58,58,58,58	0
35	NA	0	9173	1/1	0.26	3.26	58,58,58,58	0
33	MG	0	8023	1/1	0.17	3.25	48,48,48,48	0
35	NA	0	9101	1/1	0.16	2.67	47,47,47,47	0
35	NA	0	9178	1/1	0.17	2.65	57,57,57,57	0
37	CD	O	9205	1/1	0.26	2.60	200,200,200,200	0
33	MG	0	8100	1/1	0.16	2.56	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	CL	0	9305	1/1	0.20	2.45	71,71,71,71	0
35	NA	M	9147	1/1	0.21	2.34	33,33,33,33	0
33	MG	0	8081	1/1	0.17	2.12	54,54,54,54	0
35	NA	Q	9148	1/1	0.26	2.04	43,43,43,43	0
33	MG	0	8097	1/1	0.14	1.99	40,40,40,40	0
33	MG	0	8040	1/1	0.18	1.94	52,52,52,52	0
33	MG	0	8013	1/1	0.19	1.89	41,41,41,41	0
33	MG	0	8080	1/1	0.15	1.86	46,46,46,46	0
35	NA	0	9176	1/1	0.16	1.70	42,42,42,42	0
33	MG	0	8012	1/1	0.16	1.29	32,32,32,32	0
33	MG	0	8063	1/1	0.14	1.26	84,84,84,84	0
33	MG	0	8054	1/1	0.14	1.23	39,39,39,39	0
35	NA	0	9115	1/1	0.14	1.19	39,39,39,39	0
35	NA	0	9157	1/1	0.12	1.17	69,69,69,69	0
35	NA	0	9124	1/1	0.17	1.14	67,67,67,67	0
35	NA	9	9151	1/1	0.38	1.14	87,87,87,87	0
35	NA	0	9140	1/1	0.17	1.08	45,45,45,45	0
35	NA	0	9168	1/1	0.13	1.06	56,56,56,56	0
33	MG	0	8030	1/1	0.15	0.73	26,26,26,26	0
33	MG	0	8071	1/1	0.13	0.68	72,72,72,72	0
33	MG	0	8104	1/1	0.20	0.66	73,73,73,73	0
35	NA	0	9165	1/1	0.22	0.54	42,42,42,42	0
33	MG	0	8018	1/1	0.14	0.53	47,47,47,47	0
36	CL	A	9309	1/1	0.18	0.46	77,77,77,77	0
35	NA	0	9134	1/1	0.13	0.38	37,37,37,37	0
33	MG	0	8038	1/1	0.14	0.34	26,26,26,26	0
35	NA	0	9103	1/1	0.15	0.29	39,39,39,39	0
33	MG	A	8065	1/1	0.17	0.28	52,52,52,52	0
35	NA	R	9137	1/1	0.13	0.26	50,50,50,50	0
36	CL	O	9308	1/1	0.21	0.12	81,81,81,81	0
35	NA	0	9111	1/1	0.12	0.05	59,59,59,59	0
33	MG	0	8102	1/1	0.12	-0.03	67,67,67,67	0
35	NA	0	9166	1/1	0.13	-0.17	68,68,68,68	0
36	CL	J	9301	1/1	0.15	-0.27	73,73,73,73	0
33	MG	0	8044	1/1	0.12	-0.30	49,49,49,49	0
33	MG	0	8029	1/1	0.16	-0.40	36,36,36,36	0
33	MG	0	8005	1/1	0.14	-0.48	37,37,37,37	0
33	MG	9	8095	1/1	0.12	-0.52	75,75,75,75	0
33	MG	0	8101	1/1	0.12	-0.55	74,74,74,74	0
33	MG	0	8079	1/1	0.12	-0.55	38,38,38,38	0
36	CL	L	9310	1/1	0.14	-0.60	61,61,61,61	0
35	NA	C	9104	1/1	0.14	-0.65	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	A	9145	1/1	0.15	-0.66	45,45,45,45	0
35	NA	O	9123	1/1	0.16	-0.66	43,43,43,43	0
33	MG	O	8077	1/1	0.13	-0.67	35,35,35,35	0
35	NA	H	9109	1/1	0.13	-0.68	36,36,36,36	0
35	NA	O	9133	1/1	0.11	-0.68	32,32,32,32	0
33	MG	K	8069	1/1	0.13	-0.71	49,49,49,49	0
36	CL	B	9319	1/1	0.14	-0.79	60,60,60,60	0
35	NA	H	9122	1/1	0.12	-0.80	59,59,59,59	0
33	MG	O	8033	1/1	0.13	-0.82	32,32,32,32	0
33	MG	O	8026	1/1	0.12	-0.92	31,31,31,31	0
33	MG	O	8111	1/1	0.12	-0.96	77,77,77,77	0
36	CL	M	9318	1/1	0.14	-0.96	50,50,50,50	0
33	MG	O	8107	1/1	0.09	-0.97	38,38,38,38	0
33	MG	O	8014	1/1	0.12	-0.97	41,41,41,41	0
33	MG	O	8015	1/1	0.11	-0.98	31,31,31,31	0
36	CL	J	9321	1/1	0.13	-1.00	54,54,54,54	0
33	MG	O	8057	1/1	0.13	-1.01	45,45,45,45	0
33	MG	O	8027	1/1	0.12	-1.02	55,55,55,55	0
33	MG	B	8055	1/1	0.12	-1.02	52,52,52,52	0
33	MG	O	8036	1/1	0.10	-1.03	35,35,35,35	0
35	NA	9	9183	1/1	0.12	-1.06	49,49,49,49	0
37	CD	U	9201	1/1	0.09	-1.08	69,69,69,69	0
33	MG	O	8058	1/1	0.13	-1.09	57,57,57,57	0
34	K	O	9003	1/1	0.12	-1.11	66,66,66,66	0
37	CD	Z	9203	1/1	0.09	-1.13	68,68,68,68	0
33	MG	O	8062	1/1	0.12	-1.15	57,57,57,57	0
36	CL	N	9307	1/1	0.16	-1.16	66,66,66,66	0
33	MG	O	8106	1/1	0.09	-1.25	63,63,63,63	0
36	CL	3	9304	1/1	0.16	-1.26	70,70,70,70	0
35	NA	O	9132	1/1	0.10	-1.29	35,35,35,35	0
33	MG	O	8048	1/1	0.12	-1.30	62,62,62,62	0
36	CL	O	9313	1/1	0.10	-1.53	61,61,61,61	0
33	MG	O	8086	1/1	0.05	-1.64	47,47,47,47	0
33	MG	O	8017	1/1	0.08	-1.64	33,33,33,33	0
35	NA	O	9117	1/1	0.09	-1.73	46,46,46,46	0
33	MG	O	8003	1/1	0.14	-1.73	40,40,40,40	0
36	CL	R	9306	1/1	0.11	-1.74	48,48,48,48	0
33	MG	O	8074	1/1	0.08	-1.77	40,40,40,40	0
33	MG	O	8064	1/1	0.10	-1.78	33,33,33,33	0
33	MG	O	8108	1/1	0.11	-1.79	75,75,75,75	0
36	CL	O	9311	1/1	0.09	-1.83	52,52,52,52	0
35	NA	O	9149	1/1	0.14	-1.83	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8056	1/1	0.13	-1.90	51,51,51,51	0
35	NA	0	9114	1/1	0.10	-2.00	51,51,51,51	0
36	CL	K	9312	1/1	0.09	-2.06	55,55,55,55	0
37	CD	1	9202	1/1	0.05	-2.06	68,68,68,68	0
35	NA	0	9141	1/1	0.07	-2.07	47,47,47,47	0
33	MG	T	8073	1/1	0.06	-2.09	66,66,66,66	0
33	MG	0	8103	1/1	0.11	-2.09	81,81,81,81	0
33	MG	0	8070	1/1	0.05	-2.11	45,45,45,45	0
35	NA	0	9181	1/1	0.07	-2.14	48,48,48,48	0
33	MG	0	8045	1/1	0.09	-2.14	62,62,62,62	0
33	MG	0	8116	1/1	0.09	-2.20	47,47,47,47	0
33	MG	0	8068	1/1	0.06	-2.23	59,59,59,59	0
33	MG	0	8020	1/1	0.12	-2.24	24,24,24,24	0
36	CL	0	9320	1/1	0.10	-2.25	48,48,48,48	0
35	NA	0	9144	1/1	0.09	-2.26	27,27,27,27	0
33	MG	0	8096	1/1	0.09	-2.31	51,51,51,51	0
36	CL	J	9302	1/1	0.05	-2.33	61,61,61,61	0
36	CL	0	9314	1/1	0.07	-2.36	53,53,53,53	0
37	CD	3	9204	1/1	0.09	-2.41	66,66,66,66	0
36	CL	0	9317	1/1	0.07	-2.47	64,64,64,64	0
35	NA	0	9127	1/1	0.10	-2.48	35,35,35,35	0
35	NA	J	9146	1/1	0.09	-2.53	35,35,35,35	0
33	MG	0	8008	1/1	0.08	-2.54	37,37,37,37	0
35	NA	0	9131	1/1	0.08	-2.60	36,36,36,36	0
35	NA	0	9119	1/1	0.08	-2.63	36,36,36,36	0
35	NA	0	9153	1/1	0.09	-2.69	25,25,25,25	0
33	MG	0	8001	1/1	0.10	-2.74	38,38,38,38	0
36	CL	0	9303	1/1	0.12	-2.83	64,64,64,64	0
33	MG	0	8042	1/1	0.08	-2.94	39,39,39,39	0
35	NA	0	9130	1/1	0.07	-3.04	44,44,44,44	0
35	NA	R	9138	1/1	0.07	-3.07	61,61,61,61	0
33	MG	3	8078	1/1	0.05	-3.10	55,55,55,55	0
33	MG	0	8099	1/1	0.10	-3.28	63,63,63,63	0
33	MG	0	8094	1/1	0.11	-3.32	86,86,86,86	0
33	MG	0	8034	1/1	0.10	-3.40	32,32,32,32	0
33	MG	0	8004	1/1	0.04	-3.54	27,27,27,27	0
33	MG	0	8112	1/1	0.08	-3.54	47,47,47,47	0
33	MG	0	8118	1/1	0.10	-3.57	40,40,40,40	0
33	MG	0	8010	1/1	0.11	-3.58	29,29,29,29	0
33	MG	0	8089	1/1	0.09	-3.63	60,60,60,60	0
35	NA	0	9116	1/1	0.10	-3.67	36,36,36,36	0
33	MG	0	8022	1/1	0.07	-3.79	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8025	1/1	0.09	-3.90	35,35,35,35	0
33	MG	0	8091	1/1	0.06	-3.95	57,57,57,57	0
33	MG	0	8084	1/1	0.11	-4.15	51,51,51,51	0
33	MG	0	8019	1/1	0.08	-4.18	38,38,38,38	0
33	MG	0	8043	1/1	0.08	-4.26	53,53,53,53	0
33	MG	0	8093	1/1	0.10	-4.34	52,52,52,52	0
33	MG	0	8032	1/1	0.04	-4.39	35,35,35,35	0
35	NA	0	9139	1/1	0.09	-4.40	22,22,22,22	0
35	NA	0	9167	1/1	0.08	-4.42	47,47,47,47	0
34	K	0	9002	1/1	0.08	-4.52	54,54,54,54	0
35	NA	0	9108	1/1	0.09	-4.52	61,61,61,61	0
33	MG	0	8028	1/1	0.10	-4.62	44,44,44,44	0
33	MG	Y	8109	1/1	0.08	-4.67	39,39,39,39	0
33	MG	0	8076	1/1	0.06	-4.83	70,70,70,70	0
33	MG	A	8066	1/1	0.04	-5.01	66,66,66,66	0
33	MG	0	8117	1/1	0.10	-5.23	40,40,40,40	0
33	MG	0	8067	1/1	0.09	-5.59	46,46,46,46	0
35	NA	0	9128	1/1	0.05	-5.67	35,35,35,35	0
33	MG	0	8007	1/1	0.07	-5.72	24,24,24,24	0
35	NA	0	9136	1/1	0.06	-5.72	56,56,56,56	0
35	NA	0	9120	1/1	0.10	-5.75	43,43,43,43	0
35	NA	0	9105	1/1	0.07	-5.80	39,39,39,39	0
33	MG	0	8006	1/1	0.05	-5.85	33,33,33,33	0
33	MG	9	8052	1/1	0.07	-5.96	47,47,47,47	0
33	MG	0	8075	1/1	0.06	-6.17	43,43,43,43	0
33	MG	0	8035	1/1	0.06	-7.30	51,51,51,51	0
33	MG	0	8009	1/1	0.10	-7.70	35,35,35,35	0
33	MG	0	8110	1/1	0.07	-8.18	40,40,40,40	0
33	MG	0	8031	1/1	0.08	-8.21	37,37,37,37	0
33	MG	0	8002	1/1	0.06	-8.43	39,39,39,39	0
33	MG	0	8039	1/1	0.06	-8.50	51,51,51,51	0
33	MG	0	8088	1/1	0.06	-8.66	36,36,36,36	0
33	MG	0	8061	1/1	0.08	-8.77	45,45,45,45	0
33	MG	0	8050	1/1	0.08	-9.07	61,61,61,61	0
33	MG	0	8059	1/1	0.07	-9.19	44,44,44,44	0
35	NA	0	9143	1/1	0.06	-10.66	36,36,36,36	0
33	MG	0	8113	1/1	0.08	-12.51	45,45,45,45	0
33	MG	0	8083	1/1	0.07	-12.70	42,42,42,42	0
33	MG	0	8051	1/1	0.07	-13.10	61,61,61,61	0
33	MG	0	8046	1/1	0.09	-14.51	54,54,54,54	0
33	MG	0	8037	1/1	0.06	-18.17	44,44,44,44	0
33	MG	0	8115	1/1	0.11	-31.00	49,49,49,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.