



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 07:48 am BST

PDB ID : 4W2F
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with amicoumacin, mRNA and three deacylated tRNAs in the A, P and E sites
Authors : Polikanov, Y.S.; Osterman, I.A.; Szal, T.; Tashlitsky, V.N.; Serebryakova, M.V.; Kusochev, P.; Bulkley, D.; Malanicheva, I.A.; Efimenko, T.A.; Efremenkova, O.V.; Konevega, A.L.; Shaw, K.J.; Bogdanov, A.A.; Rodnina, M.V.; Dontsova, O.A.; Mankin, A.S.; Steitz, T.A.; Sergiev, P.V.
Deposited on : 2014-09-12
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

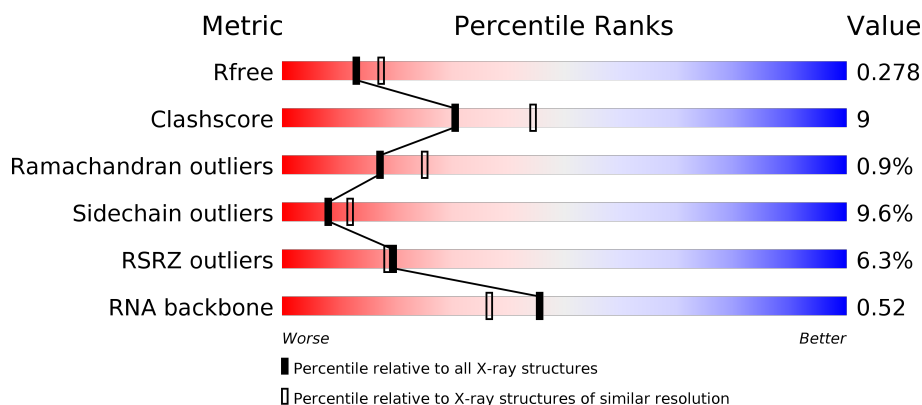
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1521	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>32%</div> <div>9%</div> <div>..</div> </div> </div>
1	CA	1521	<div> <div>5%</div> <div> <div></div> <div>52%</div> <div>37%</div> <div>9%</div> <div>..</div> </div> </div>
2	AB	256	<div> <div>6%</div> <div> <div></div> <div>52%</div> <div>31%</div> <div>7%</div> <div>10%</div> </div> </div>
2	CB	256	<div> <div>14%</div> <div> <div></div> <div>48%</div> <div>32%</div> <div>11%</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AW	76	
23	AY	76	
23	CW	76	
23	CY	76	
24	AX	77	
24	CX	77	
25	BA	2915	
25	DA	2915	
26	BB	121	
26	DB	121	











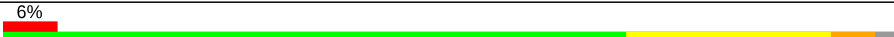


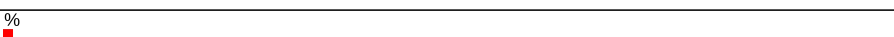








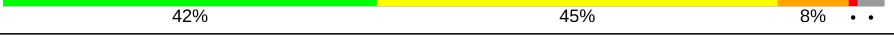


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Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	
34	DO	122	
35	BP	150	
35	DP	150	
36	BQ	141	
36	DQ	141	
37	BR	118	
37	DR	118	
38	BS	112	
38	DS	112	
39	BT	146	

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Mol	Chain	Length	Quality of chain
39	DT	146	
40	BU	118	
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	

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Mol	Chain	Length	Quality of chain
52	B6	54	
52	D6	54	
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	
55	B9	37	
55	D9	37	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 298643 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1497	Total	C	N	O	P	0	0	0
			32185	14324	5967	10397	1497			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
2	CB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
6	CF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
8	CH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			983	623	193	167				
9	CI	127	Total	C	N	O		0	0	0
			978	619	190	169				

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	97	Total	C	N	O		0	0	0
			709	440	138	131				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O			
			714	445	138	131	0	0	0

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	AK	114	Total	C	N	O	S		
			829	516	155	155	3	0	0
11	CK	114	Total	C	N	O	S		
			833	519	156	155	3	0	0

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AL	122	Total	C	N	O	S		
			930	585	185	159	1	0	0
12	CL	122	Total	C	N	O	S		
			930	585	185	159	1	0	0

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	AM	123	Total	C	N	O	S		
			958	592	198	166	2	0	0
13	CM	122	Total	C	N	O	S		
			950	586	197	165	2	0	0

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0
14	CN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0

- Molecule 15 is a protein called 30S Ribosomal Protein S15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0
15	CO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
16	CP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	CR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
19	CS	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
20	CT	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	CU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
22	CV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 23 is a RNA chain called A/P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
23	AY	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
23	CW	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
23	CY	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 24 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
24	CX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2871	Total	C	N	O	P	0	0	0
			61844	27523	11572	19878	2871			
25	DA	2800	Total	C	N	O	P	0	0	0
			60314	26840	11284	19390	2800			

- Molecule 26 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	120	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
26	DB	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- Molecule 27 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
27	DD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 28 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
28	DE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 29 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
29	DF	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 30 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	181	Total	C	N	O	S	0	0	0
			1429	916	256	253	4			
30	DG	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

- Molecule 31 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	DH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 32 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
32	DI	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	1			

- Molecule 33 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
33	DN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 34 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
34	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 35 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
35	DP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 36 is a protein called 50S Ribosomal Protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
36	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 37 is a protein called 50S Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
37	DR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 38 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BS	110	Total	C	N	O		0	0	0
			873	550	174	149				
38	DS	110	Total	C	N	O		0	0	0
			870	549	173	148				

- Molecule 39 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
39	DT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 40 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
40	DU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 41 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
41	DV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 42 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
42	DW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 43 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
43	DX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 44 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
44	DY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 45 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BZ	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
45	DZ	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

- Molecule 46 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
46	D0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 47 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	D1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 48 is a protein called 50S Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
48	D2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 49 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B3	59	Total	C	N	O	0	0	0
			469	298	90	81			
49	D3	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 50 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			
50	D4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 51 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
51	D5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 52 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
52	D6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 53 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
53	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 54 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
54	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 55 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
55	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CR	1	Total	Mg	0	0
			1	1		
56	B4	1	Total	Mg	0	0
			1	1		
56	BA	906	Total	Mg	0	0
			906	906		
56	AK	1	Total	Mg	0	0
			1	1		
56	DQ	3	Total	Mg	0	0
			3	3		
56	D3	1	Total	Mg	0	0
			1	1		
56	AB	2	Total	Mg	0	0
			2	2		
56	DF	7	Total	Mg	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CV	1	Total 1	Mg 1	0	0
56	B8	3	Total 3	Mg 3	0	0
56	BE	12	Total 12	Mg 12	0	0
56	AW	4	Total 4	Mg 4	0	0
56	DU	4	Total 4	Mg 4	0	0
56	B1	2	Total 2	Mg 2	0	0
56	DY	1	Total 1	Mg 1	0	0
56	AN	1	Total 1	Mg 1	0	0
56	BP	6	Total 6	Mg 6	0	0
56	AX	13	Total 13	Mg 13	0	0
56	DR	1	Total 1	Mg 1	0	0
56	BI	1	Total 1	Mg 1	0	0
56	CA	201	Total 201	Mg 201	0	0
56	B5	4	Total 4	Mg 4	0	0
56	BB	30	Total 30	Mg 30	0	0
56	BT	2	Total 2	Mg 2	0	0
56	D8	2	Total 2	Mg 2	0	0
56	AE	2	Total 2	Mg 2	0	0
56	DB	21	Total 21	Mg 21	0	0
56	CF	2	Total 2	Mg 2	0	0
56	DT	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B9	1	Total 1	Mg 1	0	0
56	BF	15	Total 15	Mg 15	0	0
56	BX	6	Total 6	Mg 6	0	0
56	B2	2	Total 2	Mg 2	0	0
56	AA	233	Total 233	Mg 233	0	0
56	BQ	7	Total 7	Mg 7	0	0
56	CQ	2	Total 2	Mg 2	0	0
56	D0	1	Total 1	Mg 1	0	0
56	AR	1	Total 1	Mg 1	0	0
56	DV	2	Total 2	Mg 2	0	0
56	B6	2	Total 2	Mg 2	0	0
56	AM	1	Total 1	Mg 1	0	0
56	BU	10	Total 10	Mg 10	0	0
56	AD	1	Total 1	Mg 1	0	0
56	BN	4	Total 4	Mg 4	0	0
56	CT	1	Total 1	Mg 1	0	0
56	CG	1	Total 1	Mg 1	0	0
56	BG	6	Total 6	Mg 6	0	0
56	BY	3	Total 3	Mg 3	0	0
56	DE	7	Total 7	Mg 7	0	0
56	B3	2	Total 2	Mg 2	0	0

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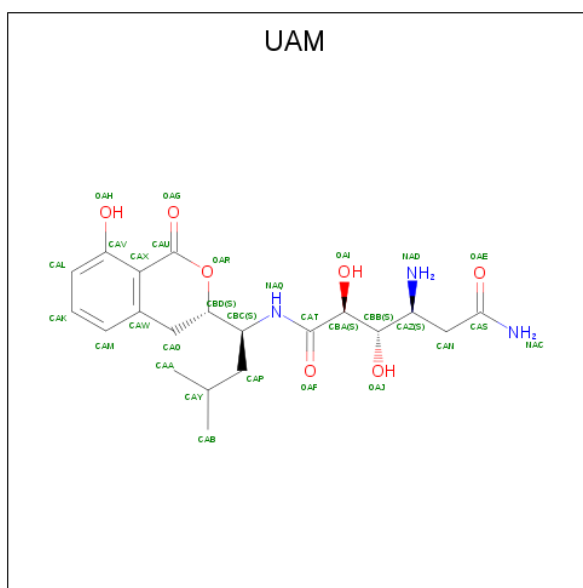
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CJ	2	Total 2	Mg 2	0	0
56	BR	3	Total 3	Mg 3	0	0
56	CP	1	Total 1	Mg 1	0	0
56	DA	673	Total 673	Mg 673	0	0
56	DP	1	Total 1	Mg 1	0	0
56	DW	3	Total 3	Mg 3	0	0
56	D5	2	Total 2	Mg 2	0	0
56	B7	3	Total 3	Mg 3	0	0
56	AL	1	Total 1	Mg 1	0	0
56	BV	5	Total 5	Mg 5	0	0
56	DO	1	Total 1	Mg 1	0	0
56	BO	5	Total 5	Mg 5	0	0
56	CX	6	Total 6	Mg 6	0	0
56	D1	1	Total 1	Mg 1	0	0
56	DX	1	Total 1	Mg 1	0	0
56	AH	1	Total 1	Mg 1	0	0
56	BZ	3	Total 3	Mg 3	0	0
56	DZ	1	Total 1	Mg 1	0	0
56	BS	3	Total 3	Mg 3	0	0
56	CW	4	Total 4	Mg 4	0	0
56	DG	1	Total 1	Mg 1	0	0

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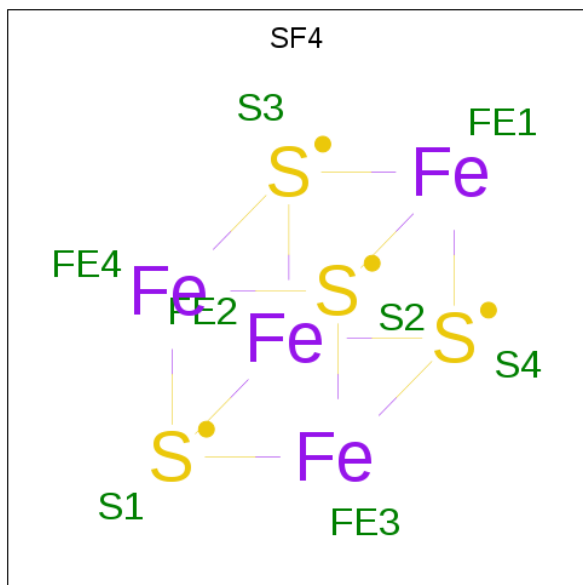
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CD	2	Total 2	Mg 2	0	0
56	BD	13	Total 13	Mg 13	0	0
56	AT	1	Total 1	Mg 1	0	0
56	CL	2	Total 2	Mg 2	0	0
56	B0	7	Total 7	Mg 7	0	0
56	CE	1	Total 1	Mg 1	0	0
56	BW	5	Total 5	Mg 5	0	0
56	AY	2	Total 2	Mg 2	0	0
56	DD	6	Total 6	Mg 6	0	0
56	CK	1	Total 1	Mg 1	0	0
56	AF	1	Total 1	Mg 1	0	0
56	BH	1	Total 1	Mg 1	0	0

- Molecule 57 is Amicoumacin A (three-letter code: UAM) (formula: $C_{20}H_{29}N_3O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	AA	1	Total	C	N	O	0	0
			30	20	3	7		
57	CA	1	Total	C	N	O	0	0
			30	20	3	7		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AD	1	Total	Fe	S	0	0
			8	4	4		
58	CD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B5	1	Total	Zn	0	0
			1	1		
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	BY	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	DY	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D5	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	D6	1	Total	Zn	0	0
			1	1		
59	D9	1	Total	Zn	0	0
			1	1		
59	B6	1	Total	Zn	0	0
			1	1		

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AX	1	Total	K	0	0
			1	1		
60	CX	1	Total	K	0	0
			1	1		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	264	Total	O	0	0
			264	264		
61	AB	1	Total	O	0	0
			1	1		
61	AE	2	Total	O	0	0
			2	2		
61	AJ	1	Total	O	0	0
			1	1		
61	AL	4	Total	O	0	0
			4	4		
61	AM	1	Total	O	0	0
			1	1		
61	AQ	1	Total	O	0	0
			1	1		
61	AV	4	Total	O	0	0
			4	4		
61	AW	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AX	11	Total 11	O 11	0	0
61	AY	1	Total 1	O 1	0	0
61	BA	1486	Total 1486	O 1486	0	0
61	BB	43	Total 43	O 43	0	0
61	BD	19	Total 19	O 19	0	0
61	BE	20	Total 20	O 20	0	0
61	BF	14	Total 14	O 14	0	0
61	BG	5	Total 5	O 5	0	0
61	BH	1	Total 1	O 1	0	0
61	BI	2	Total 2	O 2	0	0
61	BN	2	Total 2	O 2	0	0
61	BO	7	Total 7	O 7	0	0
61	BP	19	Total 19	O 19	0	0
61	BQ	5	Total 5	O 5	0	0
61	BR	5	Total 5	O 5	0	0
61	BS	5	Total 5	O 5	0	0
61	BT	5	Total 5	O 5	0	0
61	BU	8	Total 8	O 8	0	0
61	BV	6	Total 6	O 6	0	0
61	BW	1	Total 1	O 1	0	0
61	BX	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BY	3	Total 3	O 3	0	0
61	BZ	1	Total 1	O 1	0	0
61	B0	8	Total 8	O 8	0	0
61	B1	3	Total 3	O 3	0	0
61	B2	4	Total 4	O 4	0	0
61	B3	3	Total 3	O 3	0	0
61	B4	1	Total 1	O 1	0	0
61	B5	4	Total 4	O 4	0	0
61	B6	1	Total 1	O 1	0	0
61	B7	4	Total 4	O 4	0	0
61	B8	8	Total 8	O 8	0	0
61	CA	204	Total 204	O 204	0	0
61	CD	1	Total 1	O 1	0	0
61	CG	1	Total 1	O 1	0	0
61	CI	1	Total 1	O 1	0	0
61	CJ	4	Total 4	O 4	0	0
61	CL	4	Total 4	O 4	0	0
61	CO	1	Total 1	O 1	0	0
61	CP	1	Total 1	O 1	0	0
61	CR	1	Total 1	O 1	0	0
61	CT	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	CW	2	Total	O	0	0
			2	2		
61	CX	6	Total	O	0	0
			6	6		
61	DA	1039	Total	O	0	0
			1039	1039		
61	DB	10	Total	O	0	0
			10	10		
61	DD	17	Total	O	0	0
			17	17		
61	DE	8	Total	O	0	0
			8	8		
61	DF	6	Total	O	0	0
			6	6		
61	DI	2	Total	O	0	0
			2	2		
61	DN	1	Total	O	0	0
			1	1		
61	DO	3	Total	O	0	0
			3	3		
61	DP	12	Total	O	0	0
			12	12		
61	DQ	1	Total	O	0	0
			1	1		
61	DR	3	Total	O	0	0
			3	3		
61	DT	3	Total	O	0	0
			3	3		
61	DU	1	Total	O	0	0
			1	1		
61	DV	1	Total	O	0	0
			1	1		
61	DW	2	Total	O	0	0
			2	2		
61	DX	2	Total	O	0	0
			2	2		
61	DY	1	Total	O	0	0
			1	1		
61	DZ	2	Total	O	0	0
			2	2		
61	D0	4	Total	O	0	0
			4	4		

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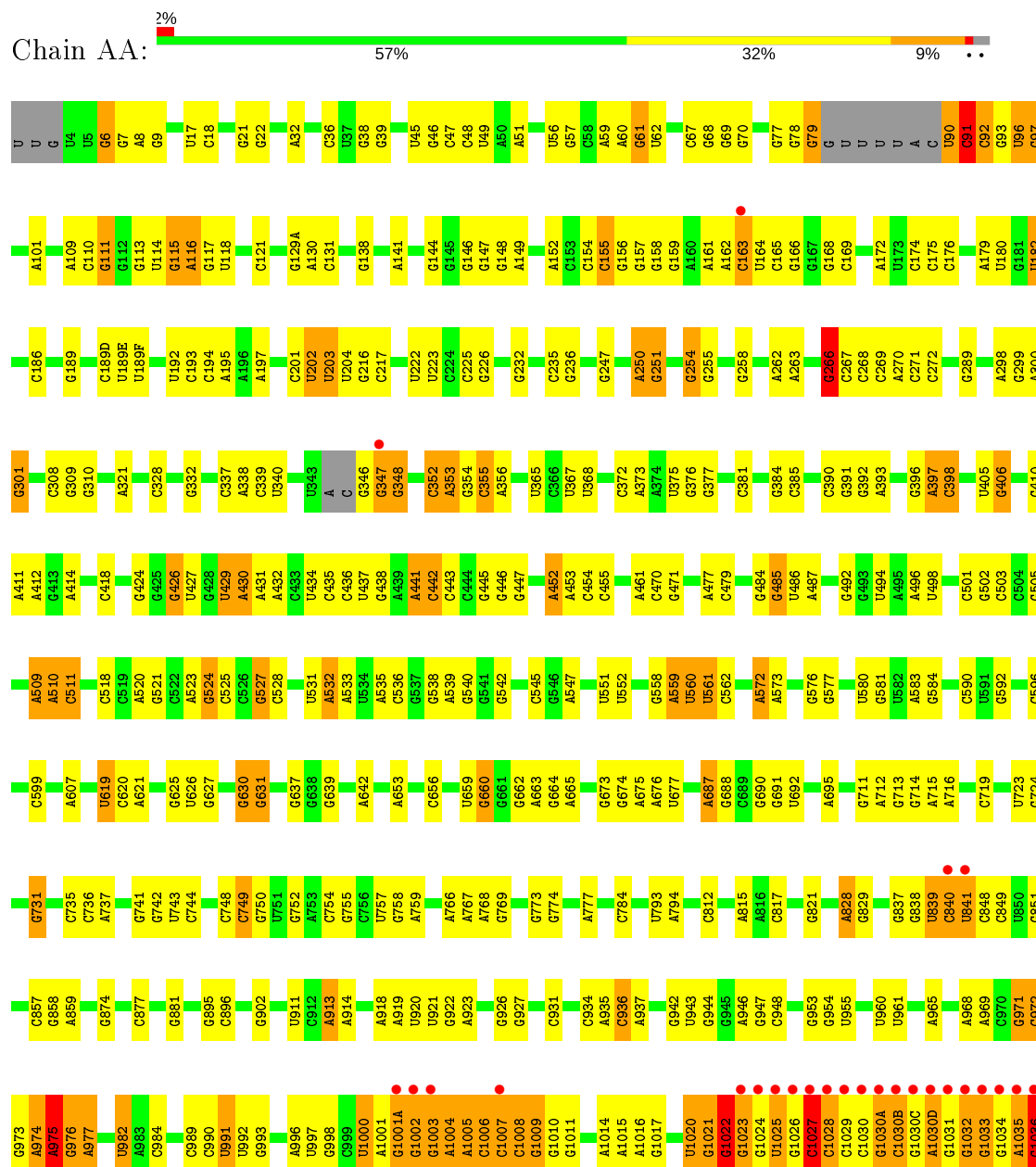
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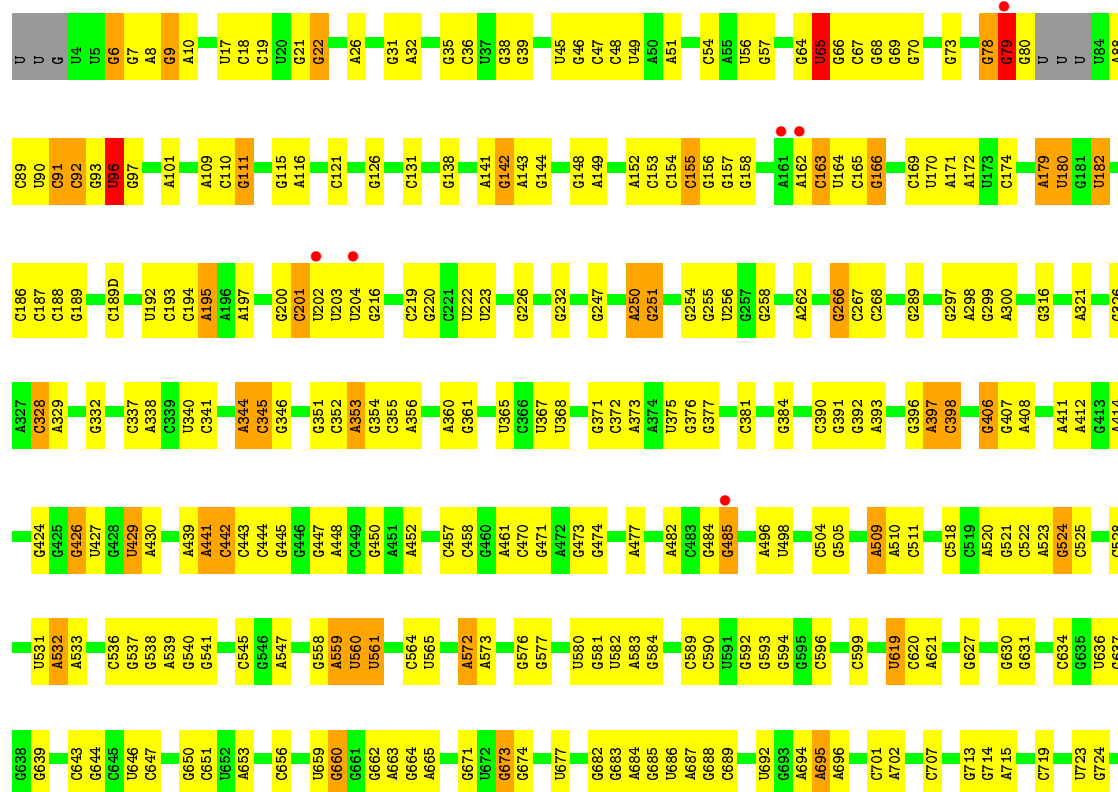
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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			4	4		
61	D2	1	Total	O	0	0
			1	1		
61	D3	1	Total	O	0	0
			1	1		
61	D5	2	Total	O	0	0
			2	2		
61	D7	5	Total	O	0	0
			5	5		
61	D8	5	Total	O	0	0
			5	5		
61	D9	1	Total	O	0	0
			1	1		

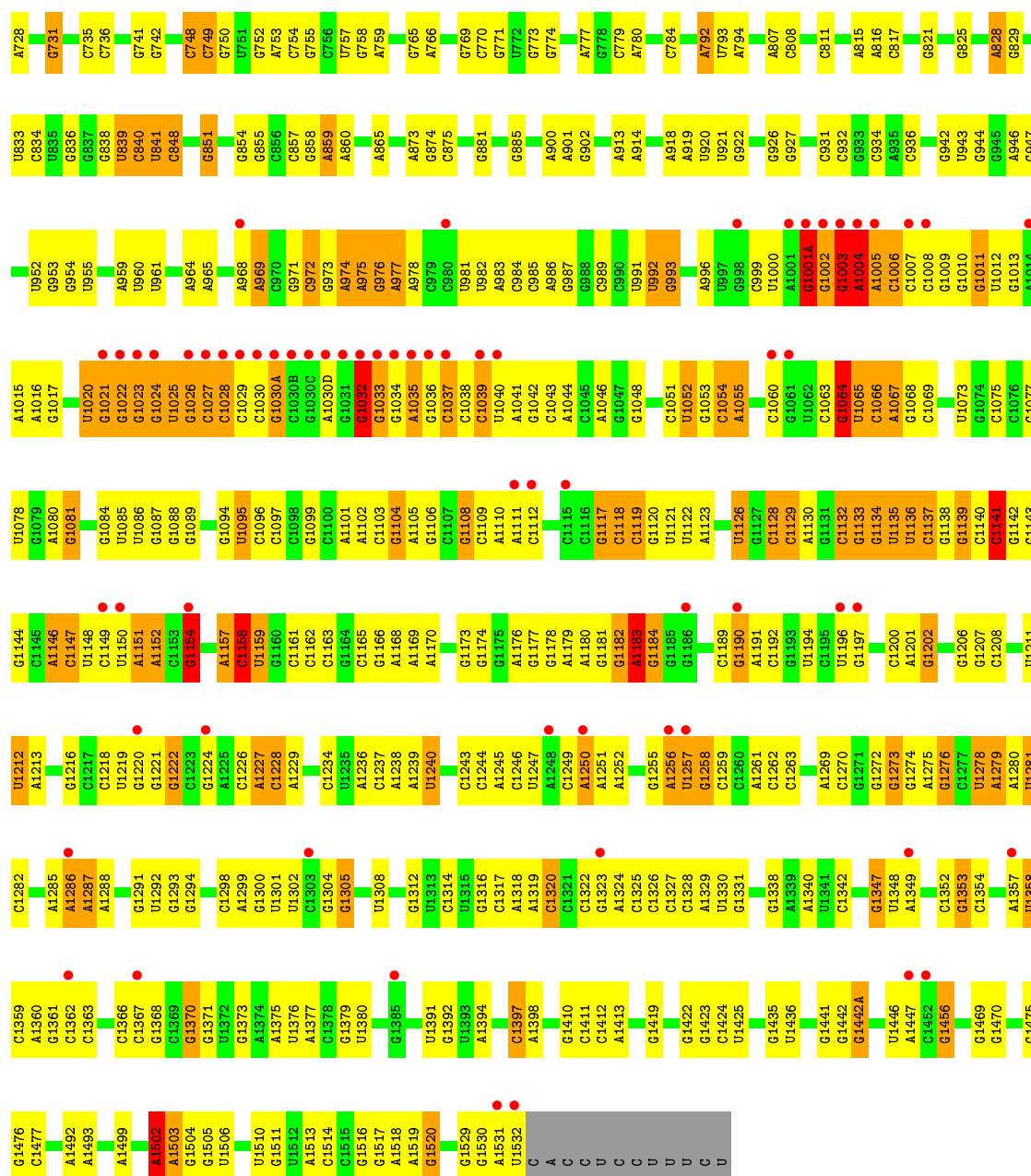
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: 16S Ribosomal RNA



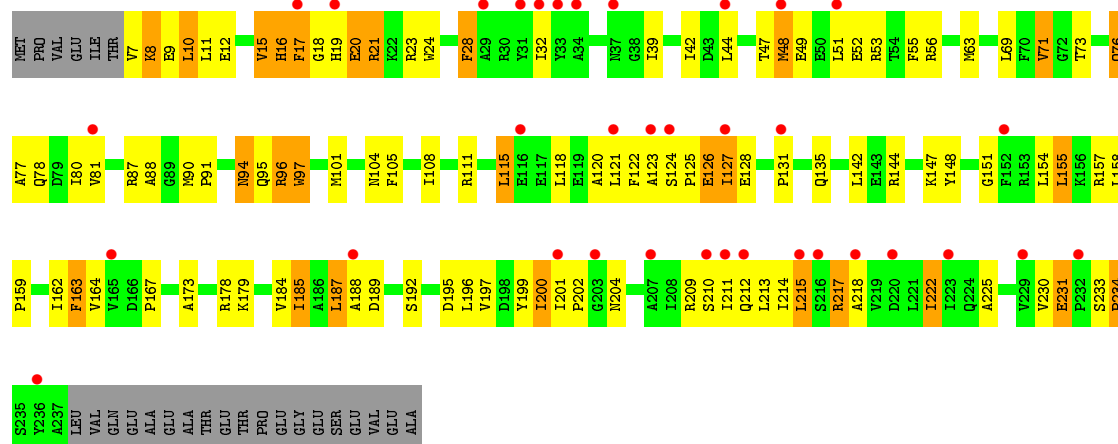




GLY
GLU
SER
GLU
VAL
GLU
ALA

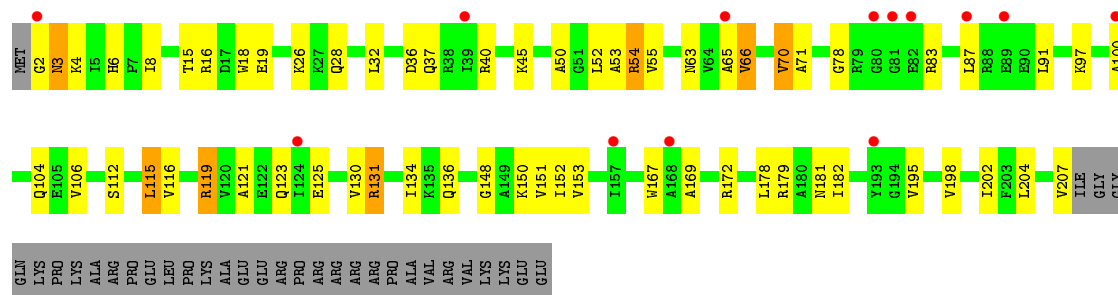
• Molecule 2: 30S Ribosomal Protein S2

Chain CB: 14% 48% 32% 11% 10%



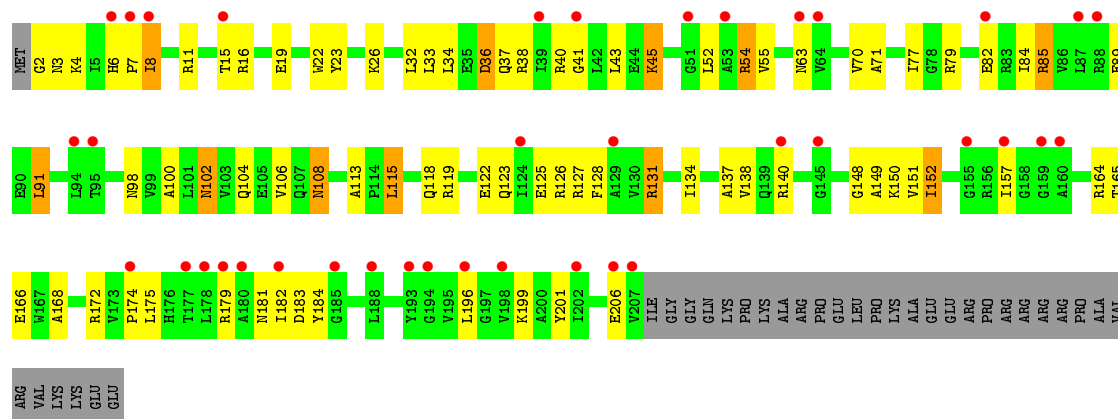
• Molecule 3: 30S Ribosomal Protein S3

Chain AC: 5% 60% 23% 14%

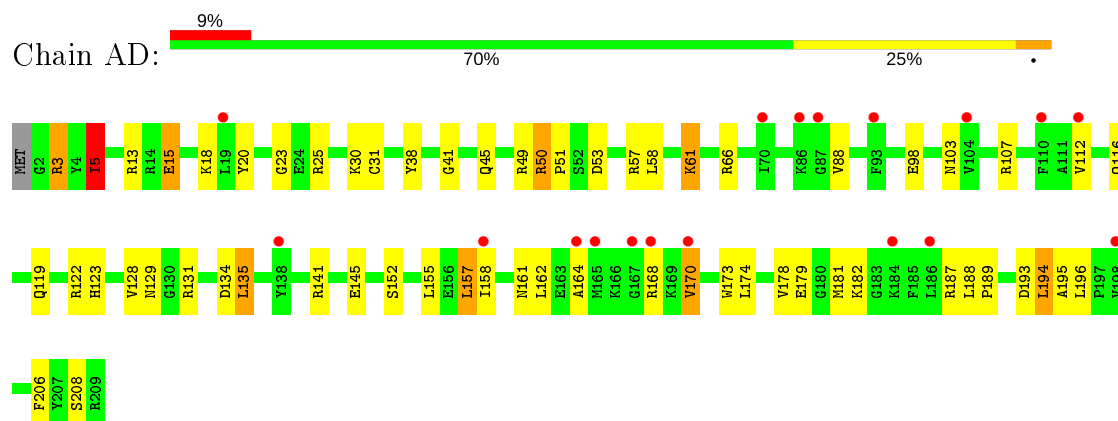


• Molecule 3: 30S Ribosomal Protein S3

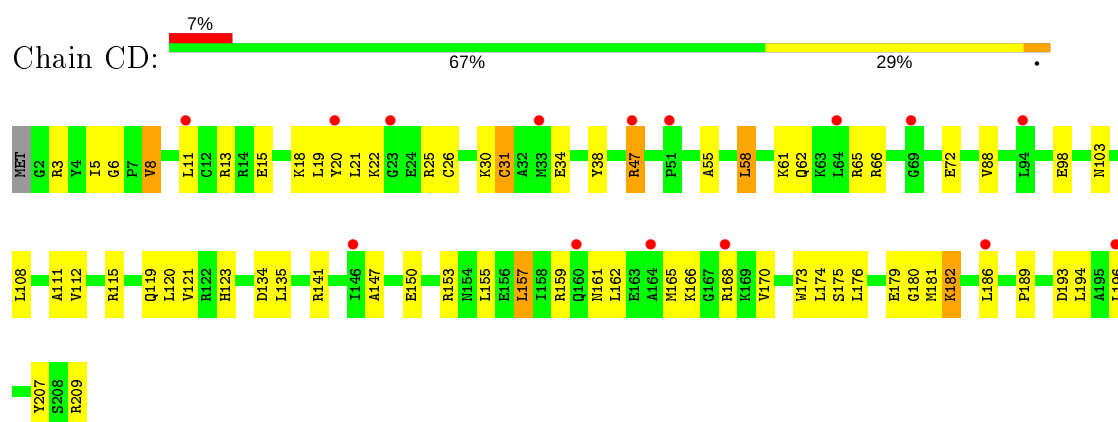
Chain CC: 16% 53% 28% 5% 14%



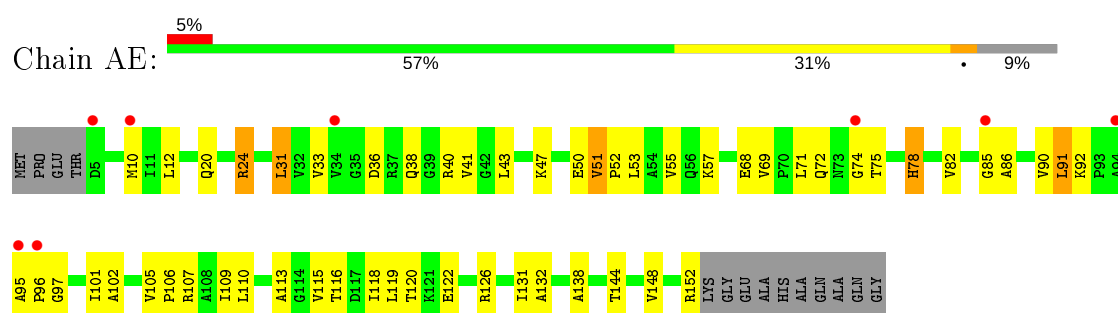
- Molecule 4: 30S Ribosomal Protein S4



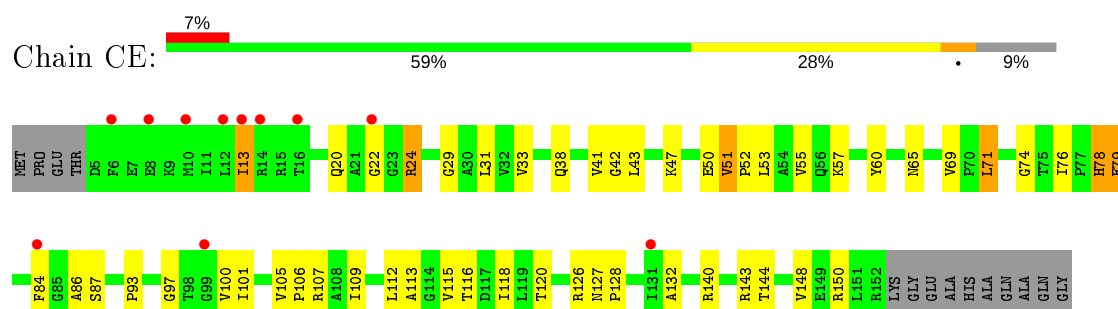
- Molecule 4: 30S Ribosomal Protein S4




- Molecule 5: 30S Ribosomal Protein S5



- Molecule 5: 30S Ribosomal Protein S5




- Molecule 6: 30S Ribosomal Protein S6

Chain AF:  73% 23% ..




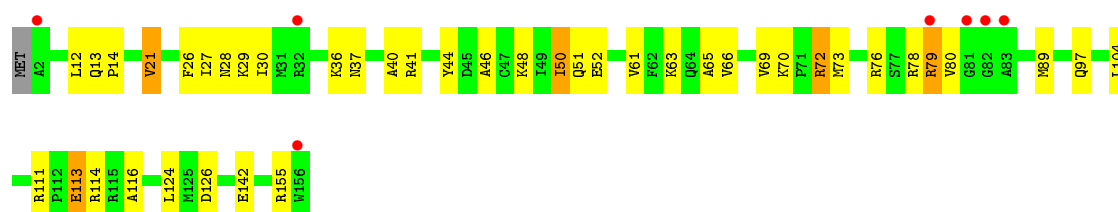
• Molecule 6: 30S Ribosomal Protein S6

Chain CF:  3% 75% 21% ..



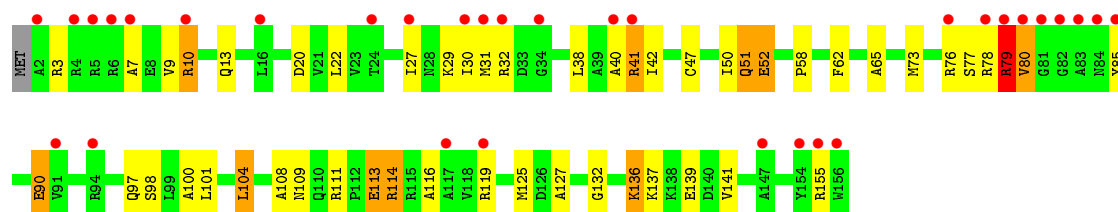
• Molecule 7: 30S Ribosomal Protein S7

Chain AG:  4% 72% 24% ..




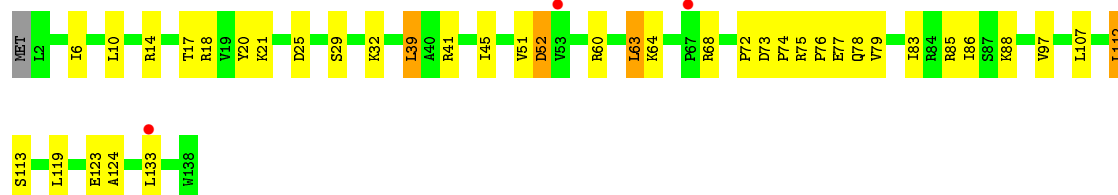
• Molecule 7: 30S Ribosomal Protein S7

Chain CG:  21% 67% 26% 6% ..



• Molecule 8: 30S Ribosomal Protein S8

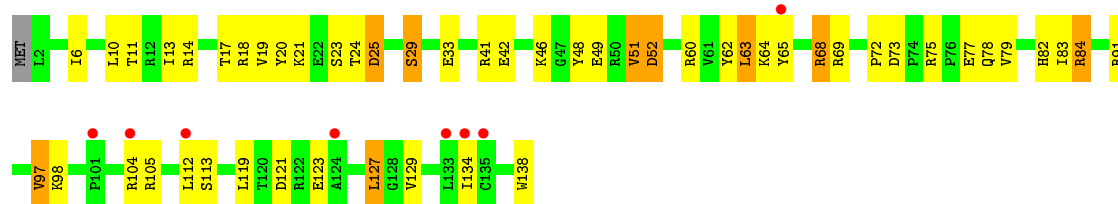
Chain AH:  2% 71% 25% ..



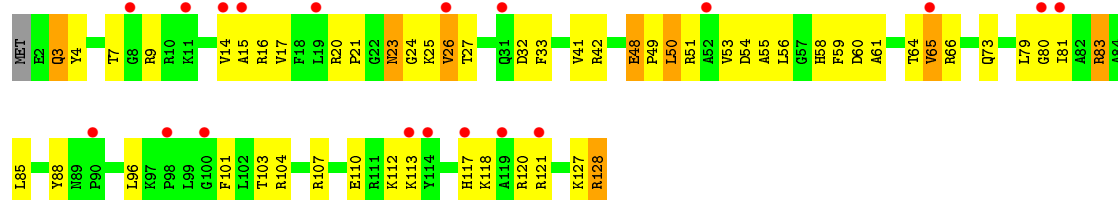
• Molecule 8: 30S Ribosomal Protein S8

Chain CH:  6% 62% 31% 7% ..

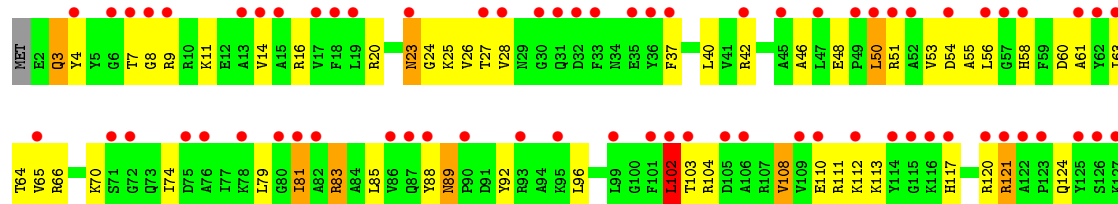




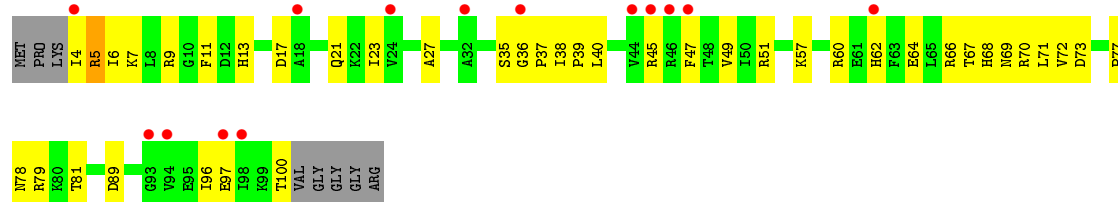
• Molecule 9: 30S Ribosomal Protein S9



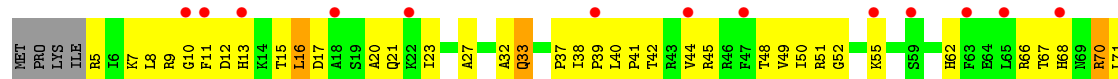
• Molecule 9: 30S Ribosomal Protein S9

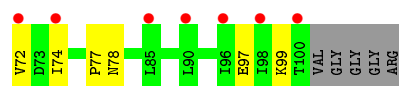


• Molecule 10: 30S Ribosomal Protein S10

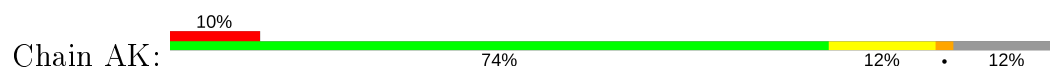


• Molecule 10: 30S Ribosomal Protein S10

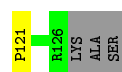
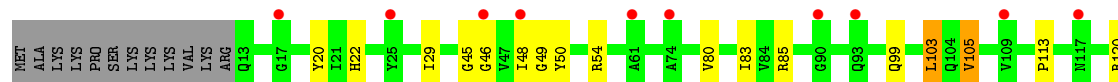
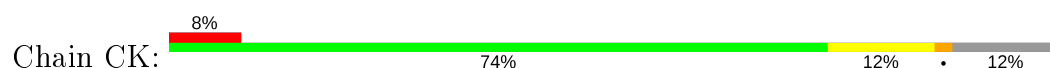




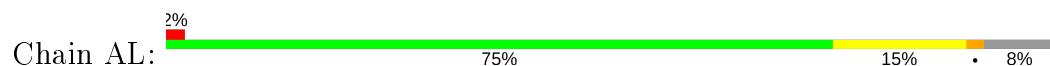
• Molecule 11: 30S Ribosomal Protein S11



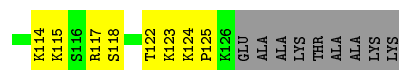
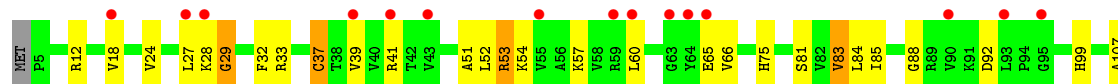
• Molecule 11: 30S Ribosomal Protein S11



• Molecule 12: 30S Ribosomal Protein S12

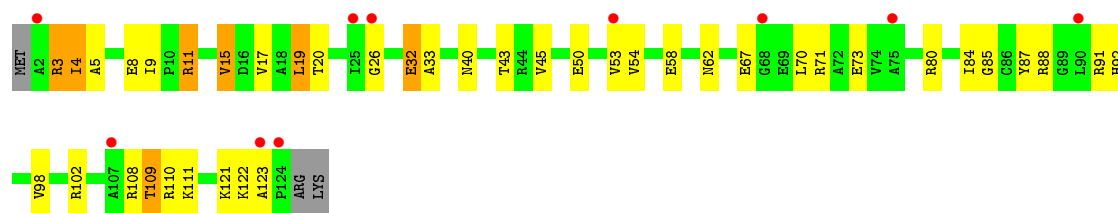


• Molecule 12: 30S Ribosomal Protein S12

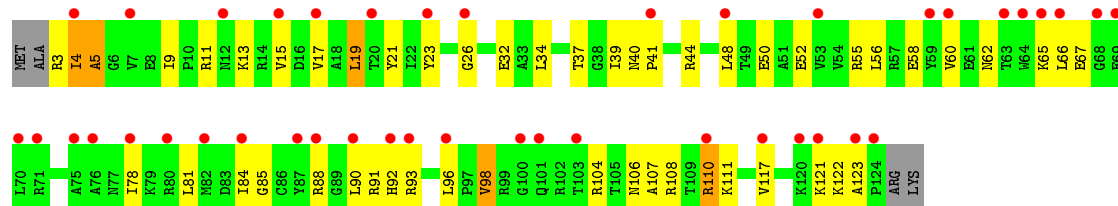


• Molecule 13: 30S Ribosomal Protein S13

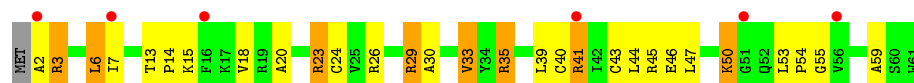




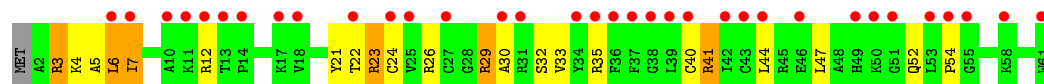
• Molecule 13: 30S Ribosomal Protein S13



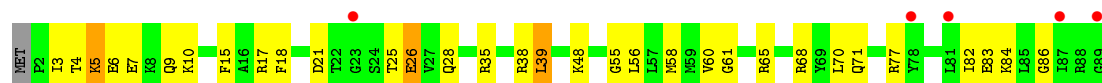
• Molecule 14: 30S Ribosomal Protein S14



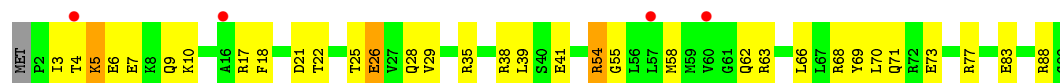
• Molecule 14: 30S Ribosomal Protein S14



• Molecule 15: 30S Ribosomal Protein S15

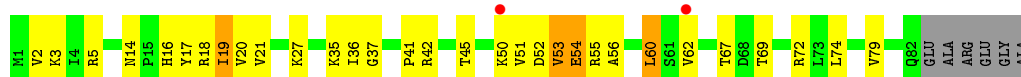


• Molecule 15: 30S Ribosomal Protein S15

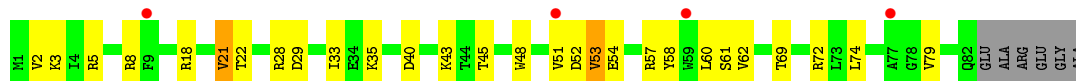


• Molecule 16: 30S Ribosomal Protein S16

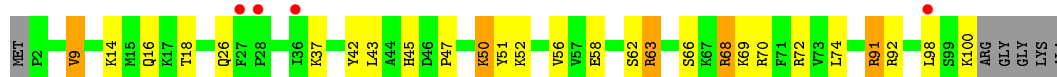




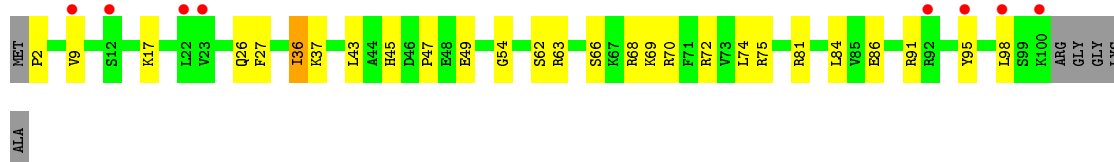
• Molecule 16: 30S Ribosomal Protein S16



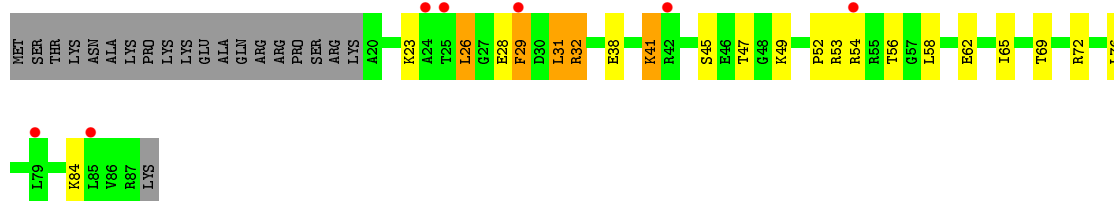
• Molecule 17: 30S Ribosomal Protein S17



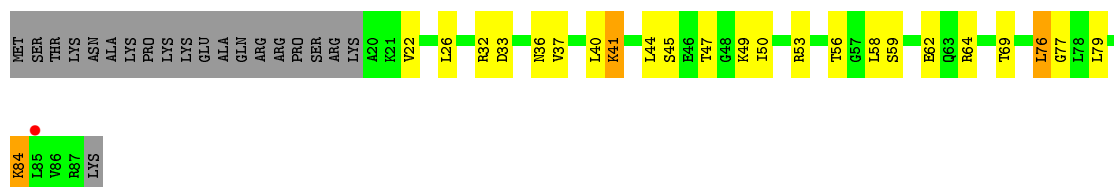
• Molecule 17: 30S Ribosomal Protein S17



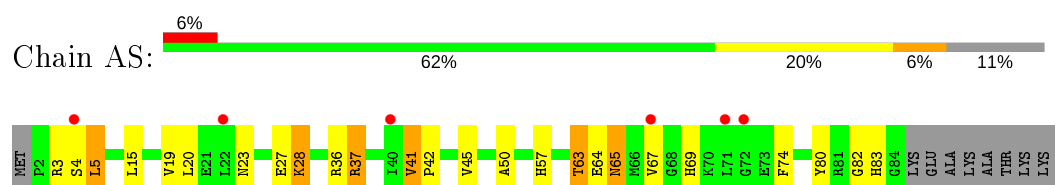
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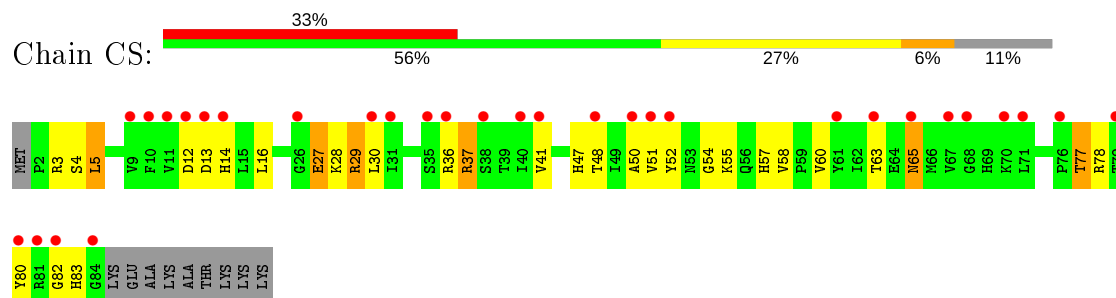
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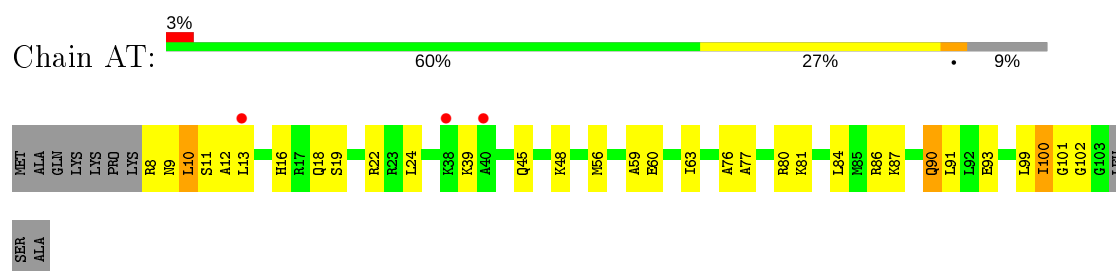
• Molecule 19: 30S Ribosomal Protein S19



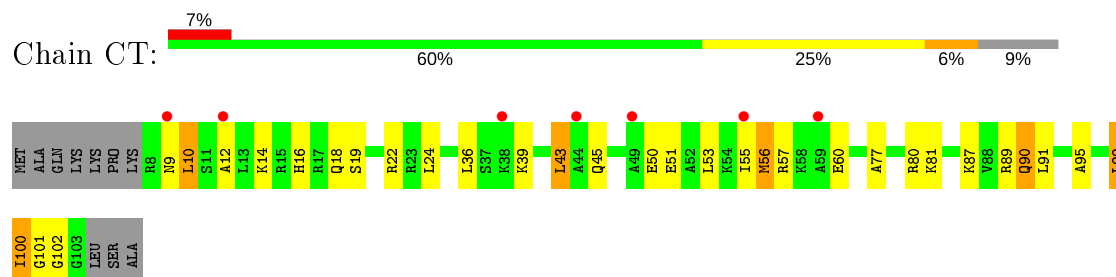
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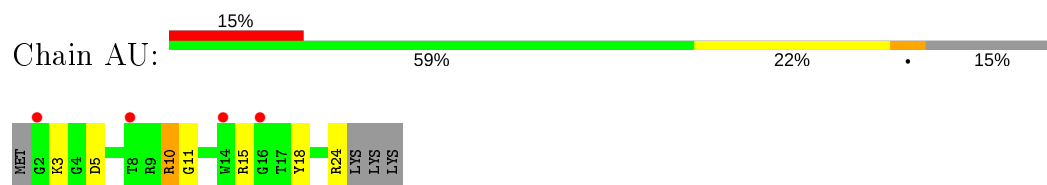
• Molecule 20: 30S Ribosomal Protein S20



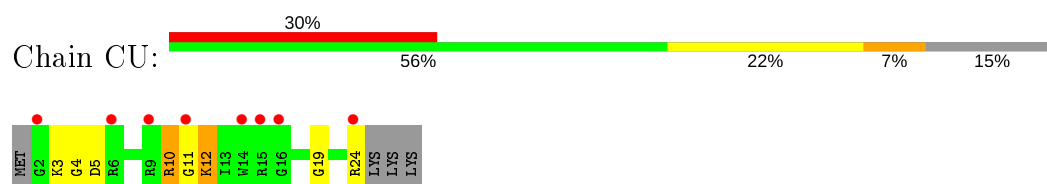
• Molecule 20: 30S Ribosomal Protein S20



• Molecule 21: 30S Ribosomal Protein THX



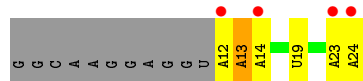
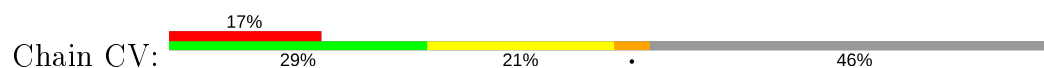
• Molecule 21: 30S Ribosomal Protein THX



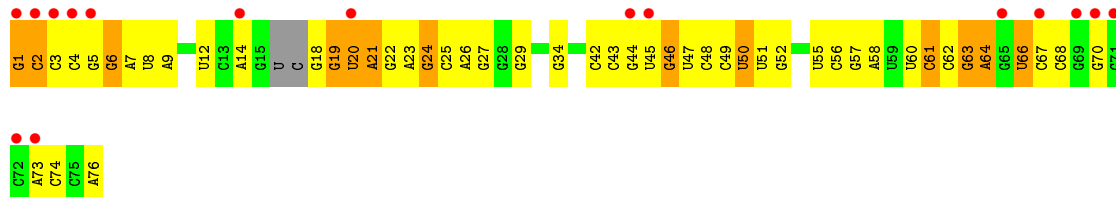
- Molecule 22: mRNA



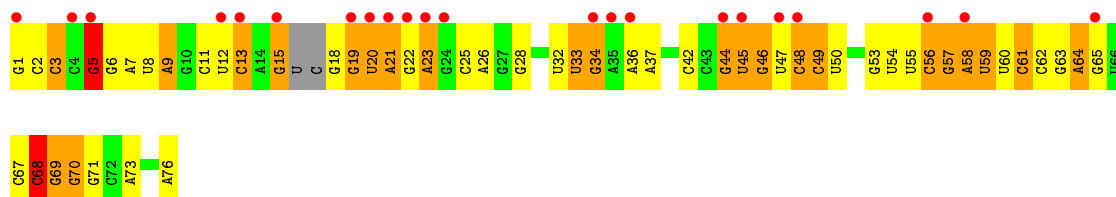
- Molecule 22: mRNA



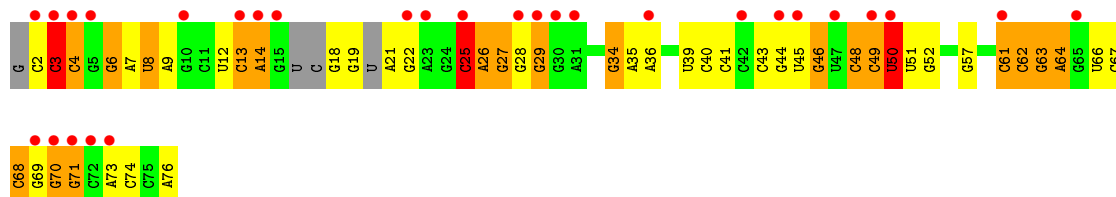
- Molecule 23: A/P-site tRNA



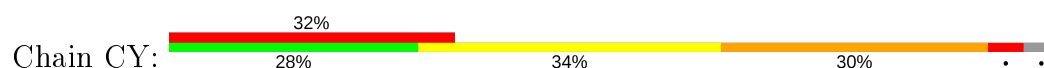
- Molecule 23: A/P-site tRNA

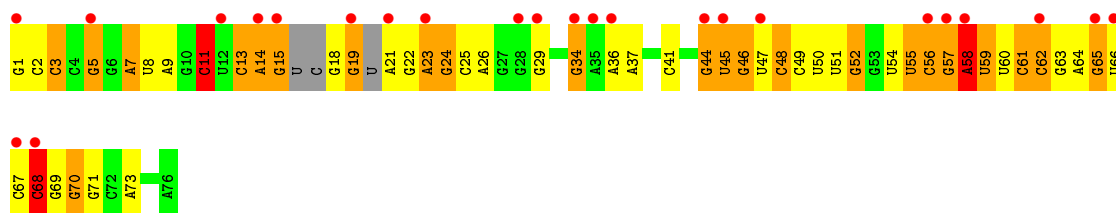


- Molecule 23: A/P-site tRNA

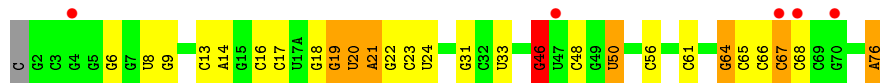


- Molecule 23: A/P-site tRNA





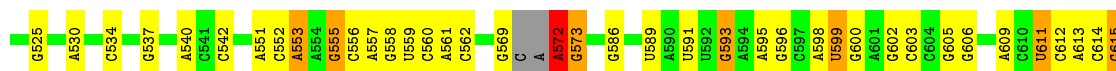
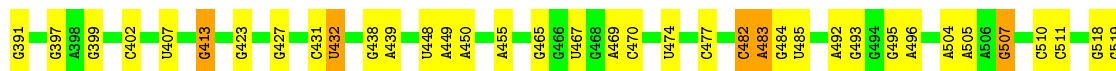
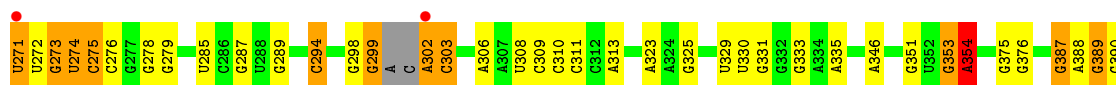
• Molecule 24: E-site tRNA

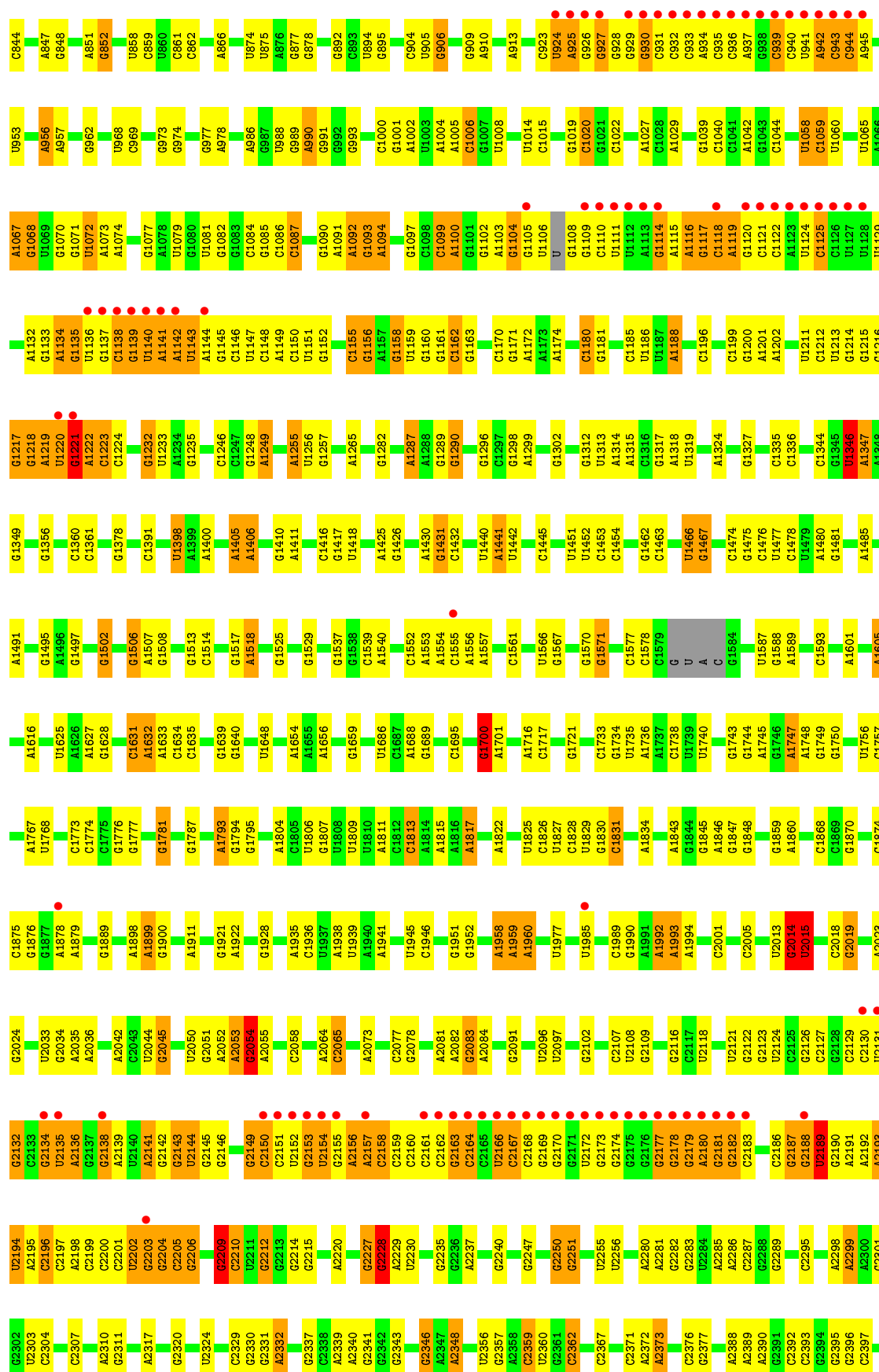


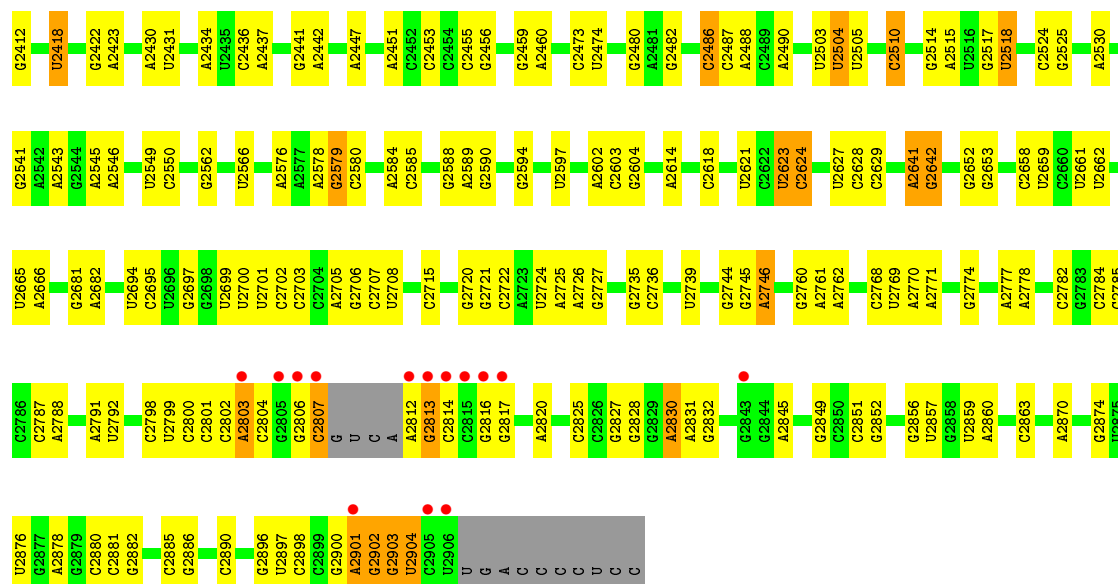
• Molecule 24: E-site tRNA



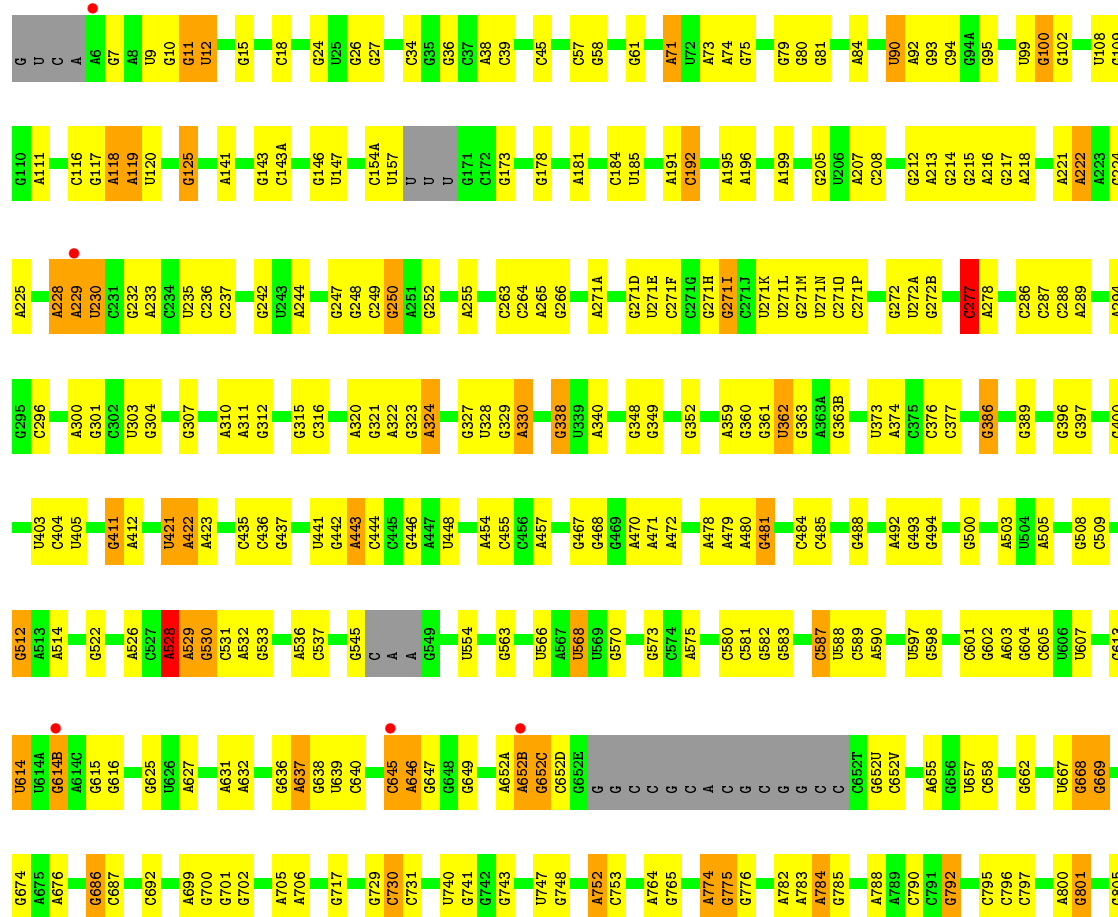
• Molecule 25: 23S Ribosomal RNA



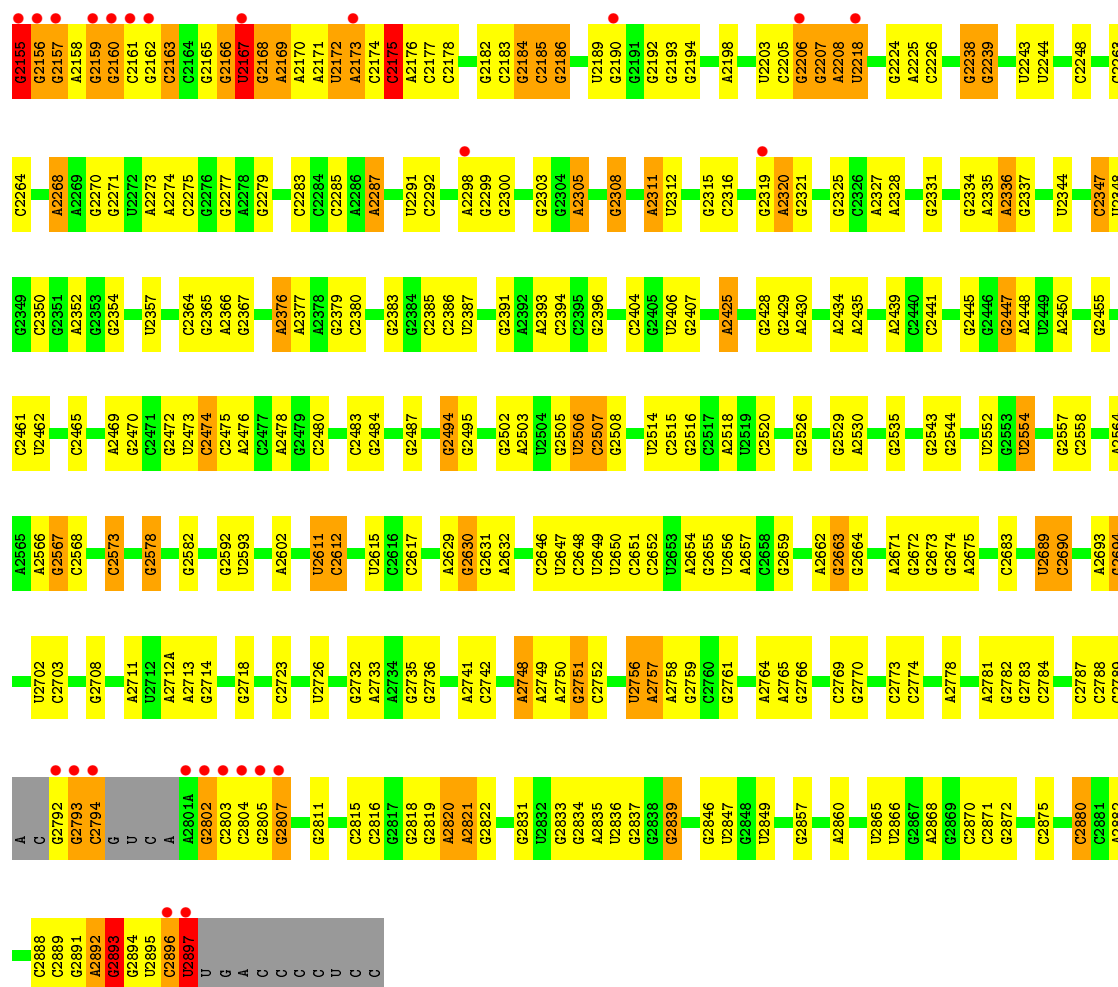




• Molecule 25: 23S Ribosomal RNA

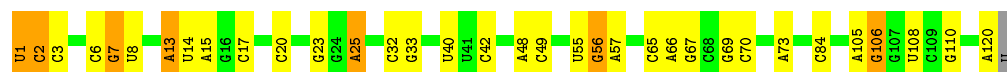


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C2097	U1993	G1837	G1756	G1623	C1530	U1420	U1314	G1212	C	U963	C884	U810
U2099	C1843	A1631A	A1759	A1631A	C1531	G1421	U1313	C1218	A	G974	C885	U811
G2100	A1847	G1836	A1759	G1836	G1533	A1427	U1314	C1219	G	C975A	C886	U812
G2101	A1848	A1637	A1762	A1637	U	C1428	C1315	A1220	C	G975A	C887	U813
U2102	C1999	G1638	G1763	G1638	A	C1428	U1335	G1223	A	A983	C888	C817
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G2146	A1965	G1718	G1718	G1718	A1590	G1467	U1391	G1274	U	U1039	C930	G874
C2147	C1966	G1719	G1719	G1719	A1591	G1467	U1392	G1275	C	A1040	C931	G875
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G2149	C1968	G1721	G1721	G1721	A1593	G1467	U1394	G1277	C	U1042	C933	U877
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C2152	A1971	G1740	G1740	G1740	A1596	G1467	U1397	G1280	U	U1045	C936	G880
G2153	A1972	G1741	G1741	G1741	A1597	G1467	U1398	G1281	C	U1046	C937	U881
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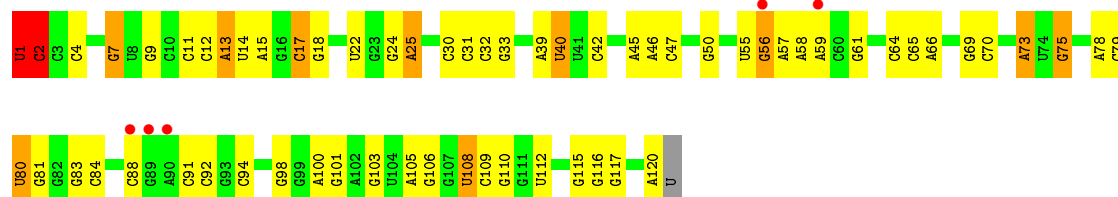
• Molecule 26: 5S Ribosomal RNA

Chain BB: 71% 22% 6%



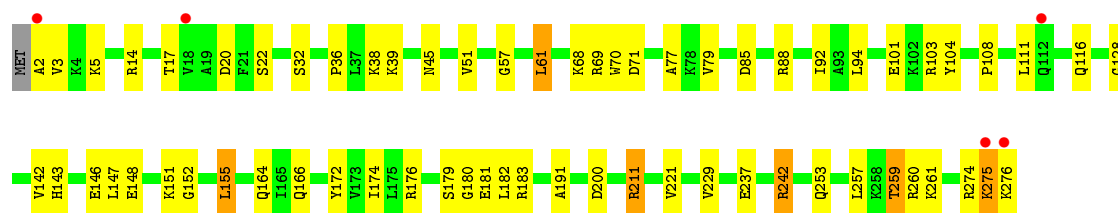
• Molecule 26: 5S Ribosomal RNA

Chain DB: 47% 42% 8%

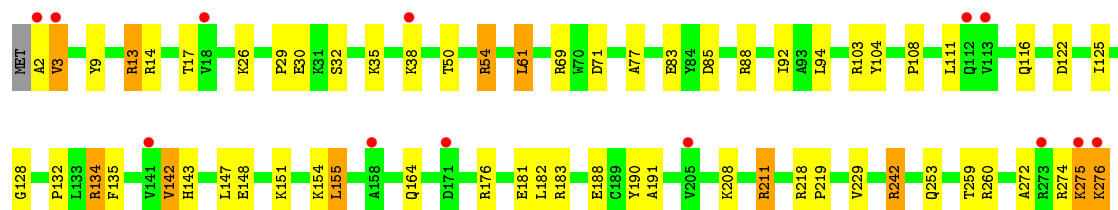
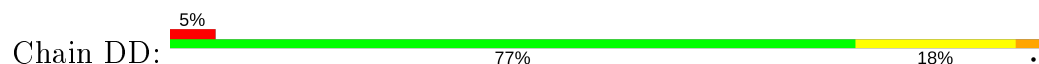


• Molecule 27: 50S Ribosomal Protein L2

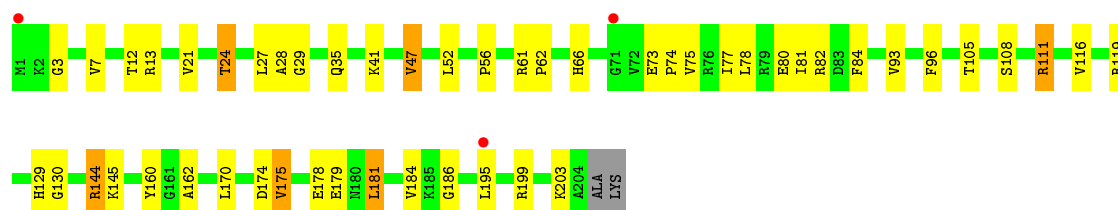
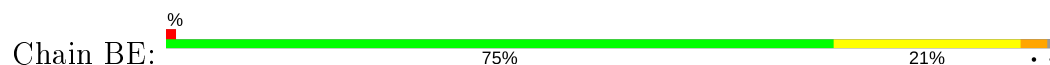
Chain BD: 76% 21% 2%



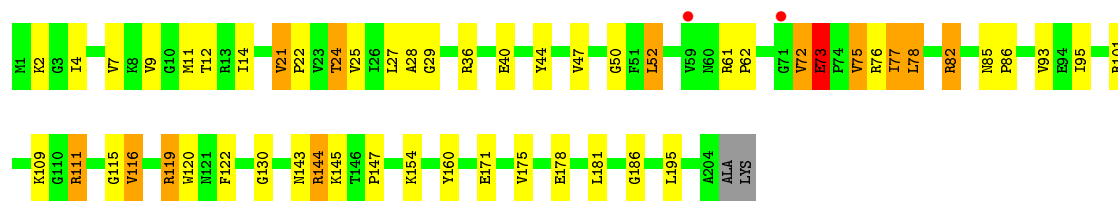
• Molecule 27: 50S Ribosomal Protein L2



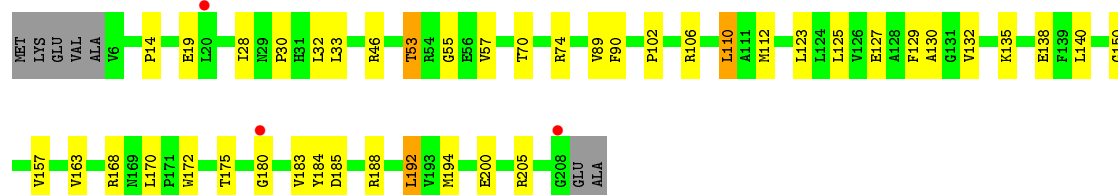
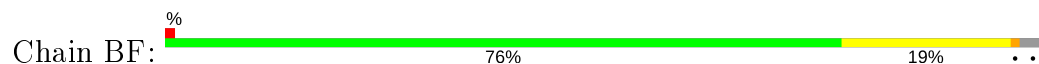
• Molecule 28: 50S Ribosomal Protein L3



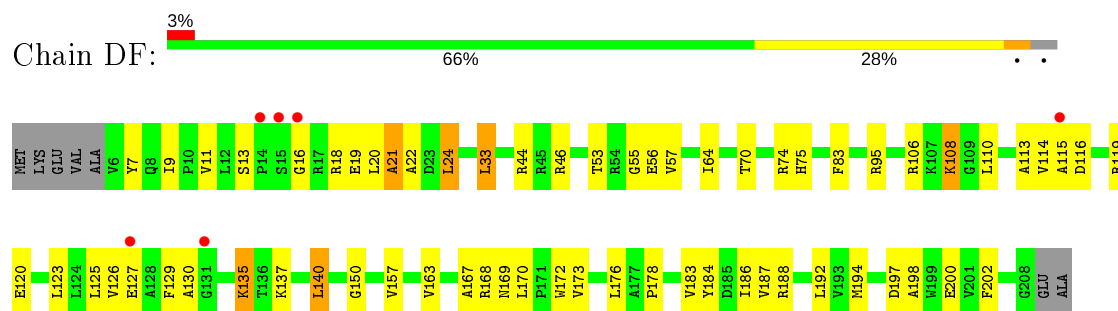
• Molecule 28: 50S Ribosomal Protein L3



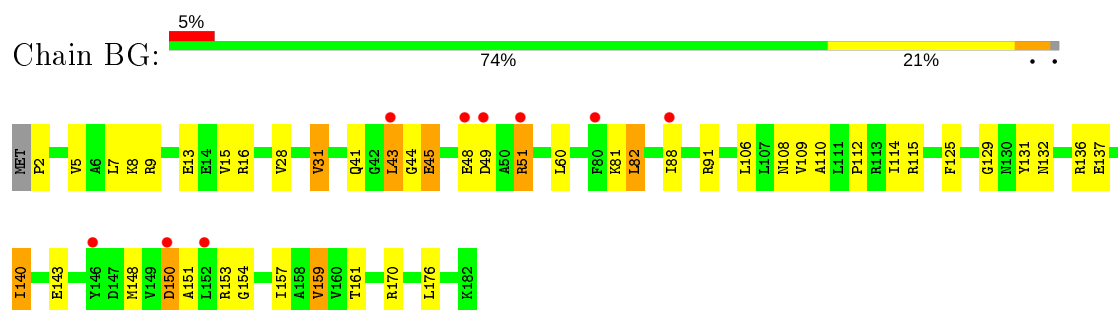
• Molecule 29: 50S Ribosomal Protein L4



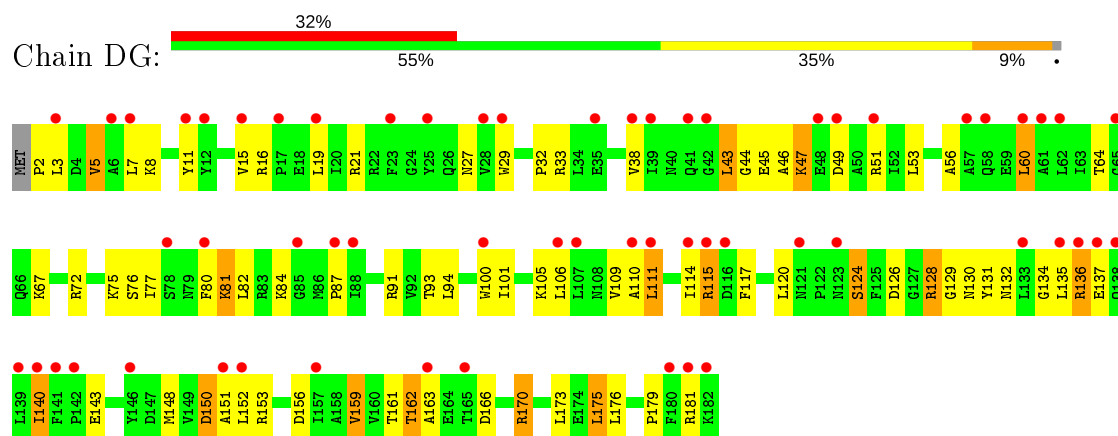
- Molecule 29: 50S Ribosomal Protein L4



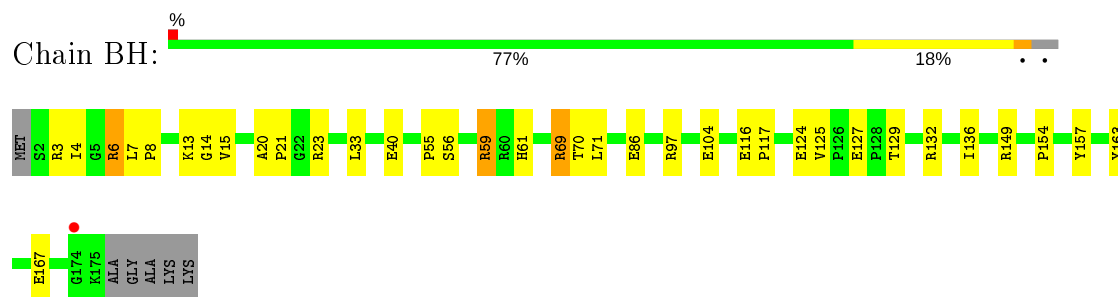
- Molecule 30: 50S Ribosomal Protein L5



- Molecule 30: 50S Ribosomal Protein L5

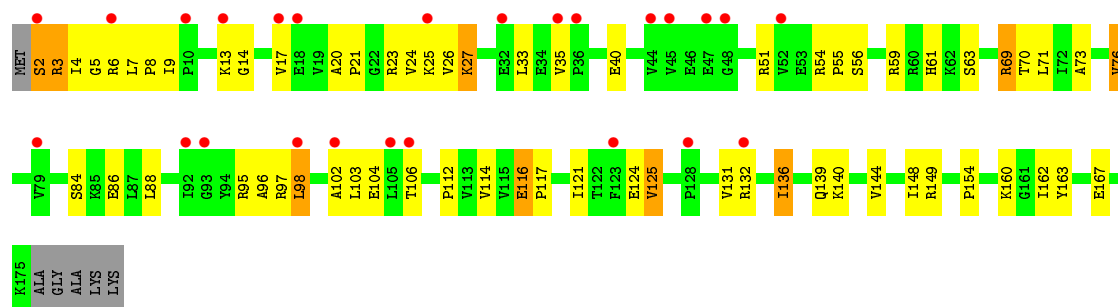


- Molecule 31: 50S Ribosomal Protein L6

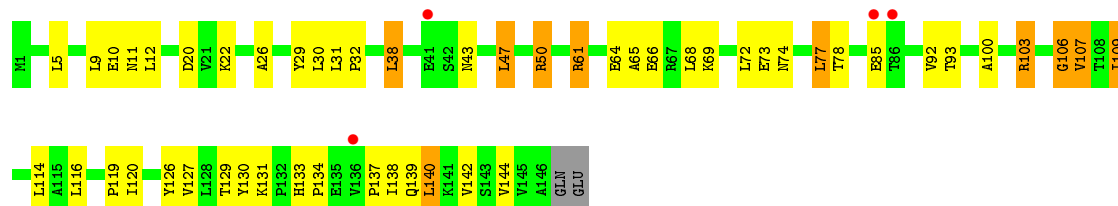


- Molecule 31: 50S Ribosomal Protein L6

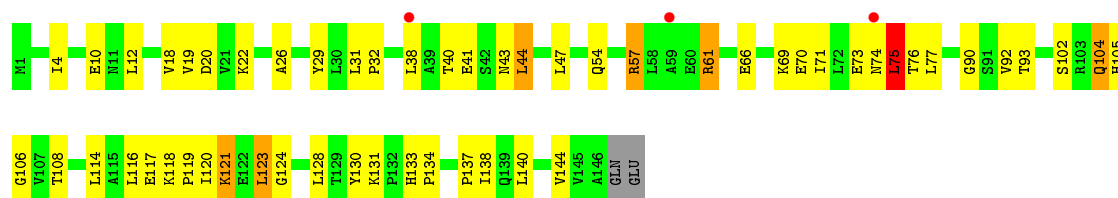




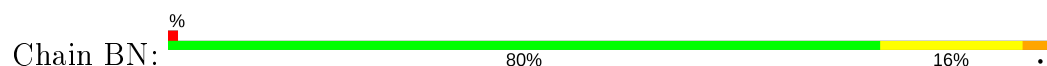
• Molecule 32: 50S Ribosomal Protein L9



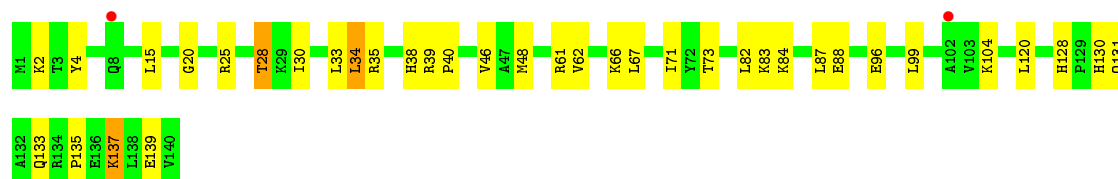
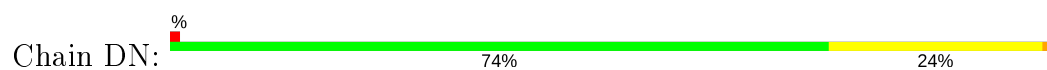
• Molecule 32: 50S Ribosomal Protein L9




• Molecule 33: 50S Ribosomal Protein L13



• Molecule 33: 50S Ribosomal Protein L13




• Molecule 34: 50S Ribosomal Protein L14

Chain BO:  78% 20% ..



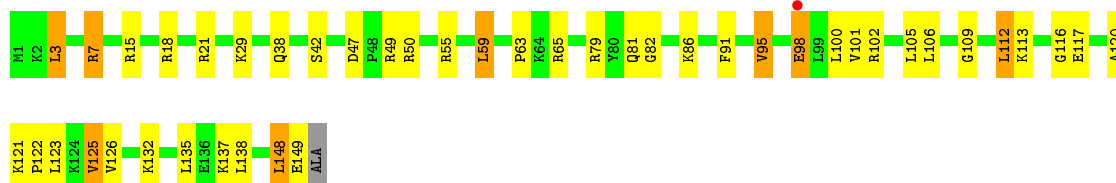
- Molecule 34: 50S Ribosomal Protein L14

Chain DO:  75% 24% .



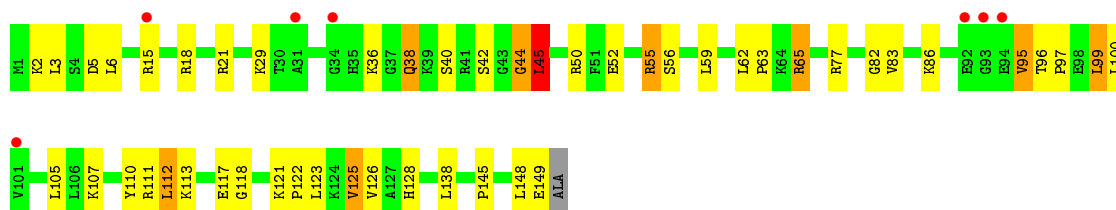
- Molecule 35: 50S Ribosomal Protein L15

Chain BP:  % 70% 24% 5% .




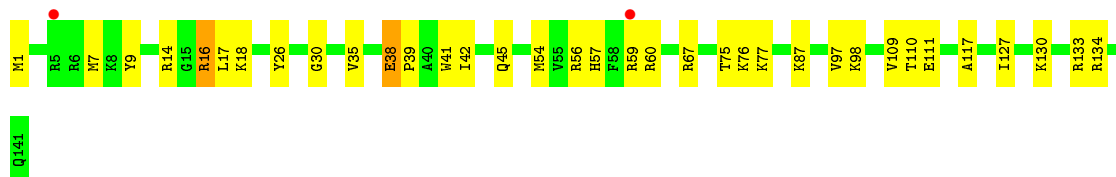
- Molecule 35: 50S Ribosomal Protein L15

Chain DP:  5% 67% 27% 5% ..




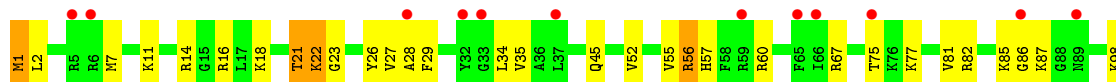
- Molecule 36: 50S Ribosomal Protein L16

Chain BQ:  % 75% 23% .



- Molecule 36: 50S Ribosomal Protein L16

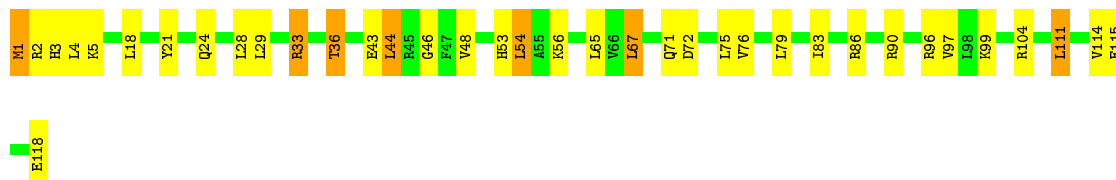
Chain DQ:  11% 72% 25% .





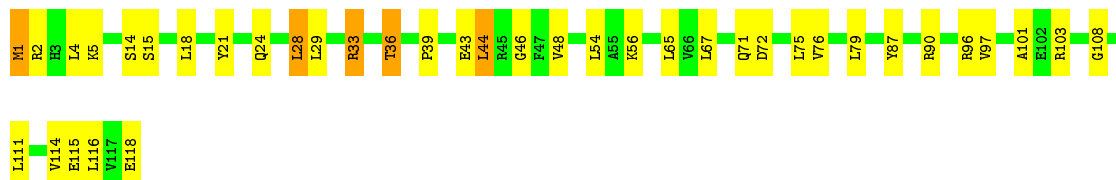
• Molecule 37: 50S Ribosomal Protein L17

Chain BR: 69% 25% 6%



• Molecule 37: 50S Ribosomal Protein L17

Chain DR: 67% 29% 4%



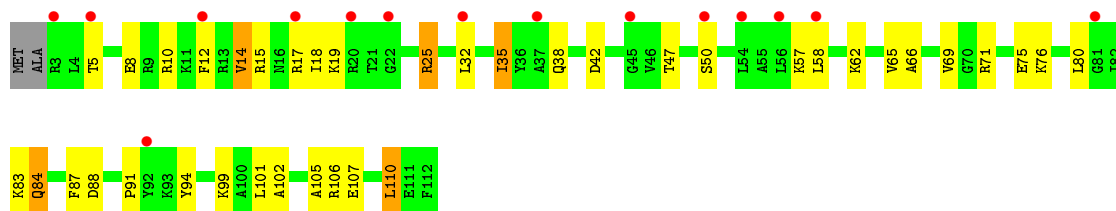
• Molecule 38: 50S Ribosomal Protein L18

Chain BS: 71% 24% 5%



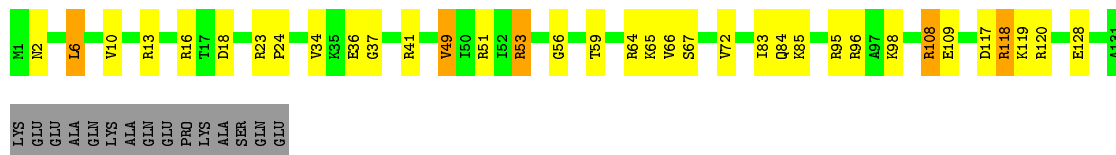
• Molecule 38: 50S Ribosomal Protein L18

Chain DS: 63% 30% 7%



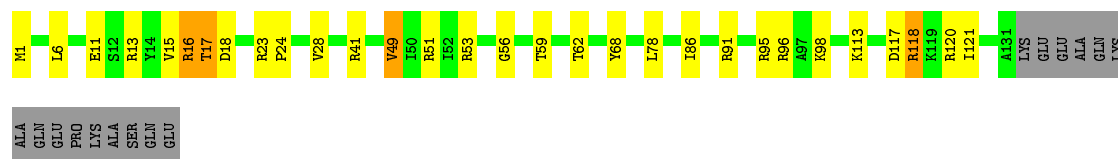
• Molecule 39: 50S Ribosomal Protein L19

Chain BT: 66% 21% 13%




- Molecule 39: 50S Ribosomal Protein L19

Chain DT: 




- Molecule 40: 50S Ribosomal Protein L20

Chain BU: 



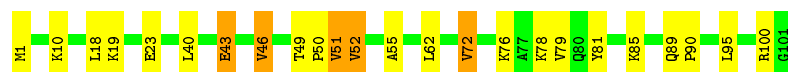
- Molecule 40: 50S Ribosomal Protein L20

Chain DU: 



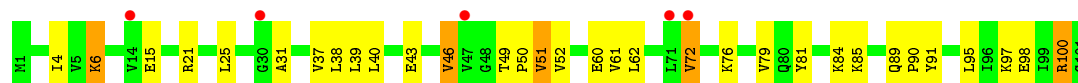
- Molecule 41: 50S Ribosomal Protein L21

Chain BV: 




- Molecule 41: 50S Ribosomal Protein L21

Chain DV: 



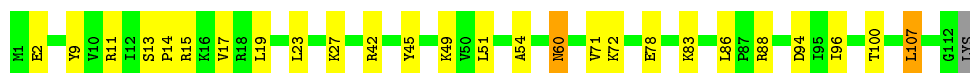
- Molecule 42: 50S Ribosomal Protein L22

Chain BW: 



- Molecule 42: 50S Ribosomal Protein L22

Chain DW: 



- Molecule 43: 50S Ribosomal Protein L23

Chain BX: 79% 19% ..



- Molecule 43: 50S Ribosomal Protein L23

Chain DX: 5% 72% 26% ..



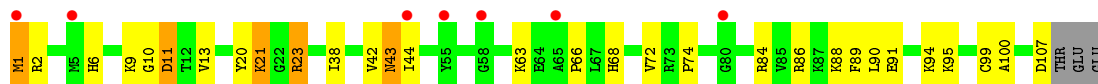
- Molecule 44: 50S Ribosomal Protein L24

Chain BY: 2% 65% 31% ..



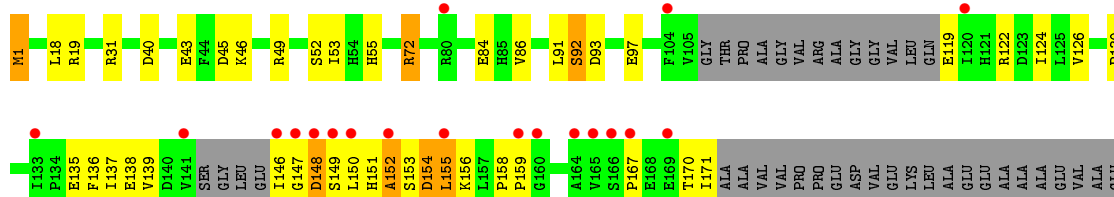
- Molecule 44: 50S Ribosomal Protein L24

Chain DY: 6% 70% 23% 5% .



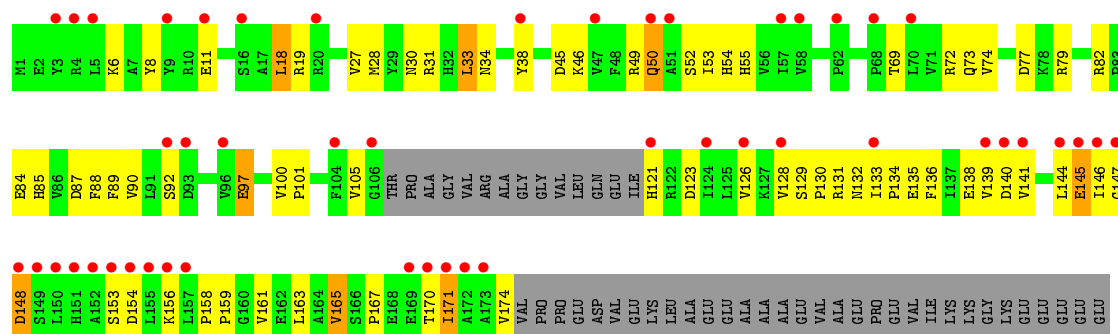
- Molecule 45: 50S Ribosomal Protein L25

Chain BZ: 9% 53% 18% 25%

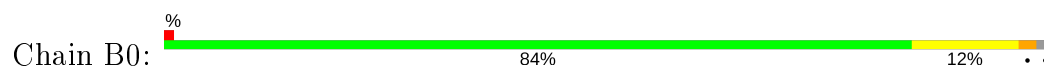


- Molecule 45: 50S Ribosomal Protein L25

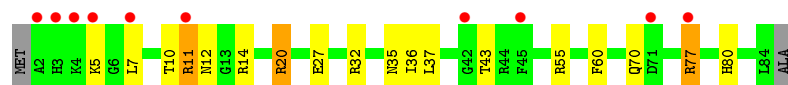
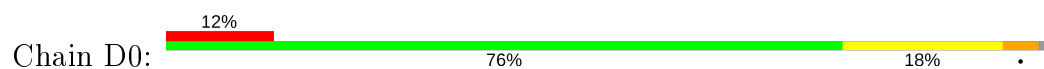
Chain DZ: 23% 43% 31% 22%



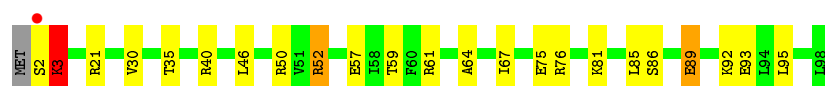
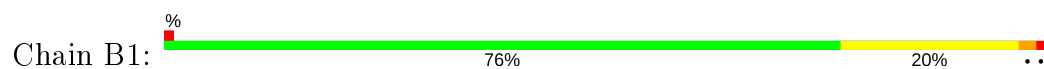
• Molecule 46: 50S Ribosomal Protein L27



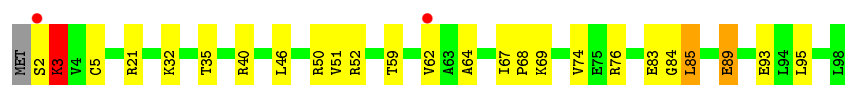
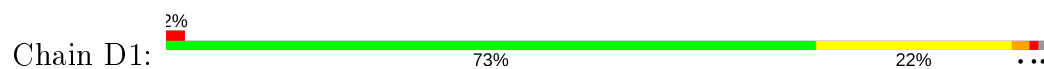
• Molecule 46: 50S Ribosomal Protein L27



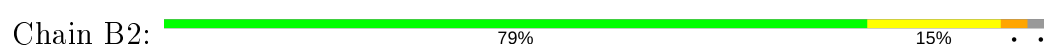
• Molecule 47: 50S Ribosomal Protein L28



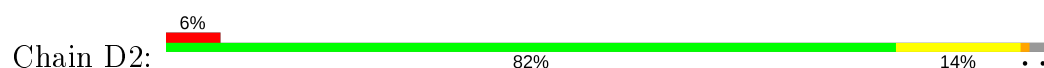
• Molecule 47: 50S Ribosomal Protein L28



• Molecule 48: 50S Ribosomal Protein L29



• Molecule 48: 50S Ribosomal Protein L29

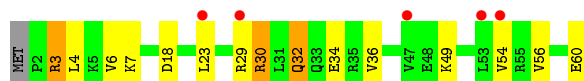
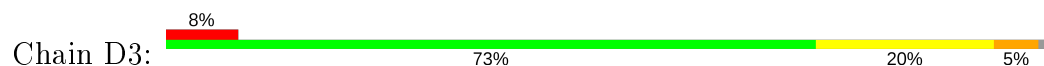




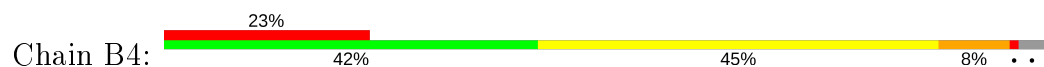
- Molecule 49: 50S Ribosomal Protein L30



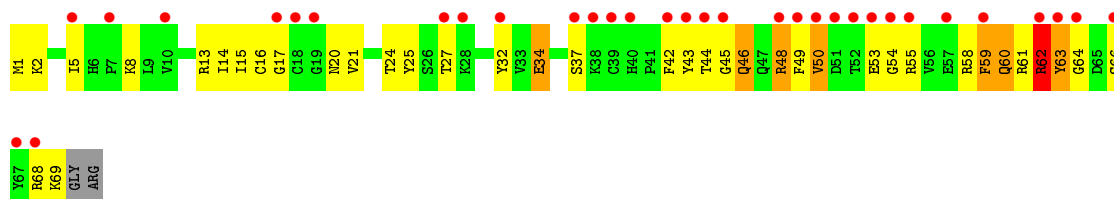
- Molecule 49: 50S Ribosomal Protein L30



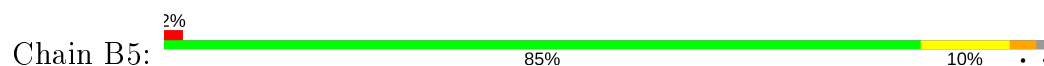
- Molecule 50: 50S Ribosomal Protein L31



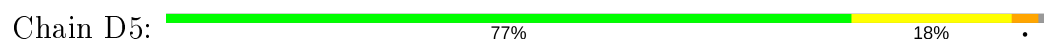
- Molecule 50: 50S Ribosomal Protein L31



- Molecule 51: 50S Ribosomal Protein L32



- Molecule 51: 50S Ribosomal Protein L32




- Molecule 52: 50S Ribosomal Protein L33

Chain B6:  70% 24% ..



- Molecule 52: 50S Ribosomal Protein L33

Chain D6:  6% 72% 24% ..




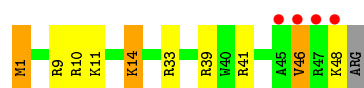
- Molecule 53: 50S Ribosomal Protein L34

Chain B7:  6% 65% 31% ..



- Molecule 53: 50S Ribosomal Protein L34

Chain D7:  8% 78% 14% 6% ..



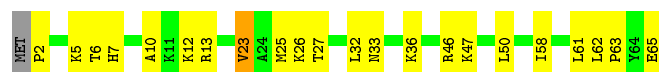
- Molecule 54: 50S Ribosomal Protein L35

Chain B8:  60% 35% ..




- Molecule 54: 50S Ribosomal Protein L35

Chain D8:  65% 32% ..



- Molecule 55: 50S Ribosomal Protein L36

Chain B9:  84% 14% ..



- Molecule 55: 50S Ribosomal Protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.06Å 448.57Å 623.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	256.12 – 2.40 311.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (256.12-2.40) 99.6 (311.98-2.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.237 , 0.277 0.237 , 0.278	Depositor DCC
R_{free} test set	113081 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	298643	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, MIA, SF4, MG, UAM, 5MC, 4SU, 7MG, K, 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	AA	0.38	0/36027	0.90	45/56227 (0.1%)
1	CA	0.37	1/36170 (0.0%)	0.91	47/56452 (0.1%)
2	AB	0.30	0/1881	0.58	0/2542
2	CB	0.30	0/1860	0.61	1/2518 (0.0%)
3	AC	0.28	0/1572	0.50	0/2126
3	CC	0.30	0/1566	0.56	0/2119
4	AD	0.29	0/1685	0.49	0/2262
4	CD	0.29	0/1704	0.50	0/2284
5	AE	0.29	0/1145	0.52	0/1543
5	CE	0.31	0/1149	0.57	0/1548
6	AF	0.30	0/823	0.49	0/1115
6	CF	0.30	0/829	0.51	0/1123
7	AG	0.28	0/1250	0.54	0/1679
7	CG	0.27	0/1254	0.53	0/1683
8	AH	0.28	0/1108	0.51	0/1494
8	CH	0.27	0/1108	0.49	0/1494
9	AI	0.29	0/1002	0.56	0/1346
9	CI	0.28	0/997	0.53	1/1343 (0.1%)
10	AJ	0.28	0/722	0.57	0/982
10	CJ	0.29	0/727	0.55	0/988
11	AK	0.29	0/844	0.50	0/1145
11	CK	0.28	0/848	0.51	0/1149
12	AL	0.30	0/946	0.51	0/1274
12	CL	0.29	0/946	0.56	1/1274 (0.1%)
13	AM	0.28	0/969	0.56	0/1302
13	CM	0.28	0/961	0.55	0/1291
14	AN	0.29	0/501	0.48	0/664
14	CN	0.30	0/501	0.55	0/664
15	AO	0.28	0/739	0.51	0/985
15	CO	0.29	0/739	0.52	0/985
16	AP	0.27	0/697	0.51	0/939
16	CP	0.28	0/693	0.50	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.30	0/836	0.53	0/1117
17	CQ	0.27	0/836	0.48	0/1117
18	AR	0.30	0/560	0.51	0/746
18	CR	0.26	0/560	0.49	0/746
19	AS	0.27	0/667	0.53	0/900
19	CS	0.31	0/661	0.64	0/893
20	AT	0.26	0/730	0.55	0/965
20	CT	0.28	0/729	0.52	0/965
21	AU	0.27	0/203	0.48	0/266
21	CU	0.30	0/203	0.51	0/266
22	AV	0.36	0/310	0.84	0/480
22	CV	0.40	0/310	0.89	1/480 (0.2%)
23	AW	0.53	1/1606 (0.1%)	1.13	2/2497 (0.1%)
23	AY	0.53	1/1606 (0.1%)	1.13	8/2497 (0.3%)
23	CW	0.51	0/1556	1.23	9/2418 (0.4%)
23	CY	0.56	1/1583 (0.1%)	1.22	12/2459 (0.5%)
24	AX	0.50	2/1725 (0.1%)	1.13	14/2689 (0.5%)
24	CX	0.49	0/1725	1.13	14/2689 (0.5%)
25	BA	0.50	5/69261 (0.0%)	0.96	91/108110 (0.1%)
25	DA	0.42	0/67545	0.92	63/105432 (0.1%)
26	BB	0.43	1/2882 (0.0%)	0.83	1/4494 (0.0%)
26	DB	0.47	1/2879 (0.0%)	0.91	2/4487 (0.0%)
27	BD	0.36	0/2186	0.60	1/2944 (0.0%)
27	DD	0.34	0/2186	0.56	0/2944
28	BE	0.36	0/1592	0.56	0/2149
28	DE	0.34	0/1592	0.61	1/2149 (0.0%)
29	BF	0.35	0/1619	0.54	0/2193
29	DF	0.33	0/1615	0.55	0/2188
30	BG	0.29	0/1454	0.51	0/1964
30	DG	0.29	0/1453	0.52	0/1963
31	BH	0.31	0/1356	0.56	0/1834
31	DH	0.30	0/1356	0.54	0/1834
32	BI	0.29	0/1112	0.56	0/1514
32	DI	0.27	0/1079	0.55	1/1475 (0.1%)
33	BN	0.33	0/1144	0.54	0/1543
33	DN	0.32	0/1144	0.53	0/1543
34	BO	0.34	0/943	0.54	1/1269 (0.1%)
34	DO	0.32	0/943	0.56	1/1269 (0.1%)
35	BP	0.32	0/1152	0.57	0/1533
35	DP	0.32	0/1152	0.59	1/1533 (0.1%)
36	BQ	0.34	0/1143	0.53	0/1527
36	DQ	0.32	0/1143	0.53	0/1527
37	BR	0.36	0/982	0.61	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DR	0.34	0/982	0.55	0/1312
38	BS	0.31	0/883	0.52	0/1176
38	DS	0.31	0/880	0.53	0/1172
39	BT	0.33	0/1105	0.56	0/1477
39	DT	0.30	0/1097	0.53	0/1468
40	BU	0.38	0/977	0.58	0/1301
40	DU	0.34	0/977	0.53	0/1301
41	BV	0.41	0/782	0.62	0/1049
41	DV	0.29	0/782	0.54	0/1049
42	BW	0.38	0/897	0.57	0/1205
42	DW	0.33	0/897	0.55	0/1205
43	BX	0.37	0/764	0.63	1/1025 (0.1%)
43	DX	0.34	0/764	0.53	1/1025 (0.1%)
44	BY	0.34	0/819	0.56	0/1095
44	DY	0.33	0/819	0.54	0/1095
45	BZ	0.31	0/1267	0.57	0/1717
45	DZ	0.30	0/1299	0.55	0/1763
46	B0	0.35	0/662	0.60	0/881
46	D0	0.30	0/662	0.49	0/881
47	B1	0.32	0/762	0.52	0/1014
47	D1	0.33	0/762	0.52	0/1014
48	B2	0.32	0/590	0.56	0/781
48	D2	0.28	0/590	0.47	0/781
49	B3	0.37	0/474	0.60	0/635
49	D3	0.27	0/469	0.50	0/630
50	B4	0.34	0/565	0.63	0/761
50	D4	0.33	0/545	0.65	0/737
51	B5	0.36	0/469	0.54	0/635
51	D5	0.33	0/469	0.59	0/635
52	B6	0.36	0/460	0.57	0/613
52	D6	0.29	0/456	0.49	0/608
53	B7	0.39	0/426	0.59	0/561
53	D7	0.34	0/426	0.54	0/561
54	B8	0.36	0/525	0.58	0/691
54	D8	0.30	0/525	0.51	0/691
55	B9	0.34	0/310	0.49	0/407
55	D9	0.31	0/310	0.53	0/407
All	All	0.41	13/317730 (0.0%)	0.85	320/475754 (0.1%)

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
2	AB	0	1
7	AG	0	1
7	CG	0	1
50	B4	0	2
All	All	0	5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AY	1	G	OP3-P	-10.51	1.48	1.61
26	BB	1	U	OP3-P	-10.37	1.48	1.61
23	CY	1	G	OP3-P	-10.36	1.48	1.61
26	DB	1	U	OP3-P	-10.22	1.48	1.61
23	AW	1	G	OP3-P	-9.85	1.49	1.61
25	BA	354	A	N9-C4	-6.71	1.33	1.37
25	BA	553	A	N9-C4	-6.02	1.34	1.37
25	BA	1067	A	N9-C4	-5.86	1.34	1.37
24	AX	14	A	N7-C5	-5.77	1.35	1.39
1	CA	1154	G	C6-N1	-5.24	1.35	1.39
24	AX	14	A	C8-N7	-5.22	1.27	1.31
25	BA	1188	A	N9-C4	-5.12	1.34	1.37
25	BA	593	G	C6-O6	-5.03	1.19	1.24

All (320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1154	G	C5-C6-O6	12.79	136.28	128.60
24	AX	46	G	C6-N1-C2	-10.27	118.94	125.10
24	AX	14	A	C4-C5-C6	10.10	122.05	117.00
25	BA	1807	G	O5'-P-OP2	-9.98	96.71	105.70
1	AA	1002	G	N3-C4-N9	9.53	131.72	126.00
24	CX	46	G	C6-N1-C2	-9.19	119.59	125.10
1	AA	1002	G	C4-N9-C1'	9.15	138.40	126.50
1	CA	1004	A	O4'-C1'-N9	8.95	115.36	108.20
1	CA	1119	C	C2-N3-C4	8.93	124.36	119.90
25	BA	599	U	O5'-P-OP1	-8.88	97.71	105.70
1	AA	1002	G	N3-C4-C5	-8.82	124.19	128.60
1	CA	1001(A)	G	N3-C4-N9	8.73	131.24	126.00
24	AX	14	A	C5-N7-C8	8.65	108.22	103.90
25	BA	354	A	C2-N3-C4	-8.59	106.31	110.60
25	DA	1614	A	O5'-P-OP1	-8.54	98.02	105.70
25	BA	187	C	O5'-P-OP2	-8.52	98.03	105.70
1	CA	1154	G	N1-C6-O6	-8.44	114.84	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	22	G	C5-N7-C8	-8.38	100.11	104.30
25	BA	848	G	O5'-P-OP2	-8.33	98.21	105.70
25	BA	993	G	O5'-P-OP1	-8.26	98.27	105.70
24	CX	14	A	C4-C5-C6	8.25	121.13	117.00
25	BA	593	G	C5-C6-O6	-8.16	123.70	128.60
1	AA	1002	G	C8-N9-C1'	-8.07	116.51	127.00
25	BA	2158	C	N1-C2-O2	8.02	123.71	118.90
24	AX	14	A	C5-C6-N1	-7.83	113.79	117.70
1	CA	1001(A)	G	C8-N9-C1'	-7.80	116.85	127.00
23	AY	33	U	C2-N1-C1'	7.79	127.04	117.70
25	BA	611	U	O5'-P-OP2	-7.78	98.70	105.70
25	BA	139	A	N7-C8-N9	7.72	117.66	113.80
1	AA	1030(B)	C	C2-N1-C1'	7.69	127.26	118.80
1	CA	1001(A)	G	C4-N9-C1'	7.67	136.47	126.50
25	DA	2897	U	C2-N1-C1'	7.67	126.90	117.70
25	BA	537	G	O4'-C1'-N9	7.62	114.30	108.20
25	BA	2172	U	N1-C2-O2	-7.57	117.50	122.80
23	AY	33	U	N1-C2-O2	7.56	128.09	122.80
1	CA	79	G	C5-C6-O6	7.41	133.04	128.60
25	BA	591	U	C5-C4-O4	-7.40	121.46	125.90
25	DA	2139	C	N1-C2-O2	7.39	123.33	118.90
25	BA	2163	G	C5-C6-O6	7.37	133.02	128.60
25	DA	1298	C	O5'-P-OP2	-7.32	99.11	105.70
25	BA	1686	U	O5'-P-OP2	-7.27	99.16	105.70
25	BA	593	G	C5-C6-N1	7.24	115.12	111.50
1	CA	1119	C	C5-C4-N4	7.24	125.27	120.20
25	BA	2189	U	C2-N1-C1'	7.22	126.36	117.70
25	DA	645	C	C2-N1-C1'	7.22	126.74	118.80
24	AX	46	G	C5-C6-N1	7.21	115.11	111.50
25	BA	12	U	C2-N1-C1'	7.21	126.36	117.70
24	CX	14	A	C5-N7-C8	7.20	107.50	103.90
25	BA	1232	G	N1-C6-O6	-7.20	115.58	119.90
25	DA	2167	U	C2-N1-C1'	7.19	126.33	117.70
25	BA	1813	C	O5'-P-OP1	-7.17	99.24	105.70
25	BA	2058	C	O5'-P-OP1	-7.17	99.24	105.70
1	CA	754	C	C2-N1-C1'	7.16	126.68	118.80
1	CA	1119	C	N3-C4-C5	-7.16	119.04	121.90
25	BA	2015	U	O5'-P-OP1	-7.16	99.26	105.70
25	DA	2167	U	N1-C2-O2	7.08	127.76	122.80
25	BA	1067	A	C2-N3-C4	-7.07	107.07	110.60
25	DA	277	C	N1-C2-O2	6.98	123.09	118.90
1	CA	96	U	O4'-C1'-N1	6.89	113.71	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	1346	U	P-O3'-C3'	6.87	127.94	119.70
1	AA	1007	C	N1-C2-O2	6.86	123.02	118.90
25	BA	2694	U	O5'-P-OP2	-6.86	99.53	105.70
25	BA	1020	C	N1-C2-O2	-6.82	114.81	118.90
1	CA	1003	G	C4-N9-C1'	6.81	135.35	126.50
1	AA	90	U	C2-N1-C1'	6.80	125.87	117.70
1	AA	1027	C	C5-C6-N1	6.76	124.38	121.00
25	BA	139	A	C8-N9-C4	-6.75	103.10	105.80
25	DA	2893	G	C5-C6-O6	-6.74	124.56	128.60
25	DA	512	G	O4'-C1'-N9	6.74	113.59	108.20
25	BA	988	U	O5'-P-OP2	-6.73	99.64	105.70
23	CW	50	U	C5-C4-O4	-6.70	121.88	125.90
1	CA	1183	A	P-O3'-C3'	6.67	127.71	119.70
1	AA	1036	G	C4-N9-C1'	6.65	135.15	126.50
23	AY	64	A	C5-C6-N6	6.63	129.00	123.70
23	AY	64	A	N1-C6-N6	-6.62	114.63	118.60
1	AA	254	G	O5'-P-OP1	-6.62	99.75	105.70
25	DA	801	G	O5'-P-OP2	-6.61	99.75	105.70
25	BA	2050	U	N1-C2-O2	6.60	127.42	122.80
24	CX	14	A	C5-C6-N1	-6.59	114.41	117.70
25	BA	978	A	O4'-C1'-N9	6.54	113.43	108.20
24	AX	46	G	N3-C2-N2	-6.52	115.33	119.90
23	CY	22	G	C8-N9-C1'	-6.52	118.53	127.00
23	CY	22	G	C4-N9-C1'	6.51	134.96	126.50
23	AY	68	C	N1-C2-O2	6.51	122.80	118.90
1	CA	1003	G	N7-C8-N9	6.50	116.35	113.10
1	AA	91	C	C2-N1-C1'	6.49	125.94	118.80
1	CA	754	C	N1-C2-O2	6.45	122.77	118.90
1	AA	1027	C	C6-N1-C2	-6.45	117.72	120.30
25	BA	553	A	C2-N3-C4	-6.44	107.38	110.60
25	BA	591	U	N3-C4-C5	6.44	118.46	114.60
25	BA	2189	U	N1-C2-O2	6.43	127.30	122.80
24	CX	22	G	N1-C6-O6	-6.40	116.06	119.90
1	CA	1020	U	N1-C2-O2	6.39	127.27	122.80
25	BA	2189	U	N3-C2-O2	-6.37	117.74	122.20
23	CW	25	C	C6-N1-C2	-6.36	117.76	120.30
1	AA	91	C	C5-C4-N4	-6.36	115.75	120.20
1	AA	1002	G	C6-C5-N7	-6.35	126.59	130.40
24	CX	46	G	C5-C6-N1	6.34	114.67	111.50
25	BA	2050	U	N3-C4-O4	-6.32	114.97	119.40
1	AA	1027	C	C2-N1-C1'	6.32	125.75	118.80
23	CY	11	C	C5-C6-N1	6.32	124.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	558	G	O5'-P-OP1	-6.30	100.03	105.70
25	BA	2163	G	C6-N1-C2	6.26	128.86	125.10
25	BA	1344	C	O5'-P-OP2	-6.26	100.07	105.70
1	CA	1001(A)	G	N9-C4-C5	-6.26	102.90	105.40
1	AA	91	C	N3-C4-N4	6.25	122.38	118.00
25	DA	2136	C	N1-C2-O2	6.23	122.64	118.90
32	DI	75	LEU	CA-CB-CG	6.20	129.55	115.30
34	DO	8	LEU	CA-CB-CG	6.20	129.55	115.30
43	BX	57	LEU	CA-CB-CG	6.18	129.52	115.30
23	AY	33	U	N3-C2-O2	-6.14	117.90	122.20
1	AA	754	C	C2-N1-C1'	6.14	125.55	118.80
25	BA	990	A	C5-N7-C8	-6.13	100.83	103.90
25	DA	1372	U	C5-C4-O4	-6.13	122.22	125.90
25	BA	793	A	O4'-C1'-N9	6.13	113.11	108.20
25	DA	2473	U	C2-N1-C1'	6.13	125.06	117.70
25	BA	990	A	C2-N3-C4	-6.13	107.54	110.60
25	BA	831	A	OP1-P-O3'	6.11	118.63	105.20
28	DE	72	VAL	C-N-CA	6.10	136.95	121.70
1	AA	91	C	C6-N1-C1'	-6.09	113.49	120.80
1	CA	1064	G	P-O3'-C3'	6.08	127.00	119.70
34	BO	8	LEU	CA-CB-CG	6.08	129.28	115.30
25	DA	1992	G	P-O3'-C3'	6.07	126.98	119.70
25	DA	2123	G	C5-C6-O6	-6.07	124.96	128.60
25	DA	2893	G	N9-C4-C5	-6.06	102.97	105.40
25	DA	2893	G	C4-C5-N7	6.03	113.21	110.80
25	DA	2167	U	N3-C2-O2	-6.01	117.99	122.20
25	BA	2014	G	P-O3'-C3'	6.01	126.92	119.70
24	CX	14	A	C4-N9-C1'	6.01	137.11	126.30
25	BA	139	A	C5-N7-C8	-5.99	100.91	103.90
25	BA	354	A	N1-C2-N3	5.98	132.29	129.30
25	BA	798	A	O5'-P-OP1	-5.98	100.32	105.70
1	CA	792	A	O4'-C1'-N9	5.96	112.97	108.20
25	DA	2175	C	C5-C6-N1	5.94	123.97	121.00
1	AA	1027	C	N1-C2-O2	5.92	122.45	118.90
24	CX	22	G	C5-N7-C8	-5.90	101.35	104.30
1	AA	1022	G	N3-C2-N2	5.90	124.03	119.90
1	CA	1001(A)	G	C6-C5-N7	-5.89	126.86	130.40
1	AA	1030(B)	C	N1-C2-O2	5.88	122.43	118.90
25	BA	553	A	N3-C4-N9	-5.87	122.70	127.40
25	BA	593	G	C4-C5-N7	5.87	113.15	110.80
25	DA	1372	U	N3-C4-O4	5.86	123.50	119.40
25	BA	2166	U	N1-C2-O2	-5.85	118.70	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CX	14	A	C8-N9-C1'	-5.85	117.17	127.70
1	AA	1030(B)	C	C6-N1-C1'	-5.84	113.79	120.80
1	CA	1286	A	N7-C8-N9	5.84	116.72	113.80
1	CA	1158	C	N1-C2-O2	5.83	122.40	118.90
1	CA	1154	G	C6-N1-C2	5.83	128.59	125.10
1	AA	299	G	C5-C6-O6	-5.81	125.11	128.60
25	BA	1188	A	C2-N3-C4	-5.80	107.70	110.60
25	DA	277	C	C2-N1-C1'	5.80	125.19	118.80
24	CX	22	G	C4-C5-C6	-5.80	115.32	118.80
25	DA	1698	A	O4'-C1'-N9	5.80	112.84	108.20
23	CY	11	C	C2-N1-C1'	5.79	125.17	118.80
1	AA	1397	C	C2-N1-C1'	5.79	125.17	118.80
24	AX	22	G	C4-C5-C6	-5.79	115.33	118.80
1	AA	1132	C	C2-N1-C1'	5.78	125.16	118.80
1	AA	92	C	C5-C6-N1	5.77	123.88	121.00
1	CA	1126	U	C2-N1-C1'	5.77	124.62	117.70
25	DA	2155	G	N3-C2-N2	5.74	123.92	119.90
1	CA	1023	G	N3-C4-N9	5.73	129.44	126.00
26	DB	80	U	O4'-C1'-N1	5.72	112.78	108.20
25	BA	593	G	N9-C4-C5	-5.72	103.11	105.40
1	CA	1020	U	N3-C2-O2	-5.71	118.20	122.20
23	CW	71	G	N3-C4-N9	5.70	129.42	126.00
25	DA	2155	G	C6-N1-C2	5.70	128.52	125.10
25	BA	840	A	O5'-P-OP2	-5.69	100.58	105.70
25	DA	528	A	C2-N3-C4	-5.69	107.76	110.60
1	CA	1158	C	C2-N1-C1'	5.68	125.05	118.80
23	AW	14	A	N1-C6-N6	5.68	122.01	118.60
25	DA	2129	C	C2-N1-C1'	5.66	125.03	118.80
23	CY	11	C	C2-N3-C4	5.65	122.73	119.90
25	BA	2158	C	C5-C6-N1	5.61	123.80	121.00
25	DA	528	A	P-O3'-C3'	5.60	126.42	119.70
24	CX	17	C	C2-N1-C1'	5.60	124.96	118.80
1	CA	754	C	C6-N1-C1'	-5.59	114.09	120.80
24	AX	46	G	C5-C6-O6	-5.59	125.25	128.60
25	BA	2172	U	C2-N3-C4	-5.58	123.65	127.00
25	DA	614	U	N3-C2-O2	-5.57	118.30	122.20
25	DA	2175	C	C2-N1-C1'	5.57	124.93	118.80
25	BA	139	A	O4'-C1'-N9	5.57	112.65	108.20
25	DA	2897	U	C5-C6-N1	5.57	125.48	122.70
25	BA	1249	A	O4'-C1'-N9	5.56	112.65	108.20
24	AX	14	A	C4-N9-C1'	5.56	136.30	126.30
25	BA	1958	A	O4'-C1'-N9	5.56	112.65	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CW	71	G	C8-N9-C1'	-5.56	119.77	127.00
24	AX	22	G	C5-C6-N1	5.56	114.28	111.50
25	DA	2897	U	N1-C2-O2	5.55	126.69	122.80
25	DA	2321	G	C4-N9-C1'	5.54	133.71	126.50
1	AA	1036	G	C8-N9-C1'	-5.54	119.80	127.00
1	CA	1032	G	N3-C4-N9	-5.53	122.68	126.00
24	AX	14	A	C8-N9-C1'	-5.53	117.74	127.70
1	AA	1531	A	O4'-C1'-N9	-5.53	103.78	108.20
25	BA	553	A	N3-C4-C5	5.53	130.67	126.80
1	CA	1183	A	OP1-P-O3'	5.53	117.36	105.20
25	BA	1067	A	N1-C2-N3	5.52	132.06	129.30
1	CA	1154	G	N3-C2-N2	5.52	123.77	119.90
43	DX	57	LEU	CA-CB-CG	5.52	128.00	115.30
25	DA	1300	U	P-O3'-C3'	5.52	126.32	119.70
23	CY	7	A	O5'-P-OP2	-5.50	100.75	105.70
25	BA	354	A	N3-C4-C5	5.50	130.65	126.80
24	AX	22	G	N7-C8-N9	5.50	115.85	113.10
1	CA	1001(A)	G	N3-C4-C5	-5.49	125.85	128.60
25	BA	215	G	O4'-C1'-N9	5.49	112.59	108.20
25	BA	1006	C	O5'-P-OP2	-5.48	100.76	105.70
1	CA	1154	G	N1-C2-N2	-5.48	111.27	116.20
23	CY	5	G	C5-C6-O6	-5.48	125.31	128.60
1	CA	1286	A	C8-N9-C4	-5.48	103.61	105.80
25	DA	748	G	O4'-C1'-N9	5.47	112.58	108.20
1	CA	79	G	N1-C6-O6	-5.47	116.62	119.90
25	BA	2504	U	O5'-P-OP1	-5.46	100.78	105.70
25	DA	2163	C	C6-N1-C2	-5.46	118.12	120.30
23	CY	22	G	N3-C4-N9	5.46	129.28	126.00
1	CA	1502	A	N1-C2-N3	5.46	132.03	129.30
25	DA	587	C	C2-N1-C1'	5.45	124.80	118.80
25	BA	2054	G	C5-N7-C8	5.45	107.03	104.30
25	DA	2447	G	N3-C4-N9	-5.45	122.73	126.00
1	CA	1003	G	N3-C4-N9	5.44	129.26	126.00
25	BA	254	A	O4'-C1'-N9	5.43	112.55	108.20
1	AA	21	G	O5'-P-OP1	-5.43	100.81	105.70
25	DA	277	C	N3-C2-O2	-5.42	118.11	121.90
23	AW	66	U	C5-C4-O4	5.42	129.15	125.90
25	DA	2139	C	N3-C2-O2	-5.42	118.11	121.90
23	AY	33	U	C6-N1-C1'	-5.41	113.62	121.20
25	DA	1647	G	O4'-C1'-N9	-5.40	103.88	108.20
25	BA	2172	U	N1-C2-N3	5.40	118.14	114.90
23	AY	5	G	N3-C4-N9	5.39	129.23	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1141	C	C2-N1-C1'	-5.38	112.88	118.80
23	CY	11	C	N1-C2-O2	5.38	122.13	118.90
24	CX	20	U	C2-N1-C1'	5.38	124.16	117.70
25	DA	1791	A	O5'-P-OP1	-5.38	100.86	105.70
24	AX	22	G	C4-C5-N7	5.38	112.95	110.80
1	AA	1397	C	O4'-C1'-N1	5.37	112.50	108.20
1	CA	1032	G	C5-C6-O6	5.37	131.82	128.60
25	BA	1700	G	N3-C4-C5	-5.36	125.92	128.60
25	BA	285	U	O4'-C1'-N1	5.36	112.48	108.20
25	BA	831	A	O4'-C1'-N9	5.36	112.48	108.20
1	AA	913	A	P-O3'-C3'	5.35	126.12	119.70
1	AA	115	G	P-O3'-C3'	5.35	126.12	119.70
23	CY	68	C	N1-C2-O2	5.35	122.11	118.90
1	AA	1036	G	N3-C4-C5	-5.34	125.93	128.60
25	BA	989	G	C8-N9-C1'	-5.34	120.06	127.00
1	AA	1158	C	C2-N1-C1'	5.34	124.67	118.80
25	BA	1248	G	C5-C6-O6	-5.33	125.40	128.60
9	CI	102	LEU	CA-CB-CG	5.32	127.54	115.30
1	AA	975	A	O4'-C1'-N9	-5.32	103.95	108.20
25	BA	990	A	C4-C5-N7	5.31	113.35	110.70
25	DA	192	C	O5'-P-OP1	-5.30	100.93	105.70
25	DA	945	A	C2-N3-C4	-5.30	107.95	110.60
1	CA	1003	G	C8-N9-C1'	-5.29	120.12	127.00
25	DA	2140	C	C2-N1-C1'	5.29	124.62	118.80
1	CA	1133	G	N3-C4-N9	-5.29	122.83	126.00
26	DB	2	C	C6-N1-C2	-5.27	118.19	120.30
25	DA	645	C	C6-N1-C1'	-5.27	114.48	120.80
1	AA	1158	C	N1-C2-O2	5.26	122.06	118.90
23	CW	36	A	C6-N1-C2	5.26	121.76	118.60
23	CW	3	C	C5-C6-N1	5.26	123.63	121.00
25	DA	2689	U	P-O3'-C3'	5.25	126.00	119.70
24	CX	22	G	C5-C6-N1	5.25	114.13	111.50
25	DA	2447	G	C6-C5-N7	5.25	133.55	130.40
1	CA	65	U	P-O3'-C3'	5.24	125.99	119.70
1	CA	1154	G	C5-C6-N1	-5.24	108.88	111.50
25	DA	488	G	N1-C6-O6	5.24	123.04	119.90
1	AA	1030(B)	C	O4'-C1'-N1	5.24	112.39	108.20
25	DA	645	C	C5-C6-N1	5.23	123.62	121.00
25	DA	917	A	O5'-P-OP2	-5.23	101.00	105.70
25	BA	2050	U	N3-C2-O2	-5.22	118.54	122.20
1	AA	91	C	C5-C6-N1	5.22	123.61	121.00
1	AA	1067	A	P-O3'-C3'	5.22	125.97	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CW	25	C	O4'-C1'-N1	5.22	112.37	108.20
1	AA	754	C	N1-C2-O2	5.22	122.03	118.90
25	BA	1232	G	C5-C6-O6	5.22	131.73	128.60
1	CA	1141	C	C6-N1-C1'	5.22	127.06	120.80
25	BA	2803	A	C2-N3-C4	5.21	113.21	110.60
25	BA	989	G	C4-N9-C1'	5.21	133.27	126.50
23	CW	71	G	C4-N9-C1'	5.19	133.25	126.50
1	AA	266	G	P-O3'-C3'	5.19	125.92	119.70
12	CL	29	GLY	N-CA-C	-5.18	100.16	113.10
25	BA	572	A	P-O3'-C3'	5.17	125.91	119.70
25	BA	1700	G	C8-N9-C4	-5.16	104.33	106.40
25	BA	1398	U	O5'-P-OP1	-5.16	101.05	105.70
1	AA	687	A	P-O3'-C3'	5.16	125.89	119.70
23	CW	50	U	N3-C4-O4	5.15	123.01	119.40
25	BA	354	A	N3-C4-N9	-5.15	123.28	127.40
25	DA	1352	U	O5'-P-OP1	-5.15	101.07	105.70
25	BA	1738	C	C6-N1-C2	-5.14	118.24	120.30
25	BA	2209	G	P-O3'-C3'	5.14	125.87	119.70
25	DA	2893	G	N3-C4-N9	5.14	129.08	126.00
25	DA	2447	G	C4-N9-C1'	-5.13	119.83	126.50
22	CV	19	U	C5-C4-O4	5.13	128.98	125.90
25	DA	2139	C	C2-N1-C1'	5.13	124.44	118.80
25	BA	990	A	N1-C2-N3	5.12	131.86	129.30
1	CA	1133	G	N9-C4-C5	5.12	107.45	105.40
25	DA	192	C	OP1-P-OP2	5.12	127.28	119.60
25	DA	2110	G	P-O3'-C3'	5.11	125.84	119.70
27	BD	257	LEU	CA-CB-CG	5.11	127.05	115.30
24	CX	20	U	N1-C2-O2	5.11	126.37	122.80
25	DA	2163	C	C5-C6-N1	5.10	123.55	121.00
1	CA	1032	G	C6-C5-N7	5.08	133.45	130.40
26	BB	1	U	P-O3'-C3'	5.07	125.79	119.70
25	BA	2240	G	C5-C6-O6	5.06	131.64	128.60
35	DP	44	GLY	C-N-CA	5.06	134.36	121.70
23	CY	68	C	C2-N1-C1'	5.06	124.37	118.80
25	BA	1067	A	C5-N7-C8	-5.06	101.37	103.90
25	BA	1221	G	P-O3'-C3'	5.05	125.77	119.70
23	CY	58	A	OP1-P-O3'	5.05	116.32	105.20
25	BA	795	G	O4'-C1'-N9	5.05	112.24	108.20
1	AA	1065	U	P-O3'-C3'	5.05	125.76	119.70
25	DA	2593	U	N3-C4-O4	-5.05	115.87	119.40
25	DA	2130	U	C5-C6-N1	5.04	125.22	122.70
25	DA	277	C	C6-N1-C2	-5.04	118.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1027	C	C2-N3-C4	5.04	122.42	119.90
25	BA	2240	G	N1-C6-O6	-5.04	116.88	119.90
25	BA	2459	G	OP2-P-O3'	5.04	116.28	105.20
25	DA	488	G	C5-C6-O6	-5.04	125.58	128.60
25	BA	1235	G	C5-N7-C8	5.03	106.82	104.30
25	BA	2228	G	C4-N9-C1'	5.03	133.04	126.50
25	DA	214	G	O4'-C1'-N9	5.03	112.22	108.20
2	CB	115	LEU	CA-CB-CG	5.03	126.86	115.30
25	BA	892	G	O4'-C1'-N9	5.01	112.21	108.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	9	GLU	Peptide
7	AG	79	ARG	Peptide
50	B4	59	PHE	Peptide
50	B4	67	TYR	Peptide
7	CG	79	ARG	Peptide

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32185	0	16243	436	0
1	CA	32312	0	16307	518	0
2	AB	1846	0	1867	71	0
2	CB	1825	0	1828	83	0
3	AC	1548	0	1535	40	0
3	CC	1542	0	1517	55	0
4	AD	1655	0	1672	48	0
4	CD	1674	0	1714	43	0
5	AE	1129	0	1185	34	0
5	CE	1133	0	1191	38	0
6	AF	810	0	804	18	0
6	CF	816	0	808	12	0
7	AG	1231	0	1238	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	CG	1235	0	1249	32	0
8	AH	1088	0	1126	28	0
8	CH	1088	0	1126	39	0
9	AI	983	0	986	40	0
9	CI	978	0	966	46	0
10	AJ	709	0	650	27	0
10	CJ	714	0	672	36	0
11	AK	829	0	825	12	0
11	CK	833	0	836	10	0
12	AL	930	0	980	15	0
12	CL	930	0	980	23	0
13	AM	958	0	1002	29	0
13	CM	950	0	988	38	0
14	AN	492	0	529	23	0
14	CN	492	0	529	17	0
15	AO	728	0	760	21	0
15	CO	728	0	760	23	0
16	AP	681	0	697	17	0
16	CP	677	0	686	18	0
17	AQ	823	0	891	21	0
17	CQ	823	0	891	14	0
18	AR	555	0	618	18	0
18	CR	555	0	618	17	0
19	AS	652	0	662	27	0
19	CS	646	0	644	29	0
20	AT	728	0	798	17	0
20	CT	727	0	796	21	0
21	AU	199	0	208	4	0
21	CU	199	0	208	5	0
22	AV	277	0	140	1	0
22	CV	277	0	140	6	0
23	AW	1592	0	819	29	0
23	AY	1585	0	804	55	0
23	CW	1544	0	788	39	0
23	CY	1565	0	795	61	0
24	AX	1625	0	828	15	0
24	CX	1625	0	828	19	0
25	BA	61844	0	31181	611	0
25	DA	60314	0	30412	734	0
26	BB	2577	0	1305	15	0
26	DB	2575	0	1303	51	0
27	BD	2136	0	2218	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	DD	2136	0	2218	54	0
28	BE	1559	0	1618	31	0
28	DE	1559	0	1617	38	0
29	BF	1584	0	1625	22	0
29	DF	1580	0	1619	42	0
30	BG	1429	0	1447	25	0
30	DG	1428	0	1438	55	0
31	BH	1330	0	1407	22	0
31	DH	1330	0	1407	41	0
32	BI	1097	0	1140	32	0
32	DI	1064	0	1082	29	0
33	BN	1117	0	1184	16	0
33	DN	1117	0	1184	21	0
34	BO	933	0	996	18	0
34	DO	933	0	996	17	0
35	BP	1135	0	1212	29	0
35	DP	1135	0	1212	47	0
36	BQ	1122	0	1179	20	0
36	DQ	1122	0	1179	31	0
37	BR	968	0	1033	24	0
37	DR	968	0	1033	32	0
38	BS	873	0	927	23	0
38	DS	870	0	923	23	0
39	BT	1091	0	1151	26	0
39	DT	1083	0	1136	21	0
40	BU	959	0	1019	19	0
40	DU	959	0	1019	21	0
41	BV	771	0	830	15	0
41	DV	771	0	830	18	0
42	BW	886	0	940	10	0
42	DW	886	0	940	15	0
43	BX	750	0	814	13	0
43	DX	750	0	814	18	0
44	BY	806	0	881	19	0
44	DY	806	0	881	18	0
45	BZ	1240	0	1240	24	0
45	DZ	1271	0	1273	52	0
46	B0	653	0	674	10	0
46	D0	653	0	674	18	0
47	B1	755	0	826	15	0
47	D1	755	0	826	14	0
48	B2	588	0	643	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	D2	588	0	643	5	0
49	B3	469	0	518	5	0
49	D3	464	0	514	9	0
50	B4	552	0	533	26	0
50	D4	532	0	503	30	0
51	B5	455	0	465	6	0
51	D5	455	0	465	8	0
52	B6	453	0	473	8	0
52	D6	449	0	469	11	0
53	B7	418	0	467	9	0
53	D7	418	0	467	11	0
54	B8	517	0	582	18	0
54	D8	517	0	582	23	0
55	B9	307	0	335	4	0
55	D9	307	0	335	9	0
56	AA	233	0	0	0	0
56	AB	2	0	0	0	0
56	AD	1	0	0	0	0
56	AE	2	0	0	0	0
56	AF	1	0	0	0	0
56	AH	1	0	0	0	0
56	AK	1	0	0	0	0
56	AL	1	0	0	0	0
56	AM	1	0	0	0	0
56	AN	1	0	0	0	0
56	AR	1	0	0	0	0
56	AT	1	0	0	0	0
56	AW	4	0	0	0	0
56	AX	13	0	0	0	0
56	AY	2	0	0	0	0
56	B0	7	0	0	0	0
56	B1	2	0	0	0	0
56	B2	2	0	0	0	0
56	B3	2	0	0	0	0
56	B4	1	0	0	0	0
56	B5	4	0	0	0	0
56	B6	2	0	0	0	0
56	B7	3	0	0	0	0
56	B8	3	0	0	0	0
56	B9	1	0	0	0	0
56	BA	906	0	0	0	0
56	BB	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BD	13	0	0	0	0
56	BE	12	0	0	0	0
56	BF	15	0	0	0	0
56	BG	6	0	0	0	0
56	BH	1	0	0	0	0
56	BI	1	0	0	0	0
56	BN	4	0	0	0	0
56	BO	5	0	0	0	0
56	BP	6	0	0	0	0
56	BQ	7	0	0	0	0
56	BR	3	0	0	0	0
56	BS	3	0	0	0	0
56	BT	2	0	0	0	0
56	BU	10	0	0	0	0
56	BV	5	0	0	0	0
56	BW	5	0	0	0	0
56	BX	6	0	0	0	0
56	BY	3	0	0	0	0
56	BZ	3	0	0	0	0
56	CA	201	0	0	0	0
56	CD	2	0	0	0	0
56	CE	1	0	0	0	0
56	CF	2	0	0	0	0
56	CG	1	0	0	0	0
56	CJ	2	0	0	0	0
56	CK	1	0	0	0	0
56	CL	2	0	0	0	0
56	CP	1	0	0	0	0
56	CQ	2	0	0	0	0
56	CR	1	0	0	0	0
56	CT	1	0	0	0	0
56	CV	1	0	0	0	0
56	CW	4	0	0	0	0
56	CX	6	0	0	0	0
56	D0	1	0	0	0	0
56	D1	1	0	0	0	0
56	D3	1	0	0	0	0
56	D5	2	0	0	0	0
56	D8	2	0	0	0	0
56	DA	673	0	0	0	0
56	DB	21	0	0	0	0
56	DD	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DE	7	0	0	0	0
56	DF	7	0	0	0	0
56	DG	1	0	0	0	0
56	DO	1	0	0	0	0
56	DP	1	0	0	0	0
56	DQ	3	0	0	0	0
56	DR	1	0	0	0	0
56	DT	1	0	0	0	0
56	DU	4	0	0	0	0
56	DV	2	0	0	0	0
56	DW	3	0	0	0	0
56	DX	1	0	0	0	0
56	DY	1	0	0	0	0
56	DZ	1	0	0	0	0
57	AA	30	0	28	1	0
57	CA	30	0	29	1	0
58	AD	8	0	0	0	0
58	CD	8	0	0	0	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
60	CX	1	0	0	0	0
61	AA	264	0	0	16	0
61	AB	1	0	0	0	0
61	AE	2	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	4	0	0	0	0
61	AM	1	0	0	0	0
61	AQ	1	0	0	0	0
61	AV	4	0	0	0	0
61	AW	2	0	0	0	0
61	AX	11	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	AY	1	0	0	0	0
61	B0	8	0	0	0	0
61	B1	3	0	0	0	0
61	B2	4	0	0	2	0
61	B3	3	0	0	0	0
61	B4	1	0	0	0	0
61	B5	4	0	0	0	0
61	B6	1	0	0	0	0
61	B7	4	0	0	1	0
61	B8	8	0	0	0	0
61	BA	1486	0	0	44	0
61	BB	43	0	0	2	0
61	BD	19	0	0	2	0
61	BE	20	0	0	1	0
61	BF	14	0	0	1	0
61	BG	5	0	0	1	0
61	BH	1	0	0	0	0
61	BI	2	0	0	0	0
61	BN	2	0	0	0	0
61	BO	7	0	0	0	0
61	BP	19	0	0	1	0
61	BQ	5	0	0	1	0
61	BR	5	0	0	0	0
61	BS	5	0	0	0	0
61	BT	5	0	0	0	0
61	BU	8	0	0	1	0
61	BV	6	0	0	0	0
61	BW	1	0	0	0	0
61	BX	2	0	0	0	0
61	BY	3	0	0	0	0
61	BZ	1	0	0	0	0
61	CA	204	0	0	12	0
61	CD	1	0	0	0	0
61	CG	1	0	0	1	0
61	CI	1	0	0	0	0
61	CJ	4	0	0	0	0
61	CL	4	0	0	0	0
61	CO	1	0	0	0	0
61	CP	1	0	0	0	0
61	CR	1	0	0	0	0
61	CT	1	0	0	0	0
61	CW	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	CX	6	0	0	0	0
61	D0	4	0	0	0	0
61	D1	4	0	0	1	0
61	D2	1	0	0	0	0
61	D3	1	0	0	0	0
61	D5	2	0	0	0	0
61	D7	5	0	0	0	0
61	D8	5	0	0	0	0
61	D9	1	0	0	0	0
61	DA	1039	0	0	58	0
61	DB	10	0	0	1	0
61	DD	17	0	0	0	0
61	DE	8	0	0	1	0
61	DF	6	0	0	0	0
61	DI	2	0	0	0	0
61	DN	1	0	0	0	0
61	DO	3	0	0	0	0
61	DP	12	0	0	3	0
61	DQ	1	0	0	0	0
61	DR	3	0	0	0	0
61	DT	3	0	0	0	0
61	DU	1	0	0	0	0
61	DV	1	0	0	0	0
61	DW	2	0	0	0	0
61	DX	2	0	0	0	0
61	DY	1	0	0	1	0
61	DZ	2	0	0	0	0
All	All	298643	0	196646	4377	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (4377) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1027:C:N3	1:AA:1034:G:C6	2.18	1.10
1:CA:1002:G:H1	1:CA:1038:C:N4	1.51	1.08
23:AW:6:G:H1	23:AW:67:C:N4	1.49	1.07
1:CA:1028:C:N3	1:CA:1033:G:C6	2.23	1.06
1:AA:78:G:C6	1:AA:91:C:N4	2.29	1.00
1:AA:1027:C:C2	1:AA:1034:G:C6	2.51	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:78:G:HO2'	1:AA:79:G:H8	1.08	0.97
1:CA:1029:C:C4	1:CA:1032:G:N1	2.32	0.97
25:DA:2124:G:H1	25:DA:2174:C:H42	1.12	0.97
23:CW:50:U:H3	23:CW:64:A:N6	1.63	0.97
1:CA:947:G:H1	1:CA:1234:C:H42	0.97	0.96
1:AA:1502:A:H2	1:AA:1505:G:H1	1.12	0.96
25:BA:1065:U:HO2'	25:BA:1067:A:H2	1.06	0.95
25:BA:2121:U:H3	25:BA:2212:G:H1	1.11	0.95
1:CA:1132:C:H42	1:CA:1142:G:H1	1.14	0.95
1:CA:999:C:H42	1:CA:1042:G:H1	1.10	0.95
25:BA:2161:C:H42	25:BA:2174:G:H1	1.13	0.94
23:CW:27:G:H1	23:CW:43:C:H42	1.12	0.93
1:CA:38:G:H22	1:CA:397:A:H5''	1.32	0.93
1:CA:1030(A):G:N2	1:CA:1030(D):A:OP2	2.00	0.93
23:AY:26:A:H61	23:AY:44:G:H1	1.10	0.93
23:AW:26:A:H61	23:AW:44:G:H1	1.02	0.92
25:DA:2121:G:H1	25:DA:2177:C:H42	1.13	0.91
25:BA:2161:C:N4	25:BA:2174:G:H1	1.68	0.91
23:CY:19:G:N2	23:CY:56:C:N3	2.19	0.91
1:AA:78:G:C2	1:AA:91:C:N3	2.39	0.90
25:DA:2807:G:N1	25:DA:2893:G:O6	2.04	0.90
13:CM:122:LYS:HD3	13:CM:123:ALA:H	1.37	0.89
55:D9:25:VAL:HB	55:D9:34:GLN:HB2	1.55	0.89
26:DB:7:G:H21	38:DS:38:GLN:HE22	1.20	0.89
1:CA:1002:G:N2	1:CA:1038:C:N3	2.20	0.89
1:AA:96:U:HO2'	1:AA:97:G:H8	1.18	0.88
25:BA:2146:G:H1	25:BA:2196:C:H42	1.15	0.88
42:BW:14:PRO:HG2	42:BW:78:GLU:HG2	1.54	0.88
1:CA:947:G:H1	1:CA:1234:C:N4	1.70	0.88
23:CW:50:U:H3	23:CW:64:A:H61	0.89	0.88
7:AG:72:ARG:HG3	7:AG:72:ARG:HH11	1.35	0.88
25:DA:1689:A:H62	25:DA:1698:A:H2	1.22	0.88
25:BA:2143:G:H1	25:BA:2199:C:H42	1.16	0.88
42:DW:14:PRO:HG2	42:DW:78:GLU:HG2	1.57	0.87
1:CA:1353:G:OP1	21:CU:10:ARG:NH1	2.07	0.87
23:CY:29:G:H1	23:CY:41:C:H42	1.23	0.87
46:B0:11:ARG:O	46:B0:14:ARG:NH2	2.07	0.87
25:BA:2158:C:N4	25:BA:2177:G:N1	2.22	0.87
6:CF:81:ILE:HD11	27:DD:125:ILE:HB	1.55	0.87
25:DA:1315:C:OP2	61:DA:4472:HOH:O	1.90	0.87
25:BA:1829:U:H5'	27:BD:259:THR:HG22	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:16:HIS:HB2	2:CB:204:ASN:HB3	1.57	0.86
1:CA:656:C:O2'	15:CO:28:GLN:NE2	2.07	0.86
15:CO:54:ARG:NH1	15:CO:58:MET:SD	2.48	0.86
1:CA:999:C:N4	1:CA:1042:G:H1	1.73	0.86
25:DA:900:A:H2'	25:DA:901:A:H8	1.39	0.86
2:CB:18:GLY:HA2	2:CB:42:ILE:HG13	1.55	0.86
1:AA:1008:C:N4	1:AA:1021:G:N1	2.22	0.86
7:AG:72:ARG:NH1	7:AG:142:GLU:OE2	2.08	0.86
43:BX:31:HIS:HD2	43:BX:33:LYS:H	1.24	0.85
1:AA:1008:C:N3	1:AA:1021:G:N2	2.23	0.85
3:CC:41:GLY:O	3:CC:45:LYS:NZ	2.09	0.85
25:DA:2141:G:O6	25:DA:2150:U:O2	1.95	0.85
5:CE:143:ARG:NH1	8:CH:77:GLU:OE1	2.09	0.85
23:AY:26:A:N6	23:AY:44:G:H1	1.75	0.85
23:AW:26:A:N6	23:AW:44:G:H1	1.74	0.85
25:DA:2139:C:N4	25:DA:2152:G:H1	1.75	0.85
25:DA:948:G:OP1	61:DA:4588:HOH:O	1.94	0.84
44:BY:92:ASN:HB3	44:BY:94:LYS:H	1.43	0.84
25:BA:2331:G:H22	38:BS:3:ARG:HE	1.22	0.84
28:DE:72:VAL:HG13	28:DE:73:GLU:HG3	1.59	0.84
5:CE:100:VAL:O	5:CE:107:ARG:NH2	2.10	0.83
1:CA:1003:G:N2	1:CA:1025:U:O4	2.11	0.83
25:DA:2139:C:N4	25:DA:2152:G:N1	2.26	0.83
1:CA:1360:A:OP2	14:CN:35:ARG:NH2	2.12	0.83
1:CA:1029:C:N3	1:CA:1032:G:N2	2.27	0.83
1:CA:1502:A:H2	1:CA:1505:G:H1	1.27	0.82
25:BA:1114:G:N2	25:BA:1141:A:O2'	2.11	0.82
1:AA:1027:C:C2	1:AA:1034:G:N1	2.47	0.82
25:BA:2299:A:H62	25:BA:2356:U:H3	1.27	0.82
45:DZ:46:LYS:O	45:DZ:50:GLN:NE2	2.11	0.81
1:CA:1028:C:C2	1:CA:1033:G:C6	2.68	0.81
23:CY:26:A:N1	23:CY:44:G:C6	2.48	0.81
25:BA:2158:C:N3	25:BA:2177:G:N2	2.29	0.81
38:DS:38:GLN:NE2	38:DS:47:THR:OG1	2.13	0.81
25:DA:1568:G:N7	61:DA:5002:HOH:O	2.13	0.81
25:DA:2139:C:N3	25:DA:2152:G:N2	2.28	0.81
1:AA:1314:C:OP2	19:AS:4:SER:OG	1.98	0.81
25:BA:181:C:OP1	61:BA:4160:HOH:O	1.97	0.80
35:BP:126:VAL:HG12	35:BP:148:LEU:HD22	1.63	0.80
1:CA:1002:G:H1	1:CA:1038:C:H42	0.83	0.80
1:CA:953:G:H5'	1:CA:965:A:H61	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1060:U:OP2	61:BA:5368:HOH:O	1.99	0.80
25:BA:2044:U:OP1	61:BA:4800:HOH:O	1.97	0.80
1:CA:1003:G:O6	1:CA:1035:A:N6	2.13	0.80
43:DX:31:HIS:HD2	43:DX:33:LYS:H	1.30	0.80
1:AA:1189:C:OP1	10:AJ:51:ARG:NH2	2.14	0.80
25:BA:2015:U:OP2	61:BA:5459:HOH:O	1.99	0.80
20:AT:86:ARG:O	20:AT:90:GLN:NE2	2.15	0.80
23:AY:50:U:O4	23:AY:64:A:N1	2.13	0.80
17:AQ:26:GLN:HG2	17:AQ:37:LYS:HG2	1.63	0.80
25:DA:1973:G:OP1	61:DA:4547:HOH:O	1.99	0.80
2:AB:16:HIS:HB2	2:AB:204:ASN:HB3	1.63	0.80
25:BA:1736:A:H62	25:BA:1745:A:H2	1.29	0.80
2:AB:16:HIS:CG	2:AB:17:PHE:H	1.99	0.80
25:BA:1111:U:O2	25:BA:1119:A:N6	2.14	0.80
25:DA:2287:A:H62	25:DA:2344:U:H3	1.28	0.80
25:BA:542:C:OP1	51:B5:16:ARG:NH2	2.15	0.80
1:AA:38:G:H22	1:AA:397:A:H5''	1.47	0.80
10:AJ:35:SER:HB3	10:AJ:73:ASP:HB2	1.63	0.80
25:DA:2206:G:H3'	25:DA:2207:G:C8	2.17	0.80
25:DA:1798:U:OP2	27:DD:274:ARG:NH2	2.14	0.79
25:DA:1648:C:OP1	61:DA:4516:HOH:O	1.98	0.79
23:AW:6:G:N2	23:AW:67:C:N3	2.28	0.79
1:AA:1002:G:H3'	1:AA:1003:G:O4'	1.83	0.79
1:AA:1414:U:H3	1:AA:1486:G:H1	1.31	0.79
45:BZ:139:VAL:HG22	45:BZ:155:LEU:HD11	1.64	0.79
1:CA:1029:C:N4	1:CA:1032:G:N1	2.31	0.79
1:AA:1025:U:O2	1:AA:1036:G:O6	1.99	0.79
25:DA:900:A:H2'	25:DA:901:A:C8	2.18	0.79
1:AA:975:A:H4'	1:AA:976:G:H5''	1.63	0.79
25:DA:2683:C:OP1	39:DT:53:ARG:NH2	2.16	0.79
24:AX:6:G:H1	24:AX:67:C:H42	1.28	0.79
1:CA:992:U:H3	1:CA:1044:A:H62	1.26	0.79
1:CA:522:C:H41	12:CL:53:ARG:HH22	1.30	0.79
30:DG:80:PHE:O	30:DG:82:LEU:N	2.16	0.79
1:AA:997:U:H3	1:AA:1044:A:H61	1.28	0.78
25:DA:994:C:OP1	40:DU:53:ARG:NH2	2.15	0.78
25:BA:894:U:OP2	61:BA:4554:HOH:O	2.01	0.78
23:CW:27:G:H1	23:CW:43:C:N4	1.80	0.78
1:AA:511:C:OP2	4:AD:49:ARG:NH1	2.16	0.78
11:AK:48:ILE:HD12	11:AK:63:LEU:HB2	1.65	0.78
46:B0:10:THR:HG22	46:B0:12:ASN:H	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2158:C:N4	25:BA:2177:G:C6	2.52	0.78
1:CA:1422:G:H5''	34:DO:48:PRO:HB3	1.64	0.78
23:CY:5:G:H1	23:CY:68:C:H42	1.28	0.78
1:AA:1027:C:O2	1:AA:1034:G:C2	2.36	0.78
1:CA:346:G:OP1	39:DT:41:ARG:NH2	2.16	0.78
26:DB:92:C:OP1	45:DZ:79:ARG:NH1	2.16	0.78
1:CA:742:G:OP2	15:CO:35:ARG:NH2	2.17	0.78
25:DA:1449:A:O2'	25:DA:1529:G:N2	2.17	0.78
25:BA:1059:C:OP2	61:BA:5368:HOH:O	2.00	0.78
25:DA:963:U:OP2	61:DA:4588:HOH:O	2.02	0.78
36:DQ:22:LYS:HD3	36:DQ:23:GLY:N	1.98	0.78
24:CX:6:G:H1	24:CX:67:C:H42	1.30	0.77
25:DA:1171:G:H1	25:DA:1178:C:H42	1.29	0.77
36:DQ:26:TYR:O	36:DQ:67:ARG:NH1	2.16	0.77
25:DA:301:G:OP2	44:DY:84:ARG:NH2	2.18	0.77
1:AA:1182:G:H4'	1:AA:1183:A:H5'	1.66	0.77
11:CK:99:GLN:HG2	11:CK:105:VAL:HG21	1.66	0.77
1:AA:1086:U:H3	1:AA:1099:G:H22	1.32	0.77
25:BA:2145:G:H1	25:BA:2197:C:H42	1.32	0.77
25:DA:2121:G:H1	25:DA:2177:C:N4	1.82	0.77
42:DW:2:GLU:OE2	42:DW:72:LYS:NZ	2.17	0.77
45:DZ:72:ARG:NH2	45:DZ:97:GLU:O	2.17	0.77
23:AY:26:A:N6	23:AY:44:G:N1	2.28	0.77
25:BA:693:G:O6	25:BA:697:C:N4	2.15	0.77
23:CY:26:A:N1	23:CY:44:G:O6	2.18	0.77
25:DA:2124:G:H1	25:DA:2174:C:N4	1.83	0.77
2:AB:16:HIS:CD2	2:AB:17:PHE:H	2.02	0.77
9:AI:9:ARG:HG2	9:AI:14:VAL:HG12	1.66	0.77
25:BA:239:G:OP2	54:B8:13:ARG:NH2	2.17	0.77
25:BA:1249:A:H2	25:BA:1287:A:H62	1.31	0.77
1:CA:148:G:H2'	1:CA:149:A:H8	1.49	0.77
1:AA:1352:C:OP1	21:AU:3:LYS:NZ	2.17	0.77
1:AA:1422:G:H5''	34:BO:48:PRO:HB3	1.67	0.77
2:AB:155:LEU:HD21	2:AB:159:PRO:HG3	1.67	0.77
23:CW:4:C:N3	23:CW:69:G:N2	2.33	0.77
1:CA:975:A:H4'	1:CA:976:G:H5''	1.67	0.77
36:BQ:111:GLU:OE1	36:BQ:133:ARG:NH2	2.18	0.77
1:AA:116:A:OP1	61:AA:4254:HOH:O	2.02	0.76
1:AA:78:G:C2	1:AA:91:C:C4	2.73	0.76
1:CA:427:U:OP1	4:CD:13:ARG:NH2	2.18	0.76
1:AA:742:G:OP2	15:AO:35:ARG:NH2	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:78:G:N1	1:AA:91:C:C4	2.53	0.76
2:AB:69:LEU:HB3	2:AB:162:ILE:HG22	1.65	0.76
25:BA:2146:G:H1	25:BA:2196:C:N4	1.83	0.76
26:DB:4:C:H42	26:DB:117:G:H1	1.33	0.76
25:BA:656:A:OP1	35:BP:65:ARG:NH1	2.19	0.76
23:CY:19:G:N1	23:CY:56:C:N4	2.34	0.76
45:BZ:154:ASP:N	45:BZ:154:ASP:OD1	2.19	0.76
25:DA:1798:U:H5'	27:DD:259:THR:HG22	1.68	0.76
25:DA:2122:U:O4	25:DA:2176:A:N1	2.18	0.76
4:CD:98:GLU:OE1	4:CD:103:ASN:ND2	2.16	0.76
25:DA:7:G:N2	25:DA:2896:C:O2	2.14	0.76
1:CA:1329:A:H5''	13:CM:26:GLY:H	1.51	0.76
2:CB:88:ALA:HB1	2:CB:222:ILE:HD11	1.67	0.76
4:CD:165:MET:SD	4:CD:168:ARG:NH1	2.58	0.76
9:CI:117:HIS:HB2	9:CI:121:ARG:HG2	1.68	0.76
25:DA:2112:G:N7	25:DA:2169:A:N6	2.33	0.76
1:CA:158:G:N2	1:CA:163:C:O2	2.19	0.75
25:BA:2144:U:O4	25:BA:2198:A:N1	2.19	0.75
38:BS:25:ARG:NH1	38:BS:42:ASP:OD1	2.19	0.75
13:CM:58:GLU:O	13:CM:62:ASN:ND2	2.18	0.75
25:DA:990:A:OP2	61:DA:4499:HOH:O	2.04	0.75
2:AB:201:ILE:HG21	2:AB:214:ILE:HG21	1.68	0.75
2:AB:185:ILE:HG22	2:AB:199:TYR:HB2	1.67	0.75
13:CM:3:ARG:NH2	13:CM:9:ILE:O	2.18	0.75
25:DA:397:G:N7	61:DA:4914:HOH:O	2.18	0.75
25:BA:2157:A:N6	25:BA:2178:G:O2'	2.20	0.75
1:CA:1029:C:C2	1:CA:1032:G:N2	2.55	0.75
1:CA:1256:A:N6	1:CA:1278:U:O2	2.20	0.75
8:CH:51:VAL:HG21	8:CH:60:ARG:HB2	1.67	0.75
9:CI:7:THR:O	9:CI:83:ARG:NH1	2.20	0.75
23:CY:18:G:N2	23:CY:55:PSU:N3	2.34	0.75
30:DG:115:ARG:HD2	30:DG:136:ARG:HH21	1.51	0.75
45:BZ:72:ARG:NH2	45:BZ:97:GLU:O	2.20	0.74
40:DU:76:TYR:OH	40:DU:92:ARG:NH1	2.19	0.74
1:CA:1132:C:N4	1:CA:1142:G:H1	1.86	0.74
43:DX:11:PRO:HB3	43:DX:92:LEU:HD11	1.69	0.74
1:AA:583:A:OP2	61:AA:4028:HOH:O	2.05	0.74
53:B7:34:ARG:NH1	53:B7:41:ARG:O	2.20	0.74
23:AW:5:G:H2'	23:AW:6:G:C8	2.22	0.74
1:CA:504:C:OP1	61:CA:4006:HOH:O	2.05	0.74
25:DA:2849:U:OP2	39:DT:95:ARG:NH1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:928:G:H3'	25:BA:929:G:H8	1.53	0.74
1:AA:1183:A:H3'	1:AA:1184:G:H5''	1.68	0.74
23:AY:19:G:N2	23:AY:56:C:N3	2.36	0.74
25:BA:2736:C:OP1	37:BR:3:HIS:ND1	2.19	0.74
1:CA:1301:U:O2'	1:CA:1302:U:H5'	1.88	0.74
1:CA:922:G:H4'	5:CE:20:GLN:HA	1.69	0.74
22:CV:23:A:H4'	22:CV:24:A:H5'	1.70	0.74
25:DA:2646:C:OP2	25:DA:2732:G:O2'	2.06	0.74
25:BA:2143:G:H1	25:BA:2199:C:N4	1.85	0.74
25:BA:325:G:OP2	44:BY:84:ARG:NH2	2.21	0.74
13:CM:13:LYS:HA	13:CM:44:ARG:HH11	1.53	0.74
25:DA:1019:U:H3	25:DA:1142(A):A:H62	1.36	0.74
25:BA:2251:G:OP2	61:BA:4474:HOH:O	2.06	0.73
40:BU:104:GLN:NE2	61:BU:308:HOH:O	2.20	0.73
1:AA:90:U:H2'	1:AA:91:C:H5''	1.68	0.73
3:AC:153:VAL:HG22	3:AC:198:VAL:HG12	1.70	0.73
31:BH:86:GLU:OE2	31:BH:132:ARG:NH2	2.20	0.73
25:BA:1296:G:OP2	35:BP:21:ARG:NH1	2.21	0.73
1:CA:860:A:OP2	61:CA:4160:HOH:O	2.04	0.73
13:CM:107:ALA:HB3	13:CM:111:LYS:HD2	1.68	0.73
1:AA:1027:C:C4	1:AA:1034:G:O6	2.40	0.73
25:BA:1185:C:O3'	33:BN:25:ARG:NH1	2.21	0.73
10:CJ:11:PHE:HE1	10:CJ:67:THR:HG22	1.52	0.73
23:CY:51:U:H3	23:CY:63:G:H1	1.36	0.73
1:AA:953:G:H5'	1:AA:965:A:H61	1.52	0.73
25:BA:2161:C:N3	25:BA:2174:G:N2	2.36	0.73
1:CA:1279:A:O2'	1:CA:1281:U:OP2	2.06	0.73
25:DA:1800:C:OP2	27:DD:183:ARG:NH2	2.20	0.73
33:DN:128:HIS:O	33:DN:131:GLN:NE2	2.21	0.73
36:DQ:27:VAL:O	36:DQ:29:PHE:N	2.19	0.73
1:CA:1029:C:N4	1:CA:1032:G:C6	2.57	0.73
5:AE:74:GLY:HA3	5:AE:116:THR:HG22	1.71	0.73
25:DA:2407:G:OP1	61:DA:4203:HOH:O	2.07	0.73
1:CA:582:U:OP1	15:CO:68:ARG:NH2	2.20	0.73
2:AB:115:LEU:HD13	2:AB:145:LEU:HB3	1.71	0.73
1:CA:21:G:OP1	61:CA:4063:HOH:O	2.06	0.73
1:AA:1238:A:OP2	61:AA:4170:HOH:O	2.06	0.73
47:D1:50:ARG:HG2	47:D1:59:THR:HG22	1.70	0.73
25:DA:962:G:OP1	61:DA:4588:HOH:O	2.06	0.73
45:DZ:146:ILE:HG13	45:DZ:174:VAL:HG12	1.70	0.73
23:CY:29:G:H1	23:CY:41:C:N4	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:8:ILE:HG23	3:AC:16:ARG:HG2	1.71	0.72
17:AQ:66:SER:O	17:AQ:70:ARG:NH1	2.21	0.72
1:CA:770:C:OP1	61:CA:4118:HOH:O	2.06	0.72
25:DA:2116:G:N2	25:DA:2162:G:OP1	2.22	0.72
25:DA:467:G:OP1	53:D7:33:ARG:NH1	2.22	0.72
25:BA:1361:C:OP2	61:BA:4787:HOH:O	2.07	0.72
16:CP:52:ASP:O	16:CP:54:GLU:N	2.22	0.72
26:DB:75:G:N2	45:DZ:87:ASP:OD1	2.21	0.72
1:AA:376:G:H5''	16:AP:5:ARG:HG2	1.71	0.72
25:BA:2153:G:H5''	25:BA:2154:U:H3'	1.70	0.72
26:BB:106:G:H5'	45:BZ:31:ARG:HG2	1.68	0.72
20:CT:57:ARG:HH22	20:CT:100:ILE:HD12	1.50	0.72
25:DA:649:G:H4'	54:D8:46:ARG:HH22	1.54	0.72
25:DA:1314:C:OP1	61:DA:4472:HOH:O	2.07	0.72
25:BA:2802:C:O2	25:BA:2903:G:N1	2.18	0.72
28:DE:111:ARG:HB3	37:DR:1:MET:HE1	1.70	0.72
1:AA:1027:C:N3	1:AA:1034:G:C5	2.57	0.72
1:CA:1244:C:H42	1:CA:1293:G:H1	1.37	0.72
1:AA:1423:G:OP1	34:BO:49:ARG:NH2	2.16	0.72
25:BA:1312:G:O5'	42:BW:15:ARG:NH2	2.23	0.72
39:BT:95:ARG:HH11	39:BT:95:ARG:HG2	1.54	0.72
25:DA:2788:C:OP1	28:DE:61:ARG:NH2	2.22	0.72
29:DF:53:THR:HG23	29:DF:55:GLY:H	1.55	0.72
34:DO:35:VAL:HG11	34:DO:103:ALA:HB3	1.70	0.72
35:DP:96:THR:H	35:DP:99:LEU:HD21	1.55	0.72
1:AA:677:U:H3	1:AA:713:G:H22	1.38	0.72
12:CL:57:LYS:NZ	12:CL:65:GLU:OE2	2.21	0.72
25:DA:652(C):G:N2	25:DA:652(V):C:O2	2.17	0.72
1:AA:572:A:OP1	61:AA:4111:HOH:O	2.08	0.72
25:DA:125:G:H5'	53:D7:14:LYS:HD2	1.72	0.72
1:AA:78:G:N2	1:AA:91:C:N3	2.38	0.72
1:AA:427:U:OP1	4:AD:13:ARG:NH2	2.23	0.72
7:AG:79:ARG:HB3	7:AG:80:VAL:HG22	1.72	0.71
53:B7:24:THR:HG22	53:B7:27:GLY:H	1.55	0.71
1:AA:1103:C:OP1	2:AB:96:ARG:NH2	2.23	0.71
13:AM:84:ILE:HG13	13:AM:85:GLY:HA2	1.72	0.71
23:AY:26:A:N1	23:AY:44:G:N2	2.38	0.71
26:BB:25:A:OP2	61:BB:3142:HOH:O	2.08	0.71
9:CI:53:VAL:O	9:CI:55:ALA:N	2.22	0.71
25:DA:1171:G:N2	25:DA:1178:C:N3	2.34	0.71
25:DA:2033:A:OP1	61:DA:4237:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DH:84:SER:HB3	31:DH:132:ARG:HH11	1.55	0.71
35:DP:44:GLY:O	61:DP:301:HOH:O	2.07	0.71
1:AA:346:G:OP2	39:BT:41:ARG:NH2	2.22	0.71
50:D4:44:THR:O	50:D4:46:GLN:N	2.23	0.71
25:DA:1968:G:OP1	61:DA:4546:HOH:O	2.08	0.71
25:BA:1829:U:OP2	27:BD:274:ARG:NH2	2.24	0.71
16:CP:28:ARG:NH1	16:CP:29:ASP:OD1	2.24	0.71
25:DA:2135:A:H5'	25:DA:2159:G:O2'	1.90	0.71
25:DA:528:A:O2'	25:DA:529:A:H5''	1.90	0.71
1:AA:1183:A:O2'	1:AA:1184:G:OP1	2.08	0.71
24:AX:76:A:OP2	61:AX:3103:HOH:O	2.07	0.71
25:BA:572:A:O2'	25:BA:573:G:OP1	2.06	0.71
47:D1:51:VAL:HG11	47:D1:74:VAL:HG21	1.73	0.71
34:BO:35:VAL:HG11	34:BO:103:ALA:HB3	1.72	0.71
45:BZ:153:SER:HB3	45:BZ:167:PRO:HB3	1.71	0.71
25:BA:1360:C:OP1	61:BA:4787:HOH:O	2.07	0.71
2:CB:201:ILE:HG21	2:CB:214:ILE:HG21	1.73	0.71
15:CO:4:THR:OG1	15:CO:7:GLU:OE1	2.08	0.71
1:CA:64:G:H4'	1:CA:65:U:H3'	1.72	0.71
25:DA:2135:A:H61	25:DA:2157:G:N2	1.89	0.71
25:DA:2805:G:H2'	25:DA:2807:G:C8	2.25	0.71
30:DG:161:THR:HG22	30:DG:163:ALA:H	1.56	0.71
25:BA:71:U:OP1	61:BA:4786:HOH:O	2.08	0.71
13:CM:4:ILE:HG23	13:CM:5:ALA:H	1.55	0.71
31:DH:33:LEU:HD21	31:DH:136:ILE:HB	1.73	0.71
1:CA:664:G:H22	1:CA:741:G:H1	1.38	0.70
30:BG:125:PHE:O	61:BG:4004:HOH:O	2.09	0.70
1:CA:1314:C:OP2	19:CS:4:SER:OG	2.07	0.70
7:CG:136:LYS:NZ	7:CG:139:GLU:OE2	2.24	0.70
4:AD:122:ARG:HH21	4:AD:134:ASP:HB3	1.56	0.70
1:CA:1028:C:C4	1:CA:1033:G:O6	2.44	0.70
1:CA:1029:C:C4	1:CA:1032:G:C2	2.80	0.70
25:DA:2116:G:N7	25:DA:2166:G:N2	2.39	0.70
25:DA:2592:G:OP1	61:DA:4546:HOH:O	2.09	0.70
25:DA:775:G:O3'	61:DA:4554:HOH:O	2.08	0.70
3:AC:40:ARG:NH2	3:AC:55:VAL:O	2.23	0.70
7:AG:111:ARG:NH1	7:AG:113:GLU:OE2	2.21	0.70
25:BA:1151:U:H2'	25:BA:1152:G:H8	1.55	0.70
1:CA:1163:C:H42	1:CA:1173:G:H1	1.40	0.70
7:CG:80:VAL:HB	7:CG:85:TYR:HE2	1.57	0.70
25:DA:411:G:OP1	61:DA:4203:HOH:O	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1027:C:O2	1:AA:1034:G:N1	2.24	0.70
8:AH:41:ARG:NH2	8:AH:123:GLU:OE2	2.23	0.70
13:AM:58:GLU:O	13:AM:62:ASN:ND2	2.23	0.70
54:B8:33:ASN:HA	54:B8:36:LYS:HD2	1.74	0.70
32:BI:92:VAL:HG13	32:BI:120:ILE:HB	1.74	0.70
1:CA:1129:C:H42	1:CA:1143:G:H1	1.40	0.70
1:AA:1348:U:H4'	9:AI:120:ARG:HD2	1.73	0.70
2:CB:47:THR:HA	2:CB:202:PRO:HG2	1.74	0.70
10:CJ:52:GLY:O	14:CN:41:ARG:NH2	2.24	0.70
25:DA:1204:A:H2	25:DA:1241:A:H62	1.38	0.70
1:AA:664:G:H22	1:AA:741:G:H1	1.36	0.70
2:CB:120:ALA:O	2:CB:122:PHE:N	2.21	0.70
13:CM:39:ILE:HD12	13:CM:52:GLU:HG2	1.73	0.70
25:DA:958:U:OP2	36:DQ:14:ARG:NH1	2.24	0.70
45:DZ:92:SER:O	45:DZ:130:PRO:HG3	1.91	0.70
1:AA:78:G:N1	1:AA:91:C:N4	2.39	0.70
14:AN:47:LEU:HA	14:AN:50:LYS:HZ2	1.56	0.70
16:AP:51:VAL:HG12	16:AP:53:VAL:H	1.57	0.70
25:BA:2255:U:OP1	61:BA:4160:HOH:O	2.09	0.70
1:CA:1151:A:HO2'	1:CA:1152:A:H8	1.37	0.70
25:DA:1815:A:OP2	27:DD:54:ARG:NH2	2.24	0.70
29:DF:184:TYR:CE2	29:DF:188:ARG:HD2	2.27	0.70
1:AA:1008:C:C4	1:AA:1021:G:N1	2.60	0.70
25:BA:2518:U:OP1	28:BE:144:ARG:NH2	2.25	0.70
8:CH:69:ARG:NH2	8:CH:75:ARG:O	2.23	0.70
1:CA:1148:U:O2'	9:CI:66:ARG:NH2	2.25	0.70
31:DH:17:VAL:HG13	31:DH:26:VAL:HG22	1.72	0.70
13:AM:3:ARG:HD2	13:AM:9:ILE:HG12	1.74	0.69
15:CO:25:THR:HG21	15:CO:70:LEU:HB2	1.74	0.69
25:DA:831:G:O2'	35:DP:38:GLN:NE2	2.24	0.69
1:CA:677:U:H3	1:CA:713:G:H22	1.39	0.69
1:CA:1104:G:O3'	2:CB:111:ARG:NH2	2.25	0.69
6:AF:99:ALA:HB3	18:AR:29:PHE:HE1	1.57	0.69
25:BA:1040:C:OP1	40:BU:53:ARG:NH2	2.24	0.69
25:BA:431:C:H4'	25:BA:432:U:H5''	1.74	0.69
1:CA:1024:G:H2'	1:CA:1025:U:H5''	1.73	0.69
10:CJ:17:ASP:OD1	10:CJ:70:ARG:NH1	2.26	0.69
25:DA:1342:A:OP2	61:DA:4187:HOH:O	2.10	0.69
35:DP:52:GLU:OE1	35:DP:55:ARG:NH1	2.24	0.69
1:CA:1027:C:C2	1:CA:1034:G:N1	2.57	0.69
30:DG:5:VAL:HG22	30:DG:8:LYS:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AX:20:U:H5''	24:AX:21:A:OP2	1.92	0.69
1:CA:1228:C:OP2	13:CM:108:ARG:NH2	2.20	0.69
25:DA:741:G:OP2	61:DA:4523:HOH:O	2.11	0.69
1:AA:1008:C:N4	1:AA:1021:G:C6	2.61	0.69
25:BA:1116:A:N7	25:BA:1142:A:O2'	2.24	0.69
39:BT:16:ARG:NH2	39:BT:83:ILE:O	2.26	0.69
18:AR:38:GLU:HA	18:AR:41:LYS:HD3	1.74	0.69
25:BA:1648:U:O4	61:BA:4373:HOH:O	2.08	0.69
25:BA:2227:G:H3'	25:BA:2228:G:C8	2.28	0.69
25:BA:271:U:H1'	32:BI:50:ARG:NH1	2.08	0.69
39:BT:24:PRO:HA	39:BT:49:VAL:HG22	1.73	0.69
1:CA:1159:U:O4'	1:CA:1182:G:N2	2.26	0.69
25:DA:1378:A:OP1	53:D7:10:ARG:NH2	2.26	0.69
16:AP:52:ASP:O	16:AP:54:GLU:N	2.26	0.69
25:BA:1151:U:H2'	25:BA:1152:G:C8	2.28	0.69
25:BA:1378:G:OP1	61:BA:4787:HOH:O	2.10	0.69
9:CI:128:ARG:NH2	24:CX:33:U:OP2	2.26	0.69
25:DA:1310:G:OP2	53:D7:9:ARG:NH1	2.25	0.69
27:DD:71:ASP:HB3	27:DD:103:ARG:HH22	1.57	0.69
23:AY:28:G:H1	23:AY:42:C:H42	1.40	0.69
45:BZ:52:SER:OG	45:BZ:53:ILE:N	2.26	0.69
23:CW:4:C:N4	23:CW:69:G:N1	2.40	0.69
25:DA:2148:G:H2'	25:DA:2149:G:C8	2.28	0.69
25:BA:2801:C:OP1	28:BE:61:ARG:NH2	2.25	0.69
55:B9:25:VAL:HB	55:B9:34:GLN:HB2	1.75	0.68
25:BA:331:G:H21	25:BA:354:A:H62	1.41	0.68
25:DA:1030:G:OP2	36:DQ:128:LYS:NZ	2.26	0.68
25:DA:908:C:P	36:DQ:22:LYS:HD2	2.32	0.68
9:AI:26:VAL:HG13	9:AI:61:ALA:HB3	1.76	0.68
25:BA:2289:G:OP2	46:B0:10:THR:HG21	1.93	0.68
18:CR:32:ARG:HA	18:CR:69:THR:HG21	1.75	0.68
25:DA:2327:A:H2'	25:DA:2328:A:C8	2.28	0.68
36:BQ:18:LYS:O	36:BQ:98:LYS:NZ	2.21	0.68
1:AA:559:A:OP1	5:AE:126:ARG:NH2	2.25	0.68
25:BA:1001:G:OP2	36:BQ:14:ARG:NH2	2.23	0.68
27:BD:71:ASP:HB3	27:BD:103:ARG:HH22	1.59	0.68
1:CA:1010:G:N2	1:CA:1020:U:H1'	2.09	0.68
1:CA:539:A:OP2	12:CL:115:LYS:NZ	2.26	0.68
47:D1:21:ARG:HD3	47:D1:35:THR:HG21	1.74	0.68
1:AA:346:G:H3'	1:AA:347:G:H4'	1.75	0.68
35:BP:98:GLU:OE2	35:BP:102:ARG:NH1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DQ:110:THR:HG23	36:DQ:113:GLN:HB2	1.76	0.68
1:AA:310:G:OP2	16:AP:27:LYS:NZ	2.27	0.68
23:CY:7:A:H61	23:CY:66:U:H3	1.42	0.68
45:DZ:27:VAL:HG12	45:DZ:85:HIS:HE1	1.58	0.68
1:CA:1010:G:H2'	1:CA:1011:G:H8	1.59	0.68
25:DA:81:G:N7	61:DA:4466:HOH:O	2.25	0.68
23:AY:50:U:N3	23:AY:64:A:C2	2.62	0.68
25:DA:2447:G:OP2	61:DA:4723:HOH:O	2.10	0.68
41:DV:6:LYS:HB2	41:DV:38:LEU:HD21	1.74	0.68
25:BA:1039:G:OP1	40:BU:50:ARG:NH2	2.26	0.68
25:BA:1044:C:OP1	61:BA:4797:HOH:O	2.11	0.68
25:BA:1067:A:H62	25:BA:1186:U:H3	1.41	0.68
25:BA:2209:G:O2'	25:BA:2210:C:OP1	2.10	0.68
32:BI:72:LEU:O	32:BI:74:ASN:N	2.27	0.68
1:CA:1152:A:H5'	10:CJ:13:HIS:HB2	1.75	0.68
10:CJ:44:VAL:HG13	10:CJ:66:ARG:HG2	1.75	0.68
25:DA:1452:A:OP2	61:DA:4788:HOH:O	2.12	0.68
1:AA:812:C:N3	61:AA:4053:HOH:O	2.27	0.67
25:DA:2028:U:O4	61:DA:4237:HOH:O	2.10	0.67
25:BA:1846:A:N1	61:BA:4024:HOH:O	2.27	0.67
27:BD:108:PRO:HB3	27:BD:143:HIS:CE1	2.29	0.67
35:BP:42:SER:O	61:BP:303:HOH:O	2.10	0.67
1:CA:1189:C:OP1	10:CJ:51:ARG:NH2	2.27	0.67
31:DH:104:GLU:HG3	31:DH:114:VAL:HG22	1.75	0.67
1:AA:347:G:H2'	1:AA:348:G:H8	1.60	0.67
36:BQ:14:ARG:HG2	36:BQ:41:TRP:HH2	1.57	0.67
1:CA:1312:G:H5'	19:CS:5:LEU:HD21	1.77	0.67
35:DP:100:LEU:HD12	35:DP:112:LEU:HD11	1.75	0.67
1:AA:503:C:OP1	61:AA:4193:HOH:O	2.13	0.67
1:CA:999:C:N3	1:CA:1042:G:N2	2.37	0.67
1:CA:36:C:OP1	12:CL:123:LYS:NZ	2.28	0.67
13:CM:88:ARG:HG3	13:CM:98:VAL:HG11	1.76	0.67
25:DA:1970:A:OP1	61:DA:4259:HOH:O	2.12	0.67
1:AA:78:G:C5	1:AA:91:C:N4	2.61	0.67
1:AA:266:G:H5''	1:AA:268:C:H41	1.58	0.67
11:CK:48:ILE:O	11:CK:50:TYR:N	2.28	0.67
19:CS:50:ALA:HB1	19:CS:57:HIS:HB3	1.76	0.67
25:DA:2379:G:O2'	38:DS:17:ARG:NH2	2.25	0.67
25:DA:2839:G:H5'	37:DR:46:GLY:HA2	1.74	0.67
25:BA:237:G:OP1	61:BA:5132:HOH:O	2.13	0.67
25:BA:943:C:N3	25:BA:944:C:N4	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BZ:151:HIS:O	45:BZ:153:SER:N	2.24	0.67
1:CA:1028:C:C2	1:CA:1033:G:N1	2.62	0.67
1:CA:148:G:H2'	1:CA:149:A:C8	2.30	0.67
9:CI:9:ARG:HG2	9:CI:14:VAL:HG12	1.75	0.67
46:D0:10:THR:HG22	46:D0:12:ASN:H	1.60	0.67
23:AW:6:G:H1	23:AW:67:C:H42	0.75	0.67
25:BA:1831:C:OP2	27:BD:183:ARG:NH2	2.28	0.67
1:CA:1129:C:H2'	1:CA:1139:G:N7	2.10	0.67
2:AB:178:ARG:HG2	8:AH:72:PRO:HA	1.75	0.67
42:BW:2:GLU:OE2	42:BW:72:LYS:NZ	2.23	0.67
5:CE:50:GLU:HB2	5:CE:53:LEU:HD13	1.76	0.67
3:AC:6:HIS:HD2	3:AC:8:ILE:H	1.42	0.66
5:AE:50:GLU:HB2	5:AE:53:LEU:HD13	1.76	0.66
25:BA:1027:A:OP1	61:BA:4722:HOH:O	2.12	0.66
9:CI:23:ASN:ND2	9:CI:25:LYS:HG2	2.10	0.66
18:CR:56:THR:HB	18:CR:58:LEU:HD23	1.77	0.66
25:DA:249:C:O2	54:D8:12:LYS:NZ	2.27	0.66
54:D8:33:ASN:HA	54:D8:36:LYS:HD2	1.77	0.66
25:DA:2148:G:H2'	25:DA:2149:G:H8	1.59	0.66
25:DA:307:G:N7	61:DA:4267:HOH:O	2.27	0.66
31:DH:7:LEU:HD12	31:DH:8:PRO:HD2	1.75	0.66
25:DA:2880:C:O3'	37:DR:90:ARG:NH1	2.27	0.66
1:AA:109:A:OP1	61:AA:4230:HOH:O	2.13	0.66
3:AC:181:ASN:HD22	3:AC:204:LEU:HB2	1.60	0.66
1:CA:1129:C:N4	1:CA:1143:G:H1	1.93	0.66
25:DA:1801:G:OP2	27:DD:154:LYS:NZ	2.26	0.66
2:AB:88:ALA:HB2	2:AB:219:VAL:HG13	1.77	0.66
20:AT:10:LEU:HD13	20:AT:11:SER:H	1.61	0.66
25:BA:2081:A:OP2	61:BA:4476:HOH:O	2.11	0.66
25:DA:11:G:N7	61:DA:4575:HOH:O	2.28	0.66
3:CC:100:ALA:O	3:CC:102:ASN:ND2	2.28	0.66
25:DA:2118:U:C4	25:DA:2149:G:H1'	2.30	0.66
32:DI:93:THR:HG22	32:DI:119:PRO:HB3	1.76	0.66
1:AA:539:A:OP2	12:AL:115:LYS:NZ	2.29	0.66
47:B1:2:SER:HB3	47:B1:46:LEU:HD12	1.77	0.66
27:BD:69:ARG:NH2	27:BD:128:GLY:O	2.29	0.66
9:CI:102:LEU:HD13	9:CI:103:THR:H	1.59	0.66
9:CI:3:GLN:OE1	9:CI:20:ARG:NH2	2.25	0.66
25:DA:1783:A:OP1	61:DA:4522:HOH:O	2.12	0.66
25:DA:570:G:OP1	61:DA:4397:HOH:O	2.12	0.66
25:BA:142:G:H4'	43:BX:35:THR:HG21	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:354:A:H2	25:BA:1255:A:HO2'	1.44	0.66
1:CA:1064:G:N2	1:CA:1190:G:O2'	2.29	0.66
2:CB:125:PRO:O	2:CB:127:ILE:N	2.28	0.66
26:DB:13:A:N1	26:DB:69:G:O2'	2.24	0.66
1:AA:1278:U:H5'	1:AA:1279:A:O4'	1.96	0.66
1:AA:972:C:OP1	61:AA:4182:HOH:O	2.13	0.66
61:AX:3104:HOH:O	25:BA:2597:U:OP1	2.14	0.66
25:BA:465:G:N7	61:BA:4532:HOH:O	2.28	0.66
25:BA:655:G:OP2	54:B8:15:LYS:NZ	2.24	0.66
25:DA:252:G:P	35:DP:50:ARG:HH12	2.18	0.66
4:AD:188:LEU:H	4:AD:188:LEU:HD23	1.61	0.66
1:CA:38:G:N2	1:CA:397:A:H5''	2.09	0.66
25:DA:250:G:OP2	54:D8:13:ARG:NH2	2.29	0.66
18:AR:56:THR:HB	18:AR:58:LEU:HD23	1.77	0.66
25:BA:715:G:N7	61:BA:4012:HOH:O	2.28	0.66
1:CA:79:G:H1	1:CA:90:U:H3	1.44	0.66
10:CJ:49:VAL:HG23	14:CN:41:ARG:HB2	1.77	0.66
25:DA:2819:G:N7	61:DA:4380:HOH:O	2.29	0.66
8:AH:51:VAL:HG21	8:AH:60:ARG:HB2	1.77	0.65
28:BE:12:THR:HG22	28:BE:13:ARG:H	1.62	0.65
25:DA:1912:A:OP1	61:DA:4643:HOH:O	2.13	0.65
1:AA:545:C:OP1	4:AD:61:LYS:NZ	2.29	0.65
20:CT:10:LEU:HB3	20:CT:12:ALA:H	1.60	0.65
50:D4:59:PHE:H	50:D4:59:PHE:HD1	1.45	0.65
49:B3:5:LYS:NZ	49:B3:34:GLU:OE2	2.29	0.65
25:BA:1218:G:O2'	25:BA:1219:A:O4'	2.13	0.65
25:BA:2156:A:H62	25:BA:2179:G:H1'	1.59	0.65
25:BA:2362:C:OP2	61:BA:4195:HOH:O	2.13	0.65
25:BA:333:G:N3	25:BA:353:G:O2'	2.29	0.65
37:BR:33:ARG:NH1	37:BR:115:GLU:OE2	2.30	0.65
25:DA:1670:C:OP1	61:DA:4063:HOH:O	2.13	0.65
38:BS:15:ARG:O	38:BS:19:LYS:HG2	1.95	0.65
1:CA:1166:G:N2	1:CA:1170:A:OP2	2.29	0.65
25:DA:1434:A:H61	25:DA:1558:A:H62	1.43	0.65
25:DA:2126:A:N6	25:DA:2162:G:O2'	2.30	0.65
25:DA:568:U:H5'	25:DA:945:A:N1	2.12	0.65
1:AA:1027:C:N3	1:AA:1034:G:O6	2.30	0.65
7:CG:111:ARG:NH1	7:CG:113:GLU:OE2	2.29	0.65
14:CN:4:LYS:HA	14:CN:7:ILE:HG22	1.77	0.65
16:CP:51:VAL:HG12	16:CP:53:VAL:H	1.61	0.65
50:D4:24:THR:OG1	50:D4:25:TYR:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:886:C:H1'	25:DA:890:A:H61	1.62	0.65
28:DE:47:VAL:HG11	28:DE:86:PRO:HD2	1.79	0.65
25:BA:467:U:O2	29:BF:46:ARG:NH2	2.27	0.65
1:AA:59:A:N1	61:AA:4123:HOH:O	2.28	0.65
1:CA:390:C:O3'	16:CP:28:ARG:NH2	2.29	0.65
1:CA:947:G:N2	1:CA:1234:C:N3	2.42	0.65
1:CA:426:G:OP1	4:CD:38:TYR:OH	2.12	0.65
24:CX:47:U:N3	24:CX:50:U:OP1	2.30	0.65
25:DA:1031:G:H5''	55:D9:8:LYS:HE3	1.78	0.65
25:DA:832:G:OP1	61:DA:4580:HOH:O	2.13	0.65
1:AA:1305:G:N2	1:AA:1331:G:H1'	2.11	0.65
1:AA:1381:U:H1'	7:AG:79:ARG:HG3	1.78	0.65
4:AD:23:GLY:HA3	4:AD:112:VAL:HG12	1.78	0.65
25:BA:1219:A:H4'	25:BA:1220:U:OP1	1.97	0.65
25:BA:807:G:OP1	61:BA:5080:HOH:O	2.13	0.65
36:BQ:38:GLU:HG3	36:BQ:127:ILE:HB	1.79	0.65
23:CW:50:U:H6	23:CW:50:U:H5'	1.62	0.65
25:DA:1816:G:O6	27:DD:35:LYS:NZ	2.20	0.65
23:AY:9:A:O3'	23:AY:45:U:O2'	2.15	0.65
38:BS:34:HIS:ND1	38:BS:53:SER:OG	2.28	0.65
1:CA:1106:G:H5''	3:CC:172:ARG:HG2	1.77	0.65
4:CD:175:SER:HB3	4:CD:186:LEU:HD11	1.79	0.65
1:CA:377:G:OP1	16:CP:3:LYS:HD2	1.97	0.65
25:DA:1021:A:H62	25:DA:1141:U:H3	1.42	0.65
25:DA:2171:A:N3	25:DA:2172:U:N3	2.45	0.65
25:DA:1250:G:N7	35:DP:18:ARG:NH2	2.45	0.65
44:BY:54:LYS:H	44:BY:56:PRO:HD3	1.61	0.64
45:BZ:45:ASP:OD1	45:BZ:49:ARG:NH1	2.30	0.64
7:AG:111:ARG:NH2	7:AG:126:ASP:OD2	2.30	0.64
25:BA:2902:G:H4'	25:BA:2903:G:O5'	1.96	0.64
13:CM:78:ILE:HA	13:CM:81:LEU:HD12	1.79	0.64
15:CO:55:GLY:HA2	15:CO:58:MET:HE2	1.78	0.64
23:CY:15:G:H22	23:CY:48:C:H42	1.44	0.64
1:AA:1530:G:H2'	1:AA:1531:A:O4'	1.97	0.64
3:AC:3:ASN:OD1	3:AC:3:ASN:N	2.30	0.64
25:BA:1094:A:OP2	25:BA:1155:C:N4	2.30	0.64
25:BA:928:G:H3'	25:BA:929:G:C8	2.32	0.64
27:BD:237:GLU:OE2	61:BD:409:HOH:O	2.15	0.64
1:CA:411:A:OP2	4:CD:25:ARG:NH2	2.29	0.64
25:DA:300:A:OP1	44:DY:86:ARG:NH2	2.30	0.64
26:DB:106:G:H5'	45:DZ:31:ARG:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:38:ILE:HD11	10:AJ:71:LEU:HB3	1.78	0.64
15:AO:25:THR:HG21	15:AO:70:LEU:HB2	1.79	0.64
1:CA:1108:G:O6	61:CA:4094:HOH:O	2.11	0.64
1:CA:954:G:H21	1:CA:1227:A:H62	1.45	0.64
2:CB:15:VAL:HG21	2:CB:213:LEU:HD12	1.79	0.64
3:CC:164:ARG:NH1	3:CC:166:GLU:OE1	2.31	0.64
29:DF:21:ALA:HB3	29:DF:22:ALA:HA	1.80	0.64
1:CA:1422:G:O3'	34:DO:49:ARG:NH1	2.30	0.64
1:AA:8:A:H5'	5:AE:101:ILE:HG22	1.78	0.64
25:BA:1749:G:N7	61:BA:5142:HOH:O	2.30	0.64
27:BD:108:PRO:HB3	27:BD:143:HIS:HE1	1.62	0.64
25:BA:1296:G:N7	35:BP:18:ARG:NH2	2.45	0.64
1:CA:8:A:H5'	5:CE:101:ILE:HG22	1.79	0.64
10:CJ:38:ILE:HD11	10:CJ:71:LEU:HD23	1.79	0.64
25:DA:2291:U:OP1	25:DA:2380:C:O2'	2.16	0.64
31:DH:20:ALA:HB3	31:DH:23:ARG:HG3	1.80	0.64
13:AM:11:ARG:HA	13:AM:45:VAL:HB	1.80	0.64
10:AJ:49:VAL:HG23	14:AN:41:ARG:HB2	1.79	0.64
35:BP:86:LYS:HD3	35:BP:117:GLU:HB3	1.80	0.64
1:CA:1027:C:N3	1:CA:1034:G:O6	2.30	0.64
1:CA:1119:C:H42	1:CA:1154:G:H1	1.44	0.64
2:CB:78:GLN:NE2	2:CB:95:GLN:OE1	2.30	0.64
28:DE:77:ILE:HD13	28:DE:195:LEU:HD22	1.79	0.64
1:AA:974:A:OP2	14:AN:29:ARG:NH2	2.30	0.64
1:CA:1028:C:N3	1:CA:1033:G:O6	2.30	0.64
1:CA:1251:A:H2'	1:CA:1252:A:C8	2.33	0.64
6:CF:70:ASP:OD1	6:CF:70:ASP:N	2.28	0.64
29:DF:157:VAL:HB	29:DF:194:MET:HG2	1.79	0.64
1:CA:559:A:OP1	5:CE:126:ARG:NH2	2.27	0.64
25:DA:2632:A:HO2'	25:DA:2811:G:HO2'	1.42	0.64
25:BA:2138:G:O6	25:BA:2187:G:N2	2.31	0.63
25:BA:2145:G:H1	25:BA:2197:C:N4	1.94	0.63
1:AA:1198:G:OP1	61:AA:4206:HOH:O	2.16	0.63
4:AD:15:GLU:OE2	4:AD:66:ARG:NH1	2.31	0.63
36:DQ:1:MET:N	36:DQ:1:MET:SD	2.65	0.63
37:DR:21:TYR:CZ	37:DR:43:GLU:HG2	2.33	0.63
9:AI:20:ARG:O	9:AI:60:ASP:N	2.30	0.63
25:BA:139:A:H8	25:BA:1454:C:HO2'	1.44	0.63
2:CB:178:ARG:HH22	8:CH:68:ARG:NH1	1.96	0.63
28:DE:72:VAL:HA	28:DE:73:GLU:HB3	1.81	0.63
1:AA:1502:A:H2	1:AA:1505:G:N1	1.92	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BI:61:ARG:NH2	32:BI:64:GLU:OE2	2.31	0.63
25:DA:1420:U:O2'	25:DA:1421:G:OP1	2.16	0.63
25:BA:1485:A:OP1	61:BA:5011:HOH:O	2.14	0.63
25:BA:2624:C:OP2	51:B5:2:ALA:N	2.30	0.63
25:BA:929:G:H1	25:BA:940:C:H42	1.45	0.63
42:BW:25:ARG:NH2	42:BW:74:ALA:O	2.29	0.63
1:CA:572:A:OP1	61:CA:4047:HOH:O	2.15	0.63
25:DA:2807:G:H22	25:DA:2892:A:H62	1.47	0.63
24:CX:31:G:H3'	24:CX:32:5MC:HM51	1.81	0.63
25:DA:1266:G:O5'	42:DW:15:ARG:NH2	2.31	0.63
24:AX:6:G:H1	24:AX:67:C:N4	1.97	0.63
36:BQ:35:VAL:HG13	36:BQ:130:LYS:HB3	1.80	0.63
1:CA:1278:U:H5'	1:CA:1279:A:O4'	1.98	0.63
29:DF:24:LEU:HD23	29:DF:115:ALA:HA	1.81	0.63
31:DH:149:ARG:NH1	31:DH:167:GLU:OE1	2.31	0.63
41:DV:43:GLU:OE2	41:DV:43:GLU:N	2.32	0.63
25:BA:1466:U:O2'	25:BA:1467:G:OP1	2.16	0.63
31:BH:59:ARG:HG2	31:BH:59:ARG:HH11	1.63	0.63
1:CA:1026:G:H5'	1:CA:1027:C:O5'	1.98	0.63
1:CA:254:G:OP1	17:CQ:66:SER:OG	2.09	0.63
1:AA:405:U:OP2	4:AD:3:ARG:NH2	2.31	0.63
1:AA:911:U:OP2	12:AL:97:ARG:NH1	2.32	0.63
2:AB:33:TYR:HB2	2:AB:43:ASP:HB2	1.80	0.63
3:AC:78:GLY:HA3	3:AC:83:ARG:H	1.63	0.63
25:BA:553:A:N1	25:BA:2064:A:H2'	2.13	0.63
1:CA:1027:C:O2	1:CA:1034:G:N1	2.30	0.63
1:CA:1039:C:H2'	1:CA:1040:U:O4'	1.99	0.63
1:CA:811:C:O2'	1:CA:901:A:N1	2.30	0.63
26:DB:66:A:H61	26:DB:109:C:H5'	1.64	0.63
27:DD:132:PRO:HD3	27:DD:190:TYR:CZ	2.34	0.63
29:DF:24:LEU:HD21	29:DF:114:VAL:HG12	1.80	0.63
45:DZ:145:GLU:H	45:DZ:148:ASP:HB2	1.62	0.63
1:AA:1435:G:H2'	1:AA:1436:U:C6	2.33	0.62
25:BA:1071:G:C4	25:BA:1180:C:H1'	2.34	0.62
25:BA:1125:C:H41	25:BA:1134:A:P	2.22	0.62
25:BA:2807:C:H42	25:BA:2813:G:H1	1.48	0.62
20:CT:9:ASN:O	20:CT:10:LEU:HB2	1.99	0.62
32:DI:31:LEU:HD21	32:DI:38:LEU:HG	1.81	0.62
38:DS:71:ARG:NH1	38:DS:107:GLU:OE1	2.32	0.62
23:AY:50:U:C4	23:AY:64:A:N1	2.68	0.62
1:CA:1499:A:H1'	1:CA:1520:G:H5'	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:155:LEU:HD21	2:CB:159:PRO:HG3	1.80	0.62
23:CY:44:G:H2'	23:CY:45:U:H5'	1.81	0.62
1:AA:353:A:H5'	1:AA:353:A:H8	1.63	0.62
9:CI:20:ARG:O	9:CI:60:ASP:N	2.29	0.62
23:CY:18:G:N2	23:CY:55:PSU:C4	2.66	0.62
28:DE:36:ARG:HG2	28:DE:47:VAL:HG12	1.81	0.62
9:AI:110:GLU:OE2	9:AI:113:LYS:NZ	2.33	0.62
25:BA:2849:G:H5'	37:BR:46:GLY:HA2	1.82	0.62
25:DA:2308:G:O6	25:DA:2311:A:N6	2.20	0.62
25:DA:625:G:O6	35:DP:107:LYS:NZ	2.30	0.62
25:DA:2316:C:O2'	30:DG:128:ARG:NH2	2.31	0.62
2:AB:51:LEU:HD23	2:AB:201:ILE:HD12	1.80	0.62
50:B4:46:GLN:O	50:B4:48:ARG:N	2.32	0.62
25:DA:2870:C:H2'	25:DA:2871:C:O4'	2.00	0.62
27:DD:85:ASP:OD2	27:DD:88:ARG:NH1	2.32	0.62
45:DZ:156:LYS:HE3	45:DZ:158:PRO:HD3	1.81	0.62
45:DZ:159:PRO:HA	45:DZ:161:VAL:H	1.63	0.62
1:AA:1030(A):G:O2'	1:AA:1031:G:N2	2.32	0.62
25:BA:1118:C:N3	25:BA:1138:C:N4	2.47	0.62
1:CA:1010:G:H2'	1:CA:1011:G:C8	2.35	0.62
1:CA:881:G:P	12:CL:12:ARG:HH22	2.22	0.62
23:CW:51:U:H2'	23:CW:52:G:C8	2.35	0.62
35:DP:50:ARG:HH21	54:D8:7:HIS:HD2	1.45	0.62
25:DA:692:C:O2'	27:DD:38:LYS:NZ	2.31	0.62
23:AY:50:U:H3	23:AY:64:A:H2	1.47	0.62
25:BA:294:C:H42	25:BA:390:G:H1	1.48	0.62
25:BA:298:G:H2'	25:BA:299:G:H8	1.65	0.62
1:CA:1221:G:OP1	1:CA:1320:C:N4	2.33	0.62
2:CB:187:LEU:HA	2:CB:201:ILE:HB	1.81	0.62
25:DA:1405:U:H2'	25:DA:1406:U:C6	2.35	0.62
25:DA:2151:G:H2'	25:DA:2152:G:H8	1.65	0.62
26:DB:24:G:N7	26:DB:56:G:H2'	2.15	0.62
36:DQ:35:VAL:HG13	36:DQ:130:LYS:HB3	1.82	0.62
1:AA:1002:G:O6	1:AA:1003:G:N2	2.32	0.62
23:AW:56:C:OP1	25:BA:943:C:H5'	1.99	0.62
25:BA:2825:C:H5'	51:B5:29:THR:HG21	1.81	0.62
1:CA:406:G:H5'	4:CD:5:ILE:HD11	1.82	0.62
3:CC:134:ILE:HG23	3:CC:151:VAL:HB	1.82	0.62
3:AC:26:LYS:HG2	10:AJ:45:ARG:HH12	1.65	0.62
23:AY:63:G:C2	23:AY:64:A:H1'	2.35	0.62
25:BA:388:A:H2'	25:BA:389:G:C8	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2720:G:H1'	37:BR:71:GLN:HE22	1.64	0.62
1:CA:771:G:N7	61:CA:4039:HOH:O	2.30	0.62
27:DD:3:VAL:HG13	27:DD:17:THR:HB	1.82	0.62
44:DY:23:ARG:HG2	44:DY:42:VAL:HG22	1.80	0.62
1:AA:922:G:H4'	5:AE:20:GLN:HA	1.81	0.62
25:BA:2126:G:H2'	25:BA:2127:C:C6	2.35	0.62
45:BZ:138:GLU:H	45:BZ:156:LYS:HE2	1.63	0.62
1:CA:1502:A:H2	1:CA:1505:G:N1	1.94	0.62
3:CC:8:ILE:HG23	3:CC:16:ARG:HG2	1.81	0.62
23:CY:11:C:N3	23:CY:24:G:O6	2.33	0.62
50:B4:53:GLU:HG3	50:B4:55:ARG:HA	1.82	0.61
51:B5:16:ARG:HG3	51:B5:17:ASP:N	2.15	0.61
25:BA:1105:G:N2	25:BA:1125:C:O2	2.29	0.61
25:BA:302:A:O2'	25:BA:303:C:OP1	2.15	0.61
5:CE:52:PRO:HG2	5:CE:53:LEU:HD12	1.82	0.61
38:DS:25:ARG:NH1	38:DS:42:ASP:OD2	2.33	0.61
45:DZ:153:SER:HB3	45:DZ:167:PRO:HB3	1.81	0.61
24:AX:50:U:H3	24:AX:64:G:H1	1.48	0.61
23:AY:53:G:H1	23:AY:61:C:N4	1.98	0.61
1:CA:448:A:P	1:CA:485:G:H22	2.23	0.61
4:CD:166:LYS:NZ	4:CD:179:GLU:OE2	2.32	0.61
25:DA:2758:A:C2	25:DA:2759:G:H1'	2.35	0.61
32:DI:92:VAL:HG13	32:DI:120:ILE:HB	1.82	0.61
43:DX:57:LEU:HD21	43:DX:78:LYS:HE2	1.81	0.61
1:AA:1353:G:OP1	21:AU:10:ARG:NH1	2.33	0.61
1:AA:165:C:H2'	1:AA:166:G:C8	2.35	0.61
9:AI:49:PRO:HG3	9:AI:101:PHE:HD2	1.66	0.61
25:BA:346:A:OP1	29:BF:168:ARG:HD2	2.00	0.61
8:CH:14:ARG:HG2	8:CH:18:ARG:HH22	1.66	0.61
25:DA:1639:U:H2'	25:DA:1640:C:H5''	1.80	0.61
44:DY:88:LYS:HZ3	44:DY:90:LEU:HA	1.64	0.61
1:AA:78:G:N2	1:AA:91:C:C2	2.68	0.61
1:AA:975:A:H8	1:AA:975:A:H5'	1.64	0.61
1:AA:997:U:H3	1:AA:1044:A:N6	1.97	0.61
1:CA:1027:C:C4	1:CA:1034:G:O6	2.53	0.61
1:CA:1240:U:N3	7:CG:30:ILE:O	2.29	0.61
37:DR:101:ALA:HB3	51:D5:47:PRO:HG3	1.83	0.61
27:DD:132:PRO:HG2	27:DD:135:PHE:CD2	2.35	0.61
2:AB:115:LEU:HD11	2:AB:146:GLN:HG3	1.81	0.61
1:AA:1152:A:OP1	10:AJ:68:HIS:ND1	2.33	0.61
1:CA:564:C:O2'	8:CH:91:ARG:NH2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2130:U:H4'	25:DA:2133:G:H4'	1.81	0.61
37:DR:2:ARG:NH1	37:DR:5:LYS:O	2.33	0.61
44:DY:94:LYS:NZ	61:DY:601:HOH:O	2.32	0.61
1:AA:1432:G:O6	61:AA:4147:HOH:O	2.13	0.61
4:AD:194:LEU:HD12	4:AD:195:ALA:H	1.65	0.61
20:AT:76:ALA:O	20:AT:80:ARG:HG2	2.00	0.61
1:AA:1503:A:O2'	22:AV:13:A:N1	2.34	0.61
25:BA:1099:C:H2'	25:BA:1100:A:O4'	2.00	0.61
48:D2:35:LEU:HD12	48:D2:53:LEU:HD12	1.82	0.61
5:AE:33:VAL:HG21	5:AE:109:ILE:HA	1.82	0.61
25:BA:2396:G:OP2	46:B0:55:ARG:NH1	2.33	0.61
45:BZ:92:SER:O	45:BZ:130:PRO:HG2	2.00	0.61
1:CA:920:U:H2'	1:CA:921:U:C6	2.36	0.61
23:CY:14:A:O2'	23:CY:15:G:OP1	2.17	0.61
25:BA:2235:G:OP1	27:BD:172:TYR:OH	2.13	0.61
45:BZ:148:ASP:N	45:BZ:148:ASP:OD1	2.33	0.61
1:CA:1005:A:H5''	1:CA:1006:C:C5	2.35	0.61
1:CA:1055:A:N7	1:CA:1200:C:N4	2.49	0.61
1:CA:986:A:N3	19:CS:52:TYR:OH	2.31	0.61
29:DF:167:ALA:HB1	29:DF:173:VAL:HG11	1.81	0.61
36:DQ:18:LYS:O	36:DQ:98:LYS:NZ	2.28	0.61
1:AA:1320:C:O2	19:AS:36:ARG:NH2	2.34	0.61
25:BA:1834:A:O2'	27:BD:259:THR:HG21	2.01	0.61
1:CA:1028:C:O2	1:CA:1033:G:N1	2.34	0.61
10:CJ:8:LEU:HB2	10:CJ:70:ARG:HB2	1.82	0.61
25:DA:1019:U:H2'	25:DA:1020:A:H8	1.64	0.61
25:DA:821:A:N1	61:DA:4395:HOH:O	2.31	0.61
1:AA:1240:U:OP2	7:AG:116:ALA:N	2.34	0.61
23:AY:8:4SU:H4'	23:AY:48:C:H4'	1.83	0.61
25:BA:2205:C:H2'	25:BA:2206:G:H8	1.65	0.61
25:BA:2859:U:OP2	39:BT:95:ARG:NH1	2.34	0.61
1:CA:17:U:H2'	1:CA:18:C:C6	2.36	0.61
1:CA:854:G:O6	61:CA:4130:HOH:O	2.16	0.61
4:CD:88:VAL:HG13	5:CE:97:GLY:HA2	1.83	0.61
23:CY:5:G:H1	23:CY:68:C:N4	1.97	0.61
25:DA:1218:C:OP2	40:DU:15:LYS:NZ	2.32	0.61
41:DV:4:ILE:HD12	41:DV:39:LEU:HB3	1.83	0.61
46:D0:11:ARG:O	46:D0:14:ARG:NH2	2.34	0.60
1:AA:538:G:H5''	12:AL:114:LYS:HB2	1.81	0.60
4:AD:128:VAL:N	4:AD:131:ARG:O	2.33	0.60
15:AO:39:LEU:HD13	15:AO:56:LEU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BZ:19:ARG:NH1	45:BZ:84:GLU:O	2.34	0.60
1:CA:1010:G:H22	1:CA:1020:U:H1'	1.65	0.60
1:CA:1216:G:H5''	14:CN:5:ALA:HB2	1.81	0.60
24:CX:6:G:H1	24:CX:67:C:N4	1.97	0.60
25:DA:1183:G:O3'	49:D3:29:ARG:NH1	2.33	0.60
1:AA:560:U:O2'	1:AA:561:U:OP2	2.16	0.60
25:BA:1513:G:O2'	25:BA:1593:C:O2'	2.18	0.60
25:BA:2227:G:H5''	25:BA:2228:G:C5	2.36	0.60
25:BA:2761:A:H5'	31:BH:4:ILE:HD13	1.82	0.60
46:D0:32:ARG:H	46:D0:35:ASN:ND2	2.00	0.60
50:D4:59:PHE:HA	50:D4:61:ARG:N	2.16	0.60
25:DA:2364:C:OP1	46:D0:55:ARG:NH1	2.32	0.60
7:AG:72:ARG:NH1	7:AG:72:ARG:HG3	2.12	0.60
29:BF:157:VAL:HB	29:BF:194:MET:HG2	1.82	0.60
25:DA:2615:U:OP1	61:DA:4305:HOH:O	2.16	0.60
50:B4:15:ILE:HB	50:B4:32:TYR:HD1	1.65	0.60
9:AI:53:VAL:O	9:AI:55:ALA:N	2.33	0.60
25:BA:1480:A:H61	25:BA:1605:A:H62	1.48	0.60
25:BA:2299:A:N6	25:BA:2356:U:H3	1.98	0.60
41:BV:72:VAL:HG13	41:BV:85:LYS:HB3	1.81	0.60
5:CE:140:ARG:O	5:CE:143:ARG:NH2	2.35	0.60
25:BA:83:A:H5'	44:BY:8:LYS:HG2	1.82	0.60
1:CA:1120:G:C5	1:CA:1154:G:N2	2.70	0.60
20:CT:10:LEU:HD23	20:CT:12:ALA:HB2	1.83	0.60
25:DA:2655:G:O2'	25:DA:2664:G:O6	2.15	0.60
1:AA:1064:G:H4'	1:AA:1065:U:OP1	2.01	0.60
1:AA:1191:A:OP1	3:AC:4:LYS:NZ	2.35	0.60
1:AA:377:G:OP1	16:AP:3:LYS:HD2	2.01	0.60
23:AY:58:A:O2'	23:AY:59:U:H5'	2.02	0.60
1:CA:1126:U:H3	10:CJ:40:LEU:HD11	1.66	0.60
8:CH:119:LEU:HB3	8:CH:123:GLU:HB3	1.82	0.60
11:CK:22:HIS:HB3	11:CK:29:ILE:HB	1.84	0.60
23:CW:13:C:O2'	23:CW:14:A:O5'	2.16	0.60
23:CY:50:U:O2	23:CY:64:A:N1	2.34	0.60
26:DB:14:U:OP2	26:DB:70:C:O2'	2.17	0.60
30:DG:150:ASP:OD1	30:DG:150:ASP:N	2.25	0.60
25:BA:2045:G:H5'	25:BA:2629:C:H4'	1.83	0.60
9:AI:9:ARG:H	9:AI:79:LEU:HD23	1.66	0.60
17:AQ:50:LYS:HD2	17:AQ:51:TYR:CZ	2.37	0.60
20:AT:87:LYS:O	20:AT:91:LEU:HG	2.01	0.60
36:BQ:16:ARG:HG2	36:BQ:18:LYS:HE2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:6:G:H4'	1:CA:298:A:H4'	1.84	0.60
25:DA:974:G:OP1	25:DA:1187:G:O2'	2.14	0.60
35:DP:138:LEU:HD23	35:DP:145:PRO:HB3	1.83	0.60
4:AD:157:LEU:HD22	4:AD:161:ASN:HD21	1.67	0.59
25:BA:1587:U:O4	61:BA:5372:HOH:O	2.16	0.59
1:CA:1183:A:O2'	1:CA:1184:G:OP1	2.16	0.59
1:CA:1286:A:C8	1:CA:1287:A:H4'	2.37	0.59
25:DA:1891:G:O6	61:DA:4758:HOH:O	2.16	0.59
1:AA:17:U:H2'	1:AA:18:C:C6	2.37	0.59
1:AA:619:U:H3	4:AD:134:ASP:HB2	1.67	0.59
41:BV:40:LEU:HB2	41:BV:46:VAL:HG13	1.84	0.59
1:CA:1086:U:H3	1:CA:1099:G:H22	1.47	0.59
25:DA:848:G:N3	25:DA:933:A:H1'	2.17	0.59
25:DA:2751:G:H8	31:DH:2:SER:HA	1.66	0.59
1:AA:148:G:H2'	1:AA:149:A:H8	1.66	0.59
47:B1:85:LEU:HB3	47:B1:89:GLU:HG3	1.84	0.59
28:BE:7:VAL:HG12	28:BE:27:LEU:HB3	1.84	0.59
1:CA:1103:C:OP1	2:CB:96:ARG:NH2	2.34	0.59
25:DA:2183:C:H2'	25:DA:2184:G:C8	2.37	0.59
25:DA:2507:C:H5"	25:DA:2573:C:N4	2.17	0.59
1:AA:1126:U:O2	1:AA:1280:A:H2'	2.03	0.59
5:AE:122:GLU:O	5:AE:126:ARG:NH1	2.35	0.59
18:AR:52:PRO:HB2	18:AR:54:ARG:HG2	1.85	0.59
25:BA:1218:G:O2'	25:BA:1219:A:O5'	2.20	0.59
25:BA:1539:C:N4	25:BA:2227:G:O2'	2.35	0.59
27:BD:85:ASP:OD2	27:BD:88:ARG:NH1	2.34	0.59
25:DA:1033:U:OP1	55:D9:9:ARG:NH2	2.36	0.59
25:DA:1803:A:O2'	27:DD:259:THR:HG21	2.02	0.59
25:DA:2162:G:H4'	25:DA:2172:U:H2'	1.83	0.59
25:DA:2206:G:H8	25:DA:2207:G:N7	1.99	0.59
25:DA:322:A:OP2	29:DF:169:ASN:HB2	2.02	0.59
39:DT:117:ASP:OD2	39:DT:120:ARG:NE	2.29	0.59
40:DU:83:LEU:HD12	40:DU:88:ILE:HB	1.83	0.59
1:AA:406:G:H5'	4:AD:5:ILE:HD11	1.84	0.59
1:AA:1456:G:O3'	20:AT:39:LYS:NZ	2.36	0.59
28:BE:28:ALA:HB3	28:BE:93:VAL:HG12	1.85	0.59
25:DA:1159:U:H2'	25:DA:1160:G:H8	1.67	0.59
25:DA:1448:G:H4'	25:DA:1542:A:OP1	2.03	0.59
25:DA:2285:C:OP2	52:D6:6:ARG:NH1	2.35	0.59
37:DR:67:LEU:HD13	37:DR:76:VAL:HG21	1.83	0.59
1:AA:976:G:H5'	1:AA:1358:U:O2'	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BR:44:LEU:HD22	37:BR:48:VAL:HG23	1.84	0.59
1:CA:1029:C:N3	1:CA:1032:G:C2	2.70	0.59
1:CA:67:C:H2'	1:CA:68:G:C8	2.37	0.59
8:AH:39:LEU:HB3	8:AH:45:ILE:HG12	1.83	0.59
25:BA:239:G:P	54:B8:13:ARG:HH22	2.25	0.59
45:BZ:155:LEU:HD12	45:BZ:156:LYS:H	1.66	0.59
1:CA:1128:C:H1'	1:CA:1147:C:H42	1.67	0.59
3:CC:19:GLU:HA	3:CC:54:ARG:HH22	1.68	0.59
25:DA:1530:C:O2'	25:DA:1531:C:O5'	2.15	0.59
25:DA:1762:A:N1	61:DA:4594:HOH:O	2.31	0.59
25:DA:2447:G:N2	25:DA:2450:A:OP2	2.35	0.59
23:AY:19:G:N1	23:AY:56:C:N4	2.50	0.59
25:BA:1740:U:O2'	27:BD:14:ARG:NH2	2.36	0.59
25:DA:1239:G:H2'	25:DA:1240:U:O4'	2.02	0.59
25:DA:1261:C:OP2	42:DW:83:LYS:NZ	2.29	0.59
30:DG:131:TYR:HB3	30:DG:159:VAL:HG13	1.85	0.59
9:AI:3:GLN:OE1	9:AI:20:ARG:NH2	2.31	0.59
19:AS:27:GLU:HB3	19:AS:28:LYS:HA	1.84	0.59
25:BA:1116:A:N6	25:BA:1142:A:N3	2.51	0.59
28:BE:29:GLY:HA3	61:BE:409:HOH:O	2.02	0.59
31:BH:7:LEU:HD12	31:BH:8:PRO:HD2	1.85	0.59
23:CW:43:C:H2'	23:CW:44:G:C8	2.36	0.59
41:DV:72:VAL:HG13	41:DV:85:LYS:HB3	1.85	0.59
4:AD:122:ARG:NH2	4:AD:134:ASP:HB3	2.18	0.59
4:CD:147:ALA:HB2	4:CD:182:LYS:HG3	1.85	0.59
13:CM:37:THR:O	13:CM:55:ARG:NH1	2.36	0.59
23:CW:25:C:H2'	23:CW:26:A:H5"	1.84	0.59
25:DA:324:A:N6	25:DA:338:G:O2'	2.36	0.59
26:DB:101:G:OP2	61:DB:3105:HOH:O	2.17	0.59
41:DV:76:LYS:HB2	41:DV:81:TYR:HB3	1.84	0.59
1:AA:347:G:H2'	1:AA:348:G:C8	2.38	0.58
1:CA:1286:A:H2'	1:CA:1287:A:H4'	1.85	0.58
1:CA:344:A:H5"	1:CA:345:C:H5	1.68	0.58
1:CA:942:G:H21	9:CI:124:GLN:NE2	2.01	0.58
28:DE:111:ARG:HG3	28:DE:160:TYR:CD2	2.38	0.58
25:DA:674:G:H1'	29:DF:74:ARG:HD3	1.84	0.58
32:DI:124:GLY:H	32:DI:144:VAL:HG23	1.68	0.58
1:AA:1136:U:H5"	1:AA:1137:C:N3	2.17	0.58
25:BA:1211:U:H2'	25:BA:1212:C:C6	2.38	0.58
25:BA:1990:G:OP1	61:BA:4942:HOH:O	2.17	0.58
35:BP:121:LYS:O	35:BP:123:LEU:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1503:A:O2'	22:CV:13:A:N1	2.35	0.58
23:CY:51:U:H2'	23:CY:52:G:O4'	2.03	0.58
30:DG:15:VAL:HG22	30:DG:175:LEU:HB3	1.85	0.58
23:AY:50:U:N3	23:AY:64:A:H2	1.99	0.58
25:BA:1346:U:H4'	25:BA:1347:A:C5'	2.32	0.58
1:CA:1147:C:H1'	9:CI:16:ARG:HH21	1.68	0.58
25:DA:2176:A:H2'	25:DA:2177:C:C6	2.38	0.58
25:DA:2299:G:H2'	25:DA:2300:G:H8	1.68	0.58
29:DF:135:LYS:HG2	29:DF:137:LYS:HZ3	1.68	0.58
25:DA:631:A:OP1	35:DP:65:ARG:NH1	2.37	0.58
38:DS:15:ARG:O	38:DS:19:LYS:HG2	2.02	0.58
1:AA:189(F):U:O2'	17:AQ:63:ARG:NH2	2.36	0.58
26:BB:23:G:O6	61:BB:3128:HOH:O	2.16	0.58
1:CA:662:G:H2'	1:CA:663:A:C8	2.38	0.58
28:DE:116:VAL:HG13	28:DE:122:PHE:HB2	1.85	0.58
32:DI:4:ILE:HD11	32:DI:44:LEU:HD13	1.84	0.58
44:DY:86:ARG:HD2	44:DY:100:ALA:HA	1.84	0.58
50:B4:24:THR:OG1	50:B4:25:TYR:N	2.36	0.58
31:BH:33:LEU:HD21	31:BH:136:ILE:HG13	1.85	0.58
32:BI:92:VAL:HG11	32:BI:144:VAL:HG11	1.85	0.58
1:CA:673:G:H2'	1:CA:674:G:C8	2.38	0.58
1:CA:1119:C:OP2	9:CI:9:ARG:NH1	2.37	0.58
25:DA:1012:U:H5	33:DN:28:THR:HG21	1.67	0.58
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.52	0.58
1:AA:1166:G:N2	1:AA:1170:A:OP2	2.37	0.58
25:BA:2130:C:H2'	25:BA:2131:U:C6	2.39	0.58
15:CO:4:THR:N	15:CO:7:GLU:OE2	2.35	0.58
23:CW:44:G:O5'	23:CW:44:G:H8	1.87	0.58
23:CW:61:C:O2'	23:CW:62:C:O5'	2.12	0.58
25:DA:1010:A:OP2	61:DA:4488:HOH:O	2.17	0.58
25:DA:1693:U:O2'	27:DD:14:ARG:NH2	2.36	0.58
32:DI:102:SER:O	32:DI:106:GLY:N	2.36	0.58
1:AA:1316:G:N1	1:AA:1319:A:OP2	2.36	0.58
25:BA:2880:C:H2'	25:BA:2881:C:O4'	2.04	0.58
40:BU:108:GLU:O	40:BU:112:ARG:HG2	2.04	0.58
5:CE:71:LEU:HD11	5:CE:115:VAL:HG22	1.85	0.58
47:D1:32:LYS:O	61:D1:202:HOH:O	2.16	0.58
25:DA:1589:C:H2'	25:DA:1590:U:H6	1.69	0.58
25:DA:2693:A:H2'	25:DA:2694:G:H8	1.68	0.58
25:DA:526:A:OP1	61:DA:4494:HOH:O	2.17	0.58
1:AA:1036:G:H3'	1:AA:1037:C:C6	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:36:ASP:OD2	5:AE:40:ARG:HB2	2.04	0.58
15:AO:17:ARG:HH11	15:AO:17:ARG:HG3	1.68	0.58
25:BA:1793:A:N1	61:BA:4975:HOH:O	2.32	0.58
35:BP:91:PHE:O	35:BP:121:LYS:NZ	2.35	0.58
23:CY:36:A:H2'	23:CY:37:MIA:O4'	2.03	0.58
47:D1:85:LEU:HB3	47:D1:89:GLU:HB3	1.85	0.58
25:DA:2136:C:HO2'	25:DA:2137:C:H6	1.52	0.58
25:DA:2836:U:H2'	25:DA:2837:G:C8	2.39	0.58
34:DO:8:LEU:HD12	34:DO:84:ALA:HB2	1.84	0.58
39:DT:17:THR:OG1	39:DT:17:THR:O	2.21	0.58
42:DW:60:ASN:HD22	42:DW:60:ASN:N	2.02	0.58
2:AB:185:ILE:CG2	2:AB:199:TYR:HB2	2.32	0.58
50:B4:63:TYR:N	50:B4:64:GLY:HA2	2.18	0.58
1:CA:976:G:H5'	1:CA:1358:U:O2'	2.04	0.58
23:CW:63:G:H2'	23:CW:64:A:O4'	2.04	0.58
25:DA:880:G:H2'	25:DA:881:G:H8	1.69	0.58
25:DA:886:C:O2'	25:DA:889:C:N4	2.37	0.58
1:AA:232:G:H1'	1:AA:262:A:N1	2.19	0.58
25:BA:1502:G:O2'	25:BA:2863:C:OP1	2.13	0.58
25:BA:721:G:H1'	29:BF:74:ARG:HD3	1.85	0.58
45:BZ:1:MET:HG2	45:BZ:55:HIS:ND1	2.18	0.58
1:CA:1133:G:H2'	1:CA:1134:G:O4'	2.04	0.58
1:CA:1348:U:H4'	9:CI:120:ARG:HD2	1.86	0.58
25:DA:1823:G:OP1	27:DD:54:ARG:NH1	2.36	0.58
30:DG:114:ILE:HA	30:DG:140:ILE:HD11	1.86	0.58
1:AA:8:A:N7	4:AD:208:SER:OG	2.37	0.57
2:AB:93:VAL:HG21	2:AB:97:TRP:HD1	1.69	0.57
5:AE:95:ALA:HB1	5:AE:96:PRO:HD2	1.86	0.57
50:B4:55:ARG:N	50:B4:56:VAL:HA	2.19	0.57
25:BA:1139:G:H3'	25:BA:1140:U:H5''	1.86	0.57
25:BA:70:A:N7	43:BX:31:HIS:HE1	2.02	0.57
1:CA:1244:C:N4	1:CA:1293:G:H1	2.00	0.57
2:CB:185:ILE:HG22	2:CB:199:TYR:HD2	1.69	0.57
7:CG:27:ILE:HD12	7:CG:40:ALA:HA	1.85	0.57
25:DA:2141:G:H2'	25:DA:2142:C:O4'	2.03	0.57
25:DA:2478:A:OP2	55:D9:2:LYS:NZ	2.28	0.57
35:DP:95:VAL:HA	35:DP:99:LEU:HD21	1.85	0.57
45:DZ:55:HIS:CE1	45:DZ:135:GLU:HB2	2.39	0.57
8:AH:73:ASP:OD1	8:AH:75:ARG:HD3	2.03	0.57
9:AI:24:GLY:HA2	9:AI:59:PHE:O	2.05	0.57
25:DA:2114:A:N6	25:DA:2115:G:H21	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1002:G:C4	1:AA:1003:G:H1'	2.38	0.57
2:AB:213:LEU:HD22	2:AB:214:ILE:HD13	1.86	0.57
25:BA:2340:A:H2'	25:BA:2341:G:C8	2.40	0.57
5:CE:43:LEU:HD21	5:CE:132:ALA:HB1	1.86	0.57
30:DG:137:GLU:HG2	30:DG:152:LEU:HD13	1.86	0.57
40:DU:49:HIS:HA	40:DU:52:ARG:HB3	1.86	0.57
23:AW:51:U:H2'	23:AW:52:G:C8	2.39	0.57
39:BT:51:ARG:HG3	39:BT:98:LYS:HD2	1.85	0.57
15:CO:5:LYS:N	15:CO:5:LYS:HD3	2.19	0.57
23:CW:2:C:N3	23:CW:71:G:O6	2.37	0.57
23:CW:4:C:N4	23:CW:69:G:H1	2.02	0.57
48:D2:65:ASN:OD1	48:D2:69:ARG:NH1	2.38	0.57
1:AA:1118:C:OP1	9:AI:104:ARG:NH1	2.37	0.57
3:AC:6:HIS:CD2	3:AC:8:ILE:H	2.22	0.57
25:BA:555:G:N1	25:BA:2045:G:OP1	2.24	0.57
25:BA:2735:G:OP2	61:BA:4257:HOH:O	2.17	0.57
10:CJ:5:ARG:N	10:CJ:99:LYS:O	2.37	0.57
25:DA:1037:G:H1	25:DA:1118:C:H42	1.52	0.57
17:AQ:45:HIS:NE2	17:AQ:47:PRO:HG3	2.20	0.57
25:BA:1633:A:H2'	25:BA:1634:C:C6	2.39	0.57
25:BA:2146:G:N2	25:BA:2196:C:N3	2.43	0.57
25:BA:2699:U:OP2	61:BA:4996:HOH:O	2.17	0.57
49:D3:7:LYS:HG3	49:D3:34:GLU:HG3	1.87	0.57
37:DR:44:LEU:HD22	37:DR:48:VAL:HG23	1.85	0.57
1:AA:838:G:H2'	1:AA:839:U:H2'	1.85	0.57
2:AB:100:GLY:N	2:AB:176:GLU:OE2	2.28	0.57
5:AE:43:LEU:HD21	5:AE:132:ALA:HB1	1.87	0.57
23:AW:19:G:H1	23:AW:56:C:H42	1.53	0.57
35:BP:116:GLY:O	35:BP:137:LYS:NZ	2.34	0.57
36:BQ:30:GLY:O	36:BQ:134:ARG:NH1	2.36	0.57
36:BQ:42:ILE:HD13	36:BQ:97:VAL:HB	1.85	0.57
1:CA:978:A:O2'	1:CA:1322:C:N3	2.31	0.57
23:CY:50:U:C2	23:CY:64:A:N1	2.73	0.57
25:DA:2128:C:H1'	25:DA:2173:A:O2'	2.05	0.57
25:DA:403:U:H4'	25:DA:404:C:H5'	1.87	0.57
29:DF:11:VAL:HG22	29:DF:125:LEU:HD13	1.86	0.57
29:DF:21:ALA:CB	29:DF:22:ALA:HA	2.35	0.57
45:DZ:19:ARG:NH1	45:DZ:84:GLU:O	2.37	0.57
1:AA:346:G:N1	1:AA:347:G:N3	2.53	0.57
8:AH:119:LEU:HB3	8:AH:123:GLU:HB3	1.86	0.57
23:AW:66:U:H2'	23:AW:67:C:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1140:U:H3	25:BA:1142:A:H3'	1.69	0.57
25:BA:2490:A:OP2	55:B9:2:LYS:NZ	2.32	0.57
28:BE:179:GLU:HB3	28:BE:181:LEU:HD22	1.87	0.57
30:BG:131:TYR:HB3	30:BG:159:VAL:HG13	1.86	0.57
24:CX:5:G:H1	24:CX:68:C:H42	1.52	0.57
25:DA:1364:G:N7	47:D1:3:LYS:HE2	2.20	0.57
25:DA:2103:C:H42	25:DA:2186:G:H1	1.52	0.57
36:DQ:34:LEU:HB2	36:DQ:118:LEU:HD22	1.87	0.57
5:AE:110:LEU:HD13	5:AE:118:ILE:HG21	1.85	0.57
13:AM:4:ILE:HG12	13:AM:5:ALA:HA	1.85	0.57
25:BA:1221:G:H1'	25:BA:1222:A:H5'	1.86	0.57
1:CA:1054:C:C4	23:CW:34:G:H1'	2.40	0.57
4:CD:162:LEU:HD13	4:CD:181:MET:HG2	1.85	0.57
25:DA:2122:U:H3	25:DA:2176:A:H2	1.51	0.57
25:DA:2023:G:H5'	25:DA:2617:C:H4'	1.86	0.57
25:DA:2693:A:H2'	25:DA:2694:G:C8	2.40	0.57
45:DZ:105:VAL:N	45:DZ:139:VAL:O	2.37	0.57
1:AA:1000:U:O4	1:AA:1041:A:N1	2.38	0.57
2:AB:19:HIS:NE2	2:AB:206:ASP:OD2	2.30	0.57
2:AB:97:TRP:HZ2	2:AB:102:LEU:HD13	1.70	0.57
13:AM:122:LYS:HD3	13:AM:123:ALA:H	1.69	0.57
27:BD:2:ALA:N	27:BD:200:ASP:OD2	2.38	0.57
29:DF:135:LYS:HG2	29:DF:137:LYS:NZ	2.20	0.57
33:DN:20:GLY:HA2	33:DN:61:ARG:HE	1.70	0.57
1:AA:60:A:H4'	1:AA:61:G:H5'	1.86	0.56
6:AF:82:ARG:HB3	6:AF:85:VAL:HG23	1.86	0.56
23:AY:12:U:H2'	23:AY:13:C:O4'	2.04	0.56
25:BA:2367:C:H1'	46:B0:39:ARG:HH21	1.70	0.56
35:BP:59:LEU:HD21	54:B8:10:ALA:HA	1.86	0.56
25:BA:2807:C:N4	25:BA:2813:G:H1	2.02	0.56
2:CB:131:PRO:O	2:CB:135:GLN:HB2	2.05	0.56
19:CS:30:LEU:HD11	19:CS:50:ALA:HB2	1.87	0.56
39:DT:16:ARG:NH1	39:DT:18:ASP:OD1	2.38	0.56
1:AA:67:C:H2'	1:AA:68:G:C8	2.40	0.56
25:BA:794:U:H4'	42:BW:92:ARG:HH22	1.71	0.56
25:DA:2892:A:H2'	25:DA:2893:G:H5'	1.85	0.56
26:DB:66:A:N6	26:DB:108:U:H3'	2.20	0.56
26:DB:57:A:H1'	30:DG:29:TRP:HB2	1.87	0.56
31:DH:56:SER:HB3	31:DH:61:HIS:ND1	2.19	0.56
8:AH:10:LEU:HD22	8:AH:83:ILE:HD11	1.87	0.56
10:AJ:17:ASP:OD1	10:AJ:70:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BF:53:THR:HG22	29:BF:55:GLY:H	1.69	0.56
1:CA:1239:A:H4'	1:CA:1240:U:H5''	1.88	0.56
1:CA:1348:U:H2'	1:CA:1349:A:H8	1.70	0.56
1:CA:828:A:OP1	8:CH:21:LYS:NZ	2.38	0.56
17:CQ:95:TYR:HA	17:CQ:98:LEU:HD12	1.85	0.56
25:DA:1019:U:H2'	25:DA:1020:A:C8	2.40	0.56
39:DT:24:PRO:HA	39:DT:49:VAL:HG22	1.87	0.56
15:AO:55:GLY:HA2	15:AO:58:MET:HE2	1.87	0.56
48:B2:59:ARG:NH2	61:B2:4003:HOH:O	2.38	0.56
25:BA:1100:A:H4'	25:BA:1100:A:OP1	2.05	0.56
25:BA:1117:G:O2'	25:BA:1135:G:H2'	2.06	0.56
28:BE:56:PRO:HG3	28:BE:74:PRO:HG2	1.86	0.56
29:BF:185:ASP:HA	29:BF:188:ARG:HD3	1.87	0.56
32:BI:131:LYS:HA	32:BI:137:PRO:HA	1.87	0.56
1:CA:1004:A:N6	1:CA:1037:C:C2	2.74	0.56
9:CI:110:GLU:OE2	9:CI:113:LYS:NZ	2.38	0.56
25:DA:1220:A:OP2	40:DU:19:LYS:NZ	2.33	0.56
47:B1:3:LYS:HB2	47:B1:61:ARG:HH12	1.69	0.56
25:BA:611:U:H2'	25:BA:612:C:C6	2.41	0.56
44:BY:18:GLY:O	44:BY:21:LYS:NZ	2.32	0.56
3:CC:71:ALA:HA	3:CC:106:VAL:HB	1.88	0.56
9:CI:9:ARG:O	9:CI:104:ARG:HG3	2.06	0.56
1:CA:1255:G:OP1	10:CJ:45:ARG:NH2	2.35	0.56
12:CL:117:ARG:HB3	12:CL:122:THR:O	2.04	0.56
25:DA:2291:U:H2'	25:DA:2292:C:C6	2.40	0.56
17:AQ:43:LEU:HD12	17:AQ:68:ARG:HG2	1.88	0.56
23:AW:50:U:H5'	23:AW:50:U:H6	1.70	0.56
23:AW:5:G:H2'	23:AW:6:G:H8	1.66	0.56
23:AY:19:G:H4'	23:AY:57:G:H22	1.69	0.56
23:AY:56:C:H2'	23:AY:57:G:O4'	2.06	0.56
26:BB:33:G:H5'	30:BG:2:PRO:HD3	1.87	0.56
1:CA:1064:G:O6	1:CA:1191:A:N6	2.39	0.56
25:DA:1183:G:H5''	49:D3:30:ARG:HH22	1.71	0.56
25:DA:108:U:H2'	25:DA:109:G:C8	2.40	0.56
1:AA:642:A:N3	8:AH:113:SER:OG	2.32	0.56
7:AG:79:ARG:HB3	7:AG:80:VAL:CG2	2.35	0.56
25:BA:1817:A:H1'	25:BA:1960:A:N6	2.21	0.56
25:BA:2303:U:OP1	25:BA:2392:C:O2'	2.23	0.56
1:CA:1305:G:N2	1:CA:1331:G:H1'	2.20	0.56
4:CD:157:LEU:O	4:CD:161:ASN:ND2	2.38	0.56
7:CG:113:GLU:CG	7:CG:119:ARG:HG2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:CS:28:LYS:HB3	19:CS:29:ARG:HA	1.88	0.56
50:D4:16:CYS:SG	50:D4:17:GLY:N	2.79	0.56
25:DA:400:G:N7	61:DA:4696:HOH:O	2.32	0.56
27:DD:17:THR:O	27:DD:211:ARG:NH2	2.35	0.56
1:AA:532:A:H2	1:AA:1206:G:H21	1.54	0.56
1:AA:96:U:O2'	1:AA:97:G:H8	1.83	0.56
29:BF:14:PRO:HD2	29:BF:127:GLU:OE2	2.06	0.56
41:BV:10:LYS:NZ	41:BV:23:GLU:OE2	2.38	0.56
1:CA:1151:A:O2'	1:CA:1152:A:H8	1.88	0.56
2:CB:73:THR:HA	2:CB:94:ASN:O	2.06	0.56
3:CC:43:LEU:HD21	3:CC:91:LEU:HD13	1.88	0.56
8:CH:14:ARG:HG2	8:CH:18:ARG:NH2	2.20	0.56
11:CK:85:ARG:HD3	11:CK:113:PRO:HD3	1.88	0.56
25:DA:1005:C:H2'	25:DA:1006:C:C6	2.40	0.56
38:DS:87:PHE:CE1	38:DS:102:ALA:HB2	2.41	0.56
7:AG:26:PHE:O	7:AG:30:ILE:HD12	2.05	0.56
23:AY:2:C:H42	23:AY:71:G:H1	1.53	0.56
52:B6:6:ARG:NH1	52:B6:26:ASN:HB2	2.21	0.56
25:BA:1159:U:H2'	25:BA:1160:G:C8	2.40	0.56
30:BG:16:ARG:HH21	30:BG:31:VAL:HG11	1.71	0.56
32:BI:72:LEU:C	32:BI:74:ASN:H	2.09	0.56
3:CC:152:ILE:HG23	3:CC:199:LYS:HB2	1.87	0.56
13:CM:91:ARG:HB2	13:CM:98:VAL:HG13	1.87	0.56
25:DA:2165:G:H2'	25:DA:2166:G:H5''	1.88	0.56
26:DB:103:G:N3	45:DZ:73:GLN:NE2	2.43	0.56
30:DG:32:PRO:HB3	30:DG:163:ALA:HB2	1.88	0.56
41:DV:40:LEU:HB2	41:DV:46:VAL:HG13	1.88	0.56
38:BS:10:ARG:O	38:BS:14:VAL:HG13	2.06	0.56
23:CY:19:G:C6	23:CY:56:C:N4	2.73	0.56
23:CY:19:G:C2	23:CY:56:C:N3	2.74	0.56
25:DA:1717:G:H2'	25:DA:1718:G:H8	1.70	0.56
25:DA:1799:G:O2'	27:DD:181:GLU:OE2	2.20	0.56
1:AA:438:G:O2'	1:AA:494:U:O4	2.20	0.56
25:BA:2298:A:H4'	25:BA:2299:A:O4'	2.06	0.56
2:CB:233:SER:HB2	2:CB:234:PRO:HD2	1.86	0.56
19:CS:27:GLU:HG2	19:CS:47:HIS:CE1	2.40	0.56
52:D6:6:ARG:NH1	52:D6:26:ASN:HB2	2.20	0.56
25:DA:1507:A:O2'	25:DA:1508:A:O5'	2.24	0.56
37:BR:96:ARG:NH2	37:BR:118:GLU:OE2	2.35	0.55
1:CA:1028:C:O2	1:CA:1033:G:C2	2.60	0.55
25:DA:2166:G:H3'	25:DA:2167:U:H5''	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2472:G:H2'	25:DA:2475:C:H42	1.70	0.55
45:DZ:52:SER:OG	45:DZ:53:ILE:N	2.26	0.55
1:AA:356:A:N3	1:AA:368:U:O2'	2.34	0.55
1:AA:38:G:N2	1:AA:397:A:H5''	2.19	0.55
2:AB:178:ARG:HH22	8:AH:68:ARG:NH1	2.04	0.55
25:BA:742:G:OP1	25:BA:1426:G:O2'	2.23	0.55
36:BQ:57:HIS:HD2	36:BQ:117:ALA:HB2	1.71	0.55
25:BA:2307:C:OP1	38:BS:10:ARG:NH1	2.39	0.55
8:CH:41:ARG:NH2	8:CH:123:GLU:OE2	2.38	0.55
25:DA:143:G:H4'	43:DX:35:THR:HG21	1.88	0.55
25:DA:2376:A:N3	38:DS:106:ARG:NH2	2.52	0.55
25:DA:2815:C:H5'	51:D5:29:THR:HG21	1.88	0.55
25:DA:307:G:N1	25:DA:310:A:OP2	2.35	0.55
1:AA:62:U:OP1	1:AA:385:C:O2'	2.23	0.55
2:AB:16:HIS:CG	2:AB:17:PHE:N	2.70	0.55
23:AY:36:A:H2'	23:AY:37:MIA:O4'	2.06	0.55
25:BA:1475:G:H2'	25:BA:1476:C:C6	2.40	0.55
25:BA:2482:G:OP1	36:BQ:56:ARG:NH2	2.39	0.55
38:BS:14:VAL:O	38:BS:18:ILE:HG12	2.07	0.55
1:CA:1239:A:H62	1:CA:1299:A:H62	1.52	0.55
1:CA:256:U:OP1	17:CQ:17:LYS:NZ	2.34	0.55
1:CA:646:U:H2'	1:CA:647:C:C6	2.42	0.55
3:CC:26:LYS:HG3	10:CJ:45:ARG:HH12	1.72	0.55
1:CA:1221:G:O3'	19:CS:77:THR:OG1	2.24	0.55
25:DA:902:C:H2'	25:DA:903:C:H6	1.71	0.55
38:DS:15:ARG:NE	38:DS:88:ASP:OD2	2.31	0.55
1:AA:346:G:C3'	1:AA:347:G:H4'	2.35	0.55
8:AH:29:SER:HB3	8:AH:32:LYS:HG3	1.88	0.55
19:AS:20:LEU:HD23	19:AS:23:ASN:HD22	1.70	0.55
20:AT:10:LEU:HB3	20:AT:12:ALA:H	1.70	0.55
23:AW:58:A:O2'	23:AW:60:U:OP2	2.19	0.55
23:AY:19:G:O4'	23:AY:57:G:N1	2.40	0.55
25:BA:1148:C:H2'	25:BA:1149:A:H8	1.72	0.55
25:BA:1298:G:OP1	40:BU:36:ARG:NH2	2.39	0.55
1:CA:1318:A:OP1	19:CS:3:ARG:NH2	2.38	0.55
1:CA:532:A:H2	1:CA:1206:G:H21	1.54	0.55
15:CO:17:ARG:HG3	15:CO:17:ARG:HH11	1.71	0.55
1:CA:450:G:OP1	16:CP:43:LYS:NZ	2.38	0.55
25:DA:108:U:H2'	25:DA:109:G:H8	1.70	0.55
25:DA:897:C:H3'	25:DA:898:C:C6	2.41	0.55
31:DH:6:ARG:HH21	31:DH:54:ARG:HH12	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1012:U:C5	33:DN:28:THR:HG21	2.40	0.55
1:AA:130:A:OP2	17:AQ:63:ARG:NE	2.39	0.55
1:AA:662:G:H2'	1:AA:663:A:C8	2.41	0.55
3:CC:52:LEU:HD11	3:CC:55:VAL:HG23	1.88	0.55
23:CY:9:A:H5'	23:CY:46:7MG:N3	2.22	0.55
25:DA:1359:A:H61	25:DA:1372:U:H3	1.55	0.55
17:AQ:9:VAL:HG13	17:AQ:56:VAL:HG22	1.87	0.55
23:AY:8:4SU:H1'	23:AY:48:C:H1'	1.88	0.55
25:BA:1217:G:O6	25:BA:1223:C:N4	2.22	0.55
2:CB:144:ARG:NH2	2:CB:148:TYR:OH	2.39	0.55
25:DA:1352:U:OP1	61:DA:4122:HOH:O	2.18	0.55
25:DA:2769:C:H2'	25:DA:2770:G:O4'	2.07	0.55
1:AA:1002:G:N1	1:AA:1004:A:O2'	2.38	0.55
11:AK:20:TYR:HB2	11:AK:31:THR:HG23	1.88	0.55
49:B3:3:ARG:NH1	49:B3:60:GLU:OE2	2.34	0.55
50:B4:16:CYS:SG	50:B4:17:GLY:N	2.79	0.55
25:BA:2138:G:H8	25:BA:2188:G:H22	1.55	0.55
25:BA:2695:C:OP1	39:BT:53:ARG:NH2	2.40	0.55
1:CA:1075:C:OP1	2:CB:179:LYS:NZ	2.31	0.55
1:CA:1299:A:H2'	1:CA:1299:A:N3	2.22	0.55
1:CA:538:G:H5''	12:CL:114:LYS:HB2	1.88	0.55
15:CO:5:LYS:O	15:CO:9:GLN:HG2	2.07	0.55
25:DA:1796:U:H2'	25:DA:1797:C:C6	2.42	0.55
1:AA:154:C:C2'	1:AA:155:C:H5'	2.37	0.55
2:AB:195:ASP:O	8:AH:68:ARG:NH2	2.30	0.55
25:BA:2798:C:OP1	28:BE:41:LYS:NZ	2.28	0.55
32:BI:109:ILE:HG13	32:BI:130:TYR:CZ	2.42	0.55
44:BY:92:ASN:N	44:BY:93:GLY:HA2	2.21	0.55
1:CA:942:G:H21	9:CI:124:GLN:HE22	1.54	0.55
23:CW:27:G:N2	23:CW:43:C:N3	2.48	0.55
25:DA:1778:U:H2'	25:DA:1784:A:N6	2.22	0.55
25:DA:1847:A:H3'	25:DA:1848:A:H5'	1.88	0.55
1:AA:1003:G:H21	1:AA:1038:C:H42	1.54	0.55
4:AD:107:ARG:HH22	4:AD:194:LEU:HD11	1.72	0.55
4:AD:173:TRP:CE3	4:AD:174:LEU:HG	2.42	0.55
5:AE:78:HIS:HD2	8:AH:107:LEU:HD12	1.72	0.55
19:AS:23:ASN:HA	19:AS:27:GLU:CD	2.26	0.55
23:AY:58:A:H2'	23:AY:60:U:OP2	2.06	0.55
25:BA:298:G:H2'	25:BA:299:G:C8	2.40	0.55
25:BA:493:G:OP1	53:B7:33:ARG:NH1	2.40	0.55
28:BE:111:ARG:HG3	28:BE:160:TYR:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BF:89:VAL:O	61:BF:406:HOH:O	2.18	0.55
1:CA:1028:C:C4	1:CA:1033:G:C6	2.94	0.55
1:CA:1060:C:N4	3:CC:2:GLY:HA2	2.22	0.55
3:CC:79:ARG:O	3:CC:82:GLU:HB2	2.06	0.55
25:DA:271(H):G:O2'	25:DA:271(I):G:OP2	2.25	0.55
41:DV:60:GLU:HB2	41:DV:97:LYS:HE2	1.87	0.55
43:DX:31:HIS:CD2	43:DX:33:LYS:H	2.16	0.55
1:AA:1272:G:H2'	1:AA:1273:G:O4'	2.06	0.55
1:AA:757:U:H2'	1:AA:758:G:O4'	2.07	0.55
1:AA:984:C:H42	1:AA:1221:G:H1	1.55	0.55
23:AY:33:U:H2'	23:AY:34:G:H5''	1.87	0.55
26:BB:105:A:OP1	45:BZ:72:ARG:NH1	2.40	0.55
1:CA:953:G:H5'	1:CA:965:A:N6	2.19	0.55
1:CA:973:G:H3'	1:CA:974:A:H5''	1.88	0.55
12:CL:117:ARG:NH2	12:CL:124:LYS:HG2	2.22	0.55
25:DA:330:A:H2	25:DA:1210:A:HO2'	1.56	0.55
25:DA:471:A:H2'	25:DA:472:A:O4'	2.07	0.55
39:DT:95:ARG:HG2	39:DT:95:ARG:HH11	1.72	0.55
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.42	0.54
1:AA:1457:G:OP1	20:AT:39:LYS:NZ	2.40	0.54
5:AE:102:ALA:O	5:AE:107:ARG:NH1	2.39	0.54
8:AH:51:VAL:HG12	8:AH:52:ASP:H	1.71	0.54
23:AW:76:A:H4'	25:BA:2518:U:O2'	2.06	0.54
49:B3:7:LYS:HG3	49:B3:34:GLU:HG3	1.89	0.54
25:BA:139:A:H8	25:BA:1454:C:O2'	1.90	0.54
25:BA:2603:C:H2'	25:BA:2604:G:C8	2.42	0.54
40:BU:58:ARG:HA	40:BU:61:TRP:CE3	2.41	0.54
3:CC:179:ARG:NH1	3:CC:206:GLU:OE1	2.40	0.54
19:CS:63:THR:OG1	19:CS:65:ASN:ND2	2.40	0.54
13:CM:3:ARG:HA	50:D4:34:GLU:HG2	1.88	0.54
25:DA:2357:U:OP1	46:D0:20:ARG:NH1	2.35	0.54
25:DA:2530:A:OP2	25:DA:2535:G:N2	2.40	0.54
2:AB:178:ARG:HH22	8:AH:68:ARG:HH12	1.53	0.54
25:BA:1114:G:H2'	25:BA:1115:A:O4'	2.06	0.54
27:BD:17:THR:O	27:BD:211:ARG:NH2	2.40	0.54
1:CA:45:U:H2'	1:CA:46:G:C8	2.42	0.54
25:DA:997:G:OP1	40:DU:92:ARG:HG2	2.08	0.54
19:AS:65:ASN:HD22	19:AS:65:ASN:N	2.05	0.54
25:BA:1452:U:H2'	25:BA:1453:C:C6	2.42	0.54
44:BY:6:HIS:H	44:BY:6:HIS:CD2	2.24	0.54
1:CA:1288:A:N1	1:CA:1371:G:H1'	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1116:C:H2'	25:DA:1117:G:C8	2.42	0.54
25:DA:885:C:H2'	25:DA:886:C:H4'	1.89	0.54
35:DP:59:LEU:HD21	54:D8:10:ALA:HA	1.89	0.54
37:DR:72:ASP:O	37:DR:76:VAL:HG23	2.07	0.54
1:AA:1292:U:P	7:AG:41:ARG:HH22	2.30	0.54
1:AA:625:G:H4'	16:AP:16:HIS:CD2	2.42	0.54
23:AY:5:G:H1'	23:AY:69:G:C2	2.42	0.54
25:BA:815:G:O2'	25:BA:1425:A:N1	2.35	0.54
32:BI:133:HIS:ND1	32:BI:134:PRO:O	2.40	0.54
1:CA:54:C:N4	1:CA:353:A:OP2	2.38	0.54
2:CB:178:ARG:HH22	8:CH:68:ARG:HH12	1.56	0.54
20:CT:53:LEU:HA	20:CT:56:MET:HG2	1.90	0.54
25:DA:2167:U:H2'	25:DA:2168:G:H21	1.71	0.54
25:DA:323:G:O2'	25:DA:1205:U:N3	2.37	0.54
25:DA:861:A:N3	26:DB:79:C:O2'	2.36	0.54
25:DA:864:G:OP2	36:DQ:22:LYS:HE3	2.08	0.54
1:CA:157:G:H1	1:CA:164:U:H3	1.54	0.54
9:CI:81:ILE:O	9:CI:85:LEU:HG	2.08	0.54
35:DP:121:LYS:O	35:DP:123:LEU:N	2.40	0.54
1:AA:1032:G:H2'	1:AA:1033:G:C8	2.42	0.54
1:AA:1149:C:H2'	1:AA:1150:U:C6	2.42	0.54
1:AA:1239:A:H4'	1:AA:1240:U:H5''	1.90	0.54
1:AA:1305:G:H22	1:AA:1331:G:H1'	1.72	0.54
4:AD:53:ASP:O	4:AD:57:ARG:HG3	2.07	0.54
25:BA:1717:C:OP1	61:BA:4143:HOH:O	2.18	0.54
25:BA:2339:A:H2'	25:BA:2340:A:C8	2.43	0.54
25:BA:2807:C:N3	25:BA:2813:G:N2	2.47	0.54
25:BA:354:A:H2	25:BA:1255:A:O2'	1.90	0.54
27:BD:164:GLN:NE2	27:BD:176:ARG:HH12	2.06	0.54
3:CC:138:VAL:HG23	3:CC:151:VAL:HG23	1.90	0.54
25:DA:2134:A:H2'	25:DA:2134:A:N3	2.23	0.54
25:DA:287:C:H2'	25:DA:288:C:H6	1.73	0.54
1:AA:202:U:O2'	1:AA:203:U:O5'	2.23	0.54
25:BA:1002:A:H5'	36:BQ:76:LYS:HG3	1.90	0.54
25:BA:2132:G:O2'	25:BA:2142:G:OP2	2.25	0.54
26:BB:7:G:H5''	26:BB:7:G:H8	1.73	0.54
1:CA:1028:C:N3	1:CA:1033:G:C5	2.74	0.54
4:CD:6:GLY:H	4:CD:115:ARG:HH12	1.56	0.54
4:CD:58:LEU:HD22	4:CD:62:GLN:HG2	1.90	0.54
13:CM:90:LEU:HD23	13:CM:93:ARG:HE	1.73	0.54
35:DP:63:PRO:HG2	54:D8:25:MET:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:116:C:H2'	25:DA:117:G:O4'	2.08	0.54
25:DA:2118:U:N3	25:DA:2149:G:H1'	2.22	0.54
25:DA:2650:U:H2'	25:DA:2651:C:C6	2.43	0.54
30:DG:19:LEU:HD13	30:DG:32:PRO:HG2	1.90	0.54
32:DI:104:GLN:O	32:DI:105:HIS:ND1	2.38	0.54
1:AA:346:G:N3	1:AA:347:G:H1'	2.22	0.54
18:AR:32:ARG:HA	18:AR:69:THR:HG21	1.89	0.54
49:B3:26:LEU:O	49:B3:35:ARG:NE	2.39	0.54
25:BA:794:U:O2	25:BA:2036:A:H1'	2.08	0.54
25:BA:215:G:H21	25:BA:217:A:H62	1.54	0.54
38:BS:61:ASN:HB3	38:BS:64:GLU:HB2	1.90	0.54
1:CA:396:G:O2'	1:CA:398:C:OP1	2.16	0.54
1:CA:93:G:O2'	1:CA:96:U:H5'	2.07	0.54
24:CX:50:U:H3	24:CX:64:G:H1	1.53	0.54
23:CY:50:U:N3	23:CY:64:A:N6	2.55	0.54
25:DA:1971:A:OP1	61:DA:4259:HOH:O	2.18	0.54
25:DA:236:C:H2'	25:DA:237:C:H6	1.72	0.54
25:DA:687:C:OP2	61:DA:4768:HOH:O	2.18	0.54
25:DA:878:A:N6	25:DA:899:A:O2'	2.41	0.54
32:DI:71:ILE:O	32:DI:75:LEU:HD13	2.08	0.54
1:AA:309:G:O2'	1:AA:607:A:N1	2.40	0.54
2:AB:59:GLU:HB2	2:AB:221:LEU:HD12	1.90	0.54
35:BP:50:ARG:HD3	54:B8:7:HIS:CD2	2.43	0.54
25:DA:1495:A:H2'	25:DA:1496:A:C8	2.43	0.54
25:DA:2630:G:H2'	25:DA:2631:G:C8	2.43	0.54
25:DA:296:C:O3'	44:DY:95:LYS:NZ	2.41	0.54
1:AA:1025:U:H3	1:AA:1036:G:H1	1.55	0.54
1:AA:974:A:OP1	1:AA:974:A:H8	1.91	0.54
32:BI:65:ALA:O	32:BI:69:LYS:N	2.38	0.54
1:CA:684:A:N6	61:CA:4138:HOH:O	2.40	0.54
16:CP:58:TYR:O	16:CP:61:SER:OG	2.19	0.54
1:CA:1456:G:O3'	20:CT:39:LYS:NZ	2.41	0.54
52:D6:14:THR:OG1	52:D6:48:VAL:O	2.26	0.54
55:D9:10:ILE:HD12	55:D9:32:HIS:HA	1.90	0.54
25:BA:2830:A:OP2	37:BR:2:ARG:NH2	2.41	0.53
32:BI:77:LEU:HB3	32:BI:142:VAL:HG12	1.88	0.53
9:CI:9:ARG:H	9:CI:79:LEU:HD23	1.73	0.53
1:CA:375:U:OP1	16:CP:69:THR:HG21	2.08	0.53
23:CW:21:A:N6	23:CW:46:7MG:C4	2.77	0.53
25:DA:1300:U:H4'	25:DA:1301:A:C5'	2.39	0.53
25:DA:882:G:H2'	25:DA:883:G:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DB:9:G:H1	26:DB:112:U:H3	1.54	0.53
39:DT:59:THR:HG23	39:DT:78:LEU:HB3	1.90	0.53
45:DZ:159:PRO:HA	45:DZ:161:VAL:N	2.23	0.53
1:AA:1008:C:N3	1:AA:1021:G:C2	2.76	0.53
1:AA:447:G:H2'	1:AA:485:G:N2	2.23	0.53
1:AA:527:G:O2'	1:AA:535:A:N1	2.31	0.53
4:AD:164:ALA:O	4:AD:168:ARG:HD3	2.07	0.53
25:BA:1044:C:P	40:BU:92:ARG:HH22	2.31	0.53
25:BA:484:G:O2'	25:BA:495:G:O6	2.25	0.53
25:BA:924:U:H2'	25:BA:925:A:H2	1.73	0.53
1:CA:328:C:H4'	1:CA:329:A:H5'	1.91	0.53
1:CA:93:G:C2'	1:CA:96:U:H5'	2.38	0.53
6:CF:23:LYS:HG2	6:CF:61:LEU:HD21	1.90	0.53
10:CJ:12:ASP:OD2	10:CJ:15:THR:HG23	2.08	0.53
20:CT:18:GLN:O	20:CT:22:ARG:HG3	2.08	0.53
27:DD:164:GLN:NE2	27:DD:176:ARG:HH22	2.05	0.53
25:DA:952:G:OP1	36:DQ:16:ARG:NH2	2.42	0.53
1:AA:1030(A):G:O2'	1:AA:1031:G:N1	2.41	0.53
1:AA:1136:U:H5''	1:AA:1137:C:C4	2.43	0.53
1:AA:117:G:OP2	61:AA:4254:HOH:O	2.19	0.53
1:AA:1399:C:C2	1:AA:1502:A:N6	2.77	0.53
23:AY:9:A:H4'	23:AY:46:7MG:OP2	2.07	0.53
25:BA:2152:U:O2'	25:BA:2180:A:N1	2.34	0.53
25:BA:236:G:H4'	25:BA:413:G:C5	2.43	0.53
25:BA:843:C:H2'	25:BA:844:C:C6	2.44	0.53
30:BG:5:VAL:HG22	30:BG:8:LYS:H	1.74	0.53
37:BR:118:GLU:H	37:BR:118:GLU:CD	2.10	0.53
38:BS:15:ARG:NE	38:BS:88:ASP:OD2	2.34	0.53
1:CA:1148:U:H2'	1:CA:1149:C:O4'	2.08	0.53
1:CA:1149:C:H2'	1:CA:1150:U:C6	2.43	0.53
1:CA:1249:C:O4'	9:CI:70:LYS:NZ	2.42	0.53
2:CB:15:VAL:HG13	2:CB:209:ARG:HB3	1.90	0.53
1:CA:1118:C:OP1	9:CI:104:ARG:NH1	2.42	0.53
24:CX:66:C:H2'	24:CX:67:C:O4'	2.08	0.53
23:CY:58:A:H1'	23:CY:60:U:H3	1.72	0.53
23:CY:52:G:O6	23:CY:62:C:N3	2.41	0.53
31:DH:69:ARG:HG3	31:DH:70:THR:N	2.23	0.53
43:DX:43:VAL:HG21	43:DX:81:VAL:HG11	1.91	0.53
1:AA:1275:A:C2'	1:AA:1276:G:H5'	2.38	0.53
11:AK:34:ASP:OD2	11:AK:38:ASN:HB2	2.09	0.53
25:BA:1014:U:H2'	25:BA:1015:C:C6	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2158:C:N3	25:BA:2177:G:C2	2.76	0.53
25:BA:265:U:H2'	25:BA:266:C:C6	2.43	0.53
27:BD:164:GLN:HE21	27:BD:176:ARG:HH12	1.56	0.53
2:CB:77:ALA:HA	2:CB:80:ILE:HG22	1.90	0.53
9:CI:8:GLY:O	9:CI:14:VAL:HA	2.08	0.53
1:CA:1152:A:OP1	10:CJ:70:ARG:NH2	2.42	0.53
23:CW:28:G:H2'	23:CW:29:G:O4'	2.08	0.53
24:CX:2:G:OP1	46:D0:5:LYS:NZ	2.38	0.53
25:DA:1713:U:H2'	25:DA:1714:G:H8	1.74	0.53
25:DA:1957:C:OP1	61:DA:4713:HOH:O	2.19	0.53
25:DA:315:G:H2'	25:DA:316:C:C6	2.44	0.53
25:DA:922:U:H2'	25:DA:923:C:C6	2.43	0.53
1:AA:841:U:C5	1:AA:848:C:H1'	2.44	0.53
1:AA:848:C:H2'	1:AA:849:C:H6	1.74	0.53
2:AB:95:GLN:OE1	2:AB:147:LYS:NZ	2.28	0.53
18:AR:58:LEU:HD12	18:AR:62:GLU:HB2	1.89	0.53
25:BA:390:G:H2'	25:BA:391:G:C8	2.44	0.53
1:CA:1192:C:OP1	3:CC:4:LYS:NZ	2.41	0.53
19:CS:52:TYR:HB2	19:CS:57:HIS:CE1	2.43	0.53
24:CX:15:G:H2'	24:CX:59:A:N1	2.24	0.53
25:DA:888:C:H5''	25:DA:889:C:OP2	2.07	0.53
26:DB:22:U:H3	26:DB:61:G:H1	1.56	0.53
30:DG:151:ALA:O	30:DG:153:ARG:NH1	2.41	0.53
1:AA:1239:A:H62	1:AA:1299:A:N6	2.06	0.53
53:B7:34:ARG:NH2	61:B7:201:HOH:O	2.41	0.53
25:BA:1077:G:H21	55:B9:36:GLN:HE22	1.57	0.53
25:BA:764:G:H2'	25:BA:765:A:O4'	2.08	0.53
25:BA:1001:G:H5''	36:BQ:77:LYS:HD2	1.90	0.53
4:CD:176:LEU:HD12	4:CD:182:LYS:O	2.08	0.53
12:CL:83:VAL:HG23	12:CL:107:ALA:HB2	1.90	0.53
25:DA:2022:U:O2'	25:DA:2617:C:H5'	2.09	0.53
26:DB:1:U:O2'	26:DB:2:C:O5'	2.20	0.53
27:DD:132:PRO:HG2	27:DD:135:PHE:HD2	1.72	0.53
25:DA:1817:G:OP1	27:DD:88:ARG:NH2	2.42	0.53
7:AG:48:LYS:O	7:AG:52:GLU:HG2	2.08	0.53
1:CA:56:U:H2'	1:CA:57:G:C8	2.43	0.53
1:CA:757:U:H2'	1:CA:758:G:O4'	2.09	0.53
10:CJ:42:THR:HG23	10:CJ:68:HIS:HA	1.91	0.53
13:CM:23:TYR:HB3	13:CM:67:GLU:HA	1.91	0.53
15:CO:6:GLU:OE2	15:CO:6:GLU:N	2.39	0.53
23:CY:18:G:N1	23:CY:55:PSU:C4	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:DG:46:ALA:HB2	30:DG:53:LEU:HG	1.91	0.53
32:DI:38:LEU:HD12	32:DI:38:LEU:H	1.73	0.53
1:AA:1027:C:C4	1:AA:1034:G:C6	2.89	0.53
3:AC:121:ALA:O	3:AC:125:GLU:HG3	2.09	0.53
25:BA:125:A:H5''	25:BA:126:C:C6	2.43	0.53
25:BA:2073:A:H5'	25:BA:2590:G:O4'	2.09	0.53
27:BD:20:ASP:OD2	27:BD:22:SER:OG	2.22	0.53
30:BG:106:LEU:HA	30:BG:110:ALA:HB3	1.91	0.53
1:CA:1121:U:C4	1:CA:1122:U:C4	2.97	0.53
6:CF:76:ALA:O	6:CF:80:ARG:HG3	2.08	0.53
12:CL:124:LYS:HD3	12:CL:125:PRO:HD2	1.91	0.53
23:CW:18:G:O2'	23:CW:57:G:N2	2.33	0.53
23:CW:50:U:H2'	23:CW:51:U:C6	2.44	0.53
25:DA:1250:G:OP2	35:DP:21:ARG:NH1	2.42	0.53
25:DA:1579:A:H2'	25:DA:1580:A:C8	2.43	0.53
25:DA:2121:G:N2	25:DA:2177:C:N3	2.46	0.53
37:DR:21:TYR:OH	37:DR:43:GLU:HG2	2.09	0.53
25:BA:1114:G:O2'	25:BA:1142:A:O2'	2.18	0.53
25:BA:2178:G:H8	25:BA:2178:G:OP2	1.92	0.53
25:BA:2486:C:OP2	25:BA:2487:C:N4	2.39	0.53
25:BA:387:G:H2'	25:BA:388:A:H8	1.74	0.53
41:BV:76:LYS:HB2	41:BV:81:TYR:HB3	1.90	0.53
1:CA:1002:G:C4	1:CA:1003:G:C8	2.97	0.53
1:CA:1435:G:H2'	1:CA:1436:U:C6	2.44	0.53
1:CA:838:G:H1	1:CA:848:C:N4	2.07	0.53
8:CH:46:LYS:HA	8:CH:64:LYS:HE3	1.90	0.53
15:CO:28:GLN:NE2	15:CO:66:LEU:HD21	2.24	0.53
23:CW:44:G:H2'	23:CW:45:U:H5'	1.90	0.53
25:DA:2135:A:H61	25:DA:2157:G:H21	1.56	0.53
25:DA:2137:C:H2'	25:DA:2138:C:H6	1.73	0.53
25:DA:2144:U:O2	25:DA:2148:G:N1	2.42	0.53
30:DG:64:THR:HB	30:DG:94:LEU:HD21	1.91	0.53
31:DH:106:THR:HG22	31:DH:112:PRO:HB3	1.91	0.53
1:AA:1179:A:H4'	9:AI:103:THR:HA	1.91	0.53
1:AA:159:G:O2'	1:AA:161:A:N7	2.33	0.53
2:AB:74:LYS:NZ	2:AB:206:ASP:OD1	2.34	0.53
23:AW:26:A:N1	23:AW:44:G:N2	2.52	0.53
25:BA:1716:A:H5''	25:BA:2562:G:OP1	2.09	0.53
1:CA:1179:A:H4'	9:CI:103:THR:HA	1.91	0.53
9:CI:26:VAL:HG13	9:CI:61:ALA:HB3	1.91	0.53
10:CJ:32:ALA:HB1	10:CJ:33:GLN:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1060:C:H5''	10:CJ:51:ARG:HB3	1.91	0.53
25:DA:2144:U:O2'	25:DA:2148:G:N2	2.42	0.53
28:DE:9:VAL:HG22	28:DE:25:VAL:HB	1.92	0.53
29:DF:150:GLY:HA2	29:DF:172:TRP:CE3	2.43	0.53
45:DZ:121:HIS:N	45:DZ:171:ILE:O	2.41	0.53
9:AI:23:ASN:HB2	9:AI:25:LYS:HE2	1.91	0.52
24:AX:66:C:H2'	24:AX:67:C:O4'	2.09	0.52
25:BA:278:G:OP1	47:B1:76:ARG:NH1	2.42	0.52
34:BO:59:LYS:NZ	34:BO:89:ASN:OD1	2.42	0.52
1:CA:141:A:H1'	1:CA:182:U:O2	2.09	0.52
2:CB:21:ARG:HA	2:CB:39:ILE:HD13	1.91	0.52
15:CO:28:GLN:HE21	15:CO:66:LEU:HD21	1.73	0.52
25:DA:1769:G:O2'	25:DA:1958:C:OP1	2.22	0.52
25:DA:2303:G:O2'	30:DG:132:ASN:ND2	2.39	0.52
1:AA:630:G:O2'	1:AA:631:G:H5'	2.09	0.52
25:BA:1845:G:H4'	27:BD:51:VAL:HG21	1.91	0.52
25:BA:2784:C:H2'	25:BA:2785:C:C6	2.44	0.52
1:CA:1151:A:H5''	10:CJ:41:PRO:HA	1.92	0.52
1:CA:200:G:H2'	1:CA:201:C:O4'	2.09	0.52
1:CA:976:G:OP1	14:CN:32:SER:N	2.38	0.52
45:DZ:77:ASP:N	45:DZ:82:ARG:O	2.36	0.52
3:AC:116:VAL:HG21	3:AC:202:ILE:HD11	1.91	0.52
5:AE:12:LEU:HB3	5:AE:31:LEU:HB2	1.91	0.52
13:AM:84:ILE:HG13	13:AM:85:GLY:CA	2.39	0.52
25:BA:671:A:H2'	25:BA:672:G:O4'	2.08	0.52
1:CA:1246:C:H2'	1:CA:1247:U:H6	1.74	0.52
1:CA:825:G:H21	8:CH:11:THR:HG21	1.73	0.52
18:CR:22:VAL:HB	18:CR:56:THR:HA	1.92	0.52
19:CS:13:ASP:HA	19:CS:16:LEU:HB3	1.91	0.52
25:DA:1607:C:N4	25:DA:1622:G:OP2	2.28	0.52
34:DO:115:VAL:HG13	34:DO:121:VAL:HG21	1.90	0.52
35:DP:38:GLN:O	35:DP:40:SER:N	2.38	0.52
35:DP:97:PRO:HD3	35:DP:126:VAL:O	2.10	0.52
23:AW:7:A:H61	23:AW:66:U:H3	1.57	0.52
25:BA:1067:A:H3'	25:BA:1067:A:C8	2.44	0.52
25:BA:1356:G:OP2	53:B7:9:ARG:HD2	2.09	0.52
25:BA:1735:U:O2	25:BA:1747:A:H5'	2.09	0.52
25:BA:2130:C:H2'	25:BA:2131:U:H6	1.75	0.52
25:BA:661:G:OP1	35:BP:132:LYS:HE2	2.09	0.52
31:BH:97:ARG:NE	31:BH:104:GLU:OE1	2.29	0.52
32:BI:100:ALA:HA	32:BI:103:ARG:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:353:A:H8	1:CA:353:A:H5'	1.74	0.52
4:CD:72:GLU:OE1	4:CD:207:TYR:OH	2.25	0.52
25:DA:1358:G:O2'	25:DA:1359:A:H5''	2.10	0.52
25:DA:2114:A:H62	25:DA:2115:G:H21	1.58	0.52
25:DA:2123:G:H1	25:DA:2175:C:H42	1.57	0.52
4:AD:107:ARG:NH2	4:AD:194:LEU:HD11	2.24	0.52
10:AJ:11:PHE:HE1	10:AJ:67:THR:HG22	1.75	0.52
23:AY:8:4SU:N3	23:AY:15:G:O6	2.43	0.52
25:BA:2186:C:H2'	25:BA:2187:G:H5'	1.91	0.52
25:BA:968:U:H2'	25:BA:969:C:C6	2.45	0.52
1:CA:986:A:H1'	19:CS:55:LYS:HA	1.90	0.52
13:CM:40:ASN:ND2	13:CM:41:PRO:HD2	2.24	0.52
20:CT:43:LEU:HD13	20:CT:51:GLU:HB3	1.92	0.52
25:DA:2037:G:H2'	25:DA:2038:G:C8	2.45	0.52
25:DA:2133:G:N2	25:DA:2157:G:H1'	2.23	0.52
25:DA:2142:C:N3	25:DA:2149:G:O6	2.42	0.52
25:DA:2239:G:OP2	61:DA:4263:HOH:O	2.19	0.52
25:DA:855:G:H2'	25:DA:856:C:C6	2.44	0.52
25:DA:890:A:H2'	25:DA:892:G:C8	2.44	0.52
7:AG:14:PRO:HG3	7:AG:21:VAL:HG13	1.91	0.52
12:AL:71:PRO:O	12:AL:102:ARG:NH1	2.41	0.52
6:AF:99:ALA:HB3	18:AR:29:PHE:CE1	2.40	0.52
25:BA:1466:U:HO2'	25:BA:1467:G:P	2.32	0.52
25:BA:510:C:H2'	25:BA:511:C:C6	2.45	0.52
39:BT:53:ARG:HH11	39:BT:53:ARG:HB3	1.75	0.52
1:CA:441:A:H5'	1:CA:442:C:OP2	2.10	0.52
3:CC:150:LYS:HB3	3:CC:201:TYR:HB2	1.92	0.52
11:CK:45:GLY:O	11:CK:50:TYR:HB2	2.10	0.52
25:DA:93:G:H2'	25:DA:94:C:C6	2.44	0.52
25:DA:784:A:C6	27:DD:229:VAL:HG11	2.45	0.52
35:DP:44:GLY:CA	35:DP:45:LEU:HB2	2.39	0.52
1:AA:1159:U:OP1	2:AB:133:LYS:NZ	2.39	0.52
1:AA:411:A:OP2	4:AD:25:ARG:NH2	2.43	0.52
7:AG:79:ARG:HB3	7:AG:80:VAL:HA	1.92	0.52
23:AY:19:G:C2	23:AY:56:C:N3	2.78	0.52
25:BA:615:G:O6	61:BA:5060:HOH:O	2.17	0.52
1:CA:1048:G:OP1	14:CN:3:ARG:NH2	2.40	0.52
1:CA:1087:G:N2	1:CA:1099:G:H1'	2.25	0.52
1:CA:1360:A:OP1	1:CA:1360:A:H8	1.92	0.52
1:CA:784:C:H4'	25:DA:1837:C:OP1	2.10	0.52
25:DA:1771:C:OP1	61:DA:4536:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2469:A:H5'	25:DA:2470:G:OP2	2.10	0.52
7:AG:46:ALA:O	7:AG:50:ILE:HG22	2.09	0.52
14:AN:24:CYS:HB2	14:AN:40:CYS:HB3	1.90	0.52
25:BA:1102:G:H5''	25:BA:1103:A:O4'	2.10	0.52
25:BA:2736:C:H4'	37:BR:1:MET:HG3	1.92	0.52
43:BX:31:HIS:CD2	43:BX:33:LYS:H	2.14	0.52
1:CA:1202:G:O4'	14:CN:29:ARG:NH1	2.42	0.52
1:CA:1352:C:H2'	1:CA:1353:G:C8	2.45	0.52
1:CA:473:G:H2'	1:CA:474:G:H8	1.75	0.52
1:CA:828:A:H5''	1:CA:859:A:C2	2.44	0.52
3:CC:113:ALA:N	3:CC:183:ASP:OD2	2.39	0.52
23:CY:15:G:N2	23:CY:48:C:H42	2.07	0.52
25:DA:2144:U:H1'	25:DA:2148:G:H22	1.75	0.52
25:DA:2787:C:H1'	28:DE:62:PRO:HG3	1.92	0.52
25:DA:883:G:C6	25:DA:884:C:C4	2.98	0.52
29:DF:129:PHE:CD2	29:DF:163:VAL:HG21	2.45	0.52
31:DH:24:VAL:HG22	31:DH:35:VAL:HB	1.91	0.52
35:DP:96:THR:H	35:DP:99:LEU:CD2	2.23	0.52
43:DX:53:LYS:HB3	43:DX:82:GLN:HB3	1.91	0.52
1:AA:442:C:H42	1:AA:492:G:H1	1.56	0.52
25:BA:1159:U:H2'	25:BA:1160:G:H8	1.73	0.52
25:BA:1451:U:H2'	25:BA:1452:U:C6	2.45	0.52
1:CA:1042:G:H2'	1:CA:1043:C:O4'	2.10	0.52
1:CA:1152:A:C5'	10:CJ:13:HIS:HB2	2.39	0.52
2:CB:167:PRO:HG2	2:CB:192:SER:HB2	1.91	0.52
2:CB:16:HIS:HB2	2:CB:204:ASN:CB	2.35	0.52
8:CH:10:LEU:HD22	8:CH:83:ILE:HD11	1.91	0.52
25:DA:1584:C:O2'	25:DA:1586:A:O5'	2.20	0.52
25:DA:184:C:H2'	25:DA:185:U:C6	2.45	0.52
25:DA:71:A:N7	43:DX:31:HIS:HE1	2.07	0.52
30:DG:106:LEU:O	30:DG:111:LEU:HD12	2.10	0.52
1:AA:78:G:O2'	1:AA:79:G:H8	1.84	0.52
9:AI:7:THR:O	9:AI:83:ARG:NH1	2.43	0.52
12:AL:53:ARG:NH1	12:AL:92:ASP:OD2	2.42	0.52
24:AX:19:G:H4'	24:AX:20:U:OP2	2.10	0.52
25:BA:551:A:O2'	25:BA:2065:C:O2	2.28	0.52
25:BA:2169:G:H3'	25:BA:2169:G:N3	2.25	0.52
1:CA:1134:G:H2'	1:CA:1135:U:H5'	1.92	0.52
2:CB:91:PRO:HG3	2:CB:154:LEU:HB2	1.92	0.52
4:CD:18:LYS:NZ	4:CD:31:CYS:SG	2.83	0.52
8:CH:24:THR:HG22	8:CH:63:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2815:C:H2'	25:DA:2816:C:H6	1.74	0.52
25:DA:668:G:H5'	25:DA:669:G:OP2	2.10	0.52
27:DD:142:VAL:HG13	27:DD:191:ALA:HB1	1.92	0.52
30:DG:115:ARG:CZ	30:DG:115:ARG:HB3	2.40	0.52
13:AM:15:VAL:HG22	13:AM:43:THR:O	2.10	0.51
25:BA:1091:A:OP1	25:BA:1092:A:H3'	2.10	0.51
1:CA:356:A:N3	1:CA:368:U:O2'	2.37	0.51
3:CC:6:HIS:HD2	3:CC:8:ILE:H	1.58	0.51
4:CD:157:LEU:HD22	4:CD:161:ASN:HD21	1.74	0.51
25:DA:1231:G:H2'	25:DA:1232:G:C8	2.44	0.51
25:DA:2507:C:H2'	25:DA:2508:G:O4'	2.10	0.51
25:DA:882:G:H2'	25:DA:883:G:H8	1.75	0.51
25:DA:887:A:H4'	25:DA:888:C:H5	1.74	0.51
27:DD:134:ARG:NH1	27:DD:188:GLU:OE2	2.43	0.51
28:DE:143:ASN:HD22	28:DE:147:PRO:HD3	1.75	0.51
28:DE:36:ARG:NH1	28:DE:85:ASN:OD1	2.44	0.51
1:AA:659:U:C2'	1:AA:660:G:H5'	2.40	0.51
25:BA:1140:U:N3	25:BA:1142:A:H3'	2.24	0.51
25:BA:1431:G:O2'	25:BA:1442:U:O2	2.24	0.51
25:BA:1552:C:H2'	25:BA:1553:A:H8	1.75	0.51
25:BA:553:A:OP1	61:BA:4814:HOH:O	2.19	0.51
25:BA:599:U:H2'	25:BA:600:G:C8	2.45	0.51
25:BA:718:C:N4	61:BA:5028:HOH:O	2.43	0.51
16:CP:18:ARG:HD3	16:CP:35:LYS:HD2	1.91	0.51
27:DD:69:ARG:NH2	27:DD:128:GLY:O	2.43	0.51
1:CA:1423:G:P	34:DO:49:ARG:HH12	2.33	0.51
1:AA:1002:G:C5	1:AA:1003:G:H1'	2.45	0.51
1:AA:154:C:H2'	1:AA:155:C:H5'	1.92	0.51
1:AA:250:A:H4'	1:AA:251:G:O5'	2.09	0.51
13:AM:80:ARG:NH2	19:AS:69:HIS:HE1	2.08	0.51
23:AY:18:G:O2'	23:AY:19:G:H5'	2.09	0.51
52:B6:10:LEU:HG	52:B6:54:ILE:HG13	1.91	0.51
25:BA:1898:A:H2'	25:BA:1899:A:C8	2.44	0.51
25:BA:1830:G:O2'	27:BD:181:GLU:OE2	2.20	0.51
1:CA:222:U:H2'	1:CA:223:U:C6	2.45	0.51
1:CA:344:A:H5''	1:CA:345:C:C5	2.44	0.51
15:CO:26:GLU:OE2	15:CO:77:ARG:NE	2.37	0.51
23:CW:51:U:H2'	23:CW:52:G:H8	1.75	0.51
23:CY:66:U:H2'	23:CY:67:C:O4'	2.10	0.51
25:DA:11:G:H2'	25:DA:12:U:H5'	1.93	0.51
25:DA:2183:C:H2'	25:DA:2184:G:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:947:G:H2'	25:DA:948:G:C8	2.45	0.51
29:DF:114:VAL:HG21	29:DF:202:PHE:CE1	2.46	0.51
30:DG:173:LEU:HD23	30:DG:176:LEU:HD12	1.92	0.51
32:DI:26:ALA:O	32:DI:31:LEU:HB2	2.11	0.51
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.92	0.51
35:BP:63:PRO:HG2	54:B8:25:MET:HB2	1.92	0.51
25:BA:2167:C:O2'	25:BA:2169:G:N7	2.38	0.51
1:CA:1095:U:H5''	1:CA:1109:C:O2	2.10	0.51
1:CA:922:G:N3	1:CA:1398:A:H2	2.08	0.51
2:CB:178:ARG:NH1	2:CB:196:LEU:O	2.43	0.51
2:CB:76:GLN:H	2:CB:76:GLN:CD	2.14	0.51
20:CT:50:GLU:HB2	20:CT:99:LEU:HD23	1.92	0.51
25:DA:1025:G:C4	25:DA:1135:C:H1'	2.45	0.51
25:DA:2646:C:H2'	25:DA:2647:U:O4'	2.10	0.51
25:DA:602:G:O2'	25:DA:655:A:N6	2.44	0.51
37:DR:33:ARG:NH1	37:DR:115:GLU:OE2	2.35	0.51
26:DB:92:C:H5''	45:DZ:79:ARG:NH1	2.25	0.51
1:AA:1036:G:N2	1:AA:1037:C:O2	2.44	0.51
9:AI:49:PRO:HG3	9:AI:101:PHE:CD2	2.46	0.51
19:AS:63:THR:OG1	19:AS:65:ASN:ND2	2.43	0.51
23:AY:3:C:H42	23:AY:70:G:H1	1.58	0.51
1:CA:1095:U:P	1:CA:1108:G:H1	2.34	0.51
1:CA:1218:C:H2'	1:CA:1219:U:C6	2.46	0.51
8:CH:82:HIS:NE2	8:CH:84:ARG:HG2	2.25	0.51
37:DR:87:TYR:OH	37:DR:116:LEU:HB3	2.10	0.51
19:AS:64:GLU:HB3	50:B4:59:PHE:CE1	2.45	0.51
25:BA:1133:G:H2'	25:BA:1135:G:C8	2.46	0.51
25:BA:1150:C:H2'	25:BA:1151:U:C6	2.46	0.51
25:BA:2156:A:N6	25:BA:2179:G:O2'	2.44	0.51
27:BD:68:LYS:HD3	27:BD:70:TRP:CZ2	2.46	0.51
25:BA:2885:C:O2'	39:BT:2:ASN:OD1	2.25	0.51
1:CA:1013:G:N2	1:CA:1016:A:OP2	2.43	0.51
11:CK:20:TYR:CZ	11:CK:83:ILE:HD12	2.46	0.51
25:DA:2110:G:H4'	25:DA:2111:C:OP2	2.10	0.51
1:AA:1030(C):G:H2'	1:AA:1030(D):A:C8	2.46	0.51
18:AR:31:LEU:HD12	18:AR:65:ILE:HB	1.92	0.51
20:AT:60:GLU:HG3	20:AT:81:LYS:HD2	1.92	0.51
25:BA:1634:C:H2'	25:BA:1635:C:H6	1.76	0.51
25:BA:2623:U:H6	25:BA:2623:U:H5'	1.76	0.51
32:BI:130:TYR:HB3	32:BI:138:ILE:HB	1.93	0.51
38:BS:25:ARG:HB3	38:BS:25:ARG:HH11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1041:A:H2'	1:CA:1042:G:C8	2.45	0.51
5:CE:74:GLY:HA3	5:CE:116:THR:HG22	1.92	0.51
7:CG:113:GLU:HG3	7:CG:119:ARG:HG2	1.93	0.51
25:DA:2031:A:N3	25:DA:2455:G:O2'	2.34	0.51
25:DA:2141:G:O6	25:DA:2150:U:C2	2.62	0.51
27:DD:108:PRO:HG2	27:DD:111:LEU:HB2	1.92	0.51
1:AA:1218:C:H2'	1:AA:1219:U:C6	2.46	0.51
1:AA:976:G:N2	1:AA:1363:C:OP2	2.40	0.51
16:AP:56:ALA:O	16:AP:60:LEU:HB2	2.10	0.51
46:B0:32:ARG:H	46:B0:35:ASN:ND2	2.09	0.51
25:BA:1137:G:C6	25:BA:1138:C:C4	2.99	0.51
25:BA:1118:C:C2	25:BA:1138:C:N4	2.79	0.51
33:BN:4:TYR:CD2	40:BU:100:VAL:HG11	2.46	0.51
37:BR:67:LEU:HD13	37:BR:76:VAL:HG21	1.91	0.51
40:BU:86:ALA:O	41:BV:49:THR:HG23	2.11	0.51
1:CA:192:U:H2'	1:CA:193:C:C6	2.46	0.51
50:D4:61:ARG:NH1	50:D4:62:ARG:O	2.44	0.51
25:DA:2139:C:H2'	25:DA:2140:C:O4'	2.11	0.51
25:DA:2208:A:O2'	25:DA:2218:U:OP2	2.28	0.51
30:DG:56:ALA:O	30:DG:60:LEU:HB2	2.11	0.51
36:DQ:52:VAL:HA	36:DQ:55:VAL:HG12	1.93	0.51
38:DS:35:ILE:HD12	38:DS:101:LEU:HD12	1.92	0.51
10:AJ:37:PRO:HA	10:AJ:72:VAL:HG12	1.92	0.51
25:BA:1700:G:H3'	37:BR:2:ARG:HD3	1.91	0.51
25:BA:2371:C:H2'	25:BA:2372:A:O4'	2.10	0.51
26:BB:13:A:N1	26:BB:69:G:O2'	2.37	0.51
2:CB:16:HIS:CB	2:CB:204:ASN:HB3	2.37	0.51
49:D3:7:LYS:HE3	49:D3:32:GLN:HG3	1.93	0.51
25:DA:1355:G:O6	61:DA:4423:HOH:O	2.18	0.51
25:DA:2149:G:C5	25:DA:2150:U:C2	2.99	0.51
25:DA:247:G:H4'	25:DA:386:G:C5	2.46	0.51
25:DA:528:A:C2	25:DA:2042:A:H2'	2.45	0.51
25:DA:796:C:H2'	25:DA:797:C:C6	2.46	0.51
38:DS:10:ARG:NE	38:DS:91:PRO:O	2.37	0.51
11:AK:99:GLN:HG2	11:AK:105:VAL:HG21	1.92	0.51
39:BT:95:ARG:NH1	39:BT:95:ARG:HG2	2.25	0.51
3:CC:77:ILE:O	3:CC:84:ILE:N	2.41	0.51
8:CH:113:SER:HB2	8:CH:134:ILE:HD11	1.92	0.51
25:DA:125:G:H1'	53:D7:48:LYS:HE2	1.92	0.51
25:DA:868:U:H2'	25:DA:869:G:O4'	2.11	0.51
27:DD:147:LEU:HD13	27:DD:155:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DO:120:GLU:HB2	39:DT:68:TYR:HE2	1.76	0.51
1:AA:1392:G:N2	1:AA:1502:A:H8	2.09	0.50
1:AA:222:U:H2'	1:AA:223:U:C6	2.46	0.50
2:AB:47:THR:HA	2:AB:202:PRO:HG2	1.93	0.50
23:AY:28:G:H1	23:AY:42:C:N4	2.08	0.50
25:BA:1827:U:H2'	25:BA:1828:C:C6	2.45	0.50
25:BA:715:G:H5'	25:BA:716:G:OP2	2.11	0.50
30:BG:41:GLN:NE2	30:BG:154:GLY:O	2.44	0.50
30:BG:48:GLU:HA	30:BG:51:ARG:NE	2.26	0.50
30:BG:9:ARG:O	30:BG:13:GLU:HG2	2.10	0.50
39:BT:56:GLY:O	39:BT:59:THR:HG22	2.11	0.50
44:BY:98:VAL:HG12	44:BY:105:ALA:HA	1.92	0.50
8:CH:20:TYR:HA	8:CH:65:TYR:CZ	2.46	0.50
23:CY:13:C:H2'	23:CY:14:A:H5''	1.93	0.50
25:DA:1580:A:H3'	25:DA:1581:G:H8	1.76	0.50
25:DA:866:A:H2	25:DA:867:C:C5	2.29	0.50
25:DA:1007:C:OP1	33:DN:35:ARG:NH1	2.37	0.50
1:AA:1124:G:OP1	10:AJ:36:GLY:N	2.40	0.50
1:AA:352:C:O2	1:AA:355:C:N4	2.45	0.50
2:AB:93:VAL:HG21	2:AB:97:TRP:CD1	2.46	0.50
9:AI:17:VAL:HG11	9:AI:80:GLY:C	2.31	0.50
50:B4:15:ILE:HD12	50:B4:21:VAL:HG22	1.93	0.50
31:BH:56:SER:HB3	31:BH:61:HIS:ND1	2.26	0.50
40:BU:17:ILE:HG13	40:BU:32:PHE:HE1	1.75	0.50
1:CA:1006:C:H2'	1:CA:1007:C:C6	2.47	0.50
1:CA:170:U:O2'	1:CA:171:A:H5'	2.11	0.50
1:CA:392:G:H2'	1:CA:393:A:H8	1.75	0.50
2:CB:16:HIS:HB3	2:CB:210:SER:CB	2.40	0.50
9:CI:16:ARG:HB2	9:CI:64:THR:HB	1.92	0.50
3:CC:37:GLN:NE2	14:CN:52:GLN:OE1	2.44	0.50
23:CY:15:G:H22	23:CY:48:C:N4	2.09	0.50
25:DA:536:A:H2'	25:DA:537:C:C6	2.46	0.50
25:DA:994:C:O2'	25:DA:996:A:OP1	2.17	0.50
44:DY:38:ILE:HD13	44:DY:66:PRO:HA	1.93	0.50
45:DZ:28:MET:HA	45:DZ:88:PHE:O	2.11	0.50
10:AJ:11:PHE:HB3	14:AN:55:GLY:HA3	1.91	0.50
23:AY:33:U:O2	23:AY:33:U:H2'	2.10	0.50
25:BA:1417:G:H2'	25:BA:1418:U:H5	1.76	0.50
1:AA:784:C:H4'	25:BA:1868:C:OP1	2.11	0.50
25:BA:2152:U:H2'	25:BA:2153:G:H21	1.77	0.50
38:BS:48:LEU:HD23	38:BS:82:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1163:C:N4	1:CA:1173:G:H1	2.07	0.50
1:CA:1376:U:H2'	1:CA:1377:A:C8	2.46	0.50
1:CA:297:G:N2	1:CA:300:A:OP2	2.43	0.50
10:CJ:37:PRO:HA	10:CJ:72:VAL:HG12	1.93	0.50
25:DA:321:G:OP2	29:DF:135:LYS:HG3	2.11	0.50
1:AA:501:C:H2'	1:AA:502:G:C8	2.46	0.50
1:AA:509:A:O2'	1:AA:510:A:OP1	2.25	0.50
2:AB:19:HIS:CD2	2:AB:20:GLU:HG3	2.47	0.50
3:AC:112:SER:HB3	3:AC:115:LEU:HB2	1.94	0.50
6:AF:91:VAL:HG11	18:AR:72:ARG:NH1	2.25	0.50
8:AH:17:THR:HG22	8:AH:63:LEU:HG	1.92	0.50
9:AI:55:ALA:HB1	9:AI:59:PHE:HD2	1.76	0.50
25:BA:1105:G:H2'	25:BA:1106:U:C5	2.46	0.50
1:CA:1412:C:H2'	1:CA:1413:A:C8	2.46	0.50
2:CB:9:GLU:O	2:CB:11:LEU:N	2.45	0.50
4:CD:25:ARG:NH1	4:CD:30:LYS:O	2.44	0.50
7:CG:132:GLY:O	7:CG:136:LYS:HG2	2.12	0.50
50:D4:42:PHE:HA	50:D4:48:ARG:HH22	1.75	0.50
25:DA:141:A:C8	25:DA:1408:C:O2'	2.65	0.50
25:DA:2119:A:H62	25:DA:2170:A:H62	1.59	0.50
25:DA:566:U:H5''	35:DP:29:LYS:HE3	1.92	0.50
33:DN:15:LEU:HB2	33:DN:135:PRO:HB2	1.92	0.50
17:AQ:18:THR:OG1	17:AQ:69:LYS:NZ	2.26	0.50
25:BA:1223:C:H2'	25:BA:1224:C:H6	1.77	0.50
25:BA:173:C:H2'	25:BA:174:U:C6	2.47	0.50
25:BA:821:A:H2'	25:BA:821:A:N3	2.27	0.50
27:BD:2:ALA:N	61:BD:415:HOH:O	2.44	0.50
28:BE:105:THR:OG1	28:BE:199:ARG:NH2	2.45	0.50
30:BG:150:ASP:OD1	30:BG:150:ASP:N	2.39	0.50
30:BG:151:ALA:O	30:BG:153:ARG:NH1	2.44	0.50
31:BH:40:GLU:O	31:BH:55:PRO:HG3	2.11	0.50
26:BB:106:G:C5'	45:BZ:31:ARG:HG2	2.40	0.50
1:CA:1226:C:H4'	19:CS:80:TYR:CZ	2.47	0.50
1:CA:537:G:H2'	1:CA:538:G:C8	2.47	0.50
23:CY:62:C:H2'	23:CY:63:G:C8	2.47	0.50
25:DA:422:A:H2'	25:DA:423:A:C8	2.46	0.50
25:DA:636:G:O2'	25:DA:638:G:O2'	2.27	0.50
25:DA:646:A:H2'	25:DA:647:G:O4'	2.11	0.50
1:AA:1318:A:H5''	19:AS:3:ARG:HH12	1.76	0.50
1:AA:946:A:H2'	1:AA:947:G:C8	2.46	0.50
2:AB:48:MET:HA	2:AB:51:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:B4:15:ILE:HB	50:B4:32:TYR:CD1	2.44	0.50
25:BA:1634:C:H2'	25:BA:1635:C:C6	2.47	0.50
25:BA:942:A:H4'	25:BA:943:C:OP1	2.10	0.50
1:CA:1039:C:N4	1:CA:1040:U:C4	2.80	0.50
46:D0:70:GLN:OE1	46:D0:80:HIS:NE2	2.44	0.50
25:DA:1270:C:H5''	25:DA:1271:G:O5'	2.11	0.50
25:DA:493:G:H2'	25:DA:494:G:O4'	2.12	0.50
23:AW:18:G:O2'	23:AW:57:G:N2	2.30	0.50
23:AY:20:U:H4'	23:AY:21:A:OP1	2.10	0.50
25:BA:1170:C:OP1	61:BA:5067:HOH:O	2.20	0.50
25:BA:1806:U:OP1	25:BA:2001:C:O2'	2.24	0.50
25:BA:2359:C:H2'	25:BA:2360:U:C6	2.47	0.50
27:BD:148:GLU:HB2	27:BD:151:LYS:HD2	1.93	0.50
32:BI:106:GLY:HA2	32:BI:107:VAL:O	2.12	0.50
37:BR:53:HIS:O	37:BR:56:LYS:HB2	2.12	0.50
1:CA:250:A:H4'	1:CA:251:G:O5'	2.11	0.50
4:CD:15:GLU:OE2	4:CD:66:ARG:NH1	2.44	0.50
31:DH:98:LEU:HD13	31:DH:102:ALA:O	2.12	0.50
35:DP:82:GLY:HA2	35:DP:113:LYS:O	2.11	0.50
44:DY:44:ILE:HA	44:DY:63:LYS:O	2.11	0.50
1:AA:161:A:O5'	1:AA:161:A:H8	1.95	0.50
1:AA:973:G:H3'	1:AA:974:A:H5''	1.93	0.50
2:AB:212:GLN:NE2	2:AB:234:PRO:O	2.45	0.50
23:AY:32:PSU:C2	23:AY:33:U:H5	2.30	0.50
47:B1:89:GLU:O	47:B1:93:GLU:HG2	2.12	0.50
25:BA:1566:U:H2'	25:BA:1567:G:O4'	2.12	0.50
25:BA:2576:A:C2	25:BA:2659:U:H4'	2.47	0.50
32:BI:38:LEU:HD12	32:BI:38:LEU:H	1.77	0.50
45:BZ:92:SER:OG	45:BZ:93:ASP:N	2.45	0.50
1:CA:1227:A:OP2	13:CM:111:LYS:NZ	2.33	0.50
51:D5:16:ARG:HG3	51:D5:17:ASP:N	2.26	0.50
35:DP:86:LYS:HB3	35:DP:118:GLY:HA3	1.93	0.50
25:DA:1335:U:OP1	43:DX:65:ARG:NH2	2.45	0.50
45:DZ:6:LYS:HD2	45:DZ:8:TYR:CE1	2.47	0.50
1:AA:1510:U:H2'	1:AA:1511:G:C8	2.46	0.50
1:AA:346:G:C2	1:AA:347:G:H1'	2.47	0.50
25:BA:1085:G:H1	25:BA:1162:C:H42	1.60	0.50
1:CA:1034:G:H3'	1:CA:1035:A:C8	2.47	0.50
19:CS:77:THR:HG22	19:CS:78:ARG:HG2	1.94	0.50
25:DA:1341:U:OP2	25:DA:1394:U:O2'	2.25	0.50
25:DA:1354:A:H2'	25:DA:1355:G:O4'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:212:G:H2'	25:DA:213:A:O4'	2.12	0.50
25:DA:829:A:N7	25:DA:2248:C:H5'	2.27	0.50
25:DA:2352:A:N6	25:DA:2365:G:O2'	2.44	0.50
35:DP:3:LEU:HD13	35:DP:6:LEU:HD12	1.93	0.50
1:AA:130:A:H5'	17:AQ:63:ARG:HE	1.77	0.49
3:AC:36:ASP:O	3:AC:40:ARG:HG3	2.11	0.49
16:AP:18:ARG:HD3	16:AP:35:LYS:HD2	1.94	0.49
48:B2:18:PRO:O	48:B2:22:GLU:HG3	2.12	0.49
25:BA:1108:G:H5''	25:BA:1116:A:H5''	1.93	0.49
25:BA:83:A:H5''	44:BY:8:LYS:HE3	1.94	0.49
1:CA:1051:C:H2'	1:CA:1052:U:C6	2.47	0.49
1:CA:1053:G:N7	1:CA:1200:C:H5''	2.26	0.49
3:CC:131:ARG:NH1	5:CE:50:GLU:HG3	2.25	0.49
3:CC:43:LEU:HD11	3:CC:91:LEU:HD11	1.94	0.49
25:DA:855:G:O2'	46:D0:27:GLU:OE2	2.30	0.49
47:D1:5:CYS:SG	47:D1:62:VAL:HG23	2.51	0.49
25:DA:1683:C:H2'	25:DA:1684:C:C6	2.47	0.49
25:DA:1717:G:H2'	25:DA:1718:G:C8	2.47	0.49
25:DA:2117:A:O2'	25:DA:2118:U:H5''	2.11	0.49
25:DA:2149:G:H3'	25:DA:2150:U:O4'	2.11	0.49
25:DA:2206:G:H3'	25:DA:2207:G:N7	2.27	0.49
25:DA:2849:U:H4'	25:DA:2868:A:C2	2.46	0.49
36:DQ:56:ARG:O	36:DQ:56:ARG:HD3	2.12	0.49
37:DR:56:LYS:NZ	37:DR:90:ARG:O	2.44	0.49
1:AA:749:C:H2'	1:AA:750:G:H8	1.77	0.49
5:AE:152:ARG:NH2	8:AH:107:LEU:O	2.46	0.49
14:AN:23:ARG:NH1	14:AN:30:ALA:HB2	2.26	0.49
20:AT:99:LEU:HA	20:AT:100:ILE:O	2.12	0.49
25:BA:1425:A:H4'	25:BA:1426:G:OP2	2.12	0.49
1:CA:1103:C:P	2:CB:96:ARG:HH22	2.34	0.49
1:CA:918:A:H2'	1:CA:919:A:O4'	2.13	0.49
3:CC:115:LEU:O	3:CC:118:GLN:HG2	2.12	0.49
50:D4:64:GLY:C	50:D4:66:SER:H	2.15	0.49
25:DA:729:G:H5'	25:DA:730:C:H5''	1.94	0.49
27:DD:108:PRO:HB3	27:DD:143:HIS:CE1	2.47	0.49
30:DG:11:TYR:CZ	30:DG:16:ARG:HD3	2.47	0.49
1:AA:1030(C):G:N7	1:AA:1031:G:N2	2.59	0.49
1:AA:767:A:H2'	1:AA:768:A:O4'	2.11	0.49
3:AC:87:LEU:O	3:AC:91:LEU:N	2.44	0.49
5:AE:91:LEU:HD12	5:AE:120:THR:HG22	1.93	0.49
13:AM:32:GLU:HG3	13:AM:33:ALA:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AY:19:G:C4'	23:AY:57:G:H22	2.25	0.49
25:BA:1140:U:H2'	25:BA:1142:A:N7	2.28	0.49
1:CA:1285:A:H4'	1:CA:1286:A:O5'	2.12	0.49
2:CB:91:PRO:HA	2:CB:151:GLY:O	2.12	0.49
3:CC:122:GLU:HA	3:CC:125:GLU:OE2	2.11	0.49
14:CN:26:ARG:NH2	14:CN:47:LEU:HD21	2.27	0.49
25:DA:1996:C:H4'	25:DA:1997:G:OP1	2.12	0.49
30:DG:126:ASP:OD1	30:DG:130:ASN:ND2	2.39	0.49
32:DI:133:HIS:HD2	32:DI:134:PRO:HD2	1.77	0.49
40:DU:86:ALA:O	41:DV:49:THR:HG23	2.12	0.49
1:AA:1251:A:H2'	1:AA:1252:A:C8	2.46	0.49
6:AF:86:ARG:O	6:AF:87:ARG:HG2	2.11	0.49
25:BA:2331:G:N2	38:BS:3:ARG:HA	2.27	0.49
25:BA:757:G:H2'	25:BA:758:G:H8	1.77	0.49
1:CA:1136:U:OP2	1:CA:1137:C:N4	2.46	0.49
1:CA:1176:A:H2'	1:CA:1177:G:O4'	2.12	0.49
1:CA:447:G:O6	1:CA:485:G:O2'	2.23	0.49
28:DE:14:ILE:HG13	28:DE:21:VAL:HG13	1.94	0.49
38:DS:15:ARG:HE	38:DS:88:ASP:CG	2.15	0.49
1:AA:1064:G:H1'	1:AA:1190:G:N2	2.28	0.49
1:AA:436:C:H2'	1:AA:437:U:H6	1.78	0.49
1:AA:943:U:H2'	1:AA:944:G:H5'	1.95	0.49
6:AF:19:LEU:HD21	6:AF:59:TYR:CE1	2.48	0.49
19:AS:42:PRO:HD3	50:B4:61:ARG:HH21	1.77	0.49
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.94	0.49
23:AW:19:G:N2	23:AW:56:C:N3	2.61	0.49
25:BA:1405:A:H2'	25:BA:1406:A:H5'	1.93	0.49
25:BA:1958:A:OP1	25:BA:1959:A:H5'	2.12	0.49
25:BA:957:A:H2'	36:BQ:9:TYR:OH	2.12	0.49
27:BD:68:LYS:HD3	27:BD:70:TRP:CH2	2.47	0.49
1:CA:152:A:N6	1:CA:169:C:N3	2.58	0.49
2:CB:48:MET:HA	2:CB:51:LEU:HD12	1.94	0.49
8:CH:119:LEU:HD13	8:CH:127:LEU:HD23	1.94	0.49
25:DA:1359:A:N6	25:DA:1372:U:H3	2.10	0.49
25:DA:811:U:H2'	35:DP:21:ARG:HA	1.94	0.49
31:DH:97:ARG:O	31:DH:103:LEU:HD12	2.12	0.49
35:DP:42:SER:O	61:DP:303:HOH:O	2.20	0.49
1:AA:1027:C:H3'	1:AA:1028:C:C6	2.47	0.49
1:AA:49:U:O4	1:AA:365:U:H5	1.95	0.49
1:AA:625:G:H2'	1:AA:626:U:C6	2.48	0.49
25:BA:2209:G:H2'	25:BA:2210:C:O4'	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2227:G:H8	25:BA:2228:G:N7	2.11	0.49
1:CA:1009:G:N2	1:CA:1010:G:H1'	2.27	0.49
1:CA:1347:G:N2	1:CA:1373:G:H2'	2.27	0.49
8:CH:73:ASP:OD1	8:CH:75:ARG:HD3	2.11	0.49
14:CN:24:CYS:HB2	14:CN:40:CYS:HB3	1.95	0.49
23:CY:23:A:H2'	23:CY:24:G:H5''	1.94	0.49
23:CY:58:A:N3	23:CY:60:U:N3	2.60	0.49
25:DA:1231:G:H2'	25:DA:1232:G:H8	1.78	0.49
25:DA:1263:U:C4	25:DA:1264:G:C6	3.01	0.49
25:DA:236:C:H2'	25:DA:237:C:C6	2.48	0.49
27:DD:108:PRO:HB3	27:DD:143:HIS:HE1	1.78	0.49
29:DF:7:TYR:O	29:DF:22:ALA:N	2.44	0.49
35:DP:63:PRO:HD3	54:D8:27:THR:HG22	1.94	0.49
43:DX:84:ALA:HB3	43:DX:87:GLN:NE2	2.28	0.49
25:BA:1525:G:O2'	25:BA:1605:A:N1	2.46	0.49
25:BA:2418:U:OP1	25:BA:2423:A:N6	2.46	0.49
25:BA:2827:G:OP1	37:BR:99:LYS:HE2	2.13	0.49
25:BA:559:U:H2'	25:BA:560:C:C6	2.47	0.49
25:BA:930:G:N2	25:BA:939:C:O2	2.45	0.49
1:CA:1024:G:H2'	1:CA:1024:G:N3	2.27	0.49
25:DA:441:U:H2'	25:DA:442:G:C8	2.47	0.49
32:DI:130:TYR:HB3	32:DI:138:ILE:HB	1.95	0.49
39:DT:51:ARG:HG3	39:DT:98:LYS:HD2	1.94	0.49
42:DW:71:VAL:HA	42:DW:107:LEU:HD12	1.94	0.49
1:AA:1077:G:N2	1:AA:1080:A:OP2	2.44	0.49
2:AB:211:ILE:O	2:AB:215:LEU:HB2	2.12	0.49
25:BA:1221:G:H1'	25:BA:1222:A:C5'	2.42	0.49
25:BA:1480:A:H2'	25:BA:1481:G:C8	2.48	0.49
25:BA:1552:C:H2'	25:BA:1553:A:C8	2.48	0.49
25:BA:2584:A:N7	28:BE:145:LYS:HB2	2.28	0.49
25:BA:2874:G:OP1	39:BT:119:LYS:HE3	2.13	0.49
41:BV:1:MET:HB2	41:BV:43:GLU:OE2	2.12	0.49
1:CA:646:U:H2'	1:CA:647:C:H6	1.76	0.49
6:CF:69:GLU:O	6:CF:72:VAL:HG12	2.13	0.49
9:CI:28:VAL:HG22	9:CI:63:ILE:HB	1.93	0.49
9:CI:89:ASN:O	9:CI:92:TYR:HB2	2.13	0.49
23:CY:2:C:N3	23:CY:71:G:O6	2.46	0.49
54:D8:6:THR:HG22	54:D8:63:PRO:HD2	1.95	0.49
25:DA:857:C:OP2	46:D0:77:ARG:NH2	2.46	0.49
26:DB:58:A:H2'	26:DB:59:A:O4'	2.13	0.49
1:AA:36:C:OP1	12:AL:123:LYS:NZ	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:454:C:H3'	1:AA:455:C:C6	2.47	0.49
1:AA:711:G:OP1	6:AF:54:LYS:NZ	2.42	0.49
13:AM:3:ARG:HG2	13:AM:8:GLU:HA	1.94	0.49
20:AT:86:ARG:C	20:AT:90:GLN:HE22	2.17	0.49
25:BA:137:G:O2'	25:BA:138:G:H5'	2.13	0.49
25:BA:2348:A:H61	46:B0:43:THR:HG22	1.78	0.49
25:BA:670:C:H5'	25:BA:671:A:OP2	2.12	0.49
32:BI:61:ARG:HH12	32:BI:64:GLU:HG3	1.78	0.49
33:BN:62:VAL:HG22	33:BN:66:LYS:HD2	1.94	0.49
34:BO:2:ILE:HD12	34:BO:6:THR:HG21	1.95	0.49
1:CA:1168:A:C6	1:CA:1169:A:C6	3.00	0.49
1:CA:1262:C:H2'	1:CA:1263:C:H6	1.78	0.49
1:CA:1359:C:H1'	1:CA:1362:C:H41	1.78	0.49
2:CB:162:ILE:HD11	2:CB:184:VAL:HG22	1.94	0.49
12:CL:60:LEU:HD21	12:CL:66:VAL:HG22	1.93	0.49
7:AG:44:TYR:HE2	9:AI:41:VAL:HG11	1.78	0.49
7:AG:79:ARG:HB3	7:AG:80:VAL:CA	2.42	0.49
10:AJ:7:LYS:HE2	10:AJ:9:ARG:HH12	1.78	0.49
14:AN:26:ARG:NH1	14:AN:46:GLU:OE2	2.44	0.49
1:AA:1312:G:H5'	19:AS:5:LEU:HD21	1.94	0.49
25:BA:1477:U:H2'	25:BA:1478:C:C6	2.48	0.49
29:BF:89:VAL:HG12	29:BF:90:PHE:CD2	2.48	0.49
38:BS:5:THR:OG1	38:BS:8:GLU:HG3	2.13	0.49
43:BX:94:GLY:CA	43:BX:95:LEU:HB2	2.42	0.49
1:CA:49:U:O4	1:CA:365:U:H5	1.96	0.49
19:CS:30:LEU:HA	19:CS:48:THR:O	2.13	0.49
19:CS:51:VAL:O	19:CS:58:VAL:N	2.35	0.49
36:DQ:81:VAL:HG12	46:D0:5:LYS:HD3	1.94	0.49
25:DA:1784:A:O2'	61:DA:4872:HOH:O	2.15	0.49
25:DA:2099:U:H3	25:DA:2190:G:H1	1.61	0.49
25:DA:2124:G:N2	25:DA:2174:C:N3	2.51	0.49
25:DA:874:G:H5'	25:DA:875:G:OP2	2.12	0.49
26:DB:40:U:H1'	26:DB:45:A:H61	1.78	0.49
29:DF:113:ALA:HB1	29:DF:186:ILE:HG21	1.94	0.49
36:DQ:77:LYS:NZ	36:DQ:86:GLY:O	2.46	0.49
1:AA:1030(C):G:H2'	1:AA:1030(D):A:H8	1.78	0.48
1:AA:953:G:H5'	1:AA:965:A:N6	2.24	0.48
1:AA:955:U:O2'	19:AS:83:HIS:HD2	1.96	0.48
2:AB:97:TRP:CZ2	2:AB:102:LEU:HD13	2.48	0.48
6:AF:69:GLU:O	6:AF:72:VAL:HG12	2.13	0.48
1:AA:1202:G:H1'	14:AN:29:ARG:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:376:G:C5'	16:AP:5:ARG:HG2	2.42	0.48
19:AS:80:TYR:CZ	19:AS:82:GLY:HA2	2.47	0.48
25:BA:1289:G:O2'	35:BP:7:ARG:NH2	2.45	0.48
25:BA:2169:G:H2'	25:BA:2170:G:O4'	2.13	0.48
25:BA:2389:A:H2'	25:BA:2390:A:C8	2.48	0.48
25:BA:2658:C:H2'	25:BA:2659:U:O4'	2.13	0.48
25:BA:2860:A:OP2	25:BA:2876:U:H5	1.94	0.48
25:BA:30:G:H2'	25:BA:31:C:C6	2.48	0.48
1:CA:1360:A:H2'	1:CA:1361:G:O4'	2.13	0.48
2:CB:120:ALA:C	2:CB:122:PHE:H	2.14	0.48
2:CB:71:VAL:HB	2:CB:164:VAL:HG13	1.94	0.48
1:CA:750:G:H1'	15:CO:22:THR:OG1	2.12	0.48
50:D4:15:ILE:HB	50:D4:32:TYR:HD1	1.77	0.48
25:DA:2137:C:H2'	25:DA:2138:C:C6	2.48	0.48
30:DG:115:ARG:HD2	30:DG:136:ARG:NH2	2.24	0.48
26:DB:55:U:H1'	30:DG:29:TRP:HE1	1.77	0.48
5:AE:144:THR:O	5:AE:148:VAL:HG23	2.12	0.48
9:AI:55:ALA:HB1	9:AI:59:PHE:CD2	2.47	0.48
25:BA:469:A:H1'	25:BA:1246:C:O4'	2.12	0.48
25:BA:1993:A:OP2	27:BD:242:ARG:NH2	2.40	0.48
25:BA:2856:G:H2'	25:BA:2857:U:O4'	2.13	0.48
1:CA:1012:U:H2'	1:CA:1013:G:C8	2.48	0.48
21:CU:12:LYS:HZ1	21:CU:19:GLY:HA3	1.78	0.48
23:CY:44:G:C2'	23:CY:45:U:H5'	2.44	0.48
28:DE:24:THR:HG22	28:DE:186:GLY:O	2.13	0.48
25:DA:801:G:O6	29:DF:53:THR:OG1	2.30	0.48
31:DH:40:GLU:O	31:DH:55:PRO:HG3	2.13	0.48
1:AA:1258:G:O2'	1:AA:1259:C:H5'	2.14	0.48
1:AA:45:U:H2'	1:AA:46:G:C8	2.48	0.48
4:AD:88:VAL:HG22	5:AE:97:GLY:HA2	1.95	0.48
9:AI:128:ARG:NH2	24:AX:33:U:OP2	2.45	0.48
23:AY:53:G:N2	23:AY:61:C:N3	2.58	0.48
53:B7:12:ARG:NH2	53:B7:44:PRO:HB3	2.27	0.48
25:BA:1829:U:H5'	27:BD:259:THR:CG2	2.36	0.48
29:BF:150:GLY:HA2	29:BF:172:TRP:CE3	2.48	0.48
1:CA:1002:G:N3	1:CA:1003:G:C8	2.81	0.48
1:CA:1352:C:OP1	21:CU:3:LYS:NZ	2.36	0.48
1:CA:692:U:O2'	1:CA:694:A:N7	2.25	0.48
2:CB:144:ARG:O	2:CB:147:LYS:HB3	2.13	0.48
2:CB:230:VAL:HG22	2:CB:231:GLU:H	1.77	0.48
6:CF:68:PRO:HG2	6:CF:71:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CF:9:VAL:HB	6:CF:87:ARG:HB2	1.94	0.48
35:DP:2:LYS:HG2	35:DP:5:ASP:OD2	2.12	0.48
45:DZ:130:PRO:HA	45:DZ:133:ILE:HG13	1.96	0.48
1:AA:1226:C:H4'	19:AS:80:TYR:CZ	2.49	0.48
9:AI:48:GLU:H	9:AI:49:PRO:CD	2.26	0.48
25:BA:1218:G:N2	25:BA:1222:A:OP2	2.47	0.48
25:BA:2303:U:H2'	25:BA:2304:C:C6	2.49	0.48
25:BA:904:C:N4	25:BA:905:U:O4	2.46	0.48
25:BA:2584:A:N7	28:BE:144:ARG:HD2	2.29	0.48
1:CA:1273:G:H3'	1:CA:1274:G:H8	1.78	0.48
2:CB:211:ILE:O	2:CB:215:LEU:HB2	2.13	0.48
2:CB:80:ILE:HD11	2:CB:212:GLN:HA	1.96	0.48
2:CB:213:LEU:HD22	2:CB:214:ILE:HD13	1.94	0.48
13:CM:106:ASN:C	13:CM:108:ARG:H	2.16	0.48
25:DA:1833:U:O2'	25:DA:1969:A:N1	2.38	0.48
25:DA:2110:G:H5''	25:DA:2111:C:H5	1.78	0.48
25:DA:2116:G:O6	25:DA:2165:G:N2	2.47	0.48
25:DA:2149:G:C6	25:DA:2150:U:C2	3.01	0.48
25:DA:2151:G:H2'	25:DA:2152:G:C8	2.46	0.48
25:DA:2273:A:H2'	25:DA:2274:A:C8	2.48	0.48
25:DA:468:G:N7	53:D7:39:ARG:NH2	2.56	0.48
25:DA:597:U:H2'	25:DA:598:G:C8	2.48	0.48
25:DA:839:U:H2'	25:DA:840:C:C6	2.48	0.48
25:DA:1155:A:H5''	40:DU:55:ARG:HD3	1.94	0.48
1:AA:1060:C:C5	3:AC:2:GLY:HA3	2.48	0.48
1:AA:1129:C:O2'	1:AA:1139:G:N7	2.35	0.48
1:AA:1516:G:H2'	1:AA:1518:A:OP2	2.13	0.48
1:AA:346:G:O6	1:AA:347:G:N2	2.47	0.48
2:AB:84:GLU:HB3	2:AB:219:VAL:HG21	1.95	0.48
2:AB:77:ALA:HB2	2:AB:211:ILE:HD13	1.95	0.48
6:AF:19:LEU:HD11	6:AF:59:TYR:CE2	2.49	0.48
1:AA:236:G:H5''	17:AQ:42:TYR:OH	2.13	0.48
25:BA:2149:G:H1	25:BA:2183:C:H42	1.61	0.48
25:BA:757:G:H2'	25:BA:758:G:C8	2.48	0.48
35:BP:100:LEU:HD12	35:BP:112:LEU:HD11	1.94	0.48
36:BQ:75:THR:HG21	36:BQ:87:LYS:NZ	2.28	0.48
1:CA:1258:G:O2'	1:CA:1259:C:H5'	2.13	0.48
1:CA:397:A:H3'	1:CA:397:A:N3	2.28	0.48
1:CA:22:G:H4'	1:CA:885:G:C8	2.48	0.48
1:CA:946:A:H2'	1:CA:947:G:C8	2.49	0.48
3:CC:85:ARG:O	3:CC:89:GLU:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CH:69:ARG:HD3	8:CH:75:ARG:O	2.14	0.48
23:CY:7:A:N6	23:CY:66:U:H3	2.08	0.48
48:D2:18:PRO:O	48:D2:22:GLU:HG3	2.13	0.48
25:DA:2320:A:N3	25:DA:2320:A:H2'	2.28	0.48
26:DB:66:A:N6	26:DB:109:C:H5'	2.28	0.48
27:DD:242:ARG:N	27:DD:242:ARG:HD3	2.28	0.48
32:DI:12:LEU:HD22	32:DI:19:VAL:HG21	1.94	0.48
33:DN:73:THR:HA	33:DN:83:LYS:O	2.14	0.48
38:DS:105:ALA:HB1	38:DS:110:LEU:HD23	1.95	0.48
1:AA:975:A:C8	1:AA:975:A:H5'	2.46	0.48
23:AY:19:G:C6	23:AY:56:C:N4	2.81	0.48
23:AY:20:U:H3'	23:AY:20:U:OP2	2.13	0.48
25:BA:2152:U:H2'	25:BA:2153:G:N2	2.28	0.48
25:BA:2187:G:H2'	25:BA:2188:G:C8	2.48	0.48
25:BA:2658:C:OP2	25:BA:2745:G:O2'	2.30	0.48
25:BA:308:U:H2'	25:BA:309:C:C6	2.49	0.48
25:BA:692:C:H2'	25:BA:693:G:O4'	2.14	0.48
33:BN:15:LEU:HB2	33:BN:135:PRO:HB2	1.95	0.48
1:CA:1005:A:C8	1:CA:1024:G:N2	2.82	0.48
1:CA:1221:G:C2'	1:CA:1222:G:H5'	2.44	0.48
1:CA:1308:U:OP1	13:CM:98:VAL:HG23	2.13	0.48
3:CC:23:TYR:CD1	10:CJ:10:GLY:HA2	2.49	0.48
25:DA:740:U:H2'	25:DA:741:G:C8	2.49	0.48
26:DB:31:C:H4'	30:DG:29:TRP:CH2	2.48	0.48
32:DI:66:GLU:OE1	32:DI:69:LYS:HD3	2.13	0.48
39:DT:51:ARG:HB3	39:DT:62:THR:HB	1.96	0.48
44:DY:1:MET:HE3	44:DY:2:ARG:H	1.77	0.48
4:AD:98:GLU:HG2	4:AD:189:PRO:HG2	1.95	0.48
9:AI:58:HIS:CD2	9:AI:58:HIS:H	2.30	0.48
16:AP:19:ILE:HG22	16:AP:37:GLY:C	2.33	0.48
17:AQ:58:GLU:O	17:AQ:74:LEU:N	2.42	0.48
25:BA:1335:C:H2'	25:BA:1336:C:H6	1.78	0.48
31:BH:125:VAL:HG12	31:BH:127:GLU:O	2.13	0.48
32:BI:93:THR:HG22	32:BI:119:PRO:HB3	1.96	0.48
1:CA:1240:U:OP2	7:CG:116:ALA:N	2.46	0.48
1:CA:1275:A:C2'	1:CA:1276:G:H5'	2.43	0.48
1:CA:1513:A:H2'	1:CA:1514:C:C6	2.48	0.48
1:CA:811:C:N4	61:CA:4019:HOH:O	2.45	0.48
1:CA:429:U:O3'	4:CD:22:LYS:NZ	2.45	0.48
10:CJ:7:LYS:HB2	10:CJ:97:GLU:HB2	1.95	0.48
18:CR:41:LYS:HB3	18:CR:41:LYS:HE3	1.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:CY:29:G:N2	23:CY:41:C:N3	2.55	0.48
23:CY:65:G:H2'	23:CY:66:U:C6	2.48	0.48
25:DA:99:U:H4'	25:DA:100:G:H5''	1.94	0.48
25:DA:2507:C:H5''	25:DA:2573:C:C4	2.49	0.48
25:DA:303:U:H2'	25:DA:304:G:C8	2.48	0.48
25:DA:775:G:N3	61:DA:4553:HOH:O	2.35	0.48
25:DA:848:G:H2'	25:DA:849:A:C8	2.48	0.48
28:DE:4:ILE:HD11	28:DE:29:GLY:HA2	1.94	0.48
40:DU:61:TRP:CH2	40:DU:93:LYS:HB2	2.48	0.48
45:DZ:45:ASP:OD1	45:DZ:49:ARG:HD2	2.12	0.48
1:AA:339:C:H2'	1:AA:340:U:H6	1.78	0.48
12:AL:24:VAL:HB	12:AL:27:LEU:HD22	1.95	0.48
13:AM:87:TYR:O	13:AM:91:ARG:HG2	2.14	0.48
27:BD:79:VAL:HG21	27:BD:111:LEU:HD11	1.95	0.48
1:CA:1073:U:O2	2:CB:104:ASN:ND2	2.38	0.48
7:CG:90:GLU:H	7:CG:90:GLU:CD	2.15	0.48
12:CL:28:LYS:N	12:CL:29:GLY:HA2	2.29	0.48
30:DG:67:LYS:HD3	50:D4:5:ILE:HD12	1.96	0.48
25:DA:1400:G:H2'	25:DA:1401:G:C8	2.48	0.48
25:DA:1548:C:H2'	25:DA:1549:C:H6	1.77	0.48
25:DA:2849:U:O4	39:DT:23:ARG:NH2	2.32	0.48
25:DA:24:G:O2'	42:DW:78:GLU:O	2.27	0.48
1:AA:1060:C:OP1	14:AN:45:ARG:NH2	2.42	0.48
1:AA:1530:G:H4'	1:AA:1530:G:OP1	2.13	0.48
20:AT:100:ILE:HB	20:AT:101:GLY:H	1.47	0.48
25:BA:1093:G:O2'	25:BA:1094:A:O5'	2.31	0.48
25:BA:1733:C:H2'	25:BA:1734:G:O4'	2.14	0.48
25:BA:2158:C:N4	25:BA:2159:C:C4	2.82	0.48
25:BA:2250:G:H2'	25:BA:2250:G:N3	2.28	0.48
25:BA:2642:G:H21	25:BA:2901:A:H1'	1.78	0.48
1:CA:1033:G:H2'	1:CA:1034:G:H8	1.78	0.48
1:CA:1292:U:P	7:CG:41:ARG:HH22	2.37	0.48
1:CA:1397:C:OP2	5:CE:24:ARG:NH2	2.46	0.48
5:CE:93:PRO:HG2	8:CH:105:ARG:NE	2.29	0.48
52:D6:13:CYS:SG	52:D6:47:THR:HG21	2.54	0.48
25:DA:1779:U:H2'	61:DA:4825:HOH:O	2.13	0.48
25:DA:2102:U:H2'	25:DA:2103:C:C6	2.48	0.48
25:DA:2103:C:N4	25:DA:2186:G:H1	2.11	0.48
25:DA:2893:G:H8	25:DA:2893:G:OP2	1.97	0.48
36:DQ:57:HIS:HD2	36:DQ:117:ALA:HB2	1.79	0.48
25:DA:2495:G:H5''	36:DQ:82:ARG:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:DX:4:ALA:HB1	43:DX:42:ALA:HA	1.95	0.48
1:AA:56:U:H2'	1:AA:57:G:C8	2.49	0.48
50:B4:49:PHE:HB3	50:B4:50:VAL:H	1.36	0.48
25:BA:231:G:C8	54:B8:5:LYS:HG2	2.49	0.48
27:BD:179:SER:O	27:BD:275:LYS:HB2	2.14	0.48
31:BH:69:ARG:HG3	31:BH:70:THR:N	2.28	0.48
35:BP:95:VAL:HG13	35:BP:125:VAL:HB	1.94	0.48
38:BS:3:ARG:HD3	38:BS:4:LEU:N	2.28	0.48
2:CB:63:MET:HG3	2:CB:225:ALA:HB1	1.95	0.48
25:DA:500:G:N1	25:DA:503:A:OP2	2.46	0.48
25:DA:910:A:N1	25:DA:2277:G:H1'	2.29	0.48
41:DV:37:VAL:HG11	41:DV:40:LEU:HG	1.96	0.48
1:AA:1009:G:O6	1:AA:1020:U:O2	2.31	0.47
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.49	0.47
1:AA:353:A:C8	1:AA:353:A:H5'	2.47	0.47
2:AB:24:TRP:HD1	2:AB:24:TRP:H	1.61	0.47
3:AC:148:GLY:HA3	3:AC:172:ARG:O	2.14	0.47
3:AC:19:GLU:HG2	3:AC:54:ARG:NH1	2.28	0.47
25:BA:1313:U:OP2	25:BA:2034:G:N1	2.33	0.47
25:BA:2255:U:H2'	25:BA:2256:U:C6	2.49	0.47
25:BA:701:A:OP2	61:BA:4864:HOH:O	2.19	0.47
25:BA:185:A:O2'	25:BA:852:G:O6	2.23	0.47
26:BB:6:C:H2'	26:BB:7:G:H5''	1.95	0.47
30:BG:15:VAL:HG21	30:BG:176:LEU:HD23	1.95	0.47
43:BX:94:GLY:N	43:BX:95:LEU:HB2	2.29	0.47
45:BZ:137:ILE:HA	45:BZ:156:LYS:HE2	1.96	0.47
1:CA:1272:G:H2'	1:CA:1273:G:O4'	2.14	0.47
1:CA:345:C:H3'	39:DT:41:ARG:NH2	2.29	0.47
1:CA:659:U:C2'	1:CA:660:G:H5'	2.44	0.47
3:CC:149:ALA:HA	3:CC:201:TYR:O	2.14	0.47
13:CM:65:LYS:N	50:D4:50:VAL:HG21	2.29	0.47
25:DA:1218:C:H42	25:DA:1231:G:H1	1.62	0.47
25:DA:2127:G:H22	25:DA:2161:C:H2'	1.78	0.47
25:DA:597:U:H2'	25:DA:598:G:H8	1.79	0.47
1:AA:339:C:OP2	34:BO:97:ARG:NH1	2.45	0.47
7:AG:28:ASN:HD21	7:AG:36:LYS:NZ	2.12	0.47
12:AL:56:ALA:HB2	12:AL:70:ILE:HD11	1.96	0.47
12:AL:88:GLY:O	12:AL:99:HIS:HD2	1.97	0.47
50:B4:63:TYR:CD1	50:B4:63:TYR:N	2.80	0.47
25:BA:1093:G:H2'	25:BA:1156:G:N1	2.28	0.47
39:BT:65:LYS:HG2	39:BT:66:VAL:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1016:A:H2'	1:CA:1017:G:O4'	2.14	0.47
1:CA:1069:C:O2'	1:CA:1192:C:H1'	2.14	0.47
2:CB:48:MET:O	2:CB:52:GLU:N	2.44	0.47
3:CC:174:PRO:HD2	3:CC:182:ILE:HD11	1.96	0.47
23:CY:61:C:H2'	23:CY:62:C:C6	2.48	0.47
50:D4:59:PHE:N	50:D4:60:GLN:HB2	2.29	0.47
25:DA:2136:C:O2'	25:DA:2137:C:H6	1.97	0.47
25:DA:589:C:H2'	25:DA:590:A:C8	2.49	0.47
45:DZ:144:LEU:HD22	45:DZ:174:VAL:HG23	1.96	0.47
1:AA:1003:G:N2	1:AA:1038:C:H42	2.13	0.47
1:AA:1004:A:N1	1:AA:1035:A:N6	2.63	0.47
1:AA:269:C:H2'	1:AA:270:A:C8	2.49	0.47
2:AB:15:VAL:HG22	2:AB:15:VAL:O	2.13	0.47
5:AE:72:GLN:O	5:AE:75:THR:HG22	2.14	0.47
10:AJ:4:ILE:HA	10:AJ:100:THR:HA	1.96	0.47
23:AY:76:A:N6	25:BA:2434:A:O4'	2.48	0.47
25:BA:595:A:OP2	41:BV:78:LYS:NZ	2.40	0.47
28:BE:47:VAL:HG22	28:BE:84:PHE:O	2.15	0.47
39:BT:108:ARG:NH1	39:BT:109:GLU:HG3	2.30	0.47
42:BW:19:LEU:HB3	51:B5:25:LEU:HD11	1.97	0.47
1:CA:1142:G:H2'	1:CA:1143:G:O4'	2.15	0.47
1:CA:1162:C:N3	1:CA:1174:G:N2	2.61	0.47
7:CG:79:ARG:HG2	7:CG:79:ARG:HH21	1.79	0.47
9:CI:85:LEU:HD12	9:CI:96:LEU:HD11	1.95	0.47
23:CY:55:PSU:HN1	23:CY:57:G:H5'	1.78	0.47
25:DA:1040:C:H2'	25:DA:1041:C:O4'	2.15	0.47
25:DA:1857:G:C6	25:DA:1858:G:C6	3.01	0.47
25:DA:2029:G:H2'	25:DA:2031:A:OP1	2.13	0.47
25:DA:373:U:H2'	25:DA:374:A:H8	1.78	0.47
31:DH:20:ALA:HB1	31:DH:21:PRO:HD2	1.96	0.47
32:DI:61:ARG:HA	32:DI:61:ARG:HD3	1.70	0.47
38:DS:50:SER:O	38:DS:76:LYS:NZ	2.30	0.47
45:DZ:30:ASN:HA	45:DZ:89:PHE:HE1	1.79	0.47
1:AA:715:A:H2'	1:AA:716:A:C8	2.49	0.47
1:AA:1345:U:OP1	9:AI:120:ARG:NH1	2.48	0.47
9:AI:16:ARG:HB2	9:AI:64:THR:HB	1.95	0.47
1:AA:656:C:O2'	15:AO:28:GLN:NE2	2.48	0.47
25:BA:1140:U:C4	25:BA:1142:A:H5''	2.49	0.47
25:BA:1315:A:N7	61:BA:4537:HOH:O	2.36	0.47
25:BA:2018:C:H4'	25:BA:2019:G:OP1	2.13	0.47
25:BA:551:A:H5''	25:BA:552:C:OP1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BD:39:LYS:NZ	27:BD:57:GLY:O	2.45	0.47
33:BN:67:LEU:HD13	33:BN:87:LEU:HD13	1.95	0.47
34:BO:87:ILE:HD12	34:BO:91:LEU:HA	1.95	0.47
2:CB:163:PHE:HA	2:CB:185:ILE:HG12	1.96	0.47
20:CT:14:LYS:O	20:CT:18:GLN:HG3	2.14	0.47
50:D4:53:GLU:O	50:D4:55:ARG:N	2.43	0.47
25:DA:1548:C:H2'	25:DA:1549:C:C6	2.49	0.47
25:DA:2010:G:H5''	42:DW:42:ARG:HB2	1.96	0.47
25:DA:956:G:H5''	36:DQ:77:LYS:HD2	1.97	0.47
43:DX:35:THR:HG22	43:DX:38:GLU:H	1.79	0.47
3:AC:19:GLU:HG2	3:AC:54:ARG:HH11	1.79	0.47
5:AE:92:LYS:HB3	5:AE:119:LEU:HB2	1.95	0.47
13:AM:92:HIS:CE1	13:AM:98:VAL:HG21	2.49	0.47
25:BA:878:G:O2'	35:BP:38:GLN:NE2	2.47	0.47
32:BI:29:TYR:O	32:BI:32:PRO:HD2	2.14	0.47
40:BU:89:GLU:HG3	41:BV:50:PRO:HB3	1.97	0.47
41:BV:49:THR:HG22	41:BV:49:THR:O	2.15	0.47
44:BY:86:ARG:HH11	44:BY:100:ALA:HB1	1.79	0.47
1:CA:1273:G:H3'	1:CA:1274:G:C8	2.49	0.47
1:CA:1330:U:H4'	13:CM:23:TYR:CE1	2.49	0.47
1:CA:1519:A:H5''	1:CA:1520:G:OP2	2.15	0.47
9:CI:23:ASN:HD22	9:CI:24:GLY:N	2.13	0.47
25:DA:987:G:O2'	25:DA:1000:A:N3	2.43	0.47
25:DA:1506:C:H2'	25:DA:1507:A:H5'	1.95	0.47
25:DA:1518:U:H2'	25:DA:1519:G:O4'	2.14	0.47
25:DA:1721:G:N1	25:DA:1739:U:OP2	2.47	0.47
25:DA:2115:G:H4'	25:DA:2167:U:O4	2.15	0.47
25:DA:927:G:H2'	25:DA:928:G:O4'	2.13	0.47
29:DF:13:SER:OG	29:DF:16:GLY:O	2.22	0.47
1:AA:1001:A:H2'	1:AA:1001(A):G:O4'	2.14	0.47
1:AA:1006:C:H2'	1:AA:1007:C:C6	2.49	0.47
1:AA:1008:C:C2	1:AA:1021:G:N2	2.79	0.47
1:AA:1239:A:H62	1:AA:1299:A:H62	1.61	0.47
5:AE:82:VAL:HG21	5:AE:138:ALA:HA	1.96	0.47
7:AG:37:ASN:O	7:AG:41:ARG:HD2	2.14	0.47
10:AJ:27:ALA:HB2	10:AJ:81:THR:HG21	1.96	0.47
11:AK:45:GLY:O	11:AK:50:TYR:HB2	2.15	0.47
25:BA:1314:A:C2	25:BA:2035:A:C4	3.03	0.47
25:BA:2149:G:C2'	25:BA:2150:C:H5'	2.45	0.47
25:BA:2762:A:OP1	31:BH:3:ARG:NH2	2.39	0.47
25:BA:572:A:H61	41:BV:19:LYS:H	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BB:48:A:H2'	26:BB:49:C:C6	2.49	0.47
7:CG:97:GLN:O	7:CG:101:LEU:HG	2.15	0.47
16:CP:8:ARG:HB3	16:CP:28:ARG:NH1	2.30	0.47
23:CW:3:C:N3	23:CW:70:G:O6	2.47	0.47
23:CW:7:A:H5'	23:CW:8:4SU:H5	1.95	0.47
50:D4:64:GLY:O	50:D4:66:SER:N	2.37	0.47
25:DA:1022:G:H22	25:DA:1142(A):A:H2	1.61	0.47
25:DA:1446:C:H42	25:DA:1465:G:H1	1.62	0.47
25:DA:747:U:O2	25:DA:2014:A:H1'	2.14	0.47
32:DI:4:ILE:HG12	32:DI:18:VAL:HG22	1.97	0.47
32:DI:40:THR:O	32:DI:44:LEU:HB2	2.15	0.47
34:DO:120:GLU:OE2	34:DO:122:LEU:HD21	2.13	0.47
1:AA:1124:G:H5''	10:AJ:35:SER:OG	2.15	0.47
1:AA:975:A:H4'	1:AA:976:G:C5'	2.40	0.47
5:AE:40:ARG:HH21	5:AE:68:GLU:HA	1.79	0.47
15:AO:18:PHE:CZ	15:AO:21:ASP:HB3	2.49	0.47
25:BA:2418:U:H2'	25:BA:2418:U:OP2	2.14	0.47
25:BA:847:A:OP1	25:BA:847:A:H8	1.97	0.47
1:CA:1194:U:H4'	5:CE:22:GLY:HA3	1.96	0.47
2:CB:71:VAL:HG21	2:CB:164:VAL:HG22	1.97	0.47
8:CH:51:VAL:HG12	8:CH:52:ASP:H	1.79	0.47
50:D4:59:PHE:N	50:D4:59:PHE:CD1	2.83	0.47
25:DA:1539:G:H2'	25:DA:1540:U:O4'	2.15	0.47
25:DA:2243:U:H2'	25:DA:2244:U:C6	2.49	0.47
25:DA:2751:G:C8	31:DH:2:SER:HA	2.47	0.47
25:DA:322:A:OP1	29:DF:168:ARG:HD2	2.15	0.47
25:DA:631:A:H2'	25:DA:632:A:O4'	2.15	0.47
31:DH:86:GLU:OE2	31:DH:132:ARG:NH2	2.47	0.47
37:DR:44:LEU:HD23	37:DR:44:LEU:HA	1.73	0.47
1:AA:1038:C:C2'	1:AA:1039:C:H5'	2.45	0.47
1:AA:1493:A:H5''	1:AA:1494:G:OP2	2.14	0.47
3:AC:134:ILE:HG23	3:AC:151:VAL:HB	1.97	0.47
3:AC:71:ALA:HA	3:AC:106:VAL:HB	1.97	0.47
53:B7:11:LYS:HE3	53:B7:15:THR:OG1	2.14	0.47
25:BA:1067:A:H3'	25:BA:1067:A:H8	1.80	0.47
25:BA:2744:G:O3'	28:BE:203:LYS:NZ	2.48	0.47
25:BA:909:G:H2'	25:BA:910:A:O4'	2.15	0.47
29:BF:184:TYR:CE2	29:BF:188:ARG:HD2	2.50	0.47
25:BA:271:U:H1'	32:BI:50:ARG:CZ	2.44	0.47
1:CA:1120:G:C6	1:CA:1121:U:C4	3.03	0.47
3:CC:152:ILE:HD12	3:CC:199:LYS:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:265:A:C8	25:DA:266:G:H1'	2.49	0.47
40:DU:85:LYS:HB3	40:DU:116:ALA:HB1	1.97	0.47
7:AG:89:MET:SD	7:AG:155:ARG:HB2	2.54	0.47
10:AJ:57:LYS:HE2	10:AJ:60:ARG:NH2	2.30	0.47
19:AS:45:VAL:HG13	19:AS:63:THR:HA	1.97	0.47
23:AW:51:U:H2'	23:AW:52:G:H8	1.78	0.47
24:AX:8:4SU:O2	24:AX:21:A:H2	1.96	0.47
25:BA:2044:U:O2'	25:BA:2629:C:H5'	2.15	0.47
32:BI:116:LEU:HD11	32:BI:120:ILE:HG13	1.96	0.47
25:BA:2830:A:C5	37:BR:4:LEU:HD11	2.50	0.47
37:BR:56:LYS:NZ	37:BR:90:ARG:O	2.46	0.47
25:BA:572:A:N6	41:BV:19:LYS:H	2.11	0.47
4:CD:111:ALA:HB2	4:CD:120:LEU:HD12	1.95	0.47
4:CD:173:TRP:CZ3	4:CD:193:ASP:HB3	2.50	0.47
4:CD:20:TYR:CD2	4:CD:26:CYS:HB3	2.50	0.47
7:CG:108:ALA:HA	7:CG:111:ARG:HD2	1.97	0.47
9:CI:128:ARG:HH21	24:CX:32:5MC:P	2.38	0.47
17:CQ:54:GLY:O	17:CQ:81:ARG:N	2.41	0.47
19:CS:27:GLU:HB3	19:CS:28:LYS:HD3	1.97	0.47
37:DR:33:ARG:NH2	51:D5:57:VAL:O	2.35	0.47
25:DA:1219:G:H1	25:DA:1230:C:H42	1.62	0.47
25:DA:2125:G:H21	25:DA:2173:A:H62	1.62	0.47
25:DA:2125:G:N2	25:DA:2173:A:H62	2.13	0.47
25:DA:2756:U:H1'	25:DA:2757:A:H5''	1.97	0.47
25:DA:2815:C:H2'	25:DA:2816:C:C6	2.50	0.47
25:DA:38:A:H2'	25:DA:39:C:C6	2.50	0.47
25:DA:866:A:H2	25:DA:867:C:C4	2.32	0.47
25:DA:985:C:H2'	25:DA:986:C:H6	1.79	0.47
26:DB:80:U:H2'	26:DB:81:G:N7	2.29	0.47
28:DE:28:ALA:HB3	28:DE:93:VAL:HG12	1.96	0.47
1:AA:1095:U:H5''	1:AA:1109:C:O2	2.15	0.47
2:AB:163:PHE:HA	2:AB:185:ILE:HG13	1.97	0.47
10:AJ:45:ARG:HG2	10:AJ:47:PHE:CZ	2.50	0.47
1:AA:581:G:OP1	15:AO:65:ARG:NH2	2.48	0.47
17:AQ:45:HIS:CD2	17:AQ:47:PRO:HG3	2.49	0.47
25:BA:1093:G:H2'	25:BA:1156:G:N2	2.30	0.47
25:BA:1335:C:H2'	25:BA:1336:C:C6	2.50	0.47
25:BA:2129:C:H42	25:BA:2204:G:H1	1.62	0.47
25:BA:2724:U:H2'	25:BA:2727:G:H5''	1.97	0.47
27:BD:71:ASP:HB3	27:BD:103:ARG:NH2	2.29	0.47
1:CA:7:G:H5'	1:CA:298:A:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CE:24:ARG:NH1	22:CV:24:A:OP2	2.48	0.47
13:CM:84:ILE:HG13	13:CM:85:GLY:N	2.29	0.47
30:DG:109:VAL:HG21	50:D4:14:ILE:HG21	1.97	0.47
50:D4:46:GLN:C	50:D4:48:ARG:H	2.17	0.47
25:DA:250:G:P	54:D8:13:ARG:HH22	2.38	0.47
25:DA:117:G:OP2	25:DA:119:A:O2'	2.22	0.47
25:DA:1183:G:H2'	25:DA:1184:G:C8	2.49	0.47
25:DA:2469:A:H3'	25:DA:2470:G:H8	1.79	0.47
25:DA:27:G:N2	25:DA:512:G:H1'	2.29	0.47
26:DB:91:C:OP2	36:DQ:16:ARG:NH1	2.47	0.47
27:DD:92:ILE:HD12	27:DD:104:TYR:CE1	2.49	0.47
29:DF:150:GLY:HA2	29:DF:172:TRP:CD2	2.50	0.47
31:DH:84:SER:HB3	31:DH:132:ARG:NH1	2.27	0.47
44:DY:89:PHE:CZ	44:DY:95:LYS:HE2	2.50	0.47
25:DA:896:A:H5''	45:DZ:147:GLY:HA3	1.96	0.47
1:AA:1025:U:C2	1:AA:1036:G:O6	2.66	0.47
1:AA:1125:U:H4'	10:AJ:5:ARG:NH2	2.30	0.47
1:AA:337:C:H2'	1:AA:338:A:C8	2.50	0.47
1:AA:690:G:C6	1:AA:691:G:C6	3.03	0.47
24:AX:8:4SU:H6	24:AX:8:4SU:O5'	2.15	0.47
52:B6:14:THR:HB	52:B6:48:VAL:O	2.15	0.47
25:BA:1346:U:H4'	25:BA:1347:A:H5'	1.95	0.47
1:CA:1034:G:H3'	1:CA:1035:A:H8	1.78	0.47
1:CA:1178:G:N2	1:CA:1180:A:H3'	2.30	0.47
1:CA:520:A:N1	1:CA:536:C:H1'	2.30	0.47
2:CB:188:ALA:HB1	2:CB:192:SER:OG	2.15	0.47
3:CC:34:LEU:O	3:CC:38:ARG:HB2	2.14	0.47
5:CE:43:LEU:O	5:CE:65:ASN:ND2	2.38	0.47
1:CA:750:G:O2'	15:CO:21:ASP:OD1	2.33	0.47
1:CA:1318:A:H5''	19:CS:3:ARG:NH2	2.30	0.47
25:DA:851:U:H5'	49:D3:49:LYS:HD2	1.97	0.47
25:DA:514:A:N3	25:DA:581:C:O2'	2.44	0.47
27:DD:218:ARG:HB3	27:DD:219:PRO:HD2	1.96	0.47
29:DF:116:ASP:OD1	29:DF:119:ARG:NH2	2.49	0.47
45:DZ:6:LYS:HD2	45:DZ:8:TYR:HE1	1.78	0.47
1:AA:1118:C:H1'	1:AA:1179:A:C4	2.51	0.46
1:AA:1531:A:H2'	1:AA:1532:U:C4	2.50	0.46
1:AA:175:C:H2'	1:AA:176:C:C6	2.49	0.46
9:AI:15:ALA:HB2	9:AI:65:VAL:HG23	1.97	0.46
13:AM:3:ARG:HG3	13:AM:4:ILE:H	1.80	0.46
6:AF:94:GLN:HG2	18:AR:32:ARG:HH21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:B4:54:GLY:N	50:B4:55:ARG:HA	2.30	0.46
25:BA:1410:G:OP2	47:B1:3:LYS:HG3	2.15	0.46
25:BA:1921:G:H2'	25:BA:1921:G:N3	2.30	0.46
25:BA:2204:G:H2'	25:BA:2205:C:C6	2.50	0.46
39:BT:117:ASP:OD2	39:BT:120:ARG:NE	2.36	0.46
1:CA:1207:G:C6	1:CA:1208:C:C4	3.03	0.46
1:CA:1239:A:H62	1:CA:1299:A:N6	2.12	0.46
1:CA:664:G:N2	1:CA:741:G:H1	2.11	0.46
1:CA:19:C:H5''	5:CE:86:ALA:HB3	1.97	0.46
22:CV:23:A:H4'	22:CV:24:A:C5'	2.42	0.46
25:DA:1021:A:H3'	25:DA:1021:A:H8	1.80	0.46
25:DA:1991:U:H2'	25:DA:1992:G:H5''	1.96	0.46
25:DA:2182:G:H2'	25:DA:2183:C:C6	2.50	0.46
25:DA:908:C:OP2	36:DQ:22:LYS:NZ	2.33	0.46
26:DB:4:C:N4	26:DB:117:G:H1	2.06	0.46
27:DD:164:GLN:HE21	27:DD:176:ARG:HH22	1.63	0.46
27:DD:276:LYS:H	27:DD:276:LYS:HD3	1.79	0.46
35:DP:50:ARG:HH21	54:D8:7:HIS:CD2	2.29	0.46
36:DQ:75:THR:HG21	36:DQ:87:LYS:NZ	2.30	0.46
39:DT:56:GLY:O	39:DT:59:THR:HG22	2.15	0.46
1:AA:1063:C:OP2	1:AA:1064:G:O2'	2.29	0.46
1:AA:1152:A:H5'	10:AJ:13:HIS:HB2	1.96	0.46
1:AA:1221:G:C2'	1:AA:1222:G:H5'	2.45	0.46
1:AA:130:A:H5'	17:AQ:63:ARG:NE	2.29	0.46
25:BA:11:G:H2'	25:BA:12:U:H5''	1.98	0.46
25:BA:2181:G:H2'	25:BA:2182:G:C8	2.51	0.46
1:CA:707:C:OP1	11:CK:85:ARG:NH1	2.48	0.46
3:CC:134:ILE:HG22	3:CC:168:ALA:HB3	1.98	0.46
23:CY:58:A:O2'	23:CY:60:U:OP2	2.31	0.46
25:DA:1899:G:N3	25:DA:1899:G:H2'	2.30	0.46
25:DA:229:A:H5'	25:DA:230:U:H5'	1.97	0.46
25:DA:2663:G:H2'	25:DA:2664:G:O4'	2.15	0.46
25:DA:2820:A:C5	37:DR:4:LEU:HD11	2.50	0.46
25:DA:582:G:H2'	25:DA:583:G:C8	2.49	0.46
1:AA:1009:G:C5	1:AA:1021:G:C6	3.03	0.46
1:AA:262:A:C6	1:AA:263:A:C6	3.02	0.46
1:AA:848:C:H2'	1:AA:849:C:C6	2.51	0.46
15:AO:6:GLU:OE2	15:AO:6:GLU:N	2.49	0.46
19:AS:20:LEU:HD23	19:AS:23:ASN:ND2	2.30	0.46
52:B6:11:LEU:HB2	52:B6:21:TYR:HB2	1.97	0.46
25:BA:1834:A:H4'	27:BD:259:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BE:170:LEU:HB3	28:BE:184:VAL:HG22	1.98	0.46
35:BP:81:GLN:NE2	35:BP:105:LEU:O	2.46	0.46
44:BY:35:TYR:CE2	44:BY:69:ALA:HB3	2.50	0.46
1:CA:1410:G:H2'	1:CA:1411:C:H6	1.80	0.46
1:CA:807:A:H2'	1:CA:808:C:C6	2.51	0.46
2:CB:118:LEU:HD13	2:CB:142:LEU:HB2	1.96	0.46
2:CB:16:HIS:CG	2:CB:17:PHE:H	2.33	0.46
1:CA:8:A:N6	4:CD:209:ARG:HB2	2.31	0.46
10:CJ:50:ILE:HB	14:CN:41:ARG:NH2	2.30	0.46
25:DA:2131:G:OP1	25:DA:2132:U:O2'	2.18	0.46
25:DA:2336:A:H61	46:D0:43:THR:HG22	1.81	0.46
25:DA:2756:U:H5''	55:D9:19:ARG:HB3	1.96	0.46
25:DA:868:U:C4	25:DA:869:G:N7	2.83	0.46
13:CM:93:ARG:NH1	25:DA:888:C:OP1	2.41	0.46
26:DB:105:A:OP1	45:DZ:72:ARG:NH1	2.49	0.46
29:DF:11:VAL:HB	29:DF:18:ARG:HB3	1.97	0.46
30:DG:33:ARG:NH2	30:DG:162:THR:HG21	2.30	0.46
33:DN:130:HIS:HB3	33:DN:133:GLN:HG2	1.97	0.46
34:DO:16:ALA:HB2	34:DO:52:VAL:HG21	1.96	0.46
37:DR:118:GLU:CD	37:DR:118:GLU:H	2.18	0.46
28:DE:111:ARG:HA	37:DR:1:MET:SD	2.56	0.46
1:AA:1226:C:O2'	13:AM:111:LYS:NZ	2.48	0.46
4:AD:18:LYS:HE3	4:AD:20:TYR:CZ	2.51	0.46
4:AD:3:ARG:O	4:AD:5:ILE:HG22	2.15	0.46
7:AG:50:ILE:HD11	7:AG:61:VAL:HG21	1.96	0.46
15:AO:6:GLU:O	15:AO:10:LYS:HG3	2.14	0.46
54:B8:23:VAL:CG1	54:B8:47:LYS:HD3	2.45	0.46
25:BA:1081:U:H2'	25:BA:1082:G:C8	2.50	0.46
25:BA:2150:C:H2'	25:BA:2151:C:O4'	2.15	0.46
30:BG:43:LEU:HB3	30:BG:44:GLY:H	1.55	0.46
1:CA:1002:G:H2'	1:CA:1003:G:H8	1.81	0.46
1:CA:1001(A):G:H3'	1:CA:1002:G:O4'	2.16	0.46
1:CA:1256:A:HO2'	1:CA:1257:U:P	2.37	0.46
1:CA:975:A:H5'	1:CA:975:A:H8	1.81	0.46
3:CC:102:ASN:HD22	3:CC:102:ASN:N	2.13	0.46
3:CC:125:GLU:O	3:CC:127:ARG:NH1	2.45	0.46
1:CA:972:C:O2'	10:CJ:55:LYS:O	2.27	0.46
25:DA:1339:G:H5''	43:DX:16:LYS:HD3	1.98	0.46
25:DA:2119:A:N6	25:DA:2170:A:H62	2.13	0.46
25:DA:2552:U:H2'	25:DA:2554:U:OP2	2.15	0.46
37:DR:24:GLN:HB3	37:DR:44:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1376:U:H2'	1:AA:1377:A:C8	2.51	0.46
1:AA:691:G:H2'	1:AA:692:U:C6	2.50	0.46
2:AB:112:VAL:HG12	2:AB:149:LEU:HD13	1.98	0.46
4:AD:162:LEU:CD1	4:AD:181:MET:HG2	2.44	0.46
10:AJ:64:GLU:OE2	10:AJ:66:ARG:NE	2.43	0.46
1:AA:719:C:O2'	18:AR:49:LYS:HB3	2.15	0.46
25:BA:1756:U:H2'	25:BA:1757:C:C6	2.50	0.46
25:BA:225:C:H2'	25:BA:226:C:C6	2.50	0.46
25:BA:2762:A:P	31:BH:3:ARG:HH21	2.38	0.46
32:BI:31:LEU:HD21	32:BI:38:LEU:HD11	1.98	0.46
37:BR:83:ILE:O	37:BR:86:ARG:HG2	2.16	0.46
1:CA:444:C:H2'	1:CA:445:G:H8	1.80	0.46
1:CA:975:A:H4'	1:CA:976:G:C5'	2.43	0.46
8:CH:49:GLU:HG2	8:CH:62:TYR:HE1	1.81	0.46
13:CM:92:HIS:CE1	13:CM:98:VAL:HG21	2.51	0.46
25:DA:1665:A:H2'	25:DA:1666:G:O4'	2.15	0.46
26:DB:14:U:H1'	26:DB:108:U:O2'	2.16	0.46
25:DA:2748:A:H5'	31:DH:4:ILE:HD13	1.97	0.46
39:DT:91:ARG:HB2	39:DT:121:ILE:HG13	1.97	0.46
1:AA:454:C:N4	1:AA:479:C:N3	2.62	0.46
2:AB:133:LYS:O	2:AB:137:ARG:HG3	2.15	0.46
1:AA:411:A:OP2	4:AD:30:LYS:HE3	2.16	0.46
4:AD:98:GLU:OE1	4:AD:103:ASN:ND2	2.43	0.46
5:AE:91:LEU:HG	5:AE:118:ILE:HD11	1.98	0.46
23:AW:63:G:H2'	23:AW:64:A:O4'	2.15	0.46
25:BA:714:U:O2	54:B8:2:PRO:HD2	2.15	0.46
25:BA:2189:U:H3	25:BA:2190:G:H21	1.64	0.46
25:BA:2602:A:H2'	25:BA:2603:C:C6	2.50	0.46
25:BA:2800:C:H1'	28:BE:62:PRO:HG3	1.96	0.46
25:BA:2033:U:OP1	42:BW:42:ARG:NH1	2.46	0.46
1:CA:165:C:H2'	1:CA:166:G:H8	1.80	0.46
1:CA:392:G:H2'	1:CA:393:A:C8	2.51	0.46
1:CA:560:U:O2'	1:CA:561:U:OP2	2.27	0.46
1:CA:735:C:H2'	1:CA:736:C:H6	1.80	0.46
1:CA:828:A:H2'	1:CA:829:G:O4'	2.16	0.46
7:CG:32:ARG:HH12	7:CG:109:ASN:ND2	2.12	0.46
10:CJ:8:LEU:HD12	10:CJ:20:ALA:HB2	1.97	0.46
20:CT:60:GLU:HG3	20:CT:81:LYS:HD2	1.98	0.46
23:CW:51:U:O5'	23:CW:51:U:H6	1.97	0.46
23:CY:8:4SU:O2	23:CY:21:A:H2	1.97	0.46
25:DA:1830:C:OP2	61:DA:4650:HOH:O	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DB:40:U:H2'	50:D4:2:LYS:HE3	1.98	0.46
26:DB:55:U:O2'	30:DG:27:ASN:ND2	2.46	0.46
27:DD:134:ARG:HD3	27:DD:135:PHE:CE1	2.51	0.46
27:DD:164:GLN:HE21	27:DD:176:ARG:HH12	1.63	0.46
30:DG:11:TYR:OH	30:DG:33:ARG:HG2	2.16	0.46
31:DH:154:PRO:HB3	31:DH:163:TYR:CE2	2.50	0.46
1:AA:1004:A:N7	1:AA:1036:G:N2	2.64	0.46
1:AA:1148:U:H2'	1:AA:1149:C:O4'	2.16	0.46
1:AA:192:U:H2'	1:AA:193:C:C6	2.50	0.46
8:AH:6:ILE:HB	8:AH:85:ARG:NH1	2.30	0.46
9:AI:96:LEU:HA	9:AI:96:LEU:HD23	1.84	0.46
15:AO:82:ILE:O	15:AO:86:GLY:N	2.48	0.46
52:B6:13:CYS:SG	52:B6:47:THR:HG21	2.56	0.46
25:BA:2156:A:N6	25:BA:2179:G:H1'	2.29	0.46
25:BA:785:G:C6	25:BA:786:G:C2	3.04	0.46
28:BE:178:GLU:OE2	28:BE:178:GLU:N	2.30	0.46
29:BF:135:LYS:HB2	29:BF:138:GLU:HG3	1.97	0.46
1:CA:1122:U:C4	1:CA:1123:A:N7	2.84	0.46
4:CD:8:VAL:HG13	4:CD:21:LEU:HD12	1.97	0.46
6:CF:36:ARG:HH11	6:CF:38:GLU:HG2	1.81	0.46
12:CL:37:CYS:SG	12:CL:81:SER:HB2	2.56	0.46
13:CM:122:LYS:HD3	13:CM:123:ALA:N	2.17	0.46
16:CP:69:THR:HB	16:CP:72:ARG:HH12	1.81	0.46
51:D5:16:ARG:HD2	51:D5:17:ASP:OD1	2.15	0.46
25:DA:1257:C:H4'	29:DF:83:PHE:CD2	2.51	0.46
25:DA:1507:A:O2'	25:DA:1508:A:O4'	2.32	0.46
25:DA:889:C:O2'	25:DA:890:A:OP2	2.30	0.46
28:DE:101:ARG:CZ	28:DE:171:GLU:HB2	2.45	0.46
31:DH:125:VAL:HG13	31:DH:131:VAL:HG22	1.98	0.46
31:DH:149:ARG:HA	31:DH:162:ILE:HB	1.98	0.46
31:DH:95:ARG:HG2	31:DH:96:ALA:N	2.30	0.46
33:DN:73:THR:OG1	33:DN:82:LEU:HD11	2.15	0.46
38:DS:65:VAL:O	38:DS:69:VAL:HG12	2.16	0.46
1:AA:1392:G:N2	1:AA:1502:A:C8	2.84	0.46
2:AB:230:VAL:HG22	2:AB:231:GLU:H	1.80	0.46
3:AC:119:ARG:O	3:AC:123:GLN:HG3	2.15	0.46
14:AN:50:LYS:HZ3	14:AN:50:LYS:HB2	1.81	0.46
21:AU:18:TYR:CD2	21:AU:24:ARG:HD3	2.51	0.46
25:BA:2096:U:H2'	25:BA:2097:U:C6	2.50	0.46
25:BA:2163:G:C5	25:BA:2173:G:C2	3.04	0.46
25:BA:2661:U:H2'	25:BA:2662:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2820:A:N6	25:BA:2900:G:O2'	2.42	0.46
25:BA:302:A:H2'	25:BA:303:C:C6	2.51	0.46
25:BA:553:A:C2	25:BA:2065:C:H4'	2.51	0.46
26:BB:2:C:H2'	26:BB:3:C:C6	2.51	0.46
31:BH:59:ARG:HH11	31:BH:59:ARG:CG	2.29	0.46
34:BO:80:ASP:OD1	39:BT:64:ARG:NH2	2.48	0.46
1:CA:1032:G:H2'	1:CA:1033:G:C8	2.51	0.46
1:CA:1380:U:C4	7:CG:3:ARG:HG2	2.50	0.46
3:CC:137:ALA:HA	3:CC:140:ARG:CZ	2.45	0.46
13:CM:19:LEU:HD11	13:CM:56:LEU:HD21	1.97	0.46
13:CM:3:ARG:N	50:D4:34:GLU:OE1	2.49	0.46
23:CW:34:G:H2'	23:CW:35:A:C8	2.51	0.46
25:DA:1114:G:C2'	25:DA:1115:G:H5'	2.45	0.46
25:DA:2270:G:H2'	25:DA:2271:G:O4'	2.15	0.46
25:DA:2708:G:H1'	37:DR:71:GLN:HE22	1.79	0.46
25:DA:795:C:H2'	25:DA:796:C:C6	2.51	0.46
35:DP:111:ARG:HG2	35:DP:128:HIS:CD2	2.51	0.46
1:AA:1392:G:H21	1:AA:1502:A:H8	1.64	0.46
1:AA:339:C:H2'	1:AA:340:U:C6	2.50	0.46
1:AA:436:C:H2'	1:AA:437:U:C6	2.51	0.46
1:AA:731:G:H5'	1:AA:766:A:H4'	1.98	0.46
8:AH:112:LEU:HD11	8:AH:124:ALA:HB2	1.98	0.46
1:AA:1343:G:H1'	9:AI:121:ARG:NH1	2.31	0.46
25:BA:1517:G:H5"	25:BA:1518:A:OP1	2.16	0.46
25:BA:153:C:OP2	47:B1:92:LYS:NZ	2.49	0.46
25:BA:2023:A:H2'	25:BA:2024:G:C8	2.51	0.46
25:BA:2156:A:OP1	25:BA:2178:G:N2	2.49	0.46
25:BA:2897:U:H2'	25:BA:2898:C:C6	2.50	0.46
27:BD:77:ALA:O	27:BD:116:GLN:HG3	2.16	0.46
1:CA:1001(A):G:C4	1:CA:1002:G:H1'	2.50	0.46
1:CA:1105:A:H2'	1:CA:1106:G:H8	1.81	0.46
1:CA:841:U:C5	1:CA:848:C:H1'	2.51	0.46
2:CB:189:ASP:N	2:CB:189:ASP:OD1	2.49	0.46
3:CC:157:ILE:HD13	3:CC:166:GLU:HG3	1.97	0.46
14:CN:21:TYR:HE1	14:CN:23:ARG:NE	2.14	0.46
16:CP:22:THR:HA	16:CP:33:ILE:HG13	1.98	0.46
16:CP:53:VAL:O	16:CP:57:ARG:HB2	2.16	0.46
23:CY:63:G:H2'	23:CY:64:A:O4'	2.16	0.46
25:DA:2173:A:H2'	25:DA:2174:C:O4'	2.16	0.46
25:DA:287:C:H2'	25:DA:288:C:C6	2.49	0.46
25:DA:882:G:N2	25:DA:894:C:N3	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:DD:148:GLU:HB2	27:DD:151:LYS:HD2	1.98	0.46
28:DE:115:GLY:O	28:DE:119:ARG:HB2	2.16	0.46
1:AA:1070:U:H2'	1:AA:1071:C:C6	2.51	0.46
1:AA:1149:C:P	9:AI:9:ARG:HH21	2.39	0.46
1:AA:954:G:H21	1:AA:1227:A:H62	1.63	0.46
2:AB:22:LYS:HA	2:AB:40:HIS:HE1	1.81	0.46
1:AA:1106:G:H5''	3:AC:172:ARG:HG2	1.98	0.46
3:AC:28:GLN:O	3:AC:32:LEU:HD23	2.16	0.46
11:AK:48:ILE:O	11:AK:50:TYR:N	2.48	0.46
25:BA:139:A:C8	25:BA:1454:C:O2'	2.65	0.46
1:CA:1004:A:C2	1:CA:1038:C:C4	3.04	0.46
1:CA:1236:A:O2'	1:CA:1304:G:H4'	2.16	0.46
1:CA:142:G:H2'	1:CA:143:A:C8	2.51	0.46
1:CA:96:U:HO2'	1:CA:97:G:H8	1.60	0.46
5:CE:42:GLY:HA2	5:CE:65:ASN:O	2.16	0.46
5:CE:53:LEU:HD12	5:CE:53:LEU:H	1.80	0.46
7:CG:10:ARG:HA	7:CG:10:ARG:HD2	1.56	0.46
24:CX:13:C:O2'	25:DA:1924:C:H4'	2.16	0.46
25:DA:2136:C:N4	25:DA:2155:G:H1	2.14	0.46
26:DB:78:A:C2	26:DB:100:A:C4	3.04	0.46
27:DD:2:ALA:O	27:DD:3:VAL:HB	2.16	0.46
28:DE:9:VAL:HG13	28:DE:25:VAL:O	2.16	0.46
33:DN:39:ARG:HA	33:DN:40:PRO:HD3	1.79	0.46
25:DA:2882:A:H5'	37:DR:96:ARG:HG3	1.96	0.46
38:DS:83:LYS:HE3	38:DS:84:GLN:HG3	1.98	0.46
41:DV:98:GLU:CD	41:DV:100:ARG:HH12	2.20	0.46
44:DY:13:VAL:HG12	44:DY:74:PRO:HA	1.98	0.46
1:AA:1021:G:O2'	1:AA:1022:G:O5'	2.27	0.45
1:AA:920:U:H2'	1:AA:921:U:C6	2.50	0.45
25:BA:1324:A:OP1	37:BR:36:THR:HG23	2.17	0.45
25:BA:1513:G:HO2'	25:BA:1593:C:HO2'	1.53	0.45
25:BA:2346:G:H5'	38:BS:9:ARG:HG2	1.98	0.45
28:BE:24:THR:HG22	28:BE:186:GLY:O	2.15	0.45
30:BG:115:ARG:HB3	30:BG:136:ARG:HH12	1.82	0.45
38:BS:52:SER:O	38:BS:56:LEU:HD12	2.16	0.45
1:CA:1302:U:OP2	13:CM:21:TYR:OH	2.13	0.45
23:CY:62:C:H2'	23:CY:63:G:H8	1.80	0.45
25:DA:2657:A:O2'	31:DH:160:LYS:NZ	2.35	0.45
25:DA:1278:A:OP1	37:DR:36:THR:HG23	2.16	0.45
45:DZ:128:VAL:HG22	45:DZ:129:SER:O	2.15	0.45
2:AB:223:ILE:HD12	2:AB:230:VAL:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:79:ARG:CB	7:AG:80:VAL:HA	2.46	0.45
1:AA:375:U:OP1	16:AP:69:THR:HG21	2.16	0.45
49:B3:5:LYS:NZ	49:B3:55:ARG:HH12	2.14	0.45
25:BA:1232:G:H5''	41:BV:81:TYR:CE1	2.52	0.45
25:BA:1495:G:H4'	25:BA:1589:A:OP1	2.16	0.45
25:BA:1875:C:H2'	25:BA:1876:G:H8	1.81	0.45
25:BA:2652:G:OP1	33:BN:97:ARG:NH2	2.44	0.45
25:BA:704:U:H2'	25:BA:705:C:C6	2.51	0.45
28:BE:144:ARG:HB3	28:BE:145:LYS:H	1.48	0.45
33:BN:68:GLU:H	33:BN:68:GLU:HG2	1.50	0.45
34:BO:8:LEU:HD13	34:BO:82:ASN:HB3	1.98	0.45
1:CA:1039:C:C4	1:CA:1040:U:C4	3.05	0.45
1:CA:232:G:H1'	1:CA:262:A:N1	2.31	0.45
1:CA:833:U:H2'	1:CA:834:C:C6	2.51	0.45
1:CA:91:C:H2'	1:CA:92:C:C6	2.51	0.45
1:CA:992:U:H4'	1:CA:993:G:O5'	2.16	0.45
2:CB:97:TRP:NE1	2:CB:173:ALA:HB2	2.31	0.45
2:CB:88:ALA:HB1	2:CB:90:MET:HG3	1.98	0.45
14:CN:23:ARG:NH1	14:CN:30:ALA:HB2	2.31	0.45
47:D1:67:ILE:N	47:D1:68:PRO:HD2	2.32	0.45
25:DA:2127:G:N1	25:DA:2161:C:C2	2.84	0.45
25:DA:2674:G:H2'	25:DA:2675:A:C8	2.50	0.45
25:DA:2888:C:H2'	25:DA:2889:C:C6	2.51	0.45
25:DA:918:A:C5	25:DA:919:G:H1'	2.51	0.45
26:DB:83:G:N2	26:DB:94:C:O2	2.43	0.45
28:DE:44:TYR:HB2	28:DE:82:ARG:HH12	1.81	0.45
36:DQ:85:LYS:HG2	46:D0:7:LEU:HB3	1.97	0.45
1:AA:1036:G:H3'	1:AA:1037:C:H6	1.82	0.45
1:AA:1181:G:H1'	1:AA:1182:G:C4	2.51	0.45
1:AA:520:A:N1	1:AA:536:C:H1'	2.32	0.45
1:AA:731:G:OP1	1:AA:766:A:H1'	2.17	0.45
2:AB:109:SER:O	2:AB:112:VAL:HG22	2.16	0.45
2:AB:221:LEU:HD22	2:AB:221:LEU:HA	1.69	0.45
10:AJ:62:HIS:HB3	14:AN:59:ALA:HB3	1.97	0.45
13:AM:50:GLU:O	13:AM:54:VAL:HG22	2.15	0.45
25:BA:1717:C:O2	28:BE:129:HIS:NE2	2.42	0.45
25:BA:2013:U:H2'	25:BA:2014:G:H5''	1.99	0.45
1:CA:1392:G:N2	1:CA:1502:A:H8	2.14	0.45
1:CA:659:U:H2'	1:CA:660:G:H5'	1.99	0.45
8:CH:19:VAL:HG23	8:CH:21:LYS:HG3	1.98	0.45
8:CH:25:ASP:N	8:CH:25:ASP:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:CI:58:HIS:CD2	9:CI:58:HIS:H	2.33	0.45
23:CW:50:U:O2	23:CW:64:A:N1	2.50	0.45
25:DA:2203:U:O2'	25:DA:2205:C:H5'	2.16	0.45
25:DA:265:A:H1'	25:DA:266:G:O4'	2.16	0.45
25:DA:484:C:H2'	25:DA:485:C:C6	2.52	0.45
25:DA:817:C:O2'	25:DA:839:U:H5''	2.16	0.45
25:DA:844:C:C5	25:DA:845:G:C6	3.05	0.45
26:DB:79:C:H2'	26:DB:80:U:O4'	2.17	0.45
29:DF:108:LYS:NZ	29:DF:108:LYS:HB2	2.31	0.45
30:DG:124:SER:OG	30:DG:124:SER:O	2.32	0.45
30:DG:75:LYS:HE3	30:DG:77:ILE:HD11	1.98	0.45
35:DP:65:ARG:HG3	54:D8:25:MET:HG2	1.99	0.45
39:DT:11:GLU:O	39:DT:15:VAL:HG23	2.17	0.45
40:DU:79:PHE:CZ	40:DU:83:LEU:HD21	2.51	0.45
1:AA:1492:A:O2'	1:AA:1493:A:O5'	2.26	0.45
1:AA:152:A:N6	1:AA:169:C:N3	2.65	0.45
4:AD:194:LEU:HD13	4:AD:194:LEU:HA	1.70	0.45
1:AA:881:G:P	12:AL:12:ARG:HH22	2.38	0.45
24:AX:13:C:O2'	25:BA:1946:C:H4'	2.17	0.45
24:AX:17:C:H5'	24:AX:61:C:OP1	2.16	0.45
47:B1:89:GLU:HG2	47:B1:89:GLU:H	1.58	0.45
25:BA:180:A:H2'	25:BA:181:C:C6	2.51	0.45
25:BA:2163:G:C6	25:BA:2164:C:C2	3.04	0.45
25:BA:2832:G:N7	61:BA:5454:HOH:O	2.36	0.45
31:BH:6:ARG:HE	31:BH:6:ARG:HB3	1.25	0.45
25:BA:2116:G:P	32:BI:22:LYS:HD2	2.56	0.45
35:BP:135:LEU:HD23	35:BP:135:LEU:HA	1.79	0.45
39:BT:6:LEU:O	39:BT:10:VAL:HG23	2.16	0.45
1:CA:187:C:H2'	1:CA:188:C:H6	1.82	0.45
1:CA:728:A:OP1	1:CA:742:G:O2'	2.34	0.45
2:CB:78:GLN:O	2:CB:94:ASN:ND2	2.49	0.45
7:CG:77:SER:HA	7:CG:85:TYR:O	2.16	0.45
12:CL:60:LEU:HD11	12:CL:85:ILE:HD13	1.98	0.45
20:CT:50:GLU:O	20:CT:100:ILE:HD11	2.15	0.45
25:DA:1187:G:H5'	41:DV:81:TYR:CE1	2.51	0.45
25:DA:1721:G:H2'	25:DA:1740:G:O6	2.17	0.45
25:DA:1932:A:H2'	25:DA:1933:G:O4'	2.17	0.45
25:DA:2139:C:N4	25:DA:2152:G:C6	2.82	0.45
25:DA:2119:A:N6	25:DA:2170:A:N7	2.64	0.45
28:DE:2:LYS:NZ	28:DE:95:ILE:O	2.32	0.45
30:DG:111:LEU:HD23	30:DG:117:PHE:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:DG:72:ARG:NH1	30:DG:87:PRO:HG3	2.31	0.45
37:DR:97:VAL:HG22	37:DR:114:VAL:HG22	1.98	0.45
1:AA:1025:U:O2	1:AA:1036:G:C6	2.69	0.45
1:AA:110:C:H2'	1:AA:111:G:O4'	2.16	0.45
1:AA:1275:A:H2'	1:AA:1276:G:H5'	1.99	0.45
1:AA:1352:C:H2'	1:AA:1353:G:C8	2.51	0.45
1:AA:984:C:N4	1:AA:1221:G:H1	2.15	0.45
2:AB:7:VAL:HG21	2:AB:221:LEU:HD21	1.98	0.45
25:BA:1093:G:H2'	25:BA:1156:G:H1	1.82	0.45
25:BA:2102:G:OP1	47:B1:35:THR:HG21	2.17	0.45
44:BY:86:ARG:NH1	44:BY:100:ALA:HB1	2.32	0.45
1:CA:1055:A:C5	1:CA:1206:G:C2	3.05	0.45
1:CA:109:A:C6	1:CA:326:G:C6	3.05	0.45
1:CA:154:C:C2'	1:CA:155:C:H5'	2.47	0.45
57:CA:3202:UAM:OAE	57:CA:3202:UAM:NAD	2.49	0.45
1:CA:955:U:O2'	19:CS:83:HIS:HD2	2.00	0.45
5:CE:13:ILE:HG13	5:CE:13:ILE:O	2.16	0.45
25:DA:111:A:H4'	48:D2:69:ARG:NH1	2.31	0.45
25:DA:1149:G:H2'	25:DA:1150:C:C6	2.51	0.45
25:DA:1561:G:H2'	25:DA:1562:A:C8	2.50	0.45
25:DA:2331:G:O2'	46:D0:43:THR:HG22	2.17	0.45
25:DA:774:A:H2'	25:DA:774:A:N3	2.31	0.45
25:DA:800:A:OP1	25:DA:800:A:H8	1.98	0.45
28:DE:11:MET:HG2	28:DE:24:THR:HB	1.98	0.45
29:DF:53:THR:HG23	29:DF:55:GLY:N	2.28	0.45
42:DW:86:LEU:HD22	42:DW:96:ILE:HD11	1.99	0.45
1:AA:953:G:H2'	1:AA:954:G:O4'	2.17	0.45
2:AB:178:ARG:NH2	8:AH:74:PRO:HB3	2.32	0.45
8:AH:14:ARG:O	8:AH:18:ARG:HD2	2.16	0.45
14:AN:39:LEU:HD11	14:AN:47:LEU:HD12	1.99	0.45
23:AW:1:G:H2'	23:AW:2:C:C6	2.51	0.45
23:AY:5:G:H1'	23:AY:69:G:N2	2.32	0.45
54:B8:23:VAL:HG11	54:B8:47:LYS:HD3	1.99	0.45
25:BA:2473:C:H2'	25:BA:2474:U:C6	2.52	0.45
25:BA:2331:G:N2	38:BS:3:ARG:HE	2.03	0.45
1:CA:1133:G:H1	1:CA:1141:C:H42	1.65	0.45
1:CA:1162:C:N4	1:CA:1174:G:N1	2.63	0.45
1:CA:509:A:H5''	4:CD:55:ALA:HB2	1.98	0.45
15:CO:18:PHE:CE2	15:CO:21:ASP:HB2	2.51	0.45
23:CY:69:G:H2'	23:CY:70:G:O4'	2.16	0.45
52:D6:14:THR:OG1	52:D6:48:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2147:G:C2	25:DA:2148:G:H1'	2.52	0.45
25:DA:224:G:H2'	25:DA:225:A:O4'	2.16	0.45
25:DA:887:A:H4'	25:DA:888:C:C5	2.50	0.45
25:DA:1803:A:H4'	27:DD:259:THR:HG23	1.98	0.45
28:DE:27:LEU:HD22	39:DT:1:MET:HE1	1.97	0.45
41:DV:25:LEU:HD23	41:DV:25:LEU:HA	1.77	0.45
43:DX:25:LYS:HZ3	43:DX:82:GLN:HE21	1.63	0.45
43:DX:50:LYS:O	43:DX:84:ALA:N	2.49	0.45
4:AD:152:SER:O	4:AD:155:LEU:HB2	2.16	0.45
4:AD:173:TRP:CD2	4:AD:189:PRO:HG3	2.51	0.45
1:AA:542:G:H5'	4:AD:41:GLY:HA3	1.98	0.45
14:AN:29:ARG:HD3	14:AN:40:CYS:SG	2.56	0.45
47:B1:21:ARG:HD2	47:B1:35:THR:HB	1.99	0.45
25:BA:485:U:H5''	53:B7:40:TRP:CD2	2.51	0.45
25:BA:1212:C:H2'	25:BA:1213:U:C6	2.51	0.45
25:BA:275:C:H2'	25:BA:276:C:C6	2.52	0.45
27:BD:92:ILE:HD12	27:BD:104:TYR:CD1	2.52	0.45
35:BP:47:ASP:OD2	35:BP:49:ARG:NH2	2.49	0.45
37:BR:21:TYR:OH	37:BR:43:GLU:HG2	2.16	0.45
38:BS:11:LYS:O	38:BS:15:ARG:HG3	2.16	0.45
38:BS:39:ILE:HB	38:BS:49:VAL:HG13	1.99	0.45
1:CA:1134:G:C2'	1:CA:1135:U:H5'	2.46	0.45
1:CA:1291:G:C6	1:CA:1292:U:C4	3.04	0.45
1:CA:836:G:C6	1:CA:851:G:C6	3.04	0.45
10:CJ:70:ARG:HD3	10:CJ:70:ARG:HA	1.84	0.45
6:CF:50:TYR:CE2	18:CR:77:GLY:HA2	2.52	0.45
19:CS:27:GLU:HG2	19:CS:47:HIS:NE2	2.32	0.45
19:CS:80:TYR:CZ	19:CS:82:GLY:HA2	2.51	0.45
23:CY:18:G:C2	23:CY:55:PSU:C4	3.05	0.45
25:DA:1810:A:H2'	25:DA:1811:G:O4'	2.17	0.45
25:DA:1999:C:H2'	25:DA:2000:G:O4'	2.17	0.45
25:DA:2723:C:OP2	28:DE:109:LYS:NZ	2.45	0.45
29:DF:20:LEU:HD13	29:DF:21:ALA:N	2.32	0.45
54:B8:62:LEU:HB3	54:B8:65:GLU:HG2	1.99	0.45
25:BA:2343:G:O2'	46:B0:43:THR:HG22	2.17	0.45
25:BA:2859:U:H4'	25:BA:2878:A:C2	2.52	0.45
25:BA:552:C:C5	25:BA:2792:U:H2'	2.52	0.45
25:BA:2799:U:O2'	28:BE:62:PRO:O	2.27	0.45
33:BN:10:GLU:OE1	33:BN:11:PRO:HD2	2.16	0.45
39:BT:84:GLN:HG2	39:BT:85:LYS:HG2	1.98	0.45
1:CA:1036:G:H2'	1:CA:1037:C:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:408:A:H4'	4:CD:112:VAL:HG21	1.99	0.45
1:CA:964:A:N3	1:CA:969:A:O2'	2.36	0.45
5:CE:100:VAL:HG22	5:CE:118:ILE:HG22	1.99	0.45
10:CJ:27:ALA:HB1	10:CJ:74:ILE:HD13	1.98	0.45
1:CA:1305:G:H5'	21:CU:4:GLY:HA3	1.98	0.45
23:CW:76:A:H4'	25:DA:2506:U:O2'	2.17	0.45
47:D1:2:SER:HB3	47:D1:46:LEU:HD12	1.99	0.45
25:DA:2133:G:O2'	25:DA:2157:G:N2	2.50	0.45
25:DA:304:G:O6	61:DA:4492:HOH:O	2.19	0.45
25:DA:492:A:H2'	25:DA:493:G:O4'	2.17	0.45
30:DG:11:TYR:OH	30:DG:16:ARG:HD3	2.17	0.45
36:DQ:21:THR:HG21	36:DQ:101:ARG:HD3	1.99	0.45
1:AA:452:A:H4'	16:AP:72:ARG:NH1	2.32	0.45
1:AA:620:C:C2	4:AD:135:LEU:HG	2.52	0.45
1:AA:735:C:H2'	1:AA:736:C:H6	1.82	0.45
18:AR:31:LEU:HD23	18:AR:31:LEU:H	1.81	0.45
19:AS:37:ARG:H	19:AS:37:ARG:HG3	1.42	0.45
25:BA:1102:G:H4'	25:BA:1132:A:C8	2.52	0.45
25:BA:2602:A:H2'	25:BA:2603:C:H6	1.82	0.45
33:BN:96:GLU:H	33:BN:96:GLU:CD	2.20	0.45
1:CA:1151:A:O4'	10:CJ:39:PRO:HB2	2.16	0.45
1:CA:188:C:O4'	20:CT:89:ARG:NH2	2.50	0.45
3:CC:8:ILE:HD13	3:CC:184:TYR:HB3	1.99	0.45
1:CA:35:G:O2'	12:CL:118:SER:O	2.25	0.45
12:CL:32:PHE:HB3	12:CL:84:LEU:HD11	1.99	0.45
17:CQ:43:LEU:HG	17:CQ:68:ARG:HH11	1.80	0.45
20:CT:57:ARG:NH1	20:CT:101:GLY:O	2.50	0.45
47:D1:89:GLU:O	47:D1:93:GLU:HG2	2.17	0.45
50:D4:15:ILE:HB	50:D4:32:TYR:CD1	2.52	0.45
25:DA:2096:U:H2'	25:DA:2097:C:C6	2.52	0.45
25:DA:2483:C:H2'	25:DA:2484:G:O4'	2.17	0.45
25:DA:2543:G:H2'	25:DA:2544:G:C8	2.52	0.45
25:DA:448:U:H5''	61:DA:4950:HOH:O	2.17	0.45
25:DA:918:A:H5''	26:DB:98:G:O2'	2.17	0.45
25:DA:1140:C:O3'	33:DN:25:ARG:NH1	2.50	0.45
33:DN:67:LEU:HB3	33:DN:88:GLU:HG3	1.99	0.45
1:AA:1027:C:H2'	1:AA:1027:C:O2	2.17	0.45
1:AA:141:A:H1'	1:AA:182:U:O2	2.17	0.45
1:AA:441:A:H5'	1:AA:442:C:OP2	2.17	0.45
1:AA:445:G:H2'	1:AA:446:G:O4'	2.17	0.45
1:AA:741:G:H2'	1:AA:742:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:23:ASN:ND2	9:AI:23:ASN:H	2.13	0.45
31:BH:149:ARG:NH1	31:BH:167:GLU:OE2	2.48	0.45
1:CA:1004:A:H5''	1:CA:1025:U:C5	2.52	0.45
1:CA:1004:A:H3'	1:CA:1005:A:C5'	2.47	0.45
1:CA:1298:C:H2'	7:CG:114:ARG:HH12	1.82	0.45
1:CA:1469:G:H2'	1:CA:1470:G:C8	2.52	0.45
2:CB:53:ARG:O	2:CB:56:ARG:HB3	2.17	0.45
3:CC:148:GLY:HA3	3:CC:172:ARG:O	2.17	0.45
3:CC:7:PRO:O	3:CC:11:ARG:NH1	2.46	0.45
5:CE:33:VAL:HG13	5:CE:112:LEU:HD12	1.98	0.45
6:CF:82:ARG:HA	6:CF:82:ARG:HD2	1.66	0.45
7:CG:38:LEU:O	7:CG:42:ILE:HG13	2.17	0.45
20:CT:43:LEU:HD12	20:CT:55:ILE:HG13	1.98	0.45
23:CY:59:U:H3'	23:CY:60:U:O2	2.17	0.45
49:D3:18:ASP:N	49:D3:18:ASP:OD1	2.45	0.45
25:DA:443:A:H1'	25:DA:1201:C:O4'	2.17	0.45
25:DA:1247:A:OP1	29:DF:95:ARG:NH2	2.45	0.45
25:DA:1653:G:H3'	37:DR:2:ARG:HD3	1.98	0.45
25:DA:2035:G:OP1	61:DA:4502:HOH:O	2.20	0.45
25:DA:2064:C:H1'	25:DA:2450:A:C2	2.52	0.45
25:DA:90:U:H1'	25:DA:92:A:C8	2.51	0.45
31:DH:25:LYS:HE2	31:DH:27:LYS:HZ3	1.82	0.45
25:DA:1226:A:OP1	41:DV:84:LYS:HE2	2.17	0.45
45:DZ:105:VAL:O	45:DZ:140:ASP:HA	2.17	0.45
2:AB:15:VAL:HG23	2:AB:209:ARG:HB3	1.99	0.44
4:AD:129:ASN:OD1	4:AD:145:GLU:N	2.38	0.44
13:AM:50:GLU:HA	13:AM:53:VAL:HB	1.99	0.44
47:B1:3:LYS:HB2	47:B1:61:ARG:NH1	2.31	0.44
25:BA:196:A:H2'	25:BA:197:C:O4'	2.16	0.44
1:CA:1080:A:H5''	1:CA:1081:G:OP2	2.17	0.44
1:CA:142:G:H2'	1:CA:143:A:H8	1.82	0.44
1:CA:162:A:H8	1:CA:162:A:O5'	2.00	0.44
2:CB:97:TRP:CZ2	2:CB:173:ALA:HA	2.52	0.44
18:CR:53:ARG:HH21	18:CR:59:SER:HA	1.82	0.44
24:CX:21:A:N6	24:CX:46:G:H2'	2.32	0.44
53:D7:9:ARG:CG	53:D7:46:VAL:HG23	2.47	0.44
25:DA:1453:U:O2'	25:DA:1455:G:N7	2.44	0.44
25:DA:1786:A:H1'	25:DA:1938:A:N6	2.32	0.44
25:DA:1915:U:H2'	25:DA:1916:A:O4'	2.17	0.44
25:DA:1999:C:H4'	25:DA:2723:C:O2	2.17	0.44
27:DD:71:ASP:HB3	27:DD:103:ARG:NH2	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:DX:12:VAL:HG22	43:DX:29:TRP:CE2	2.52	0.44
1:AA:255:G:H1'	17:AQ:16:GLN:NE2	2.32	0.44
1:AA:453:A:C5	1:AA:454:C:C4	3.05	0.44
1:AA:78:G:C2	1:AA:91:C:N4	2.85	0.44
5:AE:105:VAL:HB	5:AE:106:PRO:HD3	1.99	0.44
5:AE:31:LEU:HA	5:AE:31:LEU:HD23	1.90	0.44
23:AW:18:G:H4'	23:AW:60:U:C6	2.52	0.44
25:BA:2186:C:C3'	25:BA:2187:G:H5'	2.47	0.44
25:BA:2699:U:H2'	25:BA:2700:U:O4'	2.15	0.44
32:BI:131:LYS:H	32:BI:138:ILE:H	1.64	0.44
35:BP:82:GLY:HA2	35:BP:113:LYS:O	2.16	0.44
40:BU:86:ALA:HB2	40:BU:116:ALA:HB2	1.99	0.44
1:CA:987:G:H1	1:CA:1218:C:H42	1.65	0.44
1:CA:1246:C:H2'	1:CA:1247:U:C6	2.53	0.44
1:CA:580:U:H2'	1:CA:581:G:O4'	2.16	0.44
1:CA:651:C:N4	1:CA:753:A:OP2	2.50	0.44
20:CT:16:HIS:O	20:CT:19:SER:OG	2.26	0.44
23:CY:19:G:N1	23:CY:56:C:C4	2.85	0.44
54:D8:58:ILE:HA	54:D8:61:LEU:HD12	1.99	0.44
55:D9:17:ILE:HD12	55:D9:17:ILE:HA	1.78	0.44
25:DA:1399:C:OP1	43:DX:25:LYS:NZ	2.47	0.44
25:DA:2167:U:H2'	25:DA:2168:G:N3	2.32	0.44
25:DA:2184:G:C2'	25:DA:2185:C:H5'	2.47	0.44
25:DA:2238:G:H2'	25:DA:2238:G:N3	2.33	0.44
25:DA:848:G:C2	25:DA:933:A:H1'	2.51	0.44
32:DI:29:TYR:O	32:DI:32:PRO:HD2	2.17	0.44
34:DO:4:PRO:O	34:DO:5:GLN:HB2	2.18	0.44
1:AA:1112:C:H1'	3:AC:179:ARG:HG2	1.99	0.44
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.53	0.44
3:AC:150:LYS:HG3	3:AC:169:ALA:HB2	1.99	0.44
5:AE:52:PRO:HG2	5:AE:53:LEU:HD12	1.97	0.44
6:AF:100:ASN:HB2	18:AR:28:GLU:HA	1.99	0.44
9:AI:26:VAL:HB	9:AI:33:PHE:HB2	1.98	0.44
13:AM:17:VAL:O	13:AM:20:THR:OG1	2.20	0.44
20:AT:18:GLN:O	20:AT:22:ARG:HG3	2.16	0.44
25:BA:2745:G:H3'	25:BA:2746:A:O4'	2.16	0.44
25:BA:861:C:O2'	25:BA:862:C:H5'	2.17	0.44
29:BF:32:LEU:HD22	29:BF:112:MET:HE1	2.00	0.44
32:BI:12:LEU:HA	32:BI:12:LEU:HD23	1.74	0.44
37:BR:72:ASP:O	37:BR:76:VAL:HG23	2.18	0.44
43:BX:53:LYS:HB3	43:BX:82:GLN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1001(A):G:C5	1:CA:1002:G:H1'	2.52	0.44
1:CA:1251:A:N1	1:CA:1354:C:O2'	2.42	0.44
1:CA:1262:C:H2'	1:CA:1263:C:C6	2.53	0.44
1:CA:371:G:H1'	1:CA:482:A:H1'	2.00	0.44
9:CI:23:ASN:HD22	9:CI:24:GLY:H	1.64	0.44
9:CI:37:PHE:HD1	9:CI:40:LEU:HD12	1.82	0.44
23:CW:61:C:O2'	23:CW:62:C:O4'	2.36	0.44
49:D3:3:ARG:HD3	49:D3:60:GLU:CB	2.47	0.44
52:D6:15:GLU:HG3	52:D6:47:THR:CG2	2.48	0.44
52:D6:40:CYS:O	52:D6:44:ARG:N	2.51	0.44
25:DA:1006:C:C2	25:DA:1138:G:N2	2.85	0.44
25:DA:1204:A:N6	25:DA:1240:U:H2'	2.32	0.44
25:DA:1336:A:H2'	25:DA:1337:G:C8	2.53	0.44
25:DA:143:G:H2'	25:DA:143(A):C:C6	2.51	0.44
25:DA:1557:C:OP2	25:DA:1558:A:O2'	2.22	0.44
25:DA:2114:A:O2'	25:DA:2167:U:H1'	2.17	0.44
25:DA:271(D):G:H2'	25:DA:271(E):U:C6	2.52	0.44
25:DA:601:C:O2	25:DA:605:C:H4'	2.17	0.44
25:DA:652(A):A:C3'	25:DA:652(B):A:H5'	2.47	0.44
28:DE:72:VAL:HA	28:DE:73:GLU:CB	2.48	0.44
25:DA:614(B):G:O2'	29:DF:44:ARG:HD2	2.17	0.44
30:DG:43:LEU:HD12	30:DG:43:LEU:HA	1.80	0.44
33:DN:30:ILE:O	33:DN:34:LEU:HD22	2.17	0.44
36:DQ:16:ARG:HG2	36:DQ:18:LYS:HE2	1.98	0.44
38:DS:94:TYR:CE1	38:DS:99:LYS:HG3	2.53	0.44
45:DZ:54:HIS:ND1	45:DZ:101:PRO:HG3	2.32	0.44
1:AA:1169:A:H2'	1:AA:1170:A:C8	2.52	0.44
1:AA:426:G:OP1	4:AD:38:TYR:OH	2.29	0.44
1:AA:434:U:H2'	1:AA:435:C:C6	2.52	0.44
1:AA:93:G:C2'	1:AA:96:U:H5'	2.47	0.44
2:AB:184:VAL:HG12	2:AB:197:VAL:HG13	1.99	0.44
11:AK:82:VAL:HB	11:AK:108:ILE:HG12	1.99	0.44
15:AO:56:LEU:O	15:AO:60:VAL:HG23	2.17	0.44
16:AP:14:ASN:OD1	16:AP:42:ARG:NH2	2.50	0.44
19:AS:41:VAL:HG22	50:B4:61:ARG:HH22	1.81	0.44
23:AY:22:G:H5'	23:AY:23:A:OP2	2.17	0.44
25:BA:2695:C:O2	34:BO:70:LYS:NZ	2.48	0.44
25:BA:2812:A:H1'	25:BA:2904:U:H1'	2.00	0.44
25:BA:482:C:O2'	25:BA:483:A:OP2	2.32	0.44
25:BA:602:G:H2'	25:BA:603:C:C6	2.52	0.44
1:CA:1261:A:H3'	1:CA:1262:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:111:ARG:HD3	2:CB:111:ARG:HA	1.71	0.44
2:CB:185:ILE:HG22	2:CB:199:TYR:HB2	1.99	0.44
5:CE:144:THR:O	5:CE:148:VAL:HG23	2.18	0.44
5:CE:79:GLU:OE1	5:CE:79:GLU:N	2.38	0.44
23:CW:4:C:N3	23:CW:69:G:C2	2.85	0.44
24:CX:19:G:H4'	24:CX:20:U:OP2	2.16	0.44
23:CY:2:C:H2'	23:CY:3:C:C6	2.52	0.44
25:DA:667:U:O2	54:D8:2:PRO:HD2	2.18	0.44
25:DA:1359:A:H2'	25:DA:1360:A:H5'	2.00	0.44
25:DA:1363:C:H2'	25:DA:1364:G:H8	1.81	0.44
25:DA:2024:G:H2'	25:DA:2025:C:H6	1.81	0.44
25:DA:743:G:OP1	28:DE:130:GLY:HA2	2.16	0.44
26:DB:55:U:O3'	30:DG:27:ASN:ND2	2.51	0.44
40:DU:58:ARG:HA	40:DU:61:TRP:CE3	2.53	0.44
42:DW:9:TYR:HA	42:DW:100:THR:CG2	2.47	0.44
1:AA:922:G:C6	1:AA:923:A:C6	3.06	0.44
2:AB:208:ILE:O	2:AB:212:GLN:HB2	2.18	0.44
3:AC:65:ALA:HA	3:AC:100:ALA:HB3	1.99	0.44
4:AD:61:LYS:HE2	4:AD:206:PHE:CE2	2.52	0.44
12:AL:113:ARG:NE	12:AL:115:LYS:O	2.47	0.44
23:AW:23:A:H3'	23:AW:24:G:H8	1.83	0.44
23:AY:19:G:H1	25:BA:2191:A:N6	2.16	0.44
50:B4:48:ARG:HD3	50:B4:48:ARG:HA	1.73	0.44
52:B6:35:GLU:OE2	52:B6:50:ARG:NH1	2.44	0.44
54:B8:54:GLU:O	54:B8:58:ILE:HG13	2.17	0.44
55:B9:17:ILE:HG12	55:B9:26:ILE:HG12	1.99	0.44
25:BA:1201:A:OP1	40:BU:55:ARG:HD3	2.18	0.44
25:BA:2051:G:H2'	25:BA:2053:A:OP1	2.17	0.44
25:BA:2486:C:H5''	25:BA:2487:C:OP2	2.17	0.44
25:BA:696:C:H2'	25:BA:697:C:C6	2.53	0.44
1:CA:1022:G:H2'	1:CA:1023:G:C8	2.53	0.44
1:CA:1095:U:OP1	1:CA:1108:G:N2	2.44	0.44
5:CE:76:ILE:O	5:CE:93:PRO:HB3	2.17	0.44
20:CT:77:ALA:O	20:CT:81:LYS:HG3	2.18	0.44
24:CX:31:G:C8	24:CX:32:5MC:HM52	2.53	0.44
25:DA:2193:G:H2'	25:DA:2194:G:H8	1.83	0.44
27:DD:26:LYS:NZ	27:DD:30:GLU:OE1	2.49	0.44
30:DG:38:VAL:HG22	30:DG:93:THR:HG23	2.00	0.44
29:DF:187:VAL:HG12	35:DP:3:LEU:HD22	1.98	0.44
40:DU:61:TRP:CZ3	40:DU:93:LYS:HB2	2.53	0.44
45:DZ:126:VAL:CG1	45:DZ:161:VAL:HG23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1030(A):G:H2'	1:AA:1030(C):G:OP2	2.17	0.44
1:AA:1145:C:H4'	1:AA:1146:A:H5'	1.99	0.44
1:AA:971:G:N1	1:AA:1363(A):A:OP2	2.42	0.44
3:AC:18:TRP:HE3	3:AC:18:TRP:H	1.64	0.44
13:AM:108:ARG:HD3	13:AM:108:ARG:HA	1.80	0.44
25:BA:1085:G:H1	25:BA:1162:C:N4	2.16	0.44
25:BA:2136:A:O2'	25:BA:2189:U:H1'	2.18	0.44
25:BA:2285:A:H2'	25:BA:2286:A:C8	2.52	0.44
25:BA:273:G:O2'	25:BA:274:U:H5''	2.18	0.44
1:CA:1245:A:H61	1:CA:1292:U:H3	1.66	0.44
1:CA:920:U:H2'	1:CA:921:U:H6	1.82	0.44
1:CA:952:U:O4	13:CM:104:ARG:HD3	2.17	0.44
2:CB:197:VAL:HB	2:CB:200:ILE:HG23	2.00	0.44
2:CB:213:LEU:O	2:CB:217:ARG:HB2	2.17	0.44
17:CQ:66:SER:O	17:CQ:70:ARG:NH1	2.50	0.44
23:CY:21:A:N6	23:CY:46:7MG:H1'	2.32	0.44
25:DA:2150:U:H2'	25:DA:2151:G:C8	2.53	0.44
25:DA:613:G:H2'	25:DA:614:U:O4'	2.16	0.44
27:DD:134:ARG:HD3	27:DD:135:PHE:CZ	2.52	0.44
27:DD:182:LEU:HB2	27:DD:272:ALA:HB3	1.99	0.44
25:DA:1022:G:N7	33:DN:66:LYS:HE2	2.32	0.44
44:DY:11:ASP:OD2	44:DY:11:ASP:N	2.50	0.44
45:DZ:126:VAL:HG13	45:DZ:161:VAL:HG23	1.99	0.44
1:AA:1151:A:O4'	10:AJ:39:PRO:HB2	2.18	0.44
1:AA:308:C:H2'	1:AA:309:G:C8	2.52	0.44
1:AA:418:C:H1'	1:AA:540:G:O2'	2.17	0.44
5:AE:51:VAL:O	5:AE:55:VAL:HG23	2.18	0.44
6:AF:6:VAL:HG22	6:AF:90:VAL:HG22	1.98	0.44
14:AN:35:ARG:HB3	14:AN:35:ARG:HE	1.54	0.44
25:BA:1199:C:H2'	25:BA:1200:G:O4'	2.18	0.44
25:BA:1898:A:H2'	25:BA:1899:A:H8	1.82	0.44
25:BA:213:G:H2'	25:BA:214:A:O4'	2.17	0.44
25:BA:2186:C:C2'	25:BA:2187:G:H5'	2.47	0.44
25:BA:1874:C:H5'	27:BD:253:GLN:NE2	2.32	0.44
30:BG:108:ASN:HB3	50:B4:22:ILE:HD13	1.99	0.44
30:BG:82:LEU:HD21	30:BG:88:ILE:HG21	1.99	0.44
34:BO:104:ARG:NH1	39:BT:34:VAL:HG21	2.33	0.44
36:BQ:26:TYR:O	36:BQ:67:ARG:NH1	2.49	0.44
37:BR:2:ARG:O	37:BR:2:ARG:HG2	2.17	0.44
39:BT:23:ARG:HG3	39:BT:120:ARG:NH1	2.33	0.44
45:BZ:156:LYS:HE3	45:BZ:158:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:583:A:H2'	1:CA:584:G:O4'	2.17	0.44
1:CA:977:A:O2'	1:CA:981:U:N3	2.45	0.44
1:CA:983:A:H2	1:CA:984:C:C6	2.36	0.44
1:CA:986:A:H2'	1:CA:987:G:O4'	2.16	0.44
10:CJ:48:THR:OG1	10:CJ:62:HIS:ND1	2.46	0.44
11:CK:80:VAL:HG13	11:CK:103:LEU:HD12	1.98	0.44
18:CR:45:SER:OG	18:CR:47:THR:HG22	2.18	0.44
18:CR:76:LEU:HA	18:CR:76:LEU:HD12	1.77	0.44
18:CR:84:LYS:HG2	18:CR:84:LYS:H	1.53	0.44
24:CX:23:C:H2'	24:CX:24:U:C6	2.53	0.44
55:D9:12:ASP:N	55:D9:12:ASP:OD1	2.51	0.44
25:DA:2650:U:H2'	25:DA:2651:C:H6	1.82	0.44
25:DA:2748:A:H2'	25:DA:2749:A:O4'	2.17	0.44
25:DA:348:G:H2'	25:DA:349:G:C8	2.53	0.44
25:DA:686:G:C2	53:D7:11:LYS:HE2	2.52	0.44
25:DA:792:G:N3	25:DA:2072:G:O2'	2.42	0.44
25:DA:820:A:N3	25:DA:943:U:H4'	2.33	0.44
25:DA:975(A):G:C2	25:DA:990:A:C8	3.05	0.44
27:DD:274:ARG:O	27:DD:275:LYS:HD3	2.17	0.44
29:DF:53:THR:HG22	29:DF:56:GLU:HG3	2.00	0.44
34:DO:26:LYS:O	34:DO:30:ALA:HB2	2.18	0.44
33:DN:4:TYR:HB2	40:DU:101:ARG:NH1	2.32	0.44
45:DZ:148:ASP:OD1	45:DZ:148:ASP:N	2.50	0.44
1:AA:620:C:H2'	1:AA:621:A:O4'	2.18	0.44
9:AI:81:ILE:O	9:AI:85:LEU:HG	2.18	0.44
23:AY:55:PSU:N3	23:AY:57:G:H5'	2.33	0.44
25:BA:1084:C:H42	25:BA:1163:G:H1	1.63	0.44
25:BA:2158:C:C4	25:BA:2177:G:N1	2.86	0.44
25:BA:2329:C:H2'	25:BA:2330:G:O4'	2.18	0.44
25:BA:2083:G:H5''	25:BA:2515:A:C2	2.52	0.44
25:BA:2721:G:H2'	25:BA:2722:C:C6	2.52	0.44
25:BA:858:U:H2'	35:BP:21:ARG:HA	2.00	0.44
28:BE:3:GLY:HA3	28:BE:81:ILE:HD12	1.99	0.44
25:BA:2543:A:H5''	31:BH:157:TYR:CZ	2.53	0.44
32:BI:126:TYR:HB2	32:BI:142:VAL:HG23	1.99	0.44
33:BN:15:LEU:HD12	33:BN:137:LYS:HG3	1.98	0.44
25:BA:1058:U:C5	33:BN:28:THR:HG21	2.52	0.44
1:CA:1316:G:O2'	1:CA:1318:A:N7	2.48	0.44
3:CC:22:TRP:CZ2	14:CN:54:PRO:HG3	2.53	0.44
3:CC:36:ASP:O	3:CC:40:ARG:HG3	2.17	0.44
4:CD:47:ARG:HD3	4:CD:47:ARG:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:CI:46:ALA:HB2	9:CI:74:ILE:HG23	1.99	0.44
10:CJ:49:VAL:HG21	14:CN:41:ARG:O	2.18	0.44
25:DA:1406:U:H2'	25:DA:1407:C:C6	2.53	0.44
25:DA:570:G:H2'	25:DA:2030:A:C5	2.53	0.44
25:DA:2156:G:H8	25:DA:2156:G:O5'	2.01	0.44
25:DA:2357:U:OP1	46:D0:20:ARG:HD3	2.18	0.44
25:DA:2567:G:H2'	25:DA:2568:C:C6	2.52	0.44
25:DA:866:A:N6	25:DA:914:C:C4	2.86	0.44
26:DB:46:A:H2'	26:DB:47:C:C6	2.53	0.44
29:DF:178:PRO:HB3	29:DF:198:ALA:HA	1.99	0.44
30:DG:136:ARG:HD2	30:DG:137:GLU:N	2.33	0.44
35:DP:59:LEU:HD23	54:D8:58:ILE:HD13	1.98	0.44
1:AA:1066:C:C2'	1:AA:1067:A:H5'	2.47	0.44
1:AA:1070:U:H2'	1:AA:1071:C:H6	1.82	0.44
1:AA:713:G:H2'	1:AA:714:G:C8	2.53	0.44
1:AA:769:G:N7	61:AA:4049:HOH:O	2.37	0.44
2:AB:16:HIS:CD2	2:AB:17:PHE:N	2.80	0.44
2:AB:187:LEU:HD13	2:AB:205:ASP:HA	1.99	0.44
2:AB:8:LYS:HG2	2:AB:9:GLU:H	1.83	0.44
8:AH:64:LYS:HG2	8:AH:79:VAL:HG21	1.99	0.44
25:BA:354:A:H2	25:BA:1255:A:C2'	2.31	0.44
25:BA:2627:U:H2'	25:BA:2628:C:C6	2.53	0.44
25:BA:518:G:H2'	25:BA:519:G:O4'	2.18	0.44
25:BA:672:G:H2'	25:BA:673:G:O4'	2.17	0.44
29:BF:53:THR:CG2	29:BF:55:GLY:H	2.31	0.44
30:BG:41:GLN:HG3	30:BG:60:LEU:HD22	1.98	0.44
39:BT:128:GLU:O	39:BT:128:GLU:HG2	2.18	0.44
44:BY:14:LEU:HB2	44:BY:75:ILE:HD11	2.00	0.44
1:CA:109:A:H5'	1:CA:110:C:C5	2.53	0.44
1:CA:1157:A:H4'	1:CA:1158:C:O5'	2.18	0.44
1:CA:748:C:H4'	1:CA:749:C:O5'	2.18	0.44
5:CE:78:HIS:HA	8:CH:105:ARG:HG3	2.00	0.44
8:CH:82:HIS:HE2	8:CH:84:ARG:HG2	1.83	0.44
17:CQ:27:PHE:CE2	17:CQ:36:ILE:HD11	2.53	0.44
23:CY:9:A:O2'	23:CY:11:C:N4	2.45	0.44
52:D6:11:LEU:HB2	52:D6:21:TYR:HB2	1.99	0.44
25:DA:11:G:C2'	25:DA:12:U:H5'	2.47	0.44
25:DA:1420:U:HO2'	25:DA:1421:G:P	2.40	0.44
25:DA:1510:G:H2'	25:DA:1511:C:O4'	2.18	0.44
25:DA:1593:G:H2'	25:DA:1594:G:C8	2.53	0.44
25:DA:1835:G:H5'	25:DA:1836:C:OP2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:191:A:H2'	25:DA:192:C:C6	2.52	0.44
25:DA:2263:C:H2'	25:DA:2264:C:O4'	2.18	0.44
25:DA:2750:A:H8	25:DA:2750:A:OP1	2.01	0.44
27:DD:77:ALA:O	27:DD:116:GLN:HG3	2.17	0.44
29:DF:9:ILE:HD13	29:DF:123:LEU:HD23	1.98	0.44
35:DP:65:ARG:HG3	54:D8:25:MET:CG	2.48	0.44
45:DZ:133:ILE:HG22	45:DZ:134:PRO:O	2.18	0.44
1:AA:129(A):G:C6	1:AA:189(E):U:H4'	2.52	0.43
1:AA:501:C:H2'	1:AA:502:G:H8	1.81	0.43
1:AA:524:G:H2'	1:AA:525:C:C6	2.52	0.43
7:AG:29:LYS:HD2	7:AG:29:LYS:HA	1.72	0.43
7:AG:97:GLN:HB2	7:AG:97:GLN:HE21	1.62	0.43
9:AI:4:TYR:CE2	9:AI:88:TYR:HA	2.53	0.43
6:AF:99:ALA:HB1	18:AR:23:LYS:HZ3	1.83	0.43
20:AT:48:LYS:HD3	20:AT:48:LYS:HA	1.71	0.43
21:AU:5:ASP:O	21:AU:11:GLY:HA3	2.18	0.43
48:B2:65:ASN:OD1	48:B2:69:ARG:NH1	2.44	0.43
25:BA:2310:A:H2'	25:BA:2311:G:O4'	2.18	0.43
25:BA:323:A:N1	25:BA:346:A:O2'	2.43	0.43
25:BA:505:A:HO2'	25:BA:507:G:H8	1.66	0.43
25:BA:831:A:H5'	25:BA:832:G:OP1	2.18	0.43
30:BG:129:GLY:O	30:BG:161:THR:OG1	2.36	0.43
35:BP:3:LEU:HA	35:BP:3:LEU:HD12	1.90	0.43
1:CA:1117:G:N2	1:CA:1180:A:H1'	2.31	0.43
1:CA:1236:A:H2'	1:CA:1237:C:C6	2.53	0.43
1:CA:833:U:H2'	1:CA:834:C:H6	1.82	0.43
2:CB:55:PHE:CE1	2:CB:218:ALA:HA	2.53	0.43
3:CC:175:LEU:HD21	3:CC:201:TYR:CE1	2.53	0.43
4:CD:155:LEU:O	4:CD:159:ARG:HG3	2.17	0.43
9:CI:11:LYS:HA	9:CI:108:VAL:HG13	1.99	0.43
16:CP:40:ASP:O	16:CP:48:TRP:HB2	2.18	0.43
25:DA:1313:U:OP1	61:DA:4345:HOH:O	2.21	0.43
25:DA:1651:G:H5'	37:DR:39:PRO:HG2	2.00	0.43
25:DA:2119:A:N6	25:DA:2171:A:C6	2.86	0.43
25:DA:303:U:H2'	25:DA:304:G:H8	1.83	0.43
30:DG:129:GLY:O	30:DG:161:THR:HB	2.18	0.43
32:DI:131:LYS:HA	32:DI:137:PRO:HA	1.99	0.43
32:DI:54:GLN:HA	32:DI:57:ARG:HE	1.82	0.43
32:DI:57:ARG:O	32:DI:61:ARG:HB2	2.17	0.43
1:AA:1190:G:O2'	1:AA:1191:A:OP2	2.34	0.43
1:AA:165:C:H2'	1:AA:166:G:H8	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:6:G:H4'	1:AA:298:A:H4'	1.99	0.43
1:AA:736:C:H2'	1:AA:737:A:C8	2.53	0.43
8:AH:25:ASP:OD1	8:AH:60:ARG:HG3	2.18	0.43
9:AI:21:PRO:HA	9:AI:59:PHE:HA	1.99	0.43
13:AM:67:GLU:OE2	13:AM:71:ARG:NH2	2.51	0.43
25:BA:1232:G:HO2'	25:BA:1233:U:H6	1.66	0.43
25:BA:492:A:N3	25:BA:730:C:H1'	2.33	0.43
26:BB:66:A:H61	26:BB:108:U:H2'	1.82	0.43
27:BD:142:VAL:CG1	27:BD:191:ALA:HB1	2.48	0.43
25:BA:790:G:OP1	28:BE:130:GLY:HA2	2.18	0.43
34:BO:104:ARG:HE	39:BT:36:GLU:HG3	1.82	0.43
1:CA:1424:C:H2'	1:CA:1425:U:O4'	2.18	0.43
3:CC:131:ARG:HH11	5:CE:50:GLU:HG3	1.83	0.43
9:CI:102:LEU:HD13	9:CI:103:THR:N	2.28	0.43
10:CJ:16:LEU:HD12	10:CJ:70:ARG:HG2	1.99	0.43
13:CM:96:LEU:O	13:CM:110:ARG:NH1	2.50	0.43
18:CR:58:LEU:HD12	18:CR:62:GLU:HB2	2.00	0.43
52:D6:19:ARG:N	52:D6:19:ARG:HD2	2.33	0.43
25:DA:1291:C:H2'	25:DA:1292:U:C6	2.53	0.43
25:DA:1477:A:H2'	25:DA:1478:G:O4'	2.18	0.43
25:DA:1958:C:OP2	61:DA:4710:HOH:O	2.20	0.43
25:DA:2129:C:C2	25:DA:2160:G:N1	2.84	0.43
25:DA:2354:G:H21	46:D0:36:ILE:HD11	1.82	0.43
25:DA:307:G:H21	25:DA:330:A:H62	1.65	0.43
25:DA:359:A:H2'	25:DA:360:G:O4'	2.18	0.43
25:DA:376:C:H2'	25:DA:377:C:C6	2.53	0.43
31:DH:121:ILE:HD11	31:DH:140:LYS:HG2	2.01	0.43
31:DH:9:ILE:HG12	31:DH:69:ARG:HD2	2.00	0.43
35:DP:55:ARG:HG2	35:DP:56:SER:N	2.33	0.43
35:DP:83:VAL:HG12	35:DP:112:LEU:HD21	1.99	0.43
1:AA:1236:A:H2'	1:AA:1237:C:C6	2.53	0.43
1:AA:1327:C:O2'	1:AA:1328:C:H5'	2.18	0.43
1:AA:659:U:H2'	1:AA:660:G:H5'	2.01	0.43
6:AF:68:PRO:HG2	6:AF:71:ARG:NH1	2.34	0.43
13:AM:84:ILE:HD12	19:AS:74:PHE:CZ	2.53	0.43
14:AN:6:LEU:HA	14:AN:6:LEU:HD12	1.84	0.43
1:AA:189(F):U:C4	17:AQ:72:ARG:NH1	2.87	0.43
54:B8:6:THR:HG22	54:B8:64:TYR:HD1	1.84	0.43
26:BB:8:U:O3'	38:BS:25:ARG:NH2	2.51	0.43
25:BA:1068:G:N7	33:BN:66:LYS:HE2	2.34	0.43
40:BU:74:LEU:H	40:BU:74:LEU:HD12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BV:50:PRO:HG2	41:BV:51:VAL:HG12	2.00	0.43
1:CA:1134:G:N3	1:CA:1134:G:H2'	2.34	0.43
1:CA:1441:G:O5'	1:CA:1441:G:H8	2.02	0.43
1:CA:340:U:H2'	1:CA:341:C:C6	2.53	0.43
4:CD:11:LEU:O	4:CD:15:GLU:HG2	2.18	0.43
9:CI:50:LEU:H	9:CI:50:LEU:HG	1.46	0.43
1:CA:689:C:P	11:CK:46:GLY:HA3	2.59	0.43
20:CT:50:GLU:HB2	20:CT:99:LEU:CD2	2.47	0.43
25:DA:1268:A:C2	25:DA:2013:A:C4	3.06	0.43
25:DA:2207:G:H3'	25:DA:2208:A:H5''	2.00	0.43
25:DA:2802:G:H2'	25:DA:2803:C:O4'	2.19	0.43
25:DA:866:A:C2	25:DA:867:C:C5	3.06	0.43
34:DO:64:ARG:HB2	34:DO:83:ALA:HB3	1.99	0.43
37:DR:103:ARG:HD3	37:DR:108:GLY:O	2.17	0.43
45:DZ:163:LEU:HA	45:DZ:163:LEU:HD12	1.86	0.43
1:AA:1442:G:O2'	1:AA:1442(A):G:OP1	2.28	0.43
4:AD:178:VAL:O	4:AD:179:GLU:HB2	2.17	0.43
8:AH:10:LEU:HD12	8:AH:85:ARG:HG2	1.99	0.43
9:AI:118:LYS:HB2	9:AI:121:ARG:HB3	2.01	0.43
25:BA:1255:A:H5''	25:BA:1257:G:O4'	2.18	0.43
25:BA:2504:U:H2'	25:BA:2505:U:C6	2.53	0.43
25:BA:2588:G:H1'	61:BA:4594:HOH:O	2.16	0.43
25:BA:60:G:H5'	48:B2:50:ILE:HG21	2.01	0.43
25:BA:906:G:O2'	25:BA:962:G:O6	2.31	0.43
36:BQ:39:PRO:HA	36:BQ:97:VAL:O	2.18	0.43
40:BU:76:TYR:OH	40:BU:92:ARG:HD3	2.18	0.43
1:CA:1159:U:H5''	1:CA:1182:G:H21	1.83	0.43
1:CA:1316:G:N1	1:CA:1319:A:OP2	2.49	0.43
1:CA:179:A:H2'	1:CA:180:U:C6	2.54	0.43
1:CA:959:A:O2'	1:CA:984:C:O2'	2.33	0.43
2:CB:101:MET:HA	2:CB:108:ILE:HG12	2.00	0.43
8:CH:33:GLU:HG2	8:CH:48:TYR:CE2	2.53	0.43
10:CJ:10:GLY:HA3	10:CJ:16:LEU:HD21	2.01	0.43
19:CS:36:ARG:HD2	19:CS:52:TYR:O	2.19	0.43
52:D6:15:GLU:HG3	52:D6:47:THR:HG23	1.99	0.43
25:DA:1599:C:OP1	61:DA:5027:HOH:O	2.20	0.43
25:DA:2018:G:H2'	25:DA:2019:A:O4'	2.19	0.43
25:DA:2136:C:O2'	25:DA:2137:C:O5'	2.36	0.43
25:DA:2831:G:OP1	25:DA:2834:G:H4'	2.19	0.43
25:DA:348:G:H2'	25:DA:349:G:H8	1.82	0.43
31:DH:148:ILE:O	31:DH:162:ILE:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:DY:21:LYS:HB3	44:DY:21:LYS:NZ	2.33	0.43
45:DZ:8:TYR:HB2	45:DZ:38:TYR:CE2	2.54	0.43
1:AA:118:U:O4	61:AA:4255:HOH:O	2.21	0.43
1:AA:1239:A:C4	1:AA:1298:C:N4	2.87	0.43
1:AA:429:U:H4'	1:AA:430:A:O5'	2.18	0.43
3:AC:152:ILE:HG23	3:AC:167:TRP:HB3	2.00	0.43
4:AD:162:LEU:HD13	4:AD:181:MET:HG2	2.00	0.43
8:AH:86:ILE:HG21	8:AH:133:LEU:HD13	2.00	0.43
9:AI:32:ASP:OD1	9:AI:33:PHE:N	2.51	0.43
10:AJ:40:LEU:HB2	10:AJ:69:ASN:HB3	2.01	0.43
13:AM:88:ARG:HG3	13:AM:98:VAL:CG1	2.49	0.43
61:BA:4094:HOH:O	29:BF:74:ARG:HG2	2.18	0.43
41:BV:52:VAL:HG22	41:BV:55:ALA:HB3	2.01	0.43
44:BY:8:LYS:HD3	44:BY:97:ARG:NH1	2.34	0.43
1:CA:1133:G:C4	1:CA:1134:G:C8	3.07	0.43
1:CA:1368:G:OP1	9:CI:111:ARG:NH2	2.35	0.43
1:CA:769:G:H4'	1:CA:1513:A:H4'	2.01	0.43
1:CA:187:C:H2'	1:CA:188:C:C6	2.53	0.43
2:CB:105:PHE:CE1	2:CB:155:LEU:HD12	2.53	0.43
2:CB:12:GLU:HA	2:CB:15:VAL:HG23	2.01	0.43
2:CB:19:HIS:CG	2:CB:20:GLU:H	2.37	0.43
12:CL:24:VAL:HB	12:CL:27:LEU:HD22	1.98	0.43
1:CA:523:A:H61	12:CL:92:ASP:HB2	1.83	0.43
16:CP:57:ARG:HH21	16:CP:79:VAL:HA	1.83	0.43
19:CS:12:ASP:OD1	19:CS:37:ARG:NH1	2.51	0.43
23:CW:39:PSU:H2'	23:CW:40:C:C6	2.53	0.43
23:CW:40:C:H2'	23:CW:41:C:H6	1.82	0.43
25:DA:2612:C:OP2	51:D5:2:ALA:N	2.51	0.43
25:DA:2061:G:H5'	25:DA:2503:A:C2	2.53	0.43
25:DA:263:C:H2'	25:DA:264:C:O4'	2.19	0.43
25:DA:2735:G:H2'	25:DA:2736:G:H8	1.83	0.43
25:DA:2896:C:H2'	25:DA:2897:U:C6	2.53	0.43
25:DA:530:G:O4'	25:DA:530:G:N3	2.50	0.43
26:DB:80:U:H2'	26:DB:81:G:C8	2.53	0.43
30:DG:47:LYS:HD2	30:DG:81:LYS:O	2.19	0.43
31:DH:27:LYS:HB3	31:DH:27:LYS:HE3	1.62	0.43
1:AA:839:U:H4'	1:AA:840:C:OP2	2.19	0.43
2:AB:45:GLN:O	2:AB:49:GLU:HB2	2.19	0.43
1:AA:523:A:H61	12:AL:92:ASP:HB2	1.84	0.43
1:AA:1226:C:H4'	19:AS:80:TYR:OH	2.19	0.43
25:BA:2005:C:H4'	25:BA:2618:C:O3'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2205:C:H2'	25:BA:2206:G:C8	2.50	0.43
25:BA:927:G:H2'	25:BA:928:G:H8	1.84	0.43
27:BD:180:GLY:HA3	27:BD:275:LYS:HG3	2.01	0.43
36:BQ:17:LEU:HA	36:BQ:17:LEU:HD23	1.85	0.43
45:BZ:149:SER:OG	45:BZ:150:LEU:N	2.52	0.43
1:CA:1144:G:N2	1:CA:1146:A:H62	2.16	0.43
1:CA:1119:C:N4	1:CA:1154:G:H1	2.13	0.43
1:CA:299:G:H2'	1:CA:300:A:C8	2.53	0.43
1:CA:643:C:H2'	1:CA:644:G:H8	1.84	0.43
4:CD:180:GLY:O	4:CD:182:LYS:HD3	2.18	0.43
4:CD:196:LEU:HD12	4:CD:196:LEU:H	1.83	0.43
8:CH:6:ILE:O	8:CH:10:LEU:HG	2.18	0.43
23:CY:19:G:N2	23:CY:56:C:C2	2.83	0.43
25:DA:1021:A:C8	25:DA:1021:A:H3'	2.53	0.43
25:DA:2792:G:N3	25:DA:2792:G:H2'	2.34	0.43
25:DA:902:C:H2'	25:DA:903:C:C6	2.51	0.43
34:DO:98:VAL:HG22	34:DO:118:ALA:HA	2.00	0.43
25:DA:446:G:OP1	40:DU:3:ARG:NH1	2.52	0.43
45:DZ:73:GLN:O	45:DZ:87:ASP:N	2.47	0.43
1:AA:410:G:O6	61:AA:4018:HOH:O	2.21	0.43
3:AC:181:ASN:HD21	3:AC:204:LEU:HD12	1.83	0.43
3:AC:52:LEU:HD21	3:AC:55:VAL:HG23	2.00	0.43
14:AN:26:ARG:HD3	14:AN:43:CYS:SG	2.58	0.43
17:AQ:62:SER:OG	17:AQ:72:ARG:HD2	2.18	0.43
23:AY:55:PSU:C2	23:AY:57:G:H5'	2.53	0.43
50:B4:59:PHE:N	50:B4:59:PHE:CD1	2.86	0.43
25:BA:2142:G:O2'	25:BA:2143:G:H5'	2.19	0.43
25:BA:2376:C:H2'	25:BA:2377:G:O4'	2.19	0.43
32:BI:127:VAL:HA	32:BI:140:LEU:O	2.17	0.43
32:BI:26:ALA:HA	32:BI:30:LEU:HB2	2.01	0.43
34:BO:122:LEU:HD13	39:BT:72:VAL:HG11	1.99	0.43
42:BW:68:ARG:NH1	42:BW:112:GLY:H	2.17	0.43
45:BZ:152:ALA:O	45:BZ:155:LEU:HB2	2.17	0.43
1:CA:1020:U:C2	1:CA:1021:G:C8	3.07	0.43
1:CA:1066:C:C2'	1:CA:1067:A:H5'	2.49	0.43
2:CB:17:PHE:HA	2:CB:44:LEU:HD11	1.99	0.43
4:CD:3:ARG:O	4:CD:5:ILE:HG22	2.18	0.43
5:CE:33:VAL:HG21	5:CE:109:ILE:HA	2.00	0.43
7:CG:20:ASP:OD1	7:CG:22:LEU:HB3	2.19	0.43
15:CO:62:GLN:O	15:CO:66:LEU:HD13	2.19	0.43
16:CP:74:LEU:O	16:CP:79:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2128:C:N4	25:DA:2161:C:N3	2.67	0.43
25:DA:2376:A:H2'	25:DA:2377:A:O4'	2.18	0.43
25:DA:2526:G:H5'	25:DA:2742:C:O2'	2.19	0.43
25:DA:2659:G:N2	25:DA:2662:A:OP2	2.51	0.43
25:DA:2671:A:H2'	25:DA:2672:G:O4'	2.19	0.43
25:DA:2773:C:H2'	25:DA:2774:C:H6	1.83	0.43
25:DA:828:U:H4'	25:DA:831:G:N1	2.33	0.43
25:DA:880:G:N2	25:DA:898:C:O2	2.52	0.43
28:DE:144:ARG:HB3	28:DE:145:LYS:H	1.45	0.43
29:DF:126:VAL:HG21	29:DF:129:PHE:CZ	2.53	0.43
38:DS:62:LYS:O	38:DS:66:ALA:N	2.44	0.43
40:DU:49:HIS:O	40:DU:53:ARG:N	2.51	0.43
1:AA:1074:G:O2'	1:AA:1101:A:N1	2.44	0.43
1:AA:438:G:H4'	4:AD:123:HIS:CE1	2.54	0.43
1:AA:551:U:H2'	1:AA:552:U:C6	2.53	0.43
1:AA:743:U:H2'	1:AA:744:C:C6	2.53	0.43
1:AA:91:C:OP1	1:AA:91:C:H4'	2.18	0.43
2:AB:189:ASP:OD1	2:AB:189:ASP:N	2.47	0.43
3:AC:53:ALA:HB2	3:AC:115:LEU:HD13	2.00	0.43
7:AG:66:VAL:HG12	7:AG:70:LYS:HE3	2.01	0.43
14:AN:14:PRO:HG3	14:AN:20:ALA:HB2	2.01	0.43
15:AO:61:GLY:O	15:AO:65:ARG:HG3	2.19	0.43
17:AQ:50:LYS:HG3	17:AQ:51:TYR:N	2.33	0.43
19:AS:15:LEU:O	19:AS:19:VAL:HG23	2.19	0.43
47:B1:86:SER:OG	47:B1:89:GLU:HG2	2.19	0.43
25:BA:1809:U:H2'	25:BA:1815:A:N6	2.34	0.43
25:BA:504:A:N1	25:BA:525:G:H4'	2.34	0.43
25:BA:605:G:H2'	25:BA:606:G:C8	2.54	0.43
28:BE:108:SER:O	28:BE:162:ALA:HA	2.19	0.43
31:BH:154:PRO:HB3	31:BH:163:TYR:CE2	2.53	0.43
37:BR:97:VAL:HG22	37:BR:114:VAL:HG13	2.01	0.43
1:CA:1064:G:H4'	1:CA:1065:U:O5'	2.19	0.43
1:CA:1095:U:H2'	1:CA:1096:C:C6	2.54	0.43
1:CA:1162:C:C2	1:CA:1174:G:N2	2.86	0.43
1:CA:1375:A:H4'	7:CG:29:LYS:HD3	1.99	0.43
1:CA:539:A:H2'	1:CA:540:G:C8	2.53	0.43
2:CB:80:ILE:HD11	2:CB:212:GLN:CA	2.48	0.43
1:CA:376:G:H4'	16:CP:5:ARG:HD3	2.01	0.43
25:DA:2141:G:C6	25:DA:2150:U:O2	2.71	0.43
25:DA:2793:G:N2	25:DA:2804:C:H1'	2.34	0.43
25:DA:322:A:H5'	25:DA:340:A:H1'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:484:C:H2'	25:DA:485:C:H6	1.84	0.43
26:DB:39:A:O2'	26:DB:40:U:H5'	2.19	0.43
28:DE:178:GLU:N	28:DE:178:GLU:OE2	2.29	0.43
32:DI:12:LEU:HA	32:DI:12:LEU:HD23	1.82	0.43
33:DN:71:ILE:HG21	33:DN:84:LYS:HB3	2.01	0.43
43:DX:8:ILE:O	48:D2:36:ARG:NH2	2.52	0.43
45:DZ:33:LEU:HD21	45:DZ:90:VAL:HG21	2.01	0.43
1:AA:1183:A:H3'	1:AA:1184:G:C5'	2.45	0.43
1:AA:300:A:H2'	1:AA:301:G:O4'	2.19	0.43
1:AA:7:G:H5'	1:AA:298:A:O4'	2.19	0.43
1:AA:936:C:H2'	1:AA:937:A:O4'	2.19	0.43
1:AA:1104:G:H4'	2:AB:111:ARG:NH1	2.34	0.43
25:BA:1793:A:H2'	61:BA:5307:HOH:O	2.18	0.43
25:BA:1825:U:H2'	25:BA:1826:C:C6	2.53	0.43
25:BA:2524:C:H2'	25:BA:2525:G:O4'	2.19	0.43
25:BA:2901:A:C6	25:BA:2902:G:C6	3.07	0.43
25:BA:640:A:C4	29:BF:180:GLY:HA2	2.54	0.43
36:BQ:75:THR:HG22	61:BQ:3105:HOH:O	2.18	0.43
37:BR:104:ARG:HG3	37:BR:111:LEU:HD21	2.00	0.43
1:CA:1132:C:N3	1:CA:1142:G:N2	2.61	0.43
1:CA:620:C:H2'	1:CA:621:A:O4'	2.19	0.43
2:CB:185:ILE:HG22	2:CB:199:TYR:CD2	2.51	0.43
1:CA:619:U:N3	4:CD:134:ASP:OD1	2.46	0.43
1:CA:7:G:O2'	5:CE:120:THR:O	2.36	0.43
22:CV:14:A:C6	23:CY:34:G:C5	3.06	0.43
23:CW:67:C:H2'	23:CW:68:C:C6	2.54	0.43
25:DA:1029:A:N1	25:DA:2465:C:O2'	2.39	0.43
25:DA:118:A:N3	25:DA:178:G:H1'	2.34	0.43
25:DA:1805:U:O2	27:DD:50:THR:HB	2.19	0.43
25:DA:244:A:C2	25:DA:255:A:C4	3.07	0.43
25:DA:2741:A:H2'	25:DA:2742:C:O4'	2.19	0.43
25:DA:2811:G:N2	25:DA:2891:G:H1'	2.34	0.43
28:DE:7:VAL:HG12	28:DE:27:LEU:HB3	2.00	0.43
34:DO:7:TYR:HE1	34:DO:20:MET:HE3	1.83	0.43
1:AA:1004:A:C5	1:AA:1037:C:N3	2.87	0.43
1:AA:146:G:C2	1:AA:147:G:C4	3.06	0.43
1:AA:392:G:H2'	1:AA:393:A:H8	1.83	0.43
1:AA:69:G:H2'	1:AA:70:G:C8	2.54	0.43
1:AA:735:C:H2'	1:AA:736:C:C6	2.54	0.43
4:AD:50:ARG:HA	4:AD:51:PRO:HD3	1.82	0.43
24:AX:23:C:H2'	24:AX:24:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1537:G:O2'	27:BD:101:GLU:HB2	2.19	0.43
25:BA:1781:G:N3	25:BA:2870:A:H2	2.17	0.43
25:BA:2053:A:C6	25:BA:2510:C:H1'	2.54	0.43
25:BA:2156:A:H8	25:BA:2156:A:OP2	2.02	0.43
42:BW:13:SER:HA	42:BW:14:PRO:HD3	1.88	0.43
1:CA:1084:G:H5'	1:CA:1102:A:OP2	2.19	0.43
1:CA:1516:G:H2'	1:CA:1518:A:OP2	2.19	0.43
1:CA:545:C:OP2	4:CD:65:ARG:NH2	2.52	0.43
1:CA:701:C:OP1	1:CA:702:A:O2'	2.21	0.43
5:CE:113:ALA:HB3	5:CE:115:VAL:HG23	2.01	0.43
5:CE:13:ILE:HA	5:CE:29:GLY:O	2.19	0.43
7:CG:100:ALA:O	7:CG:104:LEU:HB2	2.18	0.43
8:CH:64:LYS:HB3	8:CH:79:VAL:HG21	2.01	0.43
17:CQ:45:HIS:CD2	17:CQ:47:PRO:HD3	2.54	0.43
25:DA:1374:G:H2'	25:DA:1375:C:C6	2.54	0.43
25:DA:2051:A:H5'	25:DA:2578:G:O4'	2.19	0.43
25:DA:286:C:H2'	25:DA:287:C:C6	2.54	0.43
25:DA:686:G:N2	25:DA:788:A:H61	2.17	0.43
34:DO:87:ILE:HD12	34:DO:91:LEU:HA	2.01	0.43
42:DW:88:ARG:NH1	42:DW:94:ASP:OD2	2.51	0.43
1:AA:1030(A):G:O2'	1:AA:1031:G:C2	2.72	0.42
1:AA:271:C:H2'	1:AA:272:C:C6	2.54	0.42
1:AA:948:C:OP1	13:AM:109:THR:OG1	2.34	0.42
2:AB:103:THR:HA	2:AB:180:LEU:HD11	2.01	0.42
6:AF:39:LYS:HE2	6:AF:39:LYS:HB3	1.83	0.42
15:AO:5:LYS:O	15:AO:9:GLN:HG2	2.20	0.42
25:BA:1000:C:OP1	36:BQ:87:LYS:HE2	2.19	0.42
25:BA:1022:C:H5'	25:BA:1202:A:N6	2.34	0.42
25:BA:1070:G:C6	25:BA:1071:G:C6	3.07	0.42
25:BA:1631:C:O2'	25:BA:1632:A:H5'	2.19	0.42
25:BA:1744:G:OP2	25:BA:1745:A:O2'	2.23	0.42
25:BA:2122:G:O2'	25:BA:2123:G:H5'	2.19	0.42
25:BA:2138:G:H2'	25:BA:2139:A:C5	2.54	0.42
25:BA:705:C:H2'	25:BA:706:C:C6	2.54	0.42
25:BA:739:C:HO2'	25:BA:1400:A:HO2'	1.61	0.42
1:CA:194:C:H2'	1:CA:195:A:H5''	2.00	0.42
1:CA:524:G:H2'	1:CA:525:C:C6	2.53	0.42
1:CA:78:G:C2'	1:CA:79:G:H5'	2.49	0.42
9:CI:4:TYR:CE2	9:CI:88:TYR:HA	2.54	0.42
13:CM:108:ARG:HD3	13:CM:108:ARG:HA	1.74	0.42
18:CR:53:ARG:HA	18:CR:56:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1220:G:N2	19:CS:54:GLY:O	2.50	0.42
23:CW:6:G:O6	23:CW:67:C:N3	2.52	0.42
25:DA:1449:A:HO2'	25:DA:1529:G:H21	1.60	0.42
25:DA:1668:A:C8	25:DA:1674:G:C6	3.07	0.42
25:DA:1777:U:O2'	25:DA:1778:U:H5'	2.19	0.42
25:DA:2142:C:H2'	25:DA:2143:C:C6	2.54	0.42
25:DA:858:U:O2	25:DA:2268:A:H2'	2.19	0.42
25:DA:2277:G:OP2	46:D0:10:THR:HG21	2.19	0.42
25:DA:2474:C:H5''	25:DA:2475:C:OP2	2.19	0.42
25:DA:2611:U:H5'	25:DA:2611:U:H6	1.84	0.42
25:DA:271(E):U:H2'	25:DA:271(F):C:C6	2.54	0.42
25:DA:478:A:N1	25:DA:500:G:H4'	2.34	0.42
25:DA:27:G:C2	25:DA:512:G:N3	2.87	0.42
35:DP:63:PRO:O	54:D8:13:ARG:HG2	2.19	0.42
37:DR:97:VAL:HG22	37:DR:114:VAL:HG13	2.00	0.42
1:AA:1064:G:H1'	1:AA:1190:G:H21	1.83	0.42
1:AA:1346:A:OP1	9:AI:120:ARG:NH1	2.40	0.42
1:AA:437:U:O2'	4:AD:123:HIS:CD2	2.72	0.42
1:AA:935:A:C2	1:AA:936:C:C2	3.07	0.42
7:AG:28:ASN:HD21	7:AG:36:LYS:HZ1	1.67	0.42
10:AJ:38:ILE:H	10:AJ:38:ILE:HG13	1.74	0.42
25:BA:1945:U:H2'	25:BA:1946:C:C6	2.54	0.42
25:BA:593:G:C6	25:BA:2052:A:C2	3.07	0.42
25:BA:2150:C:H42	25:BA:2182:G:H1	1.66	0.42
25:BA:2707:C:H2'	25:BA:2708:U:C6	2.54	0.42
27:BD:147:LEU:HD22	27:BD:155:LEU:HD11	1.99	0.42
32:BI:47:LEU:O	32:BI:50:ARG:HG2	2.18	0.42
35:BP:79:ARG:NH2	35:BP:109:GLY:O	2.52	0.42
41:BV:89:GLN:HA	41:BV:90:PRO:HD3	1.93	0.42
1:CA:1023:G:H3'	1:CA:1024:G:H8	1.84	0.42
1:CA:1228:C:H2'	1:CA:1229:A:H8	1.83	0.42
1:CA:255:G:C6	1:CA:256:U:C4	3.08	0.42
1:CA:662:G:O2'	1:CA:836:G:OP1	2.33	0.42
2:CB:16:HIS:HB3	2:CB:210:SER:HB2	2.01	0.42
8:CH:13:ILE:O	8:CH:17:THR:HG23	2.19	0.42
9:CI:7:THR:HB	9:CI:83:ARG:NH1	2.34	0.42
14:CN:6:LEU:HB3	14:CN:23:ARG:NH2	2.35	0.42
16:CP:3:LYS:O	16:CP:21:VAL:HA	2.19	0.42
23:CW:8:4SU:H1'	23:CW:48:C:H1'	2.01	0.42
23:CY:46:7MG:H82	23:CY:46:7MG:H2'	1.74	0.42
23:CY:68:C:H2'	23:CY:69:G:H5'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:CY:8:4SU:S4	23:CY:14:A:N7	2.92	0.42
47:D1:64:ALA:HA	47:D1:67:ILE:HG13	2.01	0.42
25:DA:1379:A:H4'	25:DA:1380:G:OP2	2.19	0.42
25:DA:1639:U:C2'	25:DA:1640:C:H5''	2.46	0.42
25:DA:361:G:O2'	25:DA:362:U:H5'	2.18	0.42
25:DA:652(A):A:O2'	25:DA:652(B):A:H5'	2.19	0.42
34:DO:68:GLU:HB3	34:DO:78:ARG:HB2	2.00	0.42
41:DV:21:ARG:HG2	41:DV:91:TYR:CD2	2.54	0.42
1:AA:1009:G:C6	1:AA:1010:G:C5	3.07	0.42
1:AA:1355:G:H2'	1:AA:1356:G:C8	2.55	0.42
1:AA:562:C:H1'	12:AL:15:ARG:HB3	2.01	0.42
1:AA:977:A:H1'	1:AA:982:U:O4	2.19	0.42
2:AB:67:THR:HA	2:AB:90:MET:CE	2.49	0.42
4:AD:173:TRP:CE2	4:AD:189:PRO:HG3	2.53	0.42
9:AI:117:HIS:HB2	9:AI:121:ARG:HG3	2.00	0.42
9:AI:50:LEU:HD21	9:AI:81:ILE:HD11	2.01	0.42
13:AM:80:ARG:NH2	19:AS:69:HIS:CE1	2.86	0.42
14:AN:33:VAL:HA	14:AN:40:CYS:HA	2.01	0.42
15:AO:15:PHE:CZ	15:AO:84:LYS:HD2	2.53	0.42
6:AF:100:ASN:C	18:AR:28:GLU:HG2	2.40	0.42
23:AY:2:C:N4	23:AY:71:G:H1	2.17	0.42
25:BA:1094:A:N1	25:BA:1158:G:O2'	2.36	0.42
25:BA:1843:A:O2'	27:BD:45:ASN:N	2.47	0.42
25:BA:1935:A:H4'	25:BA:1936:C:H5''	2.01	0.42
25:BA:2190:G:O6	25:BA:2193:A:H8	2.02	0.42
25:BA:2545:A:H2'	25:BA:2546:A:O4'	2.18	0.42
25:BA:2707:C:H2'	25:BA:2708:U:H6	1.85	0.42
25:BA:973:G:N7	61:BA:4553:HOH:O	2.37	0.42
45:BZ:40:ASP:OD2	45:BZ:43:GLU:HG3	2.19	0.42
1:CA:1012:U:O2	1:CA:1017:G:O6	2.37	0.42
1:CA:1135:U:H4'	1:CA:1136:U:H5	1.84	0.42
1:CA:991:U:O2'	1:CA:1212:U:C4	2.71	0.42
1:CA:1222:G:OP1	19:CS:77:THR:HG21	2.19	0.42
1:CA:457:C:H2'	1:CA:458:C:C6	2.53	0.42
1:CA:69:G:H2'	1:CA:70:G:H8	1.84	0.42
2:CB:210:SER:OG	2:CB:211:ILE:N	2.51	0.42
9:CI:48:GLU:O	9:CI:51:ARG:HB2	2.19	0.42
12:CL:39:VAL:HG11	12:CL:41:ARG:HH11	1.84	0.42
23:CY:51:U:O2	23:CY:63:G:N2	2.40	0.42
49:D3:6:VAL:HG13	49:D3:56:VAL:HG22	2.01	0.42
25:DA:1171:G:H1	25:DA:1178:C:N4	2.05	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1300:U:H4'	25:DA:1301:A:H5'	2.01	0.42
25:DA:1790:C:H5''	25:DA:1791:A:OP1	2.19	0.42
25:DA:1815:A:H8	25:DA:1815:A:OP1	2.02	0.42
25:DA:247:G:OP2	25:DA:249:C:N4	2.46	0.42
25:DA:2564:A:C2	25:DA:2647:U:H4'	2.54	0.42
25:DA:652(C):G:H2'	25:DA:652(D):C:H6	1.85	0.42
25:DA:952:G:P	36:DQ:16:ARG:HH21	2.43	0.42
31:DH:98:LEU:HB2	31:DH:125:VAL:CG2	2.49	0.42
36:DQ:21:THR:HG21	36:DQ:101:ARG:HB2	2.02	0.42
25:DA:2690:C:OP2	37:DR:14:SER:HB3	2.19	0.42
38:DS:14:VAL:O	38:DS:18:ILE:HG12	2.20	0.42
45:DZ:69:THR:HG22	45:DZ:90:VAL:HA	2.00	0.42
2:AB:197:VAL:HB	2:AB:200:ILE:HG22	2.00	0.42
4:AD:119:GLN:HG2	4:AD:123:HIS:CD2	2.54	0.42
5:AE:53:LEU:HD12	5:AE:53:LEU:H	1.84	0.42
1:AA:584:G:H5'	17:AQ:91:ARG:NH2	2.34	0.42
25:BA:1475:G:H2'	25:BA:1476:C:H6	1.85	0.42
25:BA:1525:G:O2'	25:BA:1605:A:C2	2.71	0.42
25:BA:2896:G:H2'	25:BA:2897:U:C6	2.55	0.42
25:BA:505:A:N3	25:BA:507:G:H5''	2.34	0.42
25:BA:613:A:H2'	25:BA:614:C:O4'	2.19	0.42
31:BH:3:ARG:HG2	31:BH:6:ARG:HD2	2.01	0.42
37:BR:2:ARG:HG2	37:BR:5:LYS:HB2	2.00	0.42
1:CA:1009:G:C2	1:CA:1021:G:N3	2.87	0.42
1:CA:1009:G:H22	1:CA:1021:G:H1'	1.85	0.42
1:CA:153:C:H2'	1:CA:154:C:C6	2.55	0.42
2:CB:47:THR:HA	2:CB:202:PRO:CG	2.46	0.42
4:CD:173:TRP:CD1	4:CD:174:LEU:HG	2.55	0.42
4:CD:153:ARG:HD3	4:CD:181:MET:CE	2.50	0.42
13:CM:4:ILE:HG23	13:CM:5:ALA:N	2.30	0.42
17:CQ:26:GLN:HG2	17:CQ:37:LYS:HG2	2.01	0.42
25:DA:2461:C:H2'	25:DA:2462:U:C6	2.54	0.42
25:DA:18:C:O2'	25:DA:554:U:OP1	2.32	0.42
25:DA:662:G:OP1	61:DA:4487:HOH:O	2.21	0.42
26:DB:11:C:OP2	26:DB:12:C:H5	2.02	0.42
29:DF:197:ASP:O	29:DF:200:GLU:HB2	2.20	0.42
35:DP:45:LEU:HD22	35:DP:45:LEU:HA	1.61	0.42
1:AA:262:A:H2'	1:AA:263:A:C8	2.55	0.42
1:AA:271:C:H2'	1:AA:272:C:H6	1.84	0.42
3:AC:130:VAL:O	3:AC:134:ILE:HG13	2.19	0.42
11:AK:20:TYR:CE1	11:AK:83:ILE:HD12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AP:52:ASP:HB3	16:AP:55:ARG:HB2	2.01	0.42
20:AT:59:ALA:O	20:AT:63:ILE:HG13	2.20	0.42
23:AW:42:C:O2'	23:AW:43:C:H5'	2.20	0.42
50:B4:55:ARG:H	50:B4:56:VAL:HA	1.84	0.42
25:BA:1090:G:H5'	25:BA:1091:A:OP2	2.19	0.42
25:BA:1639:G:H2'	25:BA:1640:G:C8	2.54	0.42
25:BA:174:U:H4'	25:BA:207:A:H4'	2.02	0.42
25:BA:32:C:O2'	25:BA:33:U:H5'	2.20	0.42
25:BA:439:A:H8	25:BA:439:A:O5'	2.02	0.42
25:BA:561:A:H2'	25:BA:562:C:C6	2.54	0.42
27:BD:164:GLN:HE21	27:BD:176:ARG:NH1	2.18	0.42
25:BA:2107:C:OP1	27:BD:261:LYS:NZ	2.53	0.42
28:BE:35:GLN:OE1	28:BE:66:HIS:HE1	2.02	0.42
44:BY:20:TYR:CE1	44:BY:43:ASN:HA	2.54	0.42
1:CA:300:A:H1'	1:CA:565:U:O2	2.19	0.42
4:CD:22:LYS:HB2	4:CD:26:CYS:SG	2.59	0.42
5:CE:105:VAL:HB	5:CE:106:PRO:HD3	2.01	0.42
15:CO:29:VAL:HG13	15:CO:63:ARG:HG3	2.01	0.42
1:CA:664:G:P	18:CR:64:ARG:HH21	2.41	0.42
19:CS:48:THR:HA	19:CS:60:VAL:O	2.19	0.42
25:DA:1412:A:H2'	25:DA:1413:G:C8	2.54	0.42
25:DA:1641:A:H2'	25:DA:1642:G:O4'	2.20	0.42
25:DA:2110:G:H5''	25:DA:2111:C:C5	2.53	0.42
25:DA:2335:A:C8	25:DA:2337:G:C5	3.07	0.42
25:DA:218:A:C2	25:DA:235:U:H4'	2.53	0.42
25:DA:2516:G:H1	25:DA:2568:C:H42	1.67	0.42
25:DA:71:A:H5''	25:DA:73:A:C8	2.55	0.42
30:DG:106:LEU:HA	30:DG:110:ALA:HB3	2.01	0.42
31:DH:2:SER:O	31:DH:3:ARG:HG2	2.19	0.42
1:AA:69:G:H2'	1:AA:70:G:H8	1.85	0.42
3:AC:65:ALA:O	3:AC:66:VAL:HB	2.19	0.42
11:AK:48:ILE:HG12	11:AK:48:ILE:O	2.17	0.42
16:AP:19:ILE:HG23	16:AP:36:ILE:HG13	2.02	0.42
23:AY:50:U:C4	23:AY:64:A:C2	3.08	0.42
54:B8:61:LEU:C	54:B8:63:PRO:HD3	2.40	0.42
25:BA:1223:C:H2'	25:BA:1224:C:C6	2.55	0.42
25:BA:1506:G:H5''	25:BA:1507:A:OP2	2.19	0.42
25:BA:2430:A:H2'	25:BA:2431:U:C6	2.54	0.42
25:BA:552:C:H5	61:BA:4993:HOH:O	2.02	0.42
25:BA:722:A:C8	25:BA:851:A:C6	3.08	0.42
25:BA:895:G:O6	25:BA:974:G:H2'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BB:14:U:OP2	26:BB:70:C:O2'	2.31	0.42
32:BI:106:GLY:HA2	32:BI:107:VAL:HB	2.02	0.42
38:BS:110:LEU:HD12	38:BS:110:LEU:HA	1.82	0.42
39:BT:65:LYS:HD3	39:BT:67:SER:HB2	2.00	0.42
1:CA:1286:A:H8	1:CA:1287:A:H4'	1.83	0.42
1:CA:391:G:C6	1:CA:392:G:C5	3.07	0.42
1:CA:683:G:O6	61:CA:4140:HOH:O	2.19	0.42
20:CT:87:LYS:O	20:CT:91:LEU:HG	2.19	0.42
24:CX:20:U:H5''	24:CX:21:A:OP2	2.19	0.42
25:DA:117:G:C6	25:DA:119:A:C6	3.08	0.42
25:DA:184:C:H2'	25:DA:185:U:H6	1.85	0.42
25:DA:1877:A:H5'	25:DA:1878:G:OP2	2.18	0.42
25:DA:2224:G:H4'	25:DA:2226:C:C2	2.55	0.42
25:DA:2298:A:H2'	25:DA:2299:G:O4'	2.19	0.42
40:DU:27:LEU:HB3	40:DU:31:SER:HB3	2.01	0.42
1:AA:1124:G:N7	1:AA:1145:C:O2'	2.50	0.42
57:AA:3232:UAM:OAG	57:AA:3232:UAM:OAH	2.34	0.42
2:AB:134:GLU:HA	2:AB:137:ARG:HE	1.84	0.42
4:AD:157:LEU:HD22	4:AD:161:ASN:ND2	2.32	0.42
7:AG:124:LEU:HA	7:AG:124:LEU:HD23	1.82	0.42
10:AJ:38:ILE:HG13	10:AJ:71:LEU:O	2.20	0.42
15:AO:4:THR:N	15:AO:7:GLU:OE1	2.43	0.42
23:AY:58:A:N6	23:AY:61:C:C2	2.87	0.42
47:B1:64:ALA:HA	47:B1:67:ILE:HG13	2.02	0.42
25:BA:2627:U:H2'	25:BA:2628:C:H6	1.85	0.42
25:BA:313:A:N6	25:BA:375:G:O2'	2.53	0.42
29:BF:150:GLY:HA2	29:BF:172:TRP:CD2	2.55	0.42
34:BO:108:GLU:HG3	34:BO:108:GLU:H	1.46	0.42
43:BX:12:VAL:HG22	43:BX:29:TRP:CE2	2.54	0.42
1:CA:978:A:H1'	1:CA:1322:C:O2	2.20	0.42
1:CA:942:G:C2	1:CA:1342:C:C2	3.08	0.42
1:CA:1410:G:H2'	1:CA:1411:C:C6	2.55	0.42
1:CA:337:C:H2'	1:CA:338:A:C8	2.55	0.42
1:CA:26:A:N6	1:CA:558:G:O2'	2.48	0.42
13:CM:60:VAL:HG22	13:CM:66:LEU:HD11	2.01	0.42
23:CY:55:PSU:HN1	23:CY:57:G:C5'	2.32	0.42
25:DA:1184:G:C6	25:DA:1185:C:C4	3.08	0.42
25:DA:2469:A:C6	25:DA:2470:G:C4	3.07	0.42
25:DA:277:C:H2'	25:DA:277:C:O2	2.19	0.42
25:DA:833:U:OP1	35:DP:45:LEU:HD11	2.20	0.42
28:DE:143:ASN:HD22	28:DE:147:PRO:CD	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:DE:78:LEU:HA	28:DE:78:LEU:HD12	1.93	0.42
30:DG:7:LEU:HD22	30:DG:100:TRP:HE3	1.85	0.42
31:DH:144:VAL:O	31:DH:148:ILE:HG12	2.19	0.42
33:DN:38:HIS:H	33:DN:38:HIS:CD2	2.37	0.42
36:DQ:99:PRO:HG2	45:DZ:79:ARG:HH22	1.84	0.42
1:AA:1358:U:OP1	14:AN:35:ARG:HG2	2.20	0.42
1:AA:1509:C:H2'	1:AA:1510:U:O4'	2.19	0.42
2:AB:16:HIS:HB3	2:AB:210:SER:HB2	2.02	0.42
6:AF:33:TYR:CD2	6:AF:75:LEU:HD23	2.55	0.42
14:AN:53:LEU:HA	14:AN:54:PRO:HD2	1.88	0.42
19:AS:64:GLU:O	19:AS:67:VAL:HG23	2.19	0.42
48:B2:30:ARG:NH2	61:B2:4001:HOH:O	2.52	0.42
25:BA:1222:A:H2'	25:BA:1222:A:N3	2.34	0.42
25:BA:1992:A:H4'	25:BA:1993:A:OP1	2.20	0.42
25:BA:2052:A:H4'	25:BA:2053:A:C8	2.55	0.42
25:BA:2193:A:O2'	25:BA:2194:U:H5''	2.19	0.42
27:BD:146:GLU:HG2	27:BD:152:GLY:C	2.40	0.42
31:BH:4:ILE:O	31:BH:69:ARG:HG2	2.19	0.42
35:BP:120:ALA:HB1	35:BP:138:LEU:HA	2.00	0.42
44:BY:102:CYS:SG	44:BY:103:GLY:N	2.92	0.42
1:CA:1013:G:O2'	1:CA:1015:A:N7	2.52	0.42
1:CA:1027:C:O2'	1:CA:1034:G:N2	2.53	0.42
1:CA:1510:U:H2'	1:CA:1511:G:C8	2.55	0.42
2:CB:15:VAL:HB	2:CB:16:HIS:CD2	2.54	0.42
9:CI:55:ALA:HA	9:CI:58:HIS:CD2	2.54	0.42
1:CA:881:G:OP2	12:CL:12:ARG:NH2	2.52	0.42
20:CT:90:GLN:HB2	20:CT:90:GLN:HE21	1.58	0.42
25:DA:1478:G:O2'	25:DA:1558:A:N1	2.52	0.42
25:DA:1636:C:H2'	25:DA:1637:A:C8	2.55	0.42
25:DA:1676:A:H2'	25:DA:1677:A:O4'	2.20	0.42
25:DA:2140:C:H2'	25:DA:2140:C:O2	2.19	0.42
25:DA:2366:A:H2'	25:DA:2367:G:O4'	2.19	0.42
25:DA:2783:G:H2'	25:DA:2784:C:C6	2.55	0.42
25:DA:2865:U:C4	25:DA:2866:U:C4	3.08	0.42
25:DA:479:A:N3	25:DA:481:G:H5''	2.34	0.42
25:DA:652(C):G:H2'	25:DA:652(D):C:C6	2.54	0.42
28:DE:21:VAL:HA	28:DE:22:PRO:HD3	1.88	0.42
31:DH:3:ARG:NH2	31:DH:5:GLY:H	2.18	0.42
33:DN:67:LEU:C	33:DN:88:GLU:HG3	2.40	0.42
42:DW:23:LEU:O	42:DW:27:LYS:NZ	2.53	0.42
45:DZ:18:LEU:HA	45:DZ:18:LEU:HD12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:131:ILE:HD13	5:AE:131:ILE:HA	1.94	0.42
16:AP:74:LEU:HG	16:AP:79:VAL:HG21	2.00	0.42
25:BA:1938:A:H2'	25:BA:1939:U:O4'	2.20	0.42
25:BA:2697:G:H5'	34:BO:68:GLU:OE1	2.19	0.42
25:BA:606:G:OP2	40:BU:10:ARG:NH1	2.47	0.42
27:BD:2:ALA:HB3	27:BD:20:ASP:OD2	2.19	0.42
29:BF:110:LEU:HD12	29:BF:205:ARG:HG2	2.01	0.42
30:BG:16:ARG:HH21	30:BG:31:VAL:CG1	2.32	0.42
34:BO:120:GLU:OE2	34:BO:122:LEU:HD21	2.19	0.42
1:CA:110:C:H2'	1:CA:111:G:O4'	2.20	0.42
1:CA:1250:A:N3	1:CA:1370:G:O2'	2.41	0.42
1:CA:857:C:H2'	1:CA:858:G:O4'	2.20	0.42
2:CB:69:LEU:HD13	2:CB:91:PRO:HB2	2.02	0.42
7:CG:137:LYS:O	7:CG:141:VAL:HG23	2.20	0.42
12:CL:51:ALA:O	12:CL:52:LEU:HD13	2.19	0.42
1:CA:636:U:H5'	17:CQ:2:PRO:HD3	2.02	0.42
17:CQ:74:LEU:HD13	17:CQ:75:ARG:HG2	2.01	0.42
50:D4:62:ARG:HE	50:D4:62:ARG:N	2.18	0.42
25:DA:373:U:H2'	25:DA:374:A:C8	2.54	0.42
25:DA:441:U:O2	29:DF:46:ARG:NH2	2.44	0.42
25:DA:79:G:H2'	25:DA:80:G:O4'	2.20	0.42
32:DI:124:GLY:N	32:DI:144:VAL:HG23	2.35	0.42
32:DI:70:GLU:O	32:DI:74:ASN:HB2	2.19	0.42
33:DN:15:LEU:HB3	33:DN:137:LYS:HA	2.02	0.42
36:DQ:18:LYS:HE3	36:DQ:18:LYS:HB2	1.77	0.42
37:DR:2:ARG:HG2	37:DR:5:LYS:HB2	2.01	0.42
1:AA:1262:C:H2'	1:AA:1263:C:C6	2.55	0.42
1:AA:1316:G:H22	1:AA:1319:A:H5''	1.85	0.42
1:AA:346:G:H2'	1:AA:347:G:O3'	2.20	0.42
3:AC:136:GLN:HE21	3:AC:136:GLN:HB2	1.63	0.42
1:AA:1329:A:H5''	13:AM:26:GLY:H	1.84	0.42
47:B1:50:ARG:HD2	47:B1:57:GLU:OE1	2.19	0.42
25:BA:1119:A:H2'	25:BA:1120:G:O4'	2.20	0.42
25:BA:250:G:O2'	25:BA:633:G:O2'	2.25	0.42
25:BA:2579:G:H2'	25:BA:2580:C:C6	2.55	0.42
29:BF:28:ILE:O	29:BF:30:PRO:HD3	2.20	0.42
30:BG:132:ASN:HA	30:BG:157:ILE:O	2.20	0.42
35:BP:63:PRO:HD3	54:B8:27:THR:HG22	2.01	0.42
40:BU:8:VAL:HG13	40:BU:12:ARG:HD2	2.02	0.42
1:CA:1063:C:OP2	1:CA:1064:G:O2'	2.29	0.42
1:CA:1287:A:H2	1:CA:1353:G:H1'	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1323:G:H2'	1:CA:1324:A:C8	2.55	0.42
1:CA:1366:C:H2'	1:CA:1367:C:C6	2.54	0.42
1:CA:779:C:H2'	1:CA:780:A:O4'	2.19	0.42
2:CB:16:HIS:HB3	2:CB:210:SER:HB3	2.02	0.42
1:CA:1112:C:H1'	3:CC:179:ARG:HG2	2.02	0.42
4:CD:121:VAL:O	4:CD:134:ASP:HA	2.20	0.42
8:CH:82:HIS:HB3	8:CH:138:TRP:CE2	2.55	0.42
8:CH:14:ARG:CG	8:CH:18:ARG:HH22	2.32	0.42
23:CW:49:C:O5'	23:CW:49:C:H6	2.03	0.42
46:D0:37:LEU:HG	46:D0:60:PHE:HA	2.02	0.42
47:D1:83:GLU:HA	47:D1:84:GLY:HA2	1.72	0.42
25:DA:1359:A:N1	25:DA:1372:U:O4	2.53	0.42
25:DA:1400:G:H2'	25:DA:1401:G:H8	1.84	0.42
25:DA:2114:A:N6	25:DA:2119:A:H62	2.16	0.42
25:DA:2122:U:C4	25:DA:2176:A:N1	2.88	0.42
25:DA:217:G:H2'	25:DA:218:A:O4'	2.20	0.42
25:DA:228:A:O2'	25:DA:229:A:P	2.77	0.42
25:DA:2781:A:H5''	25:DA:2782:G:H5'	2.02	0.42
25:DA:2896:C:H2'	25:DA:2897:U:H6	1.85	0.42
25:DA:328:U:H4'	44:DY:68:HIS:CE1	2.55	0.42
29:DF:33:LEU:HA	29:DF:33:LEU:HD12	1.91	0.42
32:DI:90:GLY:O	32:DI:121:LYS:HE3	2.20	0.42
35:DP:100:LEU:HD22	35:DP:105:LEU:HD12	2.02	0.42
1:AA:486:U:H2'	1:AA:487:A:H8	1.85	0.41
1:AA:714:G:H2'	1:AA:715:A:C8	2.55	0.41
1:AA:828:A:H2'	1:AA:829:G:O4'	2.20	0.41
6:AF:14:LEU:HD11	6:AF:84:ASN:ND2	2.35	0.41
20:AT:77:ALA:O	20:AT:81:LYS:HG3	2.20	0.41
53:B7:30:VAL:O	53:B7:34:ARG:HG3	2.20	0.41
25:BA:1214:G:H2'	25:BA:1215:G:O4'	2.19	0.41
25:BA:1825:U:H2'	25:BA:1826:C:H6	1.85	0.41
25:BA:2144:U:H3	25:BA:2198:A:H2	1.64	0.41
25:BA:402:C:OP1	61:BA:5278:HOH:O	2.20	0.41
25:BA:930:G:N2	25:BA:939:C:N3	2.64	0.41
23:AW:55:PSU:O3'	25:BA:943:C:H4'	2.20	0.41
40:BU:17:ILE:HG23	40:BU:39:LEU:HD12	2.02	0.41
1:CA:1035:A:H8	1:CA:1035:A:O5'	2.02	0.41
1:CA:1146:A:H8	1:CA:1146:A:H5'	1.85	0.41
1:CA:1476:G:H2'	1:CA:1477:C:C6	2.55	0.41
1:CA:735:C:H2'	1:CA:736:C:C6	2.55	0.41
1:CA:825:G:H1	1:CA:875:C:H42	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:CK:120:ARG:HA	11:CK:121:PRO:HD3	1.89	0.41
17:CQ:81:ARG:NH2	17:CQ:84:LEU:HD21	2.35	0.41
25:DA:1580:A:OP2	25:DA:1580:A:H8	2.03	0.41
25:DA:2391:G:O6	25:DA:2425:A:H8	2.03	0.41
25:DA:2648:C:H2'	25:DA:2649:U:C6	2.54	0.41
25:DA:436:C:H2'	25:DA:437:G:C8	2.55	0.41
25:DA:566:U:O2'	25:DA:809:G:OP2	2.28	0.41
26:DB:1:U:H2'	26:DB:2:C:C6	2.55	0.41
28:DE:50:GLY:HA3	28:DE:75:VAL:HG11	2.02	0.41
28:DE:76:ARG:NH1	61:DE:405:HOH:O	2.53	0.41
30:DG:76:SER:N	30:DG:84:LYS:HB2	2.35	0.41
33:DN:4:TYR:CD2	40:DU:100:VAL:HG11	2.55	0.41
41:DV:50:PRO:HG2	41:DV:51:VAL:HG12	2.01	0.41
42:DW:45:TYR:CZ	42:DW:49:LYS:HE3	2.55	0.41
45:DZ:138:GLU:H	45:DZ:156:LYS:HE2	1.84	0.41
1:AA:1022:G:H5'	1:AA:1023:G:OP2	2.20	0.41
1:AA:162:A:O5'	1:AA:162:A:H8	2.03	0.41
1:AA:193:C:H2'	1:AA:194:C:C6	2.55	0.41
4:AD:112:VAL:HG23	4:AD:116:GLN:OE1	2.20	0.41
5:AE:113:ALA:HB3	5:AE:115:VAL:HG23	2.02	0.41
16:AP:17:TYR:HE2	16:AP:41:PRO:HG3	1.84	0.41
25:BA:1289:G:H2'	25:BA:1290:G:O4'	2.19	0.41
25:BA:2760:G:O6	25:BA:2768:C:H5''	2.20	0.41
25:BA:287:G:N7	25:BA:448:U:H2'	2.35	0.41
27:BD:242:ARG:HD3	27:BD:242:ARG:N	2.35	0.41
28:BE:47:VAL:O	28:BE:80:GLU:HA	2.20	0.41
32:BI:103:ARG:HE	32:BI:103:ARG:HB3	1.58	0.41
32:BI:66:GLU:HA	32:BI:69:LYS:HB3	2.01	0.41
33:BN:14:VAL:HG11	33:BN:138:LEU:HD12	2.02	0.41
33:BN:75:TYR:CE2	33:BN:77:GLY:HA2	2.54	0.41
1:CA:1038:C:C2'	1:CA:1039:C:H5'	2.50	0.41
1:CA:1086:U:H3	1:CA:1099:G:N2	2.17	0.41
1:CA:1391:U:H2'	1:CA:1392:G:C8	2.55	0.41
1:CA:266:G:H5''	1:CA:268:C:H41	1.85	0.41
3:CC:33:LEU:HA	3:CC:36:ASP:HB2	2.03	0.41
1:CA:671:G:H5'	6:CF:77:ARG:HH22	1.85	0.41
5:CE:79:GLU:OE1	8:CH:104:ARG:HA	2.20	0.41
13:CM:13:LYS:NZ	13:CM:21:TYR:OH	2.54	0.41
25:DA:146:G:H2'	25:DA:147:U:C6	2.56	0.41
25:DA:1885:A:H2'	25:DA:1886:C:O4'	2.20	0.41
25:DA:676:A:H2	25:DA:2069:G:N3	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:705:A:H2'	25:DA:706:A:O4'	2.20	0.41
25:DA:729:G:C6	27:DD:208:LYS:HB2	2.55	0.41
31:DH:73:ALA:O	31:DH:76:VAL:HG22	2.19	0.41
31:DH:98:LEU:HD23	31:DH:125:VAL:HG22	2.02	0.41
45:DZ:121:HIS:HB3	45:DZ:123:ASP:O	2.19	0.41
1:AA:1298:C:H4'	1:AA:1299:A:O4'	2.19	0.41
1:AA:1424:C:H2'	1:AA:1425:U:O4'	2.20	0.41
1:AA:396:G:O2'	1:AA:398:C:OP1	2.24	0.41
3:AC:87:LEU:O	3:AC:91:LEU:HB2	2.19	0.41
7:AG:27:ILE:HD12	7:AG:40:ALA:HA	2.02	0.41
8:AH:39:LEU:HD12	8:AH:39:LEU:HA	1.91	0.41
8:AH:86:ILE:HG13	8:AH:133:LEU:HD22	2.01	0.41
19:AS:42:PRO:HD3	50:B4:61:ARG:NH2	2.35	0.41
25:BA:1104:G:OP1	25:BA:1104:G:H4'	2.21	0.41
25:BA:1570:G:H2'	25:BA:1571:G:O4'	2.20	0.41
25:BA:2108:U:H2'	25:BA:2109:G:C8	2.55	0.41
25:BA:2388:A:H2'	25:BA:2389:A:O4'	2.20	0.41
25:BA:2787:C:H2'	25:BA:2788:A:O4'	2.19	0.41
25:BA:310:C:H2'	25:BA:311:C:H6	1.85	0.41
35:BP:121:LYS:HB3	35:BP:121:LYS:HE2	1.87	0.41
1:CA:316:G:OP2	1:CA:351:G:O2'	2.31	0.41
1:CA:900:A:H2'	1:CA:901:A:C8	2.56	0.41
22:CV:12:A:OP2	22:CV:12:A:H8	2.03	0.41
25:DA:1027:A:O2'	25:DA:1028:A:H5'	2.20	0.41
25:DA:1198:U:H2'	25:DA:1199:U:C6	2.55	0.41
25:DA:1857:G:C6	25:DA:1858:G:N1	2.88	0.41
25:DA:2315:G:H2'	25:DA:2316:C:C6	2.55	0.41
25:DA:2365:G:H4'	46:D0:60:PHE:CZ	2.55	0.41
25:DA:657:U:H2'	25:DA:658:C:C6	2.55	0.41
30:DG:43:LEU:HB3	30:DG:44:GLY:H	1.51	0.41
25:DA:2749:A:H1'	31:DH:63:SER:HA	2.02	0.41
34:DO:36:GLY:HA2	34:DO:106:LEU:HD23	2.02	0.41
38:DS:5:THR:OG1	38:DS:8:GLU:HG3	2.20	0.41
40:DU:108:GLU:O	40:DU:112:ARG:HG2	2.20	0.41
1:AA:445:G:H2'	1:AA:446:G:C8	2.55	0.41
1:AA:711:G:O2'	1:AA:712:A:H5'	2.21	0.41
1:AA:922:G:H2'	1:AA:923:A:C8	2.55	0.41
4:AD:194:LEU:HG	4:AD:196:LEU:HD11	2.01	0.41
10:AJ:6:ILE:HA	10:AJ:97:GLU:O	2.20	0.41
11:AK:70:LYS:HB2	11:AK:70:LYS:HE2	1.86	0.41
13:AM:3:ARG:CG	13:AM:8:GLU:HA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AR:26:LEU:HA	18:AR:26:LEU:HD12	1.93	0.41
18:AR:45:SER:OG	18:AR:47:THR:HG22	2.20	0.41
20:AT:16:HIS:O	20:AT:19:SER:OG	2.38	0.41
23:AY:19:G:N2	23:AY:56:C:C2	2.88	0.41
50:B4:18:CYS:SG	50:B4:20:ASN:HB2	2.60	0.41
25:BA:1417:G:H2'	25:BA:1418:U:C5	2.55	0.41
25:BA:2054:G:O2'	28:BE:145:LYS:HE3	2.19	0.41
25:BA:207:A:C2	25:BA:224:U:H4'	2.56	0.41
25:BA:9:U:N3	25:BA:2641:A:C2	2.87	0.41
25:BA:630:U:OP1	29:BF:102:PRO:HA	2.20	0.41
25:BA:768:C:H2'	25:BA:769:A:C8	2.55	0.41
27:BD:182:LEU:HA	27:BD:182:LEU:HD23	1.79	0.41
1:CA:589:C:H5''	8:CH:29:SER:OG	2.20	0.41
2:CB:158:LEU:HA	2:CB:159:PRO:HD3	1.88	0.41
3:CC:152:ILE:CD1	3:CC:199:LYS:HD2	2.50	0.41
7:CG:51:GLN:HB3	7:CG:51:GLN:HE21	1.62	0.41
13:CM:88:ARG:HG3	13:CM:98:VAL:CG1	2.48	0.41
21:CU:5:ASP:O	21:CU:11:GLY:HA3	2.20	0.41
49:D3:4:LEU:O	49:D3:36:VAL:HA	2.20	0.41
51:D5:20:ARG:HG2	51:D5:23:HIS:CE1	2.55	0.41
25:DA:1357:U:H2'	25:DA:1358:G:O4'	2.20	0.41
25:DA:1589:C:H2'	25:DA:1590:U:C6	2.52	0.41
26:DB:24:G:H4'	26:DB:25:A:C8	2.55	0.41
27:DD:69:ARG:C	27:DD:71:ASP:H	2.23	0.41
27:DD:29:PRO:HA	27:DD:83:GLU:OE1	2.21	0.41
37:DR:67:LEU:CD1	37:DR:76:VAL:HG21	2.48	0.41
39:DT:59:THR:HG23	39:DT:78:LEU:CB	2.50	0.41
42:DW:13:SER:HA	42:DW:14:PRO:HD3	1.91	0.41
44:DY:6:HIS:H	44:DY:6:HIS:CD2	2.38	0.41
1:AA:1016:A:H2'	1:AA:1017:G:O4'	2.21	0.41
1:AA:674:G:H2'	1:AA:675:A:H8	1.85	0.41
2:AB:192:SER:O	2:AB:194:PRO:HD3	2.20	0.41
10:AJ:23:ILE:HA	10:AJ:23:ILE:HD13	1.85	0.41
15:AO:84:LYS:HD3	15:AO:84:LYS:O	2.19	0.41
18:AR:53:ARG:HG2	18:AR:58:LEU:O	2.21	0.41
23:AW:44:G:O5'	23:AW:44:G:H8	2.04	0.41
23:AY:67:C:H2'	23:AY:68:C:C6	2.55	0.41
23:AY:7:A:C6	23:AY:49:C:C4	3.08	0.41
46:B0:43:THR:O	46:B0:43:THR:HG23	2.21	0.41
25:BA:1139:G:H3'	25:BA:1140:U:C5'	2.49	0.41
25:BA:1140:U:H4'	25:BA:1140:U:OP1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2143:G:N2	25:BA:2199:C:N3	2.55	0.41
25:BA:2504:U:H2'	25:BA:2505:U:H6	1.86	0.41
25:BA:2784:C:H2'	25:BA:2785:C:H6	1.84	0.41
25:BA:923:C:H2'	25:BA:924:U:O4'	2.20	0.41
27:BD:36:PRO:HA	27:BD:61:LEU:HD12	2.02	0.41
30:BG:114:ILE:HA	30:BG:140:ILE:HD11	2.03	0.41
45:BZ:124:ILE:HG23	45:BZ:126:VAL:HG23	2.02	0.41
1:CA:1243:C:H42	1:CA:1294:G:H1	1.68	0.41
1:CA:353:A:C8	1:CA:353:A:H5'	2.55	0.41
1:CA:695:A:C6	1:CA:696:A:C6	3.09	0.41
4:CD:119:GLN:HG2	4:CD:123:HIS:CD2	2.55	0.41
1:CA:411:A:OP2	4:CD:30:LYS:HE3	2.20	0.41
5:CE:127:ASN:HA	5:CE:128:PRO:HD3	1.89	0.41
7:CG:22:LEU:HG	7:CG:62:PHE:CE2	2.56	0.41
23:CW:34:G:H2'	23:CW:35:A:H8	1.85	0.41
25:DA:1670:C:C5	25:DA:1671:U:C4	3.09	0.41
25:DA:2167:U:H2'	25:DA:2168:G:N2	2.33	0.41
25:DA:2273:A:O2'	25:DA:2274:A:H5'	2.20	0.41
25:DA:2506:U:OP1	28:DE:144:ARG:NH2	2.54	0.41
25:DA:26:G:C6	25:DA:27:G:N1	2.88	0.41
25:DA:2857:G:N2	25:DA:2860:A:OP2	2.50	0.41
25:DA:320:A:H4'	25:DA:322:A:N7	2.35	0.41
25:DA:702:G:C2	25:DA:731:C:C2	3.08	0.41
26:DB:30:C:OP2	38:DS:32:LEU:HD11	2.20	0.41
32:DI:117:GLU:HG3	32:DI:118:LYS:H	1.86	0.41
35:DP:95:VAL:HG13	35:DP:125:VAL:HB	2.02	0.41
1:AA:1005:A:H62	1:AA:1023:G:N2	2.18	0.41
1:AA:1131:G:H8	1:AA:1131:G:O5'	2.03	0.41
1:AA:254:G:OP1	17:AQ:68:ARG:HB3	2.21	0.41
1:AA:431:A:H2'	1:AA:432:A:O4'	2.21	0.41
1:AA:837:G:H1	1:AA:849:C:H42	1.67	0.41
23:AW:19:G:H4'	23:AW:20:U:OP1	2.20	0.41
50:B4:26:SER:OG	50:B4:27:THR:N	2.53	0.41
25:BA:653:G:H5''	54:B8:18:ALA:HB2	2.01	0.41
25:BA:1140:U:O2	25:BA:1143:U:H6	2.03	0.41
25:BA:1093:G:H2'	25:BA:1156:G:C2	2.55	0.41
25:BA:2141:A:O2'	25:BA:2142:G:H5''	2.21	0.41
25:BA:2346:G:O6	46:B0:74:ARG:NH2	2.50	0.41
25:BA:2455:C:H2'	25:BA:2456:G:H8	1.85	0.41
25:BA:329:U:H2'	25:BA:330:U:C6	2.56	0.41
28:BE:7:VAL:CG1	28:BE:27:LEU:HB3	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BH:20:ALA:HB1	31:BH:21:PRO:HD2	2.03	0.41
1:CA:1245:A:H2'	1:CA:1246:C:O4'	2.21	0.41
1:CA:714:G:H2'	1:CA:715:A:C8	2.55	0.41
2:CB:214:ILE:HG12	2:CB:214:ILE:H	1.70	0.41
2:CB:215:LEU:HD22	2:CB:215:LEU:HA	1.94	0.41
7:CG:50:ILE:HG22	7:CG:125:MET:HG3	2.01	0.41
17:CQ:62:SER:OG	17:CQ:72:ARG:HD3	2.21	0.41
17:CQ:66:SER:OG	17:CQ:69:LYS:HB2	2.21	0.41
54:D8:50:LEU:HD23	54:D8:50:LEU:HA	1.93	0.41
25:DA:2386:C:H2'	25:DA:2387:U:C6	2.55	0.41
25:DA:2393:A:H2'	25:DA:2394:C:O4'	2.21	0.41
26:DB:66:A:H61	26:DB:108:U:H3'	1.84	0.41
31:DH:116:GLU:HA	31:DH:117:PRO:HD3	1.89	0.41
33:DN:96:GLU:H	33:DN:96:GLU:CD	2.23	0.41
35:DP:36:LYS:O	61:DP:304:HOH:O	2.22	0.41
1:AA:113:G:H2'	1:AA:114:U:C6	2.56	0.41
1:AA:454:C:H3'	1:AA:455:C:H6	1.84	0.41
1:AA:90:U:C2'	1:AA:91:C:H5"	2.45	0.41
2:AB:91:PRO:HG3	2:AB:154:LEU:HB2	2.03	0.41
12:AL:60:LEU:HD21	12:AL:66:VAL:HG22	2.02	0.41
14:AN:3:ARG:HA	14:AN:3:ARG:HD3	1.68	0.41
20:AT:90:GLN:O	20:AT:93:GLU:HB3	2.19	0.41
23:AW:21:A:C6	23:AW:46:7MG:C6	3.08	0.41
50:B4:55:ARG:N	50:B4:56:VAL:CA	2.83	0.41
25:BA:956:A:N1	25:BA:2289:G:H1'	2.35	0.41
25:BA:2589:A:OP2	51:B5:3:LYS:NZ	2.50	0.41
26:BB:55:U:H2'	26:BB:56:G:O4'	2.20	0.41
25:BA:2331:G:H22	38:BS:3:ARG:HA	1.86	0.41
1:CA:1392:G:N2	1:CA:1502:A:C8	2.89	0.41
1:CA:407:G:H2'	1:CA:408:A:C8	2.55	0.41
1:CA:9:G:H2'	1:CA:10:A:H8	1.85	0.41
1:CA:1060:C:C4	3:CC:2:GLY:HA2	2.56	0.41
7:CG:47:CYS:HA	7:CG:50:ILE:HD11	2.03	0.41
7:CG:52:GLU:H	7:CG:52:GLU:HG2	1.45	0.41
15:CO:17:ARG:NH1	15:CO:17:ARG:HG3	2.35	0.41
20:CT:51:GLU:O	20:CT:55:ILE:HG12	2.20	0.41
25:DA:1364:G:C5	47:D1:3:LYS:HE2	2.55	0.41
54:D8:26:LYS:HZ2	54:D8:26:LYS:HB3	1.86	0.41
25:DA:1219:G:H1	25:DA:1230:C:N4	2.19	0.41
25:DA:811:U:C2	25:DA:1251:C:C5	3.09	0.41
25:DA:1272:A:H3'	25:DA:1273:U:H5"	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2347:C:H2'	25:DA:2348:U:C6	2.55	0.41
25:DA:2794:C:N4	25:DA:2802:G:O6	2.53	0.41
36:DQ:141:GLN:NE2	45:DZ:74:VAL:O	2.54	0.41
44:DY:9:LYS:HA	44:DY:10:GLY:HA2	1.58	0.41
45:DZ:163:LEU:HG	45:DZ:165:VAL:HG22	2.01	0.41
45:DZ:97:GLU:HA	45:DZ:126:VAL:O	2.20	0.41
1:AA:154:C:N3	1:AA:168:G:C2	2.89	0.41
1:AA:676:A:H1'	11:AK:115:PRO:HB3	2.03	0.41
2:AB:178:ARG:NH1	2:AB:196:LEU:O	2.54	0.41
3:AC:63:ASN:HA	3:AC:97:LYS:HB3	2.01	0.41
1:AA:1347:G:H5''	9:AI:107:ARG:HB3	2.02	0.41
13:AM:15:VAL:O	13:AM:19:LEU:HD22	2.20	0.41
13:AM:40:ASN:HB3	13:AM:43:THR:HG23	2.02	0.41
15:AO:17:ARG:HA	15:AO:17:ARG:HD2	1.85	0.41
24:AX:64:G:H2'	24:AX:65:C:C6	2.56	0.41
25:BA:1067:A:C3'	25:BA:1067:A:C8	3.04	0.41
25:BA:2282:G:H2'	25:BA:2283:G:O4'	2.19	0.41
25:BA:2851:C:H2'	25:BA:2852:G:H8	1.85	0.41
25:BA:449:A:H2'	25:BA:450:A:C8	2.55	0.41
25:BA:696:C:P	25:BA:696:C:H6	2.43	0.41
25:BA:787:U:H2'	25:BA:788:G:C8	2.55	0.41
27:BD:275:LYS:HB3	27:BD:276:LYS:H	1.22	0.41
1:CA:1423:G:C6	1:CA:1424:C:C4	3.09	0.41
1:CA:854:G:C2	1:CA:855:G:C8	3.09	0.41
1:CA:865:A:H5'	1:CA:1078:U:C5	2.56	0.41
4:CD:173:TRP:CD1	4:CD:189:PRO:HG3	2.55	0.41
6:CF:95:GLU:HA	6:CF:96:PRO:HD3	1.87	0.41
7:CG:65:ALA:HB1	7:CG:127:ALA:HB3	2.02	0.41
10:CJ:16:LEU:HA	10:CJ:16:LEU:HD22	1.84	0.41
1:CA:1060:C:C5'	10:CJ:51:ARG:HB3	2.51	0.41
1:CA:719:C:O2'	18:CR:49:LYS:HB3	2.20	0.41
18:CR:40:LEU:HB3	18:CR:79:LEU:HD11	2.02	0.41
50:D4:61:ARG:O	50:D4:61:ARG:NH1	2.49	0.41
25:DA:1594:G:H2'	25:DA:1595:G:O4'	2.21	0.41
25:DA:1794:U:H2'	25:DA:1795:C:C6	2.56	0.41
25:DA:1916:A:H2'	25:DA:1917:U:O4'	2.21	0.41
25:DA:2000:G:N7	61:DA:4385:HOH:O	2.37	0.41
25:DA:2086:U:H2'	25:DA:2087:G:C8	2.55	0.41
25:DA:699:A:H2'	25:DA:700:G:O4'	2.20	0.41
25:DA:856:C:HO2'	25:DA:857:C:P	2.43	0.41
30:DG:166:ASP:O	30:DG:170:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:DG:16:ARG:HG3	30:DG:16:ARG:HH11	1.85	0.41
32:DI:123:LEU:HA	32:DI:144:VAL:HG23	2.03	0.41
41:DV:31:ALA:O	41:DV:61:VAL:HG12	2.20	0.41
26:DB:73:A:N1	45:DZ:34:ASN:ND2	2.68	0.41
1:AA:1095:U:P	1:AA:1108:G:H1	2.44	0.41
1:AA:1412:C:H2'	1:AA:1413:A:C8	2.56	0.41
1:AA:148:G:H2'	1:AA:149:A:C8	2.51	0.41
1:AA:235:C:H2'	1:AA:236:G:H8	1.86	0.41
3:AC:131:ARG:NH1	5:AE:50:GLU:HG3	2.35	0.41
23:AY:53:G:H1	23:AY:61:C:H42	1.69	0.41
52:B6:16:CYS:SG	52:B6:18:ARG:HG2	2.61	0.41
25:BA:1091:A:H1'	25:BA:1093:G:N3	2.35	0.41
25:BA:116:A:C8	25:BA:117:A:C8	3.09	0.41
25:BA:1222:A:H3'	25:BA:1223:C:C6	2.56	0.41
25:BA:1773:C:H2'	25:BA:1774:C:H6	1.86	0.41
25:BA:2156:A:H2	25:BA:2181:G:H4'	1.85	0.41
25:BA:2372:A:H2'	25:BA:2373:A:O4'	2.21	0.41
27:BD:5:LYS:HG2	27:BD:17:THR:HG22	2.03	0.41
30:BG:16:ARG:NH2	30:BG:28:VAL:O	2.53	0.41
33:BN:89:LYS:O	33:BN:93:THR:OG1	2.32	0.41
42:BW:75:TYR:CZ	42:BW:104:THR:HG21	2.56	0.41
43:BX:11:PRO:HB3	43:BX:92:LEU:HD11	2.02	0.41
44:BY:83:THR:HG21	44:BY:99:CYS:HB2	2.02	0.41
1:CA:1191:A:H5''	3:CC:4:LYS:HD3	2.02	0.41
2:CB:28:PHE:O	2:CB:32:ILE:HG13	2.20	0.41
3:CC:63:ASN:HB3	3:CC:98:ASN:HD22	1.86	0.41
8:CH:97:VAL:HG23	8:CH:129:VAL:O	2.21	0.41
9:CI:7:THR:HB	9:CI:83:ARG:HH12	1.85	0.41
25:DA:752:A:H3'	53:D7:1:MET:SD	2.60	0.41
54:D8:62:LEU:HB3	54:D8:65:GLU:HG2	2.03	0.41
25:DA:1306:C:H1'	25:DA:1623:G:N2	2.36	0.41
25:DA:1878:G:C2	25:DA:1879:C:C2	3.08	0.41
25:DA:2114:A:H2'	25:DA:2114:A:N3	2.36	0.41
25:DA:2168:G:C8	25:DA:2170:A:N7	2.89	0.41
25:DA:686:G:N3	53:D7:11:LYS:HE2	2.36	0.41
26:DB:105:A:H2'	26:DB:106:G:O4'	2.21	0.41
26:DB:33:G:C2	26:DB:50:G:C2	3.09	0.41
26:DB:33:G:H5'	30:DG:2:PRO:HD3	2.01	0.41
26:DB:55:U:H2'	26:DB:56:G:O4'	2.21	0.41
27:DD:9:TYR:CZ	27:DD:13:ARG:HG2	2.56	0.41
27:DD:61:LEU:HA	27:DD:61:LEU:HD12	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DH:13:LYS:HA	31:DH:14:GLY:HA2	1.57	0.41
35:DP:107:LYS:O	35:DP:110:TYR:HB2	2.20	0.41
1:AA:1014:A:H2'	1:AA:1015:A:C8	2.56	0.41
1:AA:1034:G:C6	1:AA:1035:A:C5	3.09	0.41
1:AA:1181:G:H1'	1:AA:1182:G:C5	2.56	0.41
1:AA:138:G:H1	1:AA:225:C:H42	1.69	0.41
1:AA:390:C:H2'	1:AA:391:G:C8	2.56	0.41
11:AK:84:VAL:HG11	11:AK:91:ARG:HD2	2.02	0.41
1:AA:1216:G:OP1	14:AN:2:ALA:HA	2.21	0.41
1:AA:1049:U:OP1	14:AN:3:ARG:HB2	2.21	0.41
23:AW:58:A:C6	23:AW:61:C:C2	3.09	0.41
25:BA:1065:U:H3	25:BA:1188:A:H62	1.68	0.41
25:BA:1405:A:N1	25:BA:1418:U:C4	2.89	0.41
25:BA:2201:C:H2'	25:BA:2202:U:C6	2.56	0.41
25:BA:2118:U:H3	25:BA:2215:G:H1	1.69	0.41
25:BA:2412:G:H4'	52:B6:18:ARG:HD2	2.02	0.41
25:BA:939:C:H2'	25:BA:940:C:C6	2.56	0.41
31:BH:13:LYS:HA	31:BH:14:GLY:HA2	1.58	0.41
32:BI:129:THR:HG22	32:BI:139:GLN:NE2	2.36	0.41
1:AA:1442(A):G:C8	39:BT:118:ARG:HG2	2.56	0.41
25:BA:63:A:O3'	43:BX:71:GLY:HA3	2.21	0.41
44:BY:9:LYS:HA	44:BY:10:GLY:HA2	1.62	0.41
3:CC:126:ARG:HB3	3:CC:128:PHE:CE1	2.56	0.41
8:CH:121:ASP:OD1	8:CH:121:ASP:N	2.53	0.41
50:D4:20:ASN:OD1	50:D4:21:VAL:N	2.54	0.41
53:D7:9:ARG:HG3	53:D7:46:VAL:HG23	2.02	0.41
25:DA:1223:G:N2	25:DA:1226:A:OP2	2.46	0.41
25:DA:1752:C:H2'	25:DA:1753:G:C8	2.55	0.41
25:DA:271(O):C:H2'	25:DA:271(P):C:C6	2.56	0.41
25:DA:2846:G:H2'	25:DA:2847:U:O4'	2.20	0.41
26:DB:115:G:O4'	38:DS:47:THR:HB	2.21	0.41
26:DB:17:C:H2'	26:DB:18:G:O4'	2.21	0.41
25:DA:784:A:N6	27:DD:229:VAL:HG11	2.36	0.41
29:DF:176:LEU:HD23	29:DF:176:LEU:HA	1.91	0.41
25:DA:637:A:H8	35:DP:117:GLU:HG3	1.86	0.41
42:DW:54:ALA:HB1	42:DW:107:LEU:HD22	2.02	0.41
1:AA:1072:G:H2'	1:AA:1073:U:C6	2.55	0.41
1:AA:1236:A:H4'	1:AA:1304:G:H4'	2.02	0.41
1:AA:942:G:C2	1:AA:1342:C:C2	3.09	0.41
1:AA:943:U:C2'	1:AA:944:G:H5'	2.51	0.41
3:AC:115:LEU:HA	3:AC:115:LEU:HD12	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:65:VAL:HG21	9:AI:73:GLN:HB3	2.03	0.41
13:AM:80:ARG:HH21	19:AS:69:HIS:HE1	1.68	0.41
15:AO:17:ARG:NH1	15:AO:17:ARG:HG3	2.35	0.41
48:B2:69:ARG:HB3	48:B2:70:GLN:H	1.45	0.41
50:B4:62:ARG:HB2	50:B4:63:TYR:CD1	2.56	0.41
25:BA:1093:G:H2'	25:BA:1156:G:H22	1.86	0.41
25:BA:1688:A:H2'	25:BA:1689:G:O4'	2.20	0.41
25:BA:26:G:H1'	25:BA:540:A:H61	1.86	0.41
25:BA:2705:A:H2'	25:BA:2706:G:C8	2.56	0.41
28:BE:96:PHE:O	28:BE:175:VAL:HG11	2.20	0.41
30:BG:109:VAL:C	30:BG:112:PRO:HD2	2.41	0.41
31:BH:116:GLU:HA	31:BH:117:PRO:HD3	1.88	0.41
33:BN:82:LEU:HD12	33:BN:82:LEU:HA	1.90	0.41
1:CA:1027:C:H5'	1:CA:1028:C:OP2	2.21	0.41
1:CA:1032:G:C2	1:CA:1033:G:C5	3.09	0.41
1:CA:685:G:C2	1:CA:686:U:C4	3.09	0.41
1:CA:765:G:H5''	1:CA:766:A:OP1	2.21	0.41
1:CA:839:U:O3'	1:CA:840:C:H6	2.04	0.41
3:CC:32:LEU:HD13	3:CC:32:LEU:HA	1.90	0.41
5:CE:51:VAL:O	5:CE:55:VAL:HG23	2.20	0.41
5:CE:84:PHE:N	5:CE:87:SER:O	2.53	0.41
9:CI:3:GLN:HG3	9:CI:20:ARG:HE	1.86	0.41
10:CJ:23:ILE:HD13	10:CJ:23:ILE:HA	1.87	0.41
1:CA:1228:C:P	13:CM:108:ARG:HH22	2.39	0.41
47:D1:85:LEU:HA	47:D1:85:LEU:HD13	1.91	0.41
51:D5:41:PRO:O	51:D5:44:THR:OG1	2.36	0.41
25:DA:2557:G:H2'	25:DA:2558:C:H6	1.86	0.41
25:DA:2888:C:H2'	25:DA:2889:C:H6	1.86	0.41
25:DA:867:C:N4	25:DA:868:U:O4	2.54	0.41
29:DF:137:LYS:HA	29:DF:140:LEU:HB2	2.03	0.41
41:DV:40:LEU:HB2	41:DV:46:VAL:CG1	2.51	0.41
45:DZ:171:ILE:HD13	45:DZ:171:ILE:H	1.86	0.41
1:AA:1068:G:OP2	1:AA:1068:G:H8	2.04	0.40
1:AA:1517:G:H1'	25:BA:1941:A:O3'	2.21	0.40
1:AA:921:U:O4	61:AA:4075:HOH:O	2.21	0.40
8:AH:20:TYR:CE2	8:AH:76:PRO:HG2	2.56	0.40
24:AX:21:A:N6	24:AX:46:G:H2'	2.36	0.40
23:AY:5:G:C6	23:AY:6:G:C5	3.09	0.40
50:B4:28:LYS:HA	50:B4:29:PRO:HD3	1.84	0.40
25:BA:1257:G:N3	25:BA:1282:G:C2	2.89	0.40
25:BA:217:A:H8	25:BA:218:A:H5'	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2332:A:H2'	25:BA:2332:A:N3	2.36	0.40
25:BA:427:G:N7	61:BA:5129:HOH:O	2.37	0.40
25:BA:510:C:H2'	25:BA:511:C:H6	1.86	0.40
28:BE:174:ASP:OD1	28:BE:175:VAL:N	2.54	0.40
30:BG:60:LEU:HA	30:BG:60:LEU:HD12	1.89	0.40
25:BA:1445:C:OP1	43:BX:25:LYS:NZ	2.54	0.40
43:BX:41:ASN:O	43:BX:45:THR:HG23	2.21	0.40
1:CA:1179:A:H5''	9:CI:102:LEU:HD22	2.03	0.40
1:CA:1326:C:H2'	1:CA:1327:C:C6	2.56	0.40
1:CA:219:C:H2'	1:CA:220:G:O4'	2.22	0.40
1:CA:360:A:C6	1:CA:361:G:C6	3.08	0.40
1:CA:540:G:H2'	1:CA:541:G:O4'	2.21	0.40
1:CA:682:G:N7	61:CA:4142:HOH:O	2.37	0.40
1:CA:985:C:H2'	1:CA:986:A:C8	2.56	0.40
3:CC:119:ARG:O	3:CC:123:GLN:HG3	2.21	0.40
15:CO:69:TYR:CZ	15:CO:73:GLU:HG3	2.56	0.40
23:CY:9:A:C2'	23:CY:11:C:H41	2.34	0.40
50:D4:59:PHE:N	50:D4:59:PHE:HD1	2.14	0.40
25:DA:118:A:C8	25:DA:119:A:C8	3.09	0.40
25:DA:1453:U:O4	37:DR:67:LEU:HD21	2.21	0.40
25:DA:1557:C:H5''	25:DA:1558:A:OP2	2.21	0.40
25:DA:222:A:H5''	25:DA:421:U:OP1	2.21	0.40
25:DA:839:U:H2'	25:DA:840:C:H6	1.85	0.40
30:DG:111:LEU:CD2	30:DG:120:LEU:HD21	2.51	0.40
37:DR:28:LEU:HD23	37:DR:28:LEU:HA	1.91	0.40
40:DU:106:PHE:HA	40:DU:109:LEU:HD12	2.02	0.40
44:DY:20:TYR:CE1	44:DY:43:ASN:HA	2.56	0.40
1:AA:1022:G:H4'	1:AA:1022:G:OP1	2.21	0.40
1:AA:895:G:H2'	1:AA:896:C:C6	2.56	0.40
1:AA:990:C:N4	1:AA:991:U:O4	2.55	0.40
2:AB:21:ARG:HH21	2:AB:21:ARG:H	1.68	0.40
3:AC:50:ALA:HB1	3:AC:70:VAL:HG11	2.03	0.40
5:AE:90:VAL:O	5:AE:120:THR:HA	2.21	0.40
25:BA:1074:A:N6	25:BA:1171:G:H2'	2.36	0.40
25:BA:1110:C:H2'	25:BA:1111:U:O4'	2.20	0.40
25:BA:215:G:N2	25:BA:217:A:H62	2.16	0.40
25:BA:2549:U:H2'	25:BA:2550:C:C6	2.56	0.40
25:BA:354:A:H2	25:BA:1255:A:H2'	1.86	0.40
27:BD:38:LYS:HD2	27:BD:38:LYS:HA	1.92	0.40
29:BF:123:LEU:HD13	29:BF:192:LEU:HB3	2.03	0.40
34:BO:8:LEU:HB2	34:BO:19:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:BR:54:LEU:HD12	37:BR:54:LEU:HA	1.97	0.40
44:BY:65:ALA:HA	44:BY:66:PRO:HD3	1.93	0.40
1:CA:1190:G:HO2'	1:CA:1191:A:P	2.45	0.40
1:CA:390:C:H2'	1:CA:391:G:C8	2.56	0.40
1:CA:593:G:H2'	1:CA:594:G:O4'	2.22	0.40
1:CA:731:G:OP1	1:CA:766:A:H1'	2.21	0.40
1:CA:93:G:C6	1:CA:96:U:C4	3.10	0.40
2:CB:97:TRP:HE1	2:CB:173:ALA:HB2	1.86	0.40
3:CC:131:ARG:NE	3:CC:166:GLU:OE2	2.54	0.40
12:CL:54:LYS:HG2	12:CL:75:HIS:CD2	2.56	0.40
12:CL:88:GLY:O	12:CL:99:HIS:HD2	2.04	0.40
15:CO:18:PHE:CZ	15:CO:21:ASP:HB2	2.56	0.40
18:CR:33:ASP:OD2	18:CR:36:ASN:HB2	2.22	0.40
18:CR:44:LEU:HD23	18:CR:50:ILE:HA	2.03	0.40
24:CX:17:C:H2'	24:CX:17(A):U:C5	2.56	0.40
23:CY:9:A:H8	23:CY:11:C:N4	2.19	0.40
25:DA:1610:A:OP1	61:DA:4119:HOH:O	2.21	0.40
25:DA:1759:A:H1'	25:DA:2711:A:C2	2.56	0.40
25:DA:526:A:N3	25:DA:2044:C:H1'	2.36	0.40
25:DA:242:G:C8	54:D8:5:LYS:HG2	2.56	0.40
25:DA:2514:U:H2'	25:DA:2515:C:C6	2.56	0.40
30:DG:101:ILE:HG22	30:DG:105:LYS:HE2	2.03	0.40
30:DG:3:LEU:HD22	50:D4:25:TYR:CE2	2.56	0.40
31:DH:3:ARG:NH1	31:DH:5:GLY:H	2.20	0.40
25:DA:2404:C:O3'	35:DP:77:ARG:NH2	2.53	0.40
1:AA:77:G:C6	1:AA:78:G:C6	3.10	0.40
1:AA:857:C:H2'	1:AA:858:G:O4'	2.20	0.40
2:AB:44:LEU:HA	2:AB:47:THR:OG1	2.21	0.40
5:AE:71:LEU:HD21	5:AE:115:VAL:HG22	2.03	0.40
5:AE:24:ARG:HG2	5:AE:24:ARG:H	1.67	0.40
7:AG:65:ALA:O	7:AG:69:VAL:HG23	2.21	0.40
12:AL:83:VAL:HG23	12:AL:107:ALA:HB2	2.03	0.40
23:AY:36:A:C6	23:AY:37:MIA:C5	3.05	0.40
25:BA:2230:U:O2	47:B1:52:ARG:NH2	2.53	0.40
25:BA:1086:C:H2'	25:BA:1087:C:O4'	2.20	0.40
25:BA:2203:G:HO2'	25:BA:2204:G:P	2.45	0.40
25:BA:2357:G:N3	25:BA:2393:C:H2'	2.36	0.40
25:BA:388:A:H2'	25:BA:389:G:H8	1.81	0.40
25:BA:841:G:H2'	25:BA:842:C:C6	2.56	0.40
25:BA:943:C:C2	25:BA:944:C:C4	3.09	0.40
29:BF:129:PHE:CD1	29:BF:163:VAL:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BO:21:CYS:HB2	34:BO:39:ILE:HD12	2.02	0.40
38:BS:3:ARG:HH11	38:BS:3:ARG:HD2	1.75	0.40
40:BU:76:TYR:CE1	40:BU:80:ILE:HG13	2.56	0.40
1:CA:126:G:H4'	1:CA:634:C:O2	2.21	0.40
1:CA:1305:G:O2'	1:CA:1331:G:N2	2.53	0.40
1:CA:1325:C:O2'	1:CA:1326:C:H5'	2.21	0.40
1:CA:811:C:H4'	1:CA:900:A:N6	2.35	0.40
1:CA:952:U:H2'	1:CA:953:G:H8	1.86	0.40
2:CB:77:ALA:HA	2:CB:80:ILE:CG2	2.51	0.40
18:CR:33:ASP:CG	18:CR:36:ASN:HB2	2.42	0.40
19:CS:12:ASP:OD2	19:CS:14:HIS:NE2	2.55	0.40
30:DG:179:PRO:HB2	50:D4:42:PHE:HE1	1.85	0.40
30:DG:179:PRO:HG3	50:D4:43:TYR:CZ	2.56	0.40
35:DP:62:LEU:O	54:D8:13:ARG:HD3	2.22	0.40
25:DA:1031:G:H21	55:D9:36:GLN:HE22	1.69	0.40
25:DA:1856:G:H2'	25:DA:1857:G:O4'	2.21	0.40
25:DA:330:A:H2	25:DA:1210:A:H2'	1.85	0.40
27:DD:92:ILE:HD12	27:DD:104:TYR:CD1	2.56	0.40
29:DF:64:ILE:HD11	29:DF:75:HIS:HB2	2.03	0.40
25:DA:2305:A:H5''	30:DG:134:GLY:HA3	2.02	0.40
32:DI:116:LEU:HD12	32:DI:128:LEU:HD13	2.04	0.40
39:DT:28:VAL:HG13	39:DT:86:ILE:HG23	2.02	0.40
1:AA:1057:G:H2'	1:AA:1058:G:O4'	2.21	0.40
1:AA:118:U:H6	1:AA:118:U:O5'	2.04	0.40
1:AA:1241:G:H2'	1:AA:1242:C:C6	2.56	0.40
1:AA:1442:G:H3'	1:AA:1442:G:H8	1.86	0.40
1:AA:163:C:H2'	1:AA:164:U:O4'	2.21	0.40
1:AA:848:C:O2'	1:AA:849:C:H5'	2.22	0.40
1:AA:877:C:H5''	8:AH:88:LYS:HD3	2.03	0.40
1:AA:918:A:H2'	1:AA:919:A:O4'	2.21	0.40
2:AB:160:ASP:O	2:AB:183:PRO:HD2	2.21	0.40
2:AB:84:GLU:OE1	2:AB:216:SER:HA	2.21	0.40
4:AD:170:VAL:HG13	4:AD:174:LEU:HB2	2.04	0.40
4:AD:187:ARG:NH1	4:AD:193:ASP:OD2	2.40	0.40
15:AO:26:GLU:OE2	15:AO:77:ARG:NE	2.54	0.40
15:AO:68:ARG:O	15:AO:71:GLN:HB3	2.21	0.40
25:BA:1073:A:C6	25:BA:1172:A:C4	3.09	0.40
25:BA:1405:A:C2	25:BA:1418:U:O4	2.74	0.40
25:BA:1440:U:H2'	25:BA:1441:A:O4'	2.22	0.40
25:BA:2665:U:H2'	25:BA:2666:A:C8	2.56	0.40
25:BA:266:C:H2'	25:BA:267:C:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:637:U:H5'	25:BA:640:A:N6	2.35	0.40
25:BA:718:C:H2'	25:BA:719:C:C6	2.57	0.40
27:BD:69:ARG:C	27:BD:71:ASP:H	2.24	0.40
25:BA:589:U:H5''	35:BP:29:LYS:HE3	2.04	0.40
1:CA:1004:A:H2'	1:CA:1038:C:H1'	2.03	0.40
1:CA:1327:C:O2'	1:CA:1328:C:H5'	2.21	0.40
1:CA:266:G:H8	1:CA:266:G:H2'	1.71	0.40
1:CA:943:U:H2'	1:CA:944:G:H5'	2.02	0.40
3:CC:164:ARG:HG2	3:CC:165:THR:H	1.86	0.40
7:CG:125:MET:HE2	61:CG:5101:HOH:O	2.20	0.40
7:CG:50:ILE:HD11	7:CG:58:PRO:HB3	2.03	0.40
2:CB:179:LYS:HA	8:CH:72:PRO:HG3	2.04	0.40
13:CM:84:ILE:HG22	19:CS:65:ASN:HB2	2.04	0.40
50:D4:48:ARG:HD3	50:D4:48:ARG:HA	1.69	0.40
25:DA:1843:C:H5'	27:DD:253:GLN:NE2	2.36	0.40
25:DA:2070:G:H2'	25:DA:2071:A:O4'	2.21	0.40
25:DA:2184:G:O2'	25:DA:2185:C:H5'	2.21	0.40
25:DA:2821:A:H2'	25:DA:2822:G:C8	2.57	0.40
25:DA:288:C:H2'	25:DA:289:A:C8	2.57	0.40
25:DA:57:C:H2'	25:DA:58:G:O4'	2.21	0.40
25:DA:918:A:N3	26:DB:80:U:O2'	2.50	0.40
35:DP:126:VAL:HG12	35:DP:148:LEU:HD23	2.03	0.40
1:CA:1442(A):G:C8	39:DT:118:ARG:HG2	2.57	0.40
41:DV:89:GLN:HA	41:DV:90:PRO:HD3	1.91	0.40
45:DZ:100:VAL:HA	45:DZ:101:PRO:HD3	1.91	0.40
1:AA:1182:G:C4'	1:AA:1183:A:H5'	2.44	0.40
1:AA:1504:G:OP1	1:AA:1507:A:H4'	2.22	0.40
1:AA:580:U:H2'	1:AA:581:G:O4'	2.21	0.40
2:AB:200:ILE:HD13	2:AB:200:ILE:H	1.86	0.40
17:AQ:50:LYS:HD2	17:AQ:51:TYR:CE1	2.57	0.40
48:B2:53:LEU:HD23	48:B2:53:LEU:HA	1.77	0.40
50:B4:40:HIS:HB3	50:B4:43:TYR:CD1	2.56	0.40
25:BA:1071:G:H3'	25:BA:1072:U:H5'	2.04	0.40
25:BA:1587:U:H2'	25:BA:1588:G:O4'	2.22	0.40
25:BA:2045:G:H4'	25:BA:2629:C:O3'	2.21	0.40
25:BA:2134:G:C6	25:BA:2135:U:C2	3.09	0.40
27:BD:166:GLN:HB2	27:BD:174:ILE:HG22	2.03	0.40
27:BD:142:VAL:HG13	27:BD:191:ALA:HB1	2.02	0.40
30:BG:45:GLU:H	30:BG:45:GLU:HG2	1.49	0.40
39:BT:16:ARG:HD2	39:BT:18:ASP:OD1	2.21	0.40
43:BX:44:GLU:HG2	43:BX:49:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BZ:146:ILE:HA	45:BZ:147:GLY:HA2	1.65	0.40
1:CA:1032:G:H8	1:CA:1032:G:OP2	2.04	0.40
1:CA:1051:C:H2'	1:CA:1052:U:H6	1.86	0.40
1:CA:1119:C:OP1	9:CI:83:ARG:NH2	2.54	0.40
2:CB:49:GLU:O	2:CB:52:GLU:HB3	2.21	0.40
24:CX:5:G:H1	24:CX:68:C:N4	2.18	0.40
50:D4:62:ARG:HB3	50:D4:63:TYR:CD2	2.56	0.40
52:D6:18:ARG:HD2	52:D6:42:TRP:CD1	2.57	0.40
54:D8:23:VAL:CG1	54:D8:47:LYS:HD3	2.52	0.40
25:DA:1789:A:H2'	25:DA:1790:C:O4'	2.21	0.40
25:DA:207:A:H2'	25:DA:208:C:O4'	2.22	0.40
25:DA:2107:C:H42	25:DA:2182:G:H1	1.69	0.40
25:DA:2143:C:C2	25:DA:2144:U:H1'	2.57	0.40
25:DA:2149:G:C6	25:DA:2150:U:O2	2.74	0.40
25:DA:2136:C:N4	25:DA:2155:G:N1	2.69	0.40
25:DA:2494:G:C4	25:DA:2495:G:C8	3.10	0.40
25:DA:271(H):G:O2'	25:DA:271(I):G:C8	2.70	0.40
25:DA:580:C:H2'	25:DA:581:C:H6	1.87	0.40
25:DA:812:C:H2'	25:DA:813:U:H6	1.86	0.40
25:DA:836:G:C5	25:DA:837:C:C4	3.09	0.40
25:DA:848:G:C4	25:DA:933:A:H8	2.40	0.40
28:DE:119:ARG:HB3	28:DE:120:TRP:CD1	2.56	0.40
25:DA:2094:G:P	32:DI:22:LYS:HD2	2.61	0.40
38:DS:38:GLN:HE21	38:DS:47:THR:HG1	1.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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
2	AB	229/256 (90%)	204 (89%)	19 (8%)	6 (3%)	5 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CB	229/256 (90%)	201 (88%)	16 (7%)	12 (5%)	2	1
3	AC	204/239 (85%)	189 (93%)	14 (7%)	1 (0%)	29	41
3	CC	204/239 (85%)	188 (92%)	13 (6%)	3 (2%)	10	14
4	AD	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	29	41
4	CD	206/209 (99%)	201 (98%)	5 (2%)	0	100	100
5	AE	146/162 (90%)	140 (96%)	3 (2%)	3 (2%)	7	8
5	CE	146/162 (90%)	140 (96%)	5 (3%)	1 (1%)	22	32
6	AF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
6	CF	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
7	AG	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
7	CG	153/156 (98%)	144 (94%)	7 (5%)	2 (1%)	12	17
8	AH	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
8	CH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
9	AI	125/128 (98%)	114 (91%)	8 (6%)	3 (2%)	6	6
9	CI	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	19	29
10	AJ	95/105 (90%)	85 (90%)	7 (7%)	3 (3%)	4	3
10	CJ	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	7	8
11	AK	112/129 (87%)	108 (96%)	2 (2%)	2 (2%)	8	10
11	CK	112/129 (87%)	108 (96%)	2 (2%)	2 (2%)	8	10
12	AL	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
12	CL	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
13	AM	121/126 (96%)	116 (96%)	5 (4%)	0	100	100
13	CM	120/126 (95%)	114 (95%)	4 (3%)	2 (2%)	9	11
14	AN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
14	CN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
15	AO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
15	CO	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	13	19
16	AP	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	12	17
16	CP	80/88 (91%)	78 (98%)	1 (1%)	1 (1%)	12	17
17	AQ	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
17	CQ	97/105 (92%)	96 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
18	CR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
19	AS	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
19	CS	81/93 (87%)	74 (91%)	6 (7%)	1 (1%)	13	19
20	AT	94/106 (89%)	87 (93%)	4 (4%)	3 (3%)	4	3
20	CT	94/106 (89%)	87 (93%)	2 (2%)	5 (5%)	2	1
21	AU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	CU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
27	BD	273/276 (99%)	264 (97%)	8 (3%)	1 (0%)	34	48
27	DD	273/276 (99%)	265 (97%)	7 (3%)	1 (0%)	34	48
28	BE	202/206 (98%)	198 (98%)	3 (2%)	1 (0%)	29	41
28	DE	202/206 (98%)	196 (97%)	4 (2%)	2 (1%)	15	23
29	BF	201/210 (96%)	199 (99%)	1 (0%)	1 (0%)	29	41
29	DF	201/210 (96%)	198 (98%)	1 (0%)	2 (1%)	15	23
30	BG	179/182 (98%)	168 (94%)	11 (6%)	0	100	100
30	DG	179/182 (98%)	167 (93%)	10 (6%)	2 (1%)	14	20
31	BH	172/180 (96%)	166 (96%)	6 (4%)	0	100	100
31	DH	172/180 (96%)	165 (96%)	7 (4%)	0	100	100
32	BI	144/148 (97%)	128 (89%)	12 (8%)	4 (3%)	5	4
32	DI	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	22	32
33	BN	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
33	DN	138/140 (99%)	136 (99%)	1 (1%)	1 (1%)	22	32
34	BO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
34	DO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
35	BP	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	22	32
35	DP	147/150 (98%)	138 (94%)	6 (4%)	3 (2%)	7	9
36	BQ	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
36	DQ	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	32
37	BR	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
37	DR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
38	BS	108/112 (96%)	106 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DS	108/112 (96%)	106 (98%)	1 (1%)	1 (1%)	17	25
39	BT	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	19	29
39	DT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
40	BU	114/118 (97%)	114 (100%)	0	0	100	100
40	DU	114/118 (97%)	114 (100%)	0	0	100	100
41	BV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	23
41	DV	99/101 (98%)	97 (98%)	1 (1%)	1 (1%)	15	23
42	BW	110/113 (97%)	110 (100%)	0	0	100	100
42	DW	110/113 (97%)	110 (100%)	0	0	100	100
43	BX	93/96 (97%)	92 (99%)	1 (1%)	0	100	100
43	DX	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	14	20
44	BY	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
44	DY	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
45	BZ	148/206 (72%)	140 (95%)	6 (4%)	2 (1%)	11	15
45	DZ	156/206 (76%)	149 (96%)	6 (4%)	1 (1%)	25	36
46	B0	81/85 (95%)	80 (99%)	0	1 (1%)	13	19
46	D0	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
47	B1	95/98 (97%)	94 (99%)	0	1 (1%)	14	20
47	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	20
48	B2	68/72 (94%)	67 (98%)	0	1 (2%)	10	14
48	D2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
49	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
49	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
50	B4	67/71 (94%)	57 (85%)	4 (6%)	6 (9%)	1	0
50	D4	67/71 (94%)	55 (82%)	6 (9%)	6 (9%)	1	0
51	B5	57/60 (95%)	57 (100%)	0	0	100	100
51	D5	57/60 (95%)	57 (100%)	0	0	100	100
52	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
52	D6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
53	B7	46/49 (94%)	46 (100%)	0	0	100	100
53	D7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	6	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	B8	62/65 (95%)	62 (100%)	0	0	100	100
54	D8	62/65 (95%)	62 (100%)	0	0	100	100
55	B9	35/37 (95%)	35 (100%)	0	0	100	100
55	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11372/12128 (94%)	10883 (96%)	387 (3%)	102 (1%)	17	25

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	16	HIS
2	AB	17	PHE
9	AI	54	ASP
27	BD	275	LYS
45	BZ	159	PRO
47	B1	3	LYS
50	B4	47	GLN
2	CB	10	LEU
2	CB	16	HIS
2	CB	20	GLU
2	CB	21	ARG
2	CB	121	LEU
2	CB	126	GLU
7	CG	80	VAL
9	CI	54	ASP
13	CM	5	ALA
20	CT	10	LEU
20	CT	95	ALA
28	DE	52	LEU
28	DE	73	GLU
29	DF	21	ALA
29	DF	130	ALA
30	DG	81	LYS
36	DQ	28	ALA
50	D4	45	GLY
50	D4	49	PHE
50	D4	60	GLN
53	D7	46	VAL
4	AD	5	ILE
5	AE	85	GLY
9	AI	51	ARG

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Mol	Chain	Res	Type
11	AK	105	VAL
16	AP	53	VAL
20	AT	100	ILE
29	BF	130	ALA
32	BI	106	GLY
45	BZ	152	ALA
46	B0	13	GLY
48	B2	69	ARG
50	B4	54	GLY
50	B4	56	VAL
2	CB	8	LYS
2	CB	17	PHE
2	CB	234	PRO
7	CG	7	ALA
30	DG	47	LYS
32	DI	10	GLU
35	DP	45	LEU
50	D4	54	GLY
2	AB	20	GLU
2	AB	231	GLU
10	AJ	78	ASN
10	AJ	79	ARG
11	AK	49	GLY
28	BE	52	LEU
39	BT	37	GLY
50	B4	45	GLY
3	CC	181	ASN
10	CJ	78	ASN
11	CK	49	GLY
16	CP	53	VAL
20	CT	99	LEU
20	CT	102	GLY
33	DN	2	LYS
43	DX	2	LYS
50	D4	62	ARG
2	AB	126	GLU
10	AJ	77	PRO
20	AT	102	GLY
32	BI	11	ASN
32	BI	73	GLU
50	B4	48	ARG
2	CB	123	ALA

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Mol	Chain	Res	Type
3	CC	91	LEU
10	CJ	77	PRO
11	CK	105	VAL
15	CO	88	ARG
35	DP	38	GLN
41	DV	79	VAL
50	D4	46	GLN
3	AC	66	VAL
5	AE	86	ALA
9	AI	48	GLU
20	AT	9	ASN
32	BI	107	VAL
35	BP	122	PRO
41	BV	79	VAL
50	B4	57	GLU
20	CT	100	ILE
27	DD	3	VAL
38	DS	84	GLN
47	D1	3	LYS
5	AE	69	VAL
2	CB	128	GLU
2	CB	231	GLU
19	CS	29	ARG
35	DP	122	PRO
5	CE	69	VAL
3	CC	108	ASN
45	DZ	165	VAL
13	CM	4	ILE

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	
2	AB	192/220 (87%)	170 (88%)	22 (12%)	5	7
2	CB	187/220 (85%)	158 (84%)	29 (16%)	2	3
3	AC	142/188 (76%)	128 (90%)	14 (10%)	8	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	CC	140/188 (74%)	125 (89%)	15 (11%)	6	9
4	AD	169/181 (93%)	154 (91%)	15 (9%)	9	14
4	CD	173/181 (96%)	158 (91%)	15 (9%)	10	15
5	AE	113/123 (92%)	103 (91%)	10 (9%)	10	15
5	CE	114/123 (93%)	101 (89%)	13 (11%)	5	7
6	AF	84/90 (93%)	77 (92%)	7 (8%)	11	17
6	CF	85/90 (94%)	77 (91%)	8 (9%)	8	13
7	AG	119/127 (94%)	106 (89%)	13 (11%)	6	8
7	CG	120/127 (94%)	102 (85%)	18 (15%)	3	3
8	AH	114/119 (96%)	106 (93%)	8 (7%)	15	24
8	CH	114/119 (96%)	100 (88%)	14 (12%)	4	6
9	AI	90/99 (91%)	77 (86%)	13 (14%)	3	3
9	CI	89/99 (90%)	74 (83%)	15 (17%)	2	2
10	AJ	66/92 (72%)	62 (94%)	4 (6%)	18	30
10	CJ	69/92 (75%)	64 (93%)	5 (7%)	14	23
11	AK	82/99 (83%)	79 (96%)	3 (4%)	34	53
11	CK	83/99 (84%)	81 (98%)	2 (2%)	49	68
12	AL	97/109 (89%)	92 (95%)	5 (5%)	23	38
12	CL	97/109 (89%)	92 (95%)	5 (5%)	23	38
13	AM	93/101 (92%)	81 (87%)	12 (13%)	4	5
13	CM	92/101 (91%)	80 (87%)	12 (13%)	4	4
14	AN	49/50 (98%)	36 (74%)	13 (26%)	0	0
14	CN	49/50 (98%)	39 (80%)	10 (20%)	1	1
15	AO	78/80 (98%)	71 (91%)	7 (9%)	9	14
15	CO	78/80 (98%)	68 (87%)	10 (13%)	4	5
16	AP	69/74 (93%)	59 (86%)	10 (14%)	3	3
16	CP	68/74 (92%)	63 (93%)	5 (7%)	13	22
17	AQ	94/97 (97%)	84 (89%)	10 (11%)	6	9
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	17	28
18	AR	59/77 (77%)	52 (88%)	7 (12%)	5	6
18	CR	59/77 (77%)	54 (92%)	5 (8%)	10	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	AS	69/80 (86%)	63 (91%)	6 (9%)	10	15
19	CS	67/80 (84%)	61 (91%)	6 (9%)	9	14
20	AT	70/82 (85%)	62 (89%)	8 (11%)	5	7
20	CT	70/82 (85%)	63 (90%)	7 (10%)	7	11
21	AU	18/22 (82%)	16 (89%)	2 (11%)	6	8
21	CU	18/22 (82%)	15 (83%)	3 (17%)	2	2
27	BD	215/218 (99%)	204 (95%)	11 (5%)	24	39
27	DD	215/218 (99%)	201 (94%)	14 (6%)	17	27
28	BE	164/166 (99%)	149 (91%)	15 (9%)	9	14
28	DE	164/166 (99%)	147 (90%)	17 (10%)	7	10
29	BF	160/166 (96%)	145 (91%)	15 (9%)	8	13
29	DF	159/166 (96%)	144 (91%)	15 (9%)	8	13
30	BG	144/156 (92%)	128 (89%)	16 (11%)	6	8
30	DG	143/156 (92%)	119 (83%)	24 (17%)	2	2
31	BH	144/148 (97%)	136 (94%)	8 (6%)	21	34
31	DH	144/148 (97%)	129 (90%)	15 (10%)	7	10
32	BI	113/124 (91%)	96 (85%)	17 (15%)	3	3
32	DI	105/124 (85%)	88 (84%)	17 (16%)	2	3
33	BN	118/119 (99%)	107 (91%)	11 (9%)	9	13
33	DN	118/119 (99%)	106 (90%)	12 (10%)	7	10
34	BO	100/100 (100%)	94 (94%)	6 (6%)	19	31
34	DO	100/100 (100%)	97 (97%)	3 (3%)	41	61
35	BP	115/116 (99%)	102 (89%)	13 (11%)	6	8
35	DP	115/116 (99%)	106 (92%)	9 (8%)	12	19
36	BQ	111/111 (100%)	101 (91%)	10 (9%)	9	14
36	DQ	111/111 (100%)	101 (91%)	10 (9%)	9	14
37	BR	101/101 (100%)	87 (86%)	14 (14%)	3	4
37	DR	101/101 (100%)	88 (87%)	13 (13%)	4	5
38	BS	86/88 (98%)	78 (91%)	8 (9%)	9	13
38	DS	85/88 (97%)	76 (89%)	9 (11%)	6	9
39	BT	115/127 (91%)	108 (94%)	7 (6%)	18	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	DT	113/127 (89%)	105 (93%)	8 (7%)	14	23
40	BU	93/94 (99%)	86 (92%)	7 (8%)	13	21
40	DU	93/94 (99%)	88 (95%)	5 (5%)	22	36
41	BV	80/82 (98%)	71 (89%)	9 (11%)	6	8
41	DV	80/82 (98%)	71 (89%)	9 (11%)	6	8
42	BW	90/92 (98%)	85 (94%)	5 (6%)	21	34
42	DW	90/92 (98%)	84 (93%)	6 (7%)	16	26
43	BX	77/78 (99%)	75 (97%)	2 (3%)	46	66
43	DX	77/78 (99%)	74 (96%)	3 (4%)	32	50
44	BY	85/91 (93%)	76 (89%)	9 (11%)	6	9
44	DY	85/91 (93%)	76 (89%)	9 (11%)	6	9
45	BZ	135/179 (75%)	119 (88%)	16 (12%)	5	6
45	DZ	137/179 (76%)	123 (90%)	14 (10%)	7	10
46	B0	65/67 (97%)	62 (95%)	3 (5%)	27	43
46	D0	65/67 (97%)	62 (95%)	3 (5%)	27	43
47	B1	80/83 (96%)	71 (89%)	9 (11%)	6	8
47	D1	80/83 (96%)	72 (90%)	8 (10%)	7	11
48	B2	65/67 (97%)	60 (92%)	5 (8%)	13	20
48	D2	65/67 (97%)	60 (92%)	5 (8%)	13	20
49	B3	51/52 (98%)	48 (94%)	3 (6%)	19	32
49	D3	50/52 (96%)	45 (90%)	5 (10%)	7	11
50	B4	59/63 (94%)	49 (83%)	10 (17%)	2	2
50	D4	53/63 (84%)	39 (74%)	14 (26%)	0	0
51	B5	50/52 (96%)	46 (92%)	4 (8%)	12	18
51	D5	50/52 (96%)	45 (90%)	5 (10%)	7	11
52	B6	51/52 (98%)	48 (94%)	3 (6%)	19	32
52	D6	50/52 (96%)	49 (98%)	1 (2%)	55	74
53	B7	41/42 (98%)	36 (88%)	5 (12%)	5	6
53	D7	41/42 (98%)	38 (93%)	3 (7%)	14	22
54	B8	54/55 (98%)	49 (91%)	5 (9%)	9	13
54	D8	54/55 (98%)	52 (96%)	2 (4%)	34	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
55	B9	34/34 (100%)	33 (97%)	1 (3%)	42 62
55	D9	34/34 (100%)	33 (97%)	1 (3%)	42 62
All	All	9306/10066 (92%)	8408 (90%)	898 (10%)	8 12

All (898) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	8	LYS
2	AB	16	HIS
2	AB	21	ARG
2	AB	24	TRP
2	AB	94	ASN
2	AB	96	ARG
2	AB	111	ARG
2	AB	114	ARG
2	AB	127	ILE
2	AB	128	GLU
2	AB	153	ARG
2	AB	155	LEU
2	AB	156	LYS
2	AB	169	LYS
2	AB	170	GLU
2	AB	185	ILE
2	AB	187	LEU
2	AB	195	ASP
2	AB	200	ILE
2	AB	208	ILE
2	AB	217	ARG
2	AB	221	LEU
3	AC	3	ASN
3	AC	15	THR
3	AC	37	GLN
3	AC	45	LYS
3	AC	54	ARG
3	AC	70	VAL
3	AC	104	GLN
3	AC	115	LEU
3	AC	119	ARG
3	AC	131	ARG
3	AC	178	LEU
3	AC	182	ILE

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Mol	Chain	Res	Type
3	AC	195	VAL
3	AC	207	VAL
4	AD	3	ARG
4	AD	5	ILE
4	AD	15	GLU
4	AD	31	CYS
4	AD	45	GLN
4	AD	50	ARG
4	AD	58	LEU
4	AD	61	LYS
4	AD	135	LEU
4	AD	141	ARG
4	AD	157	LEU
4	AD	158	ILE
4	AD	170	VAL
4	AD	182	LYS
4	AD	194	LEU
5	AE	10	MET
5	AE	24	ARG
5	AE	31	LEU
5	AE	38	GLN
5	AE	41	VAL
5	AE	47	LYS
5	AE	51	VAL
5	AE	57	LYS
5	AE	78	HIS
5	AE	91	LEU
6	AF	10	LEU
6	AF	24	GLU
6	AF	69	GLU
6	AF	70	ASP
6	AF	74	ASP
6	AF	75	LEU
6	AF	82	ARG
7	AG	12	LEU
7	AG	13	GLN
7	AG	21	VAL
7	AG	50	ILE
7	AG	51	GLN
7	AG	63	LYS
7	AG	72	ARG
7	AG	73	MET

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Mol	Chain	Res	Type
7	AG	76	ARG
7	AG	78	ARG
7	AG	104	LEU
7	AG	113	GLU
7	AG	114	ARG
8	AH	21	LYS
8	AH	39	LEU
8	AH	52	ASP
8	AH	63	LEU
8	AH	77	GLU
8	AH	78	GLN
8	AH	97	VAL
8	AH	112	LEU
9	AI	3	GLN
9	AI	23	ASN
9	AI	26	VAL
9	AI	27	THR
9	AI	42	ARG
9	AI	50	LEU
9	AI	56	LEU
9	AI	65	VAL
9	AI	66	ARG
9	AI	83	ARG
9	AI	112	LYS
9	AI	127	LYS
9	AI	128	ARG
10	AJ	5	ARG
10	AJ	21	GLN
10	AJ	89	ASP
10	AJ	96	ILE
11	AK	16	SER
11	AK	31	THR
11	AK	48	ILE
12	AL	27	LEU
12	AL	33	ARG
12	AL	34	ARG
12	AL	53	ARG
12	AL	83	VAL
13	AM	3	ARG
13	AM	4	ILE
13	AM	11	ARG
13	AM	15	VAL

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Mol	Chain	Res	Type
13	AM	19	LEU
13	AM	32	GLU
13	AM	70	LEU
13	AM	73	GLU
13	AM	102	ARG
13	AM	109	THR
13	AM	110	ARG
13	AM	121	LYS
14	AN	3	ARG
14	AN	6	LEU
14	AN	7	ILE
14	AN	13	THR
14	AN	15	LYS
14	AN	18	VAL
14	AN	23	ARG
14	AN	29	ARG
14	AN	33	VAL
14	AN	35	ARG
14	AN	41	ARG
14	AN	44	LEU
14	AN	50	LYS
15	AO	3	ILE
15	AO	5	LYS
15	AO	26	GLU
15	AO	38	ARG
15	AO	39	LEU
15	AO	48	LYS
15	AO	83	GLU
16	AP	2	VAL
16	AP	19	ILE
16	AP	20	VAL
16	AP	21	VAL
16	AP	45	THR
16	AP	50	LYS
16	AP	54	GLU
16	AP	60	LEU
16	AP	62	VAL
16	AP	67	THR
17	AQ	9	VAL
17	AQ	14	LYS
17	AQ	50	LYS
17	AQ	52	LYS

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Mol	Chain	Res	Type
17	AQ	63	ARG
17	AQ	68	ARG
17	AQ	91	ARG
17	AQ	92	ARG
17	AQ	98	LEU
17	AQ	100	LYS
18	AR	26	LEU
18	AR	29	PHE
18	AR	31	LEU
18	AR	32	ARG
18	AR	41	LYS
18	AR	76	LEU
18	AR	84	LYS
19	AS	5	LEU
19	AS	28	LYS
19	AS	37	ARG
19	AS	41	VAL
19	AS	63	THR
19	AS	65	ASN
20	AT	8	ARG
20	AT	10	LEU
20	AT	13	LEU
20	AT	24	LEU
20	AT	45	GLN
20	AT	56	MET
20	AT	84	LEU
20	AT	90	GLN
21	AU	10	ARG
21	AU	15	ARG
27	BD	3	VAL
27	BD	32	SER
27	BD	61	LEU
27	BD	94	LEU
27	BD	155	LEU
27	BD	211	ARG
27	BD	221	VAL
27	BD	229	VAL
27	BD	242	ARG
27	BD	259	THR
27	BD	260	ARG
28	BE	21	VAL
28	BE	24	THR

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Mol	Chain	Res	Type
28	BE	47	VAL
28	BE	73	GLU
28	BE	75	VAL
28	BE	77	ILE
28	BE	78	LEU
28	BE	82	ARG
28	BE	111	ARG
28	BE	116	VAL
28	BE	119	ARG
28	BE	144	ARG
28	BE	175	VAL
28	BE	181	LEU
28	BE	195	LEU
29	BF	19	GLU
29	BF	33	LEU
29	BF	53	THR
29	BF	57	VAL
29	BF	70	THR
29	BF	106	ARG
29	BF	110	LEU
29	BF	125	LEU
29	BF	132	VAL
29	BF	140	LEU
29	BF	170	LEU
29	BF	175	THR
29	BF	183	VAL
29	BF	192	LEU
29	BF	200	GLU
30	BG	7	LEU
30	BG	31	VAL
30	BG	43	LEU
30	BG	45	GLU
30	BG	49	ASP
30	BG	51	ARG
30	BG	81	LYS
30	BG	82	LEU
30	BG	91	ARG
30	BG	137	GLU
30	BG	140	ILE
30	BG	143	GLU
30	BG	148	MET
30	BG	150	ASP

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Mol	Chain	Res	Type
30	BG	159	VAL
30	BG	170	ARG
31	BH	6	ARG
31	BH	15	VAL
31	BH	23	ARG
31	BH	59	ARG
31	BH	69	ARG
31	BH	71	LEU
31	BH	124	GLU
31	BH	129	THR
32	BI	5	LEU
32	BI	9	LEU
32	BI	10	GLU
32	BI	20	ASP
32	BI	38	LEU
32	BI	43	ASN
32	BI	47	LEU
32	BI	50	ARG
32	BI	61	ARG
32	BI	68	LEU
32	BI	77	LEU
32	BI	78	THR
32	BI	85	GLU
32	BI	103	ARG
32	BI	109	ILE
32	BI	114	LEU
32	BI	140	LEU
33	BN	28	THR
33	BN	33	LEU
33	BN	34	LEU
33	BN	48	MET
33	BN	61	ARG
33	BN	62	VAL
33	BN	67	LEU
33	BN	68	GLU
33	BN	87	LEU
33	BN	99	LEU
33	BN	120	LEU
34	BO	8	LEU
34	BO	23	ARG
34	BO	24	VAL
34	BO	69	ILE

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Mol	Chain	Res	Type
34	BO	108	GLU
34	BO	113	LYS
35	BP	3	LEU
35	BP	7	ARG
35	BP	15	ARG
35	BP	55	ARG
35	BP	59	LEU
35	BP	95	VAL
35	BP	98	GLU
35	BP	101	VAL
35	BP	106	LEU
35	BP	112	LEU
35	BP	125	VAL
35	BP	148	LEU
35	BP	149	GLU
36	BQ	1	MET
36	BQ	7	MET
36	BQ	16	ARG
36	BQ	38	GLU
36	BQ	45	GLN
36	BQ	54	MET
36	BQ	59	ARG
36	BQ	60	ARG
36	BQ	109	VAL
36	BQ	110	THR
37	BR	1	MET
37	BR	18	LEU
37	BR	24	GLN
37	BR	28	LEU
37	BR	29	LEU
37	BR	33	ARG
37	BR	36	THR
37	BR	44	LEU
37	BR	54	LEU
37	BR	65	LEU
37	BR	67	LEU
37	BR	75	LEU
37	BR	79	LEU
37	BR	111	LEU
38	BS	12	PHE
38	BS	14	VAL
38	BS	25	ARG

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Mol	Chain	Res	Type
38	BS	46	VAL
38	BS	57	LYS
38	BS	75	GLU
38	BS	83	LYS
38	BS	110	LEU
39	BT	6	LEU
39	BT	13	ARG
39	BT	49	VAL
39	BT	53	ARG
39	BT	96	ARG
39	BT	108	ARG
39	BT	118	ARG
40	BU	8	VAL
40	BU	36	ARG
40	BU	59	ARG
40	BU	74	LEU
40	BU	95	LEU
40	BU	104	GLN
40	BU	108	GLU
41	BV	18	LEU
41	BV	43	GLU
41	BV	46	VAL
41	BV	51	VAL
41	BV	52	VAL
41	BV	62	LEU
41	BV	72	VAL
41	BV	95	LEU
41	BV	100	ARG
42	BW	11	ARG
42	BW	17	VAL
42	BW	19	LEU
42	BW	51	LEU
42	BW	107	LEU
43	BX	1	MET
43	BX	57	LEU
44	BY	1	MET
44	BY	7	VAL
44	BY	23	ARG
44	BY	43	ASN
44	BY	55	TYR
44	BY	72	VAL
44	BY	90	LEU

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Mol	Chain	Res	Type
44	BY	91	GLU
44	BY	99	CYS
45	BZ	1	MET
45	BZ	18	LEU
45	BZ	46	LYS
45	BZ	72	ARG
45	BZ	86	VAL
45	BZ	91	LEU
45	BZ	92	SER
45	BZ	119	GLU
45	BZ	122	ARG
45	BZ	135	GLU
45	BZ	136	PHE
45	BZ	148	ASP
45	BZ	154	ASP
45	BZ	155	LEU
45	BZ	170	THR
45	BZ	171	ILE
46	B0	11	ARG
46	B0	20	ARG
46	B0	55	ARG
47	B1	3	LYS
47	B1	30	VAL
47	B1	40	ARG
47	B1	52	ARG
47	B1	59	THR
47	B1	75	GLU
47	B1	81	LYS
47	B1	89	GLU
47	B1	95	LEU
48	B2	28	LYS
48	B2	32	LEU
48	B2	40	SER
48	B2	52	ASP
48	B2	70	GLN
49	B3	8	LEU
49	B3	23	LEU
49	B3	54	VAL
50	B4	1	MET
50	B4	13	ARG
50	B4	27	THR
50	B4	34	GLU

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Mol	Chain	Res	Type
50	B4	50	VAL
50	B4	56	VAL
50	B4	58	ARG
50	B4	63	TYR
50	B4	66	SER
50	B4	68	ARG
51	B5	6	VAL
51	B5	16	ARG
51	B5	29	THR
51	B5	40	LYS
52	B6	4	GLU
52	B6	14	THR
52	B6	48	VAL
53	B7	1	MET
53	B7	24	THR
53	B7	43	THR
53	B7	46	VAL
53	B7	48	LYS
54	B8	6	THR
54	B8	23	VAL
54	B8	31	HIS
54	B8	32	LEU
54	B8	46	ARG
55	B9	17	ILE
2	CB	7	VAL
2	CB	8	LYS
2	CB	10	LEU
2	CB	15	VAL
2	CB	23	ARG
2	CB	24	TRP
2	CB	28	PHE
2	CB	48	MET
2	CB	71	VAL
2	CB	76	GLN
2	CB	81	VAL
2	CB	87	ARG
2	CB	94	ASN
2	CB	96	ARG
2	CB	97	TRP
2	CB	115	LEU
2	CB	124	SER
2	CB	126	GLU

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Mol	Chain	Res	Type
2	CB	127	ILE
2	CB	155	LEU
2	CB	157	ARG
2	CB	163	PHE
2	CB	185	ILE
2	CB	187	LEU
2	CB	195	ASP
2	CB	200	ILE
2	CB	215	LEU
2	CB	217	ARG
2	CB	222	ILE
3	CC	3	ASN
3	CC	8	ILE
3	CC	15	THR
3	CC	36	ASP
3	CC	45	LYS
3	CC	54	ARG
3	CC	70	VAL
3	CC	85	ARG
3	CC	102	ASN
3	CC	104	GLN
3	CC	108	ASN
3	CC	115	LEU
3	CC	131	ARG
3	CC	152	ILE
3	CC	196	LEU
4	CD	8	VAL
4	CD	19	LEU
4	CD	31	CYS
4	CD	34	GLU
4	CD	47	ARG
4	CD	58	LEU
4	CD	61	LYS
4	CD	108	LEU
4	CD	135	LEU
4	CD	141	ARG
4	CD	150	GLU
4	CD	157	LEU
4	CD	170	VAL
4	CD	182	LYS
4	CD	194	LEU
5	CE	13	ILE

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Mol	Chain	Res	Type
5	CE	24	ARG
5	CE	31	LEU
5	CE	38	GLN
5	CE	41	VAL
5	CE	47	LYS
5	CE	51	VAL
5	CE	57	LYS
5	CE	60	TYR
5	CE	71	LEU
5	CE	78	HIS
5	CE	79	GLU
5	CE	150	ARG
6	CF	21	LEU
6	CF	28	ARG
6	CF	41	GLU
6	CF	69	GLU
6	CF	70	ASP
6	CF	74	ASP
6	CF	75	LEU
6	CF	82	ARG
7	CG	9	VAL
7	CG	10	ARG
7	CG	13	GLN
7	CG	31	MET
7	CG	41	ARG
7	CG	51	GLN
7	CG	52	GLU
7	CG	73	MET
7	CG	76	ARG
7	CG	78	ARG
7	CG	79	ARG
7	CG	90	GLU
7	CG	98	SER
7	CG	104	LEU
7	CG	113	GLU
7	CG	114	ARG
7	CG	136	LYS
7	CG	155	ARG
8	CH	23	SER
8	CH	25	ASP
8	CH	29	SER
8	CH	42	GLU

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Mol	Chain	Res	Type
8	CH	51	VAL
8	CH	52	ASP
8	CH	63	LEU
8	CH	68	ARG
8	CH	78	GLN
8	CH	84	ARG
8	CH	97	VAL
8	CH	98	LYS
8	CH	112	LEU
8	CH	127	LEU
9	CI	3	GLN
9	CI	23	ASN
9	CI	27	THR
9	CI	42	ARG
9	CI	50	LEU
9	CI	56	LEU
9	CI	65	VAL
9	CI	81	ILE
9	CI	83	ARG
9	CI	89	ASN
9	CI	102	LEU
9	CI	108	VAL
9	CI	112	LYS
9	CI	121	ARG
9	CI	128	ARG
10	CJ	9	ARG
10	CJ	16	LEU
10	CJ	21	GLN
10	CJ	33	GLN
10	CJ	70	ARG
11	CK	54	ARG
11	CK	103	LEU
12	CL	18	VAL
12	CL	33	ARG
12	CL	37	CYS
12	CL	53	ARG
12	CL	83	VAL
13	CM	11	ARG
13	CM	15	VAL
13	CM	17	VAL
13	CM	19	LEU
13	CM	32	GLU

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Mol	Chain	Res	Type
13	CM	34	LEU
13	CM	48	LEU
13	CM	50	GLU
13	CM	98	VAL
13	CM	110	ARG
13	CM	117	VAL
13	CM	121	LYS
14	CN	3	ARG
14	CN	6	LEU
14	CN	7	ILE
14	CN	12	ARG
14	CN	22	THR
14	CN	23	ARG
14	CN	29	ARG
14	CN	33	VAL
14	CN	41	ARG
14	CN	44	LEU
15	CO	3	ILE
15	CO	5	LYS
15	CO	10	LYS
15	CO	26	GLU
15	CO	38	ARG
15	CO	39	LEU
15	CO	41	GLU
15	CO	54	ARG
15	CO	71	GLN
15	CO	83	GLU
16	CP	2	VAL
16	CP	21	VAL
16	CP	45	THR
16	CP	60	LEU
16	CP	62	VAL
17	CQ	9	VAL
17	CQ	36	ILE
17	CQ	49	GLU
17	CQ	63	ARG
17	CQ	86	GLU
17	CQ	91	ARG
18	CR	26	LEU
18	CR	37	VAL
18	CR	41	LYS
18	CR	76	LEU

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Mol	Chain	Res	Type
18	CR	84	LYS
19	CS	5	LEU
19	CS	27	GLU
19	CS	37	ARG
19	CS	41	VAL
19	CS	65	ASN
19	CS	77	THR
20	CT	24	LEU
20	CT	36	LEU
20	CT	43	LEU
20	CT	45	GLN
20	CT	56	MET
20	CT	80	ARG
20	CT	90	GLN
21	CU	10	ARG
21	CU	12	LYS
21	CU	24	ARG
27	DD	13	ARG
27	DD	32	SER
27	DD	54	ARG
27	DD	61	LEU
27	DD	94	LEU
27	DD	122	ASP
27	DD	134	ARG
27	DD	142	VAL
27	DD	155	LEU
27	DD	211	ARG
27	DD	242	ARG
27	DD	260	ARG
27	DD	275	LYS
27	DD	276	LYS
28	DE	12	THR
28	DE	21	VAL
28	DE	24	THR
28	DE	40	GLU
28	DE	52	LEU
28	DE	73	GLU
28	DE	75	VAL
28	DE	77	ILE
28	DE	78	LEU
28	DE	82	ARG
28	DE	111	ARG

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Mol	Chain	Res	Type
28	DE	116	VAL
28	DE	119	ARG
28	DE	144	ARG
28	DE	154	LYS
28	DE	175	VAL
28	DE	181	LEU
29	DF	19	GLU
29	DF	24	LEU
29	DF	33	LEU
29	DF	57	VAL
29	DF	70	THR
29	DF	106	ARG
29	DF	108	LYS
29	DF	110	LEU
29	DF	120	GLU
29	DF	127	GLU
29	DF	135	LYS
29	DF	140	LEU
29	DF	170	LEU
29	DF	183	VAL
29	DF	192	LEU
30	DG	5	VAL
30	DG	21	ARG
30	DG	43	LEU
30	DG	45	GLU
30	DG	49	ASP
30	DG	51	ARG
30	DG	60	LEU
30	DG	91	ARG
30	DG	111	LEU
30	DG	115	ARG
30	DG	124	SER
30	DG	128	ARG
30	DG	135	LEU
30	DG	136	ARG
30	DG	140	ILE
30	DG	143	GLU
30	DG	148	MET
30	DG	150	ASP
30	DG	156	ASP
30	DG	159	VAL
30	DG	162	THR

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Mol	Chain	Res	Type
30	DG	170	ARG
30	DG	175	LEU
30	DG	181	ARG
31	DH	2	SER
31	DH	3	ARG
31	DH	27	LYS
31	DH	51	ARG
31	DH	59	ARG
31	DH	69	ARG
31	DH	71	LEU
31	DH	76	VAL
31	DH	88	LEU
31	DH	98	LEU
31	DH	116	GLU
31	DH	124	GLU
31	DH	125	VAL
31	DH	136	ILE
31	DH	139	GLN
32	DI	20	ASP
32	DI	41	GLU
32	DI	43	ASN
32	DI	44	LEU
32	DI	47	LEU
32	DI	57	ARG
32	DI	61	ARG
32	DI	73	GLU
32	DI	75	LEU
32	DI	76	THR
32	DI	77	LEU
32	DI	104	GLN
32	DI	108	THR
32	DI	114	LEU
32	DI	121	LYS
32	DI	123	LEU
32	DI	140	LEU
33	DN	28	THR
33	DN	33	LEU
33	DN	34	LEU
33	DN	46	VAL
33	DN	48	MET
33	DN	62	VAL
33	DN	87	LEU

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Mol	Chain	Res	Type
33	DN	99	LEU
33	DN	104	LYS
33	DN	120	LEU
33	DN	137	LYS
33	DN	139	GLU
34	DO	8	LEU
34	DO	69	ILE
34	DO	108	GLU
35	DP	15	ARG
35	DP	45	LEU
35	DP	55	ARG
35	DP	65	ARG
35	DP	95	VAL
35	DP	99	LEU
35	DP	112	LEU
35	DP	125	VAL
35	DP	149	GLU
36	DQ	1	MET
36	DQ	2	LEU
36	DQ	7	MET
36	DQ	11	LYS
36	DQ	21	THR
36	DQ	22	LYS
36	DQ	45	GLN
36	DQ	56	ARG
36	DQ	60	ARG
36	DQ	110	THR
37	DR	1	MET
37	DR	15	SER
37	DR	18	LEU
37	DR	28	LEU
37	DR	29	LEU
37	DR	33	ARG
37	DR	36	THR
37	DR	44	LEU
37	DR	54	LEU
37	DR	65	LEU
37	DR	75	LEU
37	DR	79	LEU
37	DR	111	LEU
38	DS	12	PHE
38	DS	14	VAL

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Mol	Chain	Res	Type
38	DS	25	ARG
38	DS	35	ILE
38	DS	57	LYS
38	DS	58	LEU
38	DS	75	GLU
38	DS	80	LEU
38	DS	110	LEU
39	DT	6	LEU
39	DT	13	ARG
39	DT	16	ARG
39	DT	17	THR
39	DT	49	VAL
39	DT	96	ARG
39	DT	113	LYS
39	DT	118	ARG
40	DU	36	ARG
40	DU	74	LEU
40	DU	83	LEU
40	DU	92	ARG
40	DU	104	GLN
41	DV	6	LYS
41	DV	15	GLU
41	DV	46	VAL
41	DV	51	VAL
41	DV	52	VAL
41	DV	62	LEU
41	DV	72	VAL
41	DV	95	LEU
41	DV	100	ARG
42	DW	11	ARG
42	DW	17	VAL
42	DW	19	LEU
42	DW	51	LEU
42	DW	60	ASN
42	DW	107	LEU
43	DX	23	GLU
43	DX	57	LEU
43	DX	90	GLU
44	DY	1	MET
44	DY	11	ASP
44	DY	21	LYS
44	DY	23	ARG

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Mol	Chain	Res	Type
44	DY	43	ASN
44	DY	72	VAL
44	DY	91	GLU
44	DY	99	CYS
44	DY	107	ASP
45	DZ	11	GLU
45	DZ	18	LEU
45	DZ	33	LEU
45	DZ	50	GLN
45	DZ	97	GLU
45	DZ	131	ARG
45	DZ	132	ASN
45	DZ	136	PHE
45	DZ	141	VAL
45	DZ	145	GLU
45	DZ	148	ASP
45	DZ	154	ASP
45	DZ	170	THR
45	DZ	171	ILE
46	D0	11	ARG
46	D0	20	ARG
46	D0	77	ARG
47	D1	3	LYS
47	D1	40	ARG
47	D1	52	ARG
47	D1	69	LYS
47	D1	76	ARG
47	D1	85	LEU
47	D1	89	GLU
47	D1	95	LEU
48	D2	28	LYS
48	D2	32	LEU
48	D2	44	LEU
48	D2	53	LEU
48	D2	70	GLN
49	D3	3	ARG
49	D3	23	LEU
49	D3	30	ARG
49	D3	32	GLN
49	D3	54	VAL
50	D4	1	MET
50	D4	8	LYS

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Mol	Chain	Res	Type
50	D4	13	ARG
50	D4	27	THR
50	D4	34	GLU
50	D4	37	SER
50	D4	48	ARG
50	D4	50	VAL
50	D4	58	ARG
50	D4	59	PHE
50	D4	62	ARG
50	D4	63	TYR
50	D4	68	ARG
50	D4	69	LYS
51	D5	6	VAL
51	D5	16	ARG
51	D5	29	THR
51	D5	40	LYS
51	D5	48	GLU
52	D6	14	THR
53	D7	1	MET
53	D7	14	LYS
53	D7	41	ARG
54	D8	23	VAL
54	D8	32	LEU
55	D9	17	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	16	HIS
2	AB	40	HIS
2	AB	76	GLN
2	AB	78	GLN
2	AB	94	ASN
3	AC	6	HIS
3	AC	28	GLN
3	AC	37	GLN
3	AC	102	ASN
3	AC	104	GLN
3	AC	136	GLN
3	AC	162	GLN
3	AC	181	ASN
4	AD	77	ASN

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Mol	Chain	Res	Type
4	AD	123	HIS
4	AD	125	HIS
4	AD	161	ASN
5	AE	38	GLN
5	AE	73	ASN
5	AE	78	HIS
5	AE	141	GLN
6	AF	73	ASN
6	AF	100	ASN
7	AG	28	ASN
7	AG	97	GLN
9	AI	23	ASN
9	AI	58	HIS
9	AI	89	ASN
9	AI	124	GLN
10	AJ	21	GLN
10	AJ	56	HIS
12	AL	78	GLN
12	AL	99	HIS
15	AO	28	GLN
17	AQ	16	GLN
19	AS	23	ASN
19	AS	65	ASN
19	AS	69	HIS
19	AS	83	HIS
20	AT	75	ASN
20	AT	90	GLN
27	BD	164	GLN
27	BD	253	GLN
28	BE	121	ASN
29	BF	69	HIS
29	BF	169	ASN
29	BF	203	GLN
30	BG	40	ASN
32	BI	43	ASN
35	BP	38	GLN
36	BQ	12	GLN
36	BQ	57	HIS
37	BR	71	GLN
39	BT	123	GLN
43	BX	31	HIS
43	BX	82	GLN

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Mol	Chain	Res	Type
44	BY	6	HIS
44	BY	43	ASN
45	BZ	32	HIS
48	B2	38	GLN
48	B2	70	GLN
50	B4	46	GLN
50	B4	60	GLN
55	B9	36	GLN
2	CB	78	GLN
2	CB	95	GLN
3	CC	6	HIS
3	CC	28	GLN
3	CC	98	ASN
3	CC	102	ASN
3	CC	104	GLN
3	CC	118	GLN
3	CC	136	GLN
4	CD	77	ASN
4	CD	123	HIS
4	CD	125	HIS
4	CD	161	ASN
5	CE	38	GLN
5	CE	73	ASN
5	CE	141	GLN
6	CF	13	ASN
6	CF	100	ASN
7	CG	28	ASN
7	CG	51	GLN
7	CG	97	GLN
7	CG	109	ASN
8	CH	78	GLN
9	CI	23	ASN
9	CI	58	HIS
9	CI	89	ASN
9	CI	124	GLN
10	CJ	13	HIS
10	CJ	33	GLN
12	CL	78	GLN
12	CL	99	HIS
13	CM	77	ASN
13	CM	92	HIS
15	CO	28	GLN

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Mol	Chain	Res	Type
17	CQ	16	GLN
19	CS	23	ASN
19	CS	47	HIS
19	CS	65	ASN
19	CS	69	HIS
20	CT	9	ASN
20	CT	75	ASN
20	CT	90	GLN
27	DD	87	ASN
27	DD	164	GLN
27	DD	253	GLN
28	DE	143	ASN
29	DF	69	HIS
29	DF	169	ASN
29	DF	203	GLN
30	DG	132	ASN
32	DI	43	ASN
32	DI	104	GLN
32	DI	133	HIS
33	DN	38	HIS
33	DN	133	GLN
35	DP	38	GLN
36	DQ	13	GLN
36	DQ	45	GLN
36	DQ	57	HIS
36	DQ	123	HIS
37	DR	71	GLN
38	DS	38	GLN
39	DT	43	GLN
39	DT	123	GLN
41	DV	64	HIS
43	DX	31	HIS
43	DX	82	GLN
44	DY	43	ASN
45	DZ	50	GLN
48	D2	38	GLN
55	D9	36	GLN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1494/1521 (98%)	297 (19%)	24 (1%)
1	CA	1501/1521 (98%)	306 (20%)	23 (1%)
22	AV	12/24 (50%)	2 (16%)	0
22	CV	12/24 (50%)	1 (8%)	0
23	AW	71/76 (93%)	30 (42%)	2 (2%)
23	AY	71/76 (93%)	29 (40%)	1 (1%)
23	CW	68/76 (89%)	27 (39%)	1 (1%)
23	CY	69/76 (90%)	28 (40%)	3 (4%)
24	AX	75/77 (97%)	15 (20%)	1 (1%)
24	CX	75/77 (97%)	16 (21%)	1 (1%)
25	BA	2864/2915 (98%)	446 (15%)	39 (1%)
25	DA	2791/2915 (95%)	485 (17%)	29 (1%)
26	BB	120/121 (99%)	19 (15%)	1 (0%)
26	DB	119/121 (98%)	20 (16%)	1 (0%)
All	All	9342/9620 (97%)	1721 (18%)	126 (1%)

All (1721) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	51	A
1	AA	61	G
1	AA	79	G
1	AA	91	C
1	AA	92	C
1	AA	96	U
1	AA	97	G
1	AA	101	A
1	AA	111	G
1	AA	115	G
1	AA	116	A
1	AA	121	C
1	AA	131	C
1	AA	144	G
1	AA	155	C

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Mol	Chain	Res	Type
1	AA	156	G
1	AA	157	G
1	AA	158	G
1	AA	163	C
1	AA	172	A
1	AA	174	C
1	AA	179	A
1	AA	180	U
1	AA	182	U
1	AA	186	C
1	AA	189	G
1	AA	189(D)	C
1	AA	195	A
1	AA	197	A
1	AA	201	C
1	AA	202	U
1	AA	203	U
1	AA	204	U
1	AA	216	G
1	AA	217	C
1	AA	226	G
1	AA	247	G
1	AA	251	G
1	AA	258	G
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	301	G
1	AA	321	A
1	AA	328	C
1	AA	332	G
1	AA	347	G
1	AA	348	G
1	AA	352	C
1	AA	353	A
1	AA	354	G
1	AA	355	C
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	381	C
1	AA	384	G

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Mol	Chain	Res	Type
1	AA	397	A
1	AA	398	C
1	AA	406	G
1	AA	412	A
1	AA	414	A
1	AA	424	G
1	AA	426	G
1	AA	429	U
1	AA	430	A
1	AA	441	A
1	AA	442	C
1	AA	443	C
1	AA	452	A
1	AA	461	A
1	AA	470	C
1	AA	471	G
1	AA	477	A
1	AA	484	G
1	AA	485	G
1	AA	496	A
1	AA	498	U
1	AA	505	G
1	AA	509	A
1	AA	510	A
1	AA	511	C
1	AA	518	C
1	AA	521	G
1	AA	524	G
1	AA	527	G
1	AA	528	C
1	AA	531	U
1	AA	532	A
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	561	U
1	AA	572	A
1	AA	573	A
1	AA	576	G
1	AA	577	G
1	AA	590	C
1	AA	592	G

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Mol	Chain	Res	Type
1	AA	596	C
1	AA	599	C
1	AA	619	U
1	AA	627	G
1	AA	630	G
1	AA	631	G
1	AA	637	G
1	AA	639	G
1	AA	653	A
1	AA	660	G
1	AA	665	A
1	AA	673	G
1	AA	687	A
1	AA	688	G
1	AA	695	A
1	AA	723	U
1	AA	724	G
1	AA	731	G
1	AA	749	C
1	AA	752	G
1	AA	755	G
1	AA	759	A
1	AA	773	G
1	AA	774	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	815	A
1	AA	817	C
1	AA	821	G
1	AA	828	A
1	AA	840	C
1	AA	841	U
1	AA	851	G
1	AA	859	A
1	AA	874	G
1	AA	902	G
1	AA	913	A
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	931	C

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Mol	Chain	Res	Type
1	AA	934	C
1	AA	936	C
1	AA	960	U
1	AA	961	U
1	AA	968	A
1	AA	969	A
1	AA	971	G
1	AA	972	C
1	AA	974	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	982	U
1	AA	989	C
1	AA	992	U
1	AA	993	G
1	AA	996	A
1	AA	998	G
1	AA	1000	U
1	AA	1001(A)	G
1	AA	1003	G
1	AA	1004	A
1	AA	1005	A
1	AA	1006	C
1	AA	1008	C
1	AA	1009	G
1	AA	1011	G
1	AA	1020	U
1	AA	1021	G
1	AA	1022	G
1	AA	1023	G
1	AA	1024	G
1	AA	1025	U
1	AA	1026	G
1	AA	1027	C
1	AA	1028	C
1	AA	1029	C
1	AA	1030	C
1	AA	1030(A)	G
1	AA	1030(B)	C
1	AA	1030(D)	A
1	AA	1032	G

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Mol	Chain	Res	Type
1	AA	1033	G
1	AA	1035	A
1	AA	1036	G
1	AA	1037	C
1	AA	1039	C
1	AA	1044	A
1	AA	1046	A
1	AA	1052	U
1	AA	1054	C
1	AA	1064	G
1	AA	1065	U
1	AA	1066	C
1	AA	1067	A
1	AA	1068	G
1	AA	1081	G
1	AA	1085	U
1	AA	1089	G
1	AA	1094	G
1	AA	1095	U
1	AA	1097	C
1	AA	1101	A
1	AA	1104	G
1	AA	1108	G
1	AA	1110	A
1	AA	1111	A
1	AA	1123	A
1	AA	1130	A
1	AA	1132	C
1	AA	1134	G
1	AA	1135	U
1	AA	1136	U
1	AA	1137	C
1	AA	1138	G
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1146	A
1	AA	1151	A
1	AA	1152	A
1	AA	1154	G
1	AA	1157	A
1	AA	1158	C

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Mol	Chain	Res	Type
1	AA	1159	U
1	AA	1161	C
1	AA	1165	C
1	AA	1166	G
1	AA	1183	A
1	AA	1184	G
1	AA	1196	U
1	AA	1197	G
1	AA	1202	G
1	AA	1212	U
1	AA	1213	A
1	AA	1222	G
1	AA	1224	G
1	AA	1227	A
1	AA	1228	C
1	AA	1238	A
1	AA	1240	U
1	AA	1250	A
1	AA	1256	A
1	AA	1257	U
1	AA	1258	G
1	AA	1269	A
1	AA	1270	C
1	AA	1273	G
1	AA	1276	G
1	AA	1278	U
1	AA	1279	A
1	AA	1280	A
1	AA	1281	U
1	AA	1282	C
1	AA	1286	A
1	AA	1287	A
1	AA	1299	A
1	AA	1300	G
1	AA	1302	U
1	AA	1305	G
1	AA	1317	C
1	AA	1320	C
1	AA	1338	G
1	AA	1340	A
1	AA	1347	G
1	AA	1353	G

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Mol	Chain	Res	Type
1	AA	1358	U
1	AA	1363	C
1	AA	1394	A
1	AA	1397	C
1	AA	1419	G
1	AA	1442	G
1	AA	1442(A)	G
1	AA	1446	U
1	AA	1447	A
1	AA	1452	C
1	AA	1456	G
1	AA	1475	G
1	AA	1492	A
1	AA	1493	A
1	AA	1502	A
1	AA	1503	A
1	AA	1504	G
1	AA	1506	U
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1531	A
1	AA	1532	U
22	AV	13	A
22	AV	24	A
23	AW	2	C
23	AW	3	C
23	AW	4	C
23	AW	6	G
23	AW	8	4SU
23	AW	9	A
23	AW	12	U
23	AW	19	G
23	AW	20	U
23	AW	21	A
23	AW	22	G
23	AW	24	G
23	AW	25	C
23	AW	27	G
23	AW	29	G
23	AW	34	G
23	AW	45	U

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Mol	Chain	Res	Type
23	AW	46	7MG
23	AW	47	U
23	AW	48	C
23	AW	49	C
23	AW	50	U
23	AW	61	C
23	AW	62	C
23	AW	63	G
23	AW	64	A
23	AW	68	C
23	AW	70	G
23	AW	73	A
23	AW	74	C
24	AX	9	G
24	AX	16	C
24	AX	18	G
24	AX	19	G
24	AX	20	U
24	AX	21	A
24	AX	31	G
24	AX	46	G
24	AX	48	C
24	AX	50	U
24	AX	56	C
24	AX	64	G
24	AX	67	C
24	AX	68	C
24	AX	76	A
23	AY	3	C
23	AY	5	G
23	AY	9	A
23	AY	11	C
23	AY	13	C
23	AY	15	G
23	AY	19	G
23	AY	20	U
23	AY	21	A
23	AY	23	A
23	AY	25	C
23	AY	34	G
23	AY	44	G
23	AY	45	U

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Mol	Chain	Res	Type
23	AY	46	7MG
23	AY	47	U
23	AY	48	C
23	AY	49	C
23	AY	54	5MU
23	AY	56	C
23	AY	57	G
23	AY	59	U
23	AY	61	C
23	AY	62	C
23	AY	65	G
23	AY	68	C
23	AY	69	G
23	AY	70	G
23	AY	73	A
25	BA	12	U
25	BA	13	A
25	BA	34	C
25	BA	45	C
25	BA	54	G
25	BA	57	G
25	BA	60	G
25	BA	70	A
25	BA	73	A
25	BA	74	G
25	BA	83	A
25	BA	91	G
25	BA	94	G
25	BA	116	A
25	BA	117	A
25	BA	118	U
25	BA	138	G
25	BA	162	G
25	BA	170	A
25	BA	185	A
25	BA	194	G
25	BA	203	G
25	BA	204	G
25	BA	205	A
25	BA	211	A
25	BA	218	A
25	BA	222	A

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Mol	Chain	Res	Type
25	BA	237	G
25	BA	265	U
25	BA	267	C
25	BA	271	U
25	BA	272	U
25	BA	273	G
25	BA	274	U
25	BA	275	C
25	BA	279	G
25	BA	289	G
25	BA	294	C
25	BA	299	G
25	BA	303	C
25	BA	306	A
25	BA	335	A
25	BA	351	G
25	BA	353	G
25	BA	354	A
25	BA	376	G
25	BA	387	G
25	BA	389	G
25	BA	397	G
25	BA	399	G
25	BA	407	U
25	BA	413	G
25	BA	423	G
25	BA	432	U
25	BA	438	G
25	BA	455	A
25	BA	470	C
25	BA	474	U
25	BA	477	C
25	BA	482	C
25	BA	483	A
25	BA	496	A
25	BA	507	G
25	BA	530	A
25	BA	534	C
25	BA	555	G
25	BA	556	C
25	BA	557	A
25	BA	558	G

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Mol	Chain	Res	Type
25	BA	569	G
25	BA	573	G
25	BA	586	G
25	BA	596	G
25	BA	598	A
25	BA	609	A
25	BA	615	G
25	BA	626	A
25	BA	627	G
25	BA	630	U
25	BA	639	G
25	BA	641	G
25	BA	642	G
25	BA	652	A
25	BA	662	A
25	BA	670	C
25	BA	671	A
25	BA	692	C
25	BA	693	G
25	BA	697	C
25	BA	716	G
25	BA	733	G
25	BA	764	G
25	BA	777	C
25	BA	811	A
25	BA	821	A
25	BA	822	G
25	BA	823	G
25	BA	829	A
25	BA	830	A
25	BA	831	A
25	BA	832	G
25	BA	837	C
25	BA	839	G
25	BA	852	G
25	BA	859	C
25	BA	866	A
25	BA	874	U
25	BA	875	U
25	BA	877	G
25	BA	906	G
25	BA	913	A

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Mol	Chain	Res	Type
25	BA	924	U
25	BA	925	A
25	BA	926	G
25	BA	927	G
25	BA	930	G
25	BA	931	C
25	BA	932	C
25	BA	933	C
25	BA	934	A
25	BA	935	C
25	BA	936	C
25	BA	937	A
25	BA	939	C
25	BA	941	U
25	BA	942	A
25	BA	943	C
25	BA	944	C
25	BA	945	A
25	BA	953	U
25	BA	956	A
25	BA	977	G
25	BA	986	A
25	BA	990	A
25	BA	991	G
25	BA	1004	A
25	BA	1006	C
25	BA	1008	U
25	BA	1019	G
25	BA	1020	C
25	BA	1029	A
25	BA	1042	A
25	BA	1058	U
25	BA	1059	C
25	BA	1068	G
25	BA	1072	U
25	BA	1079	U
25	BA	1087	C
25	BA	1092	A
25	BA	1093	G
25	BA	1094	A
25	BA	1097	G
25	BA	1099	C

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Mol	Chain	Res	Type
25	BA	1100	A
25	BA	1104	G
25	BA	1109	G
25	BA	1114	G
25	BA	1116	A
25	BA	1117	G
25	BA	1118	C
25	BA	1119	A
25	BA	1121	C
25	BA	1122	C
25	BA	1124	U
25	BA	1125	C
25	BA	1129	U
25	BA	1134	A
25	BA	1136	U
25	BA	1138	C
25	BA	1139	G
25	BA	1140	U
25	BA	1141	A
25	BA	1142	A
25	BA	1143	U
25	BA	1144	A
25	BA	1145	G
25	BA	1146	C
25	BA	1147	U
25	BA	1155	C
25	BA	1156	G
25	BA	1158	G
25	BA	1161	G
25	BA	1162	C
25	BA	1174	A
25	BA	1180	C
25	BA	1181	G
25	BA	1196	C
25	BA	1216	G
25	BA	1217	G
25	BA	1218	G
25	BA	1219	A
25	BA	1220	U
25	BA	1221	G
25	BA	1222	A
25	BA	1223	C

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Mol	Chain	Res	Type
25	BA	1255	A
25	BA	1256	U
25	BA	1265	A
25	BA	1287	A
25	BA	1290	G
25	BA	1299	A
25	BA	1302	G
25	BA	1317	G
25	BA	1318	A
25	BA	1319	U
25	BA	1327	G
25	BA	1346	U
25	BA	1347	A
25	BA	1349	G
25	BA	1391	C
25	BA	1398	U
25	BA	1405	A
25	BA	1406	A
25	BA	1411	A
25	BA	1416	C
25	BA	1430	A
25	BA	1431	G
25	BA	1432	C
25	BA	1441	A
25	BA	1462	G
25	BA	1463	C
25	BA	1466	U
25	BA	1467	G
25	BA	1474	C
25	BA	1491	A
25	BA	1497	G
25	BA	1502	G
25	BA	1506	G
25	BA	1508	G
25	BA	1514	C
25	BA	1518	A
25	BA	1529	G
25	BA	1540	A
25	BA	1554	A
25	BA	1555	C
25	BA	1556	A
25	BA	1557	A

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Mol	Chain	Res	Type
25	BA	1561	C
25	BA	1571	G
25	BA	1578	C
25	BA	1601	A
25	BA	1605	A
25	BA	1616	A
25	BA	1625	U
25	BA	1627	A
25	BA	1628	G
25	BA	1631	C
25	BA	1632	A
25	BA	1654	A
25	BA	1656	A
25	BA	1659	G
25	BA	1695	C
25	BA	1701	A
25	BA	1721	G
25	BA	1743	G
25	BA	1747	A
25	BA	1748	A
25	BA	1750	G
25	BA	1767	A
25	BA	1768	U
25	BA	1776	G
25	BA	1777	G
25	BA	1781	G
25	BA	1787	G
25	BA	1793	A
25	BA	1794	G
25	BA	1795	G
25	BA	1804	A
25	BA	1811	A
25	BA	1813	C
25	BA	1817	A
25	BA	1822	A
25	BA	1831	C
25	BA	1847	G
25	BA	1848	G
25	BA	1859	G
25	BA	1860	A
25	BA	1870	G
25	BA	1878	A

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Mol	Chain	Res	Type
25	BA	1879	A
25	BA	1889	G
25	BA	1899	A
25	BA	1900	G
25	BA	1911	A
25	BA	1922	A
25	BA	1928	G
25	BA	1951	G
25	BA	1952	G
25	BA	1959	A
25	BA	1960	A
25	BA	1977	U
25	BA	1985	U
25	BA	1989	C
25	BA	1992	A
25	BA	1993	A
25	BA	1994	A
25	BA	2014	G
25	BA	2015	U
25	BA	2019	G
25	BA	2042	A
25	BA	2045	G
25	BA	2053	A
25	BA	2054	G
25	BA	2055	A
25	BA	2065	C
25	BA	2077	C
25	BA	2078	G
25	BA	2082	A
25	BA	2083	G
25	BA	2084	A
25	BA	2091	G
25	BA	2124	U
25	BA	2132	G
25	BA	2134	G
25	BA	2135	U
25	BA	2136	A
25	BA	2138	G
25	BA	2141	A
25	BA	2143	G
25	BA	2144	U
25	BA	2149	G

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Mol	Chain	Res	Type
25	BA	2150	C
25	BA	2153	G
25	BA	2154	U
25	BA	2155	G
25	BA	2156	A
25	BA	2157	A
25	BA	2160	C
25	BA	2162	C
25	BA	2164	C
25	BA	2166	U
25	BA	2168	C
25	BA	2177	G
25	BA	2178	G
25	BA	2179	G
25	BA	2180	A
25	BA	2181	G
25	BA	2182	G
25	BA	2187	G
25	BA	2188	G
25	BA	2189	U
25	BA	2193	A
25	BA	2194	U
25	BA	2195	A
25	BA	2196	C
25	BA	2200	C
25	BA	2202	U
25	BA	2203	G
25	BA	2204	G
25	BA	2206	G
25	BA	2210	C
25	BA	2212	G
25	BA	2214	G
25	BA	2220	A
25	BA	2227	G
25	BA	2228	G
25	BA	2229	A
25	BA	2237	A
25	BA	2247	G
25	BA	2250	G
25	BA	2251	G
25	BA	2280	A
25	BA	2281	A

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Mol	Chain	Res	Type
25	BA	2287	C
25	BA	2295	C
25	BA	2299	A
25	BA	2301	G
25	BA	2317	A
25	BA	2320	G
25	BA	2324	U
25	BA	2332	A
25	BA	2337	G
25	BA	2346	G
25	BA	2348	A
25	BA	2359	C
25	BA	2362	C
25	BA	2373	A
25	BA	2395	G
25	BA	2397	C
25	BA	2418	U
25	BA	2422	G
25	BA	2436	C
25	BA	2437	A
25	BA	2441	G
25	BA	2442	A
25	BA	2447	A
25	BA	2451	A
25	BA	2453	C
25	BA	2460	A
25	BA	2480	G
25	BA	2486	C
25	BA	2488	A
25	BA	2503	U
25	BA	2510	C
25	BA	2514	G
25	BA	2517	G
25	BA	2518	U
25	BA	2530	A
25	BA	2541	G
25	BA	2566	U
25	BA	2578	A
25	BA	2579	G
25	BA	2585	C
25	BA	2594	G
25	BA	2614	A

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Mol	Chain	Res	Type
25	BA	2621	U
25	BA	2623	U
25	BA	2624	C
25	BA	2641	A
25	BA	2642	G
25	BA	2653	G
25	BA	2681	G
25	BA	2682	A
25	BA	2701	U
25	BA	2702	C
25	BA	2703	C
25	BA	2715	C
25	BA	2725	A
25	BA	2726	A
25	BA	2739	U
25	BA	2746	A
25	BA	2770	A
25	BA	2771	A
25	BA	2774	G
25	BA	2777	A
25	BA	2778	A
25	BA	2782	C
25	BA	2791	A
25	BA	2803	A
25	BA	2804	C
25	BA	2806	G
25	BA	2807	C
25	BA	2813	G
25	BA	2814	C
25	BA	2816	G
25	BA	2817	G
25	BA	2828	G
25	BA	2830	A
25	BA	2831	A
25	BA	2845	A
25	BA	2882	G
25	BA	2886	G
25	BA	2890	C
25	BA	2901	A
25	BA	2903	G
25	BA	2904	U
26	BB	2	C

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Mol	Chain	Res	Type
26	BB	7	G
26	BB	13	A
26	BB	15	A
26	BB	17	C
26	BB	20	C
26	BB	25	A
26	BB	32	C
26	BB	40	U
26	BB	42	C
26	BB	56	G
26	BB	57	A
26	BB	65	C
26	BB	67	G
26	BB	73	A
26	BB	84	C
26	BB	106	G
26	BB	110	G
26	BB	120	A
1	CA	6	G
1	CA	9	G
1	CA	22	G
1	CA	31	G
1	CA	32	A
1	CA	39	G
1	CA	47	C
1	CA	48	C
1	CA	51	A
1	CA	66	G
1	CA	73	G
1	CA	78	G
1	CA	79	G
1	CA	80	G
1	CA	88	A
1	CA	89	C
1	CA	91	C
1	CA	92	C
1	CA	96	U
1	CA	101	A
1	CA	111	G
1	CA	116	A
1	CA	121	C
1	CA	131	C

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Mol	Chain	Res	Type
1	CA	138	G
1	CA	142	G
1	CA	144	G
1	CA	155	C
1	CA	156	G
1	CA	163	C
1	CA	166	G
1	CA	172	A
1	CA	174	C
1	CA	179	A
1	CA	180	U
1	CA	182	U
1	CA	186	C
1	CA	189	G
1	CA	189(D)	C
1	CA	195	A
1	CA	197	A
1	CA	201	C
1	CA	202	U
1	CA	203	U
1	CA	204	U
1	CA	216	G
1	CA	226	G
1	CA	247	G
1	CA	251	G
1	CA	258	G
1	CA	266	G
1	CA	267	C
1	CA	289	G
1	CA	321	A
1	CA	328	C
1	CA	332	G
1	CA	344	A
1	CA	345	C
1	CA	352	C
1	CA	353	A
1	CA	354	G
1	CA	355	C
1	CA	367	U
1	CA	372	C
1	CA	373	A
1	CA	381	C

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Mol	Chain	Res	Type
1	CA	384	G
1	CA	397	A
1	CA	398	C
1	CA	406	G
1	CA	412	A
1	CA	414	A
1	CA	424	G
1	CA	426	G
1	CA	429	U
1	CA	430	A
1	CA	439	A
1	CA	441	A
1	CA	442	C
1	CA	443	C
1	CA	452	A
1	CA	461	A
1	CA	470	C
1	CA	471	G
1	CA	477	A
1	CA	484	G
1	CA	485	G
1	CA	496	A
1	CA	498	U
1	CA	505	G
1	CA	509	A
1	CA	510	A
1	CA	511	C
1	CA	518	C
1	CA	521	G
1	CA	524	G
1	CA	528	C
1	CA	531	U
1	CA	532	A
1	CA	533	A
1	CA	547	A
1	CA	559	A
1	CA	561	U
1	CA	572	A
1	CA	573	A
1	CA	576	G
1	CA	577	G
1	CA	590	C

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Mol	Chain	Res	Type
1	CA	592	G
1	CA	596	C
1	CA	599	C
1	CA	619	U
1	CA	627	G
1	CA	630	G
1	CA	631	G
1	CA	637	G
1	CA	639	G
1	CA	650	G
1	CA	653	A
1	CA	660	G
1	CA	665	A
1	CA	673	G
1	CA	687	A
1	CA	688	G
1	CA	695	A
1	CA	723	U
1	CA	724	G
1	CA	731	G
1	CA	749	C
1	CA	752	G
1	CA	755	G
1	CA	759	A
1	CA	773	G
1	CA	774	G
1	CA	777	A
1	CA	792	A
1	CA	793	U
1	CA	794	A
1	CA	815	A
1	CA	816	A
1	CA	817	C
1	CA	821	G
1	CA	828	A
1	CA	840	C
1	CA	841	U
1	CA	848	C
1	CA	851	G
1	CA	859	A
1	CA	873	A
1	CA	874	G

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Mol	Chain	Res	Type
1	CA	902	G
1	CA	913	A
1	CA	914	A
1	CA	926	G
1	CA	927	G
1	CA	931	C
1	CA	932	C
1	CA	934	C
1	CA	936	C
1	CA	960	U
1	CA	961	U
1	CA	968	A
1	CA	969	A
1	CA	971	G
1	CA	972	C
1	CA	974	A
1	CA	975	A
1	CA	976	G
1	CA	977	A
1	CA	982	U
1	CA	989	C
1	CA	992	U
1	CA	993	G
1	CA	996	A
1	CA	1000	U
1	CA	1001(A)	G
1	CA	1002	G
1	CA	1003	G
1	CA	1004	A
1	CA	1005	A
1	CA	1006	C
1	CA	1008	C
1	CA	1011	G
1	CA	1021	G
1	CA	1022	G
1	CA	1024	G
1	CA	1025	U
1	CA	1026	G
1	CA	1027	C
1	CA	1028	C
1	CA	1030	C
1	CA	1030(A)	G

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Mol	Chain	Res	Type
1	CA	1032	G
1	CA	1033	G
1	CA	1035	A
1	CA	1037	C
1	CA	1039	C
1	CA	1046	A
1	CA	1052	U
1	CA	1054	C
1	CA	1055	A
1	CA	1065	U
1	CA	1066	C
1	CA	1067	A
1	CA	1068	G
1	CA	1077	G
1	CA	1081	G
1	CA	1085	U
1	CA	1088	G
1	CA	1089	G
1	CA	1094	G
1	CA	1095	U
1	CA	1097	C
1	CA	1101	A
1	CA	1104	G
1	CA	1108	G
1	CA	1110	A
1	CA	1111	A
1	CA	1117	G
1	CA	1118	C
1	CA	1129	C
1	CA	1130	A
1	CA	1132	C
1	CA	1134	G
1	CA	1135	U
1	CA	1136	U
1	CA	1137	C
1	CA	1138	G
1	CA	1139	G
1	CA	1140	C
1	CA	1141	C
1	CA	1146	A
1	CA	1147	C
1	CA	1151	A

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Mol	Chain	Res	Type
1	CA	1152	A
1	CA	1154	G
1	CA	1157	A
1	CA	1158	C
1	CA	1159	U
1	CA	1161	C
1	CA	1165	C
1	CA	1182	G
1	CA	1183	A
1	CA	1184	G
1	CA	1190	G
1	CA	1196	U
1	CA	1197	G
1	CA	1201	A
1	CA	1202	G
1	CA	1211	U
1	CA	1212	U
1	CA	1213	A
1	CA	1222	G
1	CA	1224	G
1	CA	1227	A
1	CA	1228	C
1	CA	1238	A
1	CA	1240	U
1	CA	1250	A
1	CA	1256	A
1	CA	1257	U
1	CA	1258	G
1	CA	1269	A
1	CA	1270	C
1	CA	1273	G
1	CA	1276	G
1	CA	1278	U
1	CA	1279	A
1	CA	1280	A
1	CA	1281	U
1	CA	1282	C
1	CA	1287	A
1	CA	1300	G
1	CA	1305	G
1	CA	1317	C
1	CA	1320	C

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Mol	Chain	Res	Type
1	CA	1338	G
1	CA	1340	A
1	CA	1347	G
1	CA	1353	G
1	CA	1357	A
1	CA	1358	U
1	CA	1363	C
1	CA	1370	G
1	CA	1379	G
1	CA	1394	A
1	CA	1397	C
1	CA	1419	G
1	CA	1442	G
1	CA	1442(A)	G
1	CA	1446	U
1	CA	1447	A
1	CA	1456	G
1	CA	1475	G
1	CA	1492	A
1	CA	1493	A
1	CA	1502	A
1	CA	1503	A
1	CA	1504	G
1	CA	1506	U
1	CA	1517	G
1	CA	1520	G
1	CA	1529	G
1	CA	1530	G
1	CA	1531	A
1	CA	1532	U
22	CV	13	A
23	CW	3	C
23	CW	4	C
23	CW	6	G
23	CW	8	4SU
23	CW	9	A
23	CW	12	U
23	CW	14	A
23	CW	19	G
23	CW	22	G
23	CW	25	C
23	CW	26	A

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Mol	Chain	Res	Type
23	CW	27	G
23	CW	29	G
23	CW	34	G
23	CW	46	7MG
23	CW	48	C
23	CW	49	C
23	CW	50	U
23	CW	61	C
23	CW	62	C
23	CW	63	G
23	CW	64	A
23	CW	66	U
23	CW	68	C
23	CW	70	G
23	CW	73	A
23	CW	74	C
24	CX	9	G
24	CX	16	C
24	CX	18	G
24	CX	19	G
24	CX	20	U
24	CX	21	A
24	CX	31	G
24	CX	46	G
24	CX	47	U
24	CX	48	C
24	CX	50	U
24	CX	54	5MU
24	CX	56	C
24	CX	64	G
24	CX	68	C
24	CX	76	A
23	CY	3	C
23	CY	11	C
23	CY	13	C
23	CY	14	A
23	CY	15	G
23	CY	19	G
23	CY	23	A
23	CY	24	G
23	CY	25	C
23	CY	34	G

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Mol	Chain	Res	Type
23	CY	44	G
23	CY	45	U
23	CY	47	U
23	CY	48	C
23	CY	49	C
23	CY	52	G
23	CY	54	5MU
23	CY	55	PSU
23	CY	56	C
23	CY	57	G
23	CY	58	A
23	CY	59	U
23	CY	61	C
23	CY	62	C
23	CY	65	G
23	CY	68	C
23	CY	70	G
23	CY	73	A
25	DA	9	U
25	DA	10	G
25	DA	11	G
25	DA	12	U
25	DA	15	G
25	DA	34	C
25	DA	36	G
25	DA	45	C
25	DA	61	G
25	DA	71	A
25	DA	74	A
25	DA	75	G
25	DA	84	A
25	DA	90	U
25	DA	95	G
25	DA	100	G
25	DA	102	G
25	DA	118	A
25	DA	119	A
25	DA	120	U
25	DA	125	G
25	DA	154(A)	C
25	DA	157	U
25	DA	173	G

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Mol	Chain	Res	Type
25	DA	181	A
25	DA	196	A
25	DA	199	A
25	DA	205	G
25	DA	215	G
25	DA	216	A
25	DA	221	A
25	DA	222	A
25	DA	228	A
25	DA	229	A
25	DA	230	U
25	DA	232	G
25	DA	233	A
25	DA	248	G
25	DA	250	G
25	DA	271(A)	A
25	DA	271(I)	G
25	DA	271(K)	U
25	DA	271(L)	U
25	DA	271(M)	G
25	DA	271(N)	U
25	DA	272	G
25	DA	272(A)	U
25	DA	272(B)	G
25	DA	277	C
25	DA	278	A
25	DA	294	A
25	DA	311	A
25	DA	312	G
25	DA	324	A
25	DA	327	G
25	DA	329	G
25	DA	330	A
25	DA	338	G
25	DA	352	G
25	DA	362	U
25	DA	363	G
25	DA	363(B)	G
25	DA	386	G
25	DA	389	G
25	DA	396	G
25	DA	405	U

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Mol	Chain	Res	Type
25	DA	411	G
25	DA	412	A
25	DA	421	U
25	DA	422	A
25	DA	435	C
25	DA	443	A
25	DA	444	C
25	DA	454	A
25	DA	455	C
25	DA	457	A
25	DA	470	A
25	DA	480	A
25	DA	481	G
25	DA	505	A
25	DA	508	G
25	DA	509	C
25	DA	522	G
25	DA	528	A
25	DA	529	A
25	DA	530	G
25	DA	531	C
25	DA	532	A
25	DA	533	G
25	DA	545	G
25	DA	563	G
25	DA	568	U
25	DA	573	G
25	DA	575	A
25	DA	587	C
25	DA	588	U
25	DA	603	A
25	DA	604	G
25	DA	607	U
25	DA	614(B)	G
25	DA	615	G
25	DA	616	G
25	DA	627	A
25	DA	637	A
25	DA	639	U
25	DA	640	C
25	DA	645	C
25	DA	646	A

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Mol	Chain	Res	Type
25	DA	652(B)	A
25	DA	652(C)	G
25	DA	652(U)	G
25	DA	668	G
25	DA	669	G
25	DA	686	G
25	DA	701	G
25	DA	717	G
25	DA	730	C
25	DA	752	A
25	DA	753	C
25	DA	765	G
25	DA	775	G
25	DA	776	G
25	DA	782	A
25	DA	783	A
25	DA	784	A
25	DA	785	G
25	DA	790	C
25	DA	792	G
25	DA	805	G
25	DA	812	C
25	DA	819	A
25	DA	827	U
25	DA	828	U
25	DA	847	U
25	DA	848	G
25	DA	857	C
25	DA	859	G
25	DA	866	A
25	DA	867	C
25	DA	873	G
25	DA	874	G
25	DA	875	G
25	DA	879	G
25	DA	884	C
25	DA	885	C
25	DA	886	C
25	DA	887	A
25	DA	888	C
25	DA	889	C
25	DA	890	A

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Mol	Chain	Res	Type
25	DA	893	C
25	DA	894	C
25	DA	896	A
25	DA	897	C
25	DA	899	A
25	DA	900	A
25	DA	901	A
25	DA	902	C
25	DA	910	A
25	DA	917	A
25	DA	932	G
25	DA	941	A
25	DA	945	A
25	DA	946	G
25	DA	950	G
25	DA	953	A
25	DA	958	U
25	DA	959	A
25	DA	961	C
25	DA	974	G
25	DA	975	C
25	DA	983	A
25	DA	996	A
25	DA	1005	C
25	DA	1012	U
25	DA	1013	C
25	DA	1017	G
25	DA	1020	A
25	DA	1022	G
25	DA	1025	G
25	DA	1026	U
25	DA	1027	A
25	DA	1033	U
25	DA	1034	G
25	DA	1038	C
25	DA	1039	G
25	DA	1040	C
25	DA	1041	C
25	DA	1043	C
25	DA	1114	G
25	DA	1115	G
25	DA	1130	U

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Mol	Chain	Res	Type
25	DA	1135	C
25	DA	1136	G
25	DA	1139	G
25	DA	1143	A
25	DA	1153	C
25	DA	1170	G
25	DA	1171	G
25	DA	1205	U
25	DA	1206	G
25	DA	1210	A
25	DA	1211	U
25	DA	1212	G
25	DA	1219	G
25	DA	1220	A
25	DA	1229	G
25	DA	1237	A
25	DA	1244	G
25	DA	1253	A
25	DA	1256	G
25	DA	1271	G
25	DA	1272	A
25	DA	1273	U
25	DA	1300	U
25	DA	1301	A
25	DA	1309	G
25	DA	1314	C
25	DA	1352	U
25	DA	1359	A
25	DA	1360	A
25	DA	1365	A
25	DA	1370	C
25	DA	1384	A
25	DA	1385	G
25	DA	1395	A
25	DA	1416	G
25	DA	1417	C
25	DA	1420	U
25	DA	1421	G
25	DA	1427	A
25	DA	1428	C
25	DA	1435	G
25	DA	1437	C

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Mol	Chain	Res	Type
25	DA	1445	A
25	DA	1449	A
25	DA	1450	G
25	DA	1455	G
25	DA	1460	A
25	DA	1461	G
25	DA	1467	C
25	DA	1471	A
25	DA	1482	G
25	DA	1490	A
25	DA	1493	C
25	DA	1494	A
25	DA	1495	A
25	DA	1496	A
25	DA	1497	U
25	DA	1508	A
25	DA	1509	C
25	DA	1509(A)	A
25	DA	1528(A)	A
25	DA	1531	C
25	DA	1532	C
25	DA	1533	G
25	DA	1541	G
25	DA	1543	C
25	DA	1554	A
25	DA	1558	A
25	DA	1559	G
25	DA	1566	A
25	DA	1569	A
25	DA	1578	U
25	DA	1582	C
25	DA	1583	A
25	DA	1584	C
25	DA	1586	A
25	DA	1591	G
25	DA	1608	A
25	DA	1610	A
25	DA	1616	A
25	DA	1631(A)	A
25	DA	1640	C
25	DA	1648	C
25	DA	1654	A

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Mol	Chain	Res	Type
25	DA	1674	G
25	DA	1696	G
25	DA	1700	A
25	DA	1721	G
25	DA	1722	A
25	DA	1746	G
25	DA	1756	G
25	DA	1762	A
25	DA	1763	G
25	DA	1764	G
25	DA	1773	A
25	DA	1780	A
25	DA	1782	C
25	DA	1791	A
25	DA	1800	C
25	DA	1801	G
25	DA	1812	A
25	DA	1816	G
25	DA	1829	A
25	DA	1847	A
25	DA	1848	A
25	DA	1877	A
25	DA	1878	G
25	DA	1900	A
25	DA	1906	G
25	DA	1913	A
25	DA	1914	C
25	DA	1929	G
25	DA	1930	G
25	DA	1936	A
25	DA	1938	A
25	DA	1955	U
25	DA	1963	U
25	DA	1967	C
25	DA	1970	A
25	DA	1971	A
25	DA	1972	A
25	DA	1993	U
25	DA	1997	G
25	DA	2023	G
25	DA	2031	A
25	DA	2032	G

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Mol	Chain	Res	Type
25	DA	2033	A
25	DA	2043	C
25	DA	2055	C
25	DA	2056	G
25	DA	2060	A
25	DA	2061	G
25	DA	2062	A
25	DA	2069	G
25	DA	2099	U
25	DA	2101	G
25	DA	2104	G
25	DA	2105	C
25	DA	2107	C
25	DA	2108	C
25	DA	2110	G
25	DA	2111	C
25	DA	2116	G
25	DA	2117	A
25	DA	2119	A
25	DA	2122	U
25	DA	2126	A
25	DA	2127	G
25	DA	2130	U
25	DA	2131	G
25	DA	2132	U
25	DA	2133	G
25	DA	2134	A
25	DA	2135	A
25	DA	2137	C
25	DA	2138	C
25	DA	2139	C
25	DA	2144	U
25	DA	2145	C
25	DA	2146	C
25	DA	2148	G
25	DA	2149	G
25	DA	2150	U
25	DA	2151	G
25	DA	2153	G
25	DA	2154	G
25	DA	2155	G
25	DA	2156	G

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Mol	Chain	Res	Type
25	DA	2157	G
25	DA	2158	A
25	DA	2159	G
25	DA	2160	G
25	DA	2163	C
25	DA	2166	G
25	DA	2167	U
25	DA	2168	G
25	DA	2169	A
25	DA	2172	U
25	DA	2173	A
25	DA	2175	C
25	DA	2178	C
25	DA	2184	G
25	DA	2185	C
25	DA	2186	G
25	DA	2189	U
25	DA	2192	G
25	DA	2198	A
25	DA	2206	G
25	DA	2207	G
25	DA	2208	A
25	DA	2218	U
25	DA	2225	A
25	DA	2238	G
25	DA	2239	G
25	DA	2268	A
25	DA	2275	C
25	DA	2279	G
25	DA	2283	C
25	DA	2287	A
25	DA	2305	A
25	DA	2308	G
25	DA	2311	A
25	DA	2312	U
25	DA	2319	G
25	DA	2320	A
25	DA	2325	G
25	DA	2334	G
25	DA	2336	A
25	DA	2347	C
25	DA	2350	C

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Mol	Chain	Res	Type
25	DA	2376	A
25	DA	2383	G
25	DA	2385	C
25	DA	2396	G
25	DA	2406	U
25	DA	2425	A
25	DA	2428	G
25	DA	2429	G
25	DA	2430	A
25	DA	2434	A
25	DA	2435	A
25	DA	2439	A
25	DA	2441	C
25	DA	2445	G
25	DA	2448	A
25	DA	2474	C
25	DA	2476	A
25	DA	2480	C
25	DA	2487	G
25	DA	2494	G
25	DA	2502	G
25	DA	2505	G
25	DA	2506	U
25	DA	2507	C
25	DA	2518	A
25	DA	2520	C
25	DA	2529	G
25	DA	2554	U
25	DA	2566	A
25	DA	2567	G
25	DA	2573	C
25	DA	2578	G
25	DA	2582	G
25	DA	2602	A
25	DA	2611	U
25	DA	2612	C
25	DA	2629	A
25	DA	2630	G
25	DA	2652	C
25	DA	2654	A
25	DA	2656	U
25	DA	2663	G

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Mol	Chain	Res	Type
25	DA	2673	G
25	DA	2689	U
25	DA	2690	C
25	DA	2694	G
25	DA	2702	U
25	DA	2703	C
25	DA	2712(A)	A
25	DA	2713	A
25	DA	2714	G
25	DA	2718	G
25	DA	2726	U
25	DA	2733	A
25	DA	2748	A
25	DA	2751	G
25	DA	2752	C
25	DA	2757	A
25	DA	2761	G
25	DA	2764	A
25	DA	2765	A
25	DA	2766	G
25	DA	2778	A
25	DA	2789	C
25	DA	2793	G
25	DA	2794	C
25	DA	2802	G
25	DA	2807	G
25	DA	2818	G
25	DA	2820	A
25	DA	2821	A
25	DA	2833	G
25	DA	2835	A
25	DA	2839	G
25	DA	2872	G
25	DA	2875	C
25	DA	2880	C
25	DA	2892	A
25	DA	2893	G
25	DA	2894	G
25	DA	2895	U
25	DA	2896	C
25	DA	2897	U
26	DB	2	C

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Mol	Chain	Res	Type
26	DB	7	G
26	DB	13	A
26	DB	15	A
26	DB	17	C
26	DB	25	A
26	DB	32	C
26	DB	40	U
26	DB	42	C
26	DB	56	G
26	DB	64	C
26	DB	65	C
26	DB	73	A
26	DB	75	G
26	DB	84	C
26	DB	88	C
26	DB	108	U
26	DB	110	G
26	DB	116	G
26	DB	120	A

All (126) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	96	U
1	AA	115	G
1	AA	250	A
1	AA	266	G
1	AA	347	G
1	AA	429	U
1	AA	509	A
1	AA	560	U
1	AA	687	A
1	AA	748	C
1	AA	839	U
1	AA	913	A
1	AA	991	U
1	AA	1026	G
1	AA	1036	G
1	AA	1064	G
1	AA	1065	U
1	AA	1067	A
1	AA	1181	G

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Mol	Chain	Res	Type
1	AA	1201	A
1	AA	1281	U
1	AA	1285	A
1	AA	1442	G
1	AA	1492	A
23	AW	45	U
23	AW	47	U
24	AX	16	C
23	AY	58	A
25	BA	184	A
25	BA	185	A
25	BA	271	U
25	BA	302	A
25	BA	572	A
25	BA	596	G
25	BA	793	A
25	BA	811	A
25	BA	821	A
25	BA	941	U
25	BA	1005	A
25	BA	1019	G
25	BA	1093	G
25	BA	1099	C
25	BA	1135	G
25	BA	1219	A
25	BA	1220	U
25	BA	1221	G
25	BA	1255	A
25	BA	1346	U
25	BA	1347	A
25	BA	1466	U
25	BA	1554	A
25	BA	1577	C
25	BA	1700	G
25	BA	2014	G
25	BA	2153	G
25	BA	2156	A
25	BA	2166	U
25	BA	2167	C
25	BA	2192	A
25	BA	2203	G
25	BA	2205	C

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Mol	Chain	Res	Type
25	BA	2209	G
25	BA	2418	U
25	BA	2623	U
25	BA	2701	U
25	BA	2769	U
25	BA	2902	G
26	BB	1	U
1	CA	65	U
1	CA	115	G
1	CA	250	A
1	CA	266	G
1	CA	429	U
1	CA	509	A
1	CA	560	U
1	CA	687	A
1	CA	748	C
1	CA	839	U
1	CA	913	A
1	CA	1027	C
1	CA	1064	G
1	CA	1065	U
1	CA	1067	A
1	CA	1128	C
1	CA	1181	G
1	CA	1183	A
1	CA	1190	G
1	CA	1201	A
1	CA	1212	U
1	CA	1442	G
1	CA	1492	A
23	CW	13	C
24	CX	16	C
23	CY	14	A
23	CY	46	7MG
23	CY	58	A
25	DA	195	A
25	DA	196	A
25	DA	228	A
25	DA	271(K)	U
25	DA	271(M)	G
25	DA	277	C
25	DA	528	A

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Mol	Chain	Res	Type
25	DA	529	A
25	DA	587	C
25	DA	752	A
25	DA	764	A
25	DA	774	A
25	DA	827	U
25	DA	856	C
25	DA	900	A
25	DA	1210	A
25	DA	1300	U
25	DA	1420	U
25	DA	1493	C
25	DA	1530	C
25	DA	1653	G
25	DA	1913	A
25	DA	1992	G
25	DA	2110	G
25	DA	2119	A
25	DA	2126	A
25	DA	2406	U
25	DA	2689	U
25	DA	2756	U
26	DB	1	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

36 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	$\# Z > 2$
23	4SU	CW	8	23	14,21,22	1.28	1 (7%)	15,30,33	1.61	2 (13%)
23	5MU	AY	54	23	15,22,23	1.15	1 (6%)	16,32,35	1.67	2 (12%)
23	4SU	CY	8	23	14,21,22	1.33	1 (7%)	15,30,33	1.42	2 (13%)
23	MIA	AY	37	23	18,24,32	1.15	2 (11%)	18,35,47	1.23	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	4SU	AX	8	24	14,21,22	1.43	2 (14%)	15,30,33	2.78	2 (13%)
23	PSU	AW	55	23	17,21,22	1.46	3 (17%)	20,30,33	3.34	6 (30%)
23	PSU	CY	32	23	17,21,22	1.47	2 (11%)	20,30,33	3.17	6 (30%)
23	PSU	AW	32	23	17,21,22	1.55	2 (11%)	20,30,33	3.09	6 (30%)
23	5MU	CY	54	23	15,22,23	1.10	1 (6%)	16,32,35	1.83	2 (12%)
23	PSU	AY	55	23	17,21,22	1.47	3 (17%)	20,30,33	2.98	5 (25%)
23	PSU	CW	55	23	17,21,22	1.38	2 (11%)	20,30,33	3.27	6 (30%)
23	4SU	AW	8	23	14,21,22	1.26	1 (7%)	15,30,33	1.76	2 (13%)
23	PSU	AY	32	23	17,21,22	1.51	2 (11%)	20,30,33	3.20	6 (30%)
24	PSU	CX	55	24	17,21,22	1.45	2 (11%)	20,30,33	3.08	5 (25%)
23	PSU	CY	55	23	17,21,22	1.62	5 (29%)	20,30,33	3.12	7 (35%)
23	5MU	AW	54	23	15,22,23	1.05	1 (6%)	16,32,35	1.90	1 (6%)
23	4SU	AY	8	23	14,21,22	1.24	1 (7%)	15,30,33	1.51	2 (13%)
23	MIA	AW	37	23	24,31,32	2.29	4 (16%)	26,44,47	2.43	9 (34%)
24	4SU	CX	8	24	14,21,22	1.36	2 (14%)	15,30,33	2.59	2 (13%)
23	7MG	AW	46	23	22,26,27	1.75	4 (18%)	28,39,42	2.81	8 (28%)
23	PSU	CY	39	23	17,21,22	1.57	2 (11%)	20,30,33	3.43	6 (30%)
23	7MG	CY	46	23	22,26,27	1.76	3 (13%)	28,39,42	3.20	11 (39%)
24	5MC	CX	32	24	15,22,23	1.37	1 (6%)	19,32,35	1.29	3 (15%)
24	5MU	CX	54	24	15,22,23	1.16	1 (6%)	16,32,35	1.80	2 (12%)
23	PSU	CW	39	23	17,21,22	1.49	2 (11%)	20,30,33	3.31	6 (30%)
24	5MU	AX	54	24,56	15,22,23	1.10	1 (6%)	16,32,35	2.03	2 (12%)
24	PSU	AX	55	24	17,21,22	1.69	3 (17%)	20,30,33	3.24	7 (35%)
23	7MG	AY	46	23	22,26,27	1.85	3 (13%)	28,39,42	2.88	10 (35%)
23	5MU	CW	54	23	15,22,23	1.07	1 (6%)	16,32,35	2.02	1 (6%)
23	7MG	CW	46	23	22,26,27	1.77	4 (18%)	28,39,42	2.69	8 (28%)
23	PSU	CW	32	23	17,21,22	1.52	2 (11%)	20,30,33	3.18	6 (30%)
23	PSU	AW	39	23	17,21,22	1.55	3 (17%)	20,30,33	3.15	6 (30%)
24	5MC	AX	32	24	15,22,23	1.35	1 (6%)	19,32,35	1.37	3 (15%)
23	PSU	AY	39	23	17,21,22	1.45	2 (11%)	20,30,33	3.27	6 (30%)
23	MIA	CY	37	23	18,24,32	1.10	2 (11%)	18,35,47	1.24	2 (11%)
23	MIA	CW	37	23	20,27,32	1.69	3 (15%)	22,39,47	1.94	7 (31%)

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
23	4SU	CW	8	23	-	1/5/25/26	0/2/2/2
23	5MU	AY	54	23	-	3/5/25/26	0/2/2/2
23	4SU	CY	8	23	-	0/5/25/26	0/2/2/2
23	MIA	AY	37	23	-	2/3/25/34	0/3/3/3
24	4SU	AX	8	24	-	0/5/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
23	PSU	CY	32	23	-	0/7/25/26	0/2/2/2
23	PSU	AW	32	23	-	0/7/25/26	0/2/2/2
23	5MU	CY	54	23	-	2/5/25/26	0/2/2/2
23	PSU	AY	55	23	-	0/7/25/26	0/2/2/2
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	0/5/25/26	0/2/2/2
23	PSU	AY	32	23	-	0/7/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2
23	PSU	CY	55	23	-	5/7/25/26	0/2/2/2
23	5MU	AW	54	23	-	0/5/25/26	0/2/2/2
23	4SU	AY	8	23	-	1/5/25/26	0/2/2/2
23	MIA	AW	37	23	-	4/11/33/34	0/3/3/3
24	4SU	CX	8	24	-	0/5/25/26	0/2/2/2
23	7MG	AW	46	23	-	1/7/37/38	0/3/3/3
23	PSU	CY	39	23	-	0/7/25/26	0/2/2/2
23	7MG	CY	46	23	-	4/7/37/38	0/3/3/3
24	5MC	CX	32	24	-	0/5/25/26	0/2/2/2
24	5MU	CX	54	24	-	2/5/25/26	0/2/2/2
23	PSU	CW	39	23	-	0/7/25/26	0/2/2/2
24	5MU	AX	54	24,56	-	0/5/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
23	7MG	AY	46	23	-	1/7/37/38	0/3/3/3
23	5MU	CW	54	23	-	0/5/25/26	0/2/2/2
23	7MG	CW	46	23	-	2/7/37/38	0/3/3/3
23	PSU	CW	32	23	-	1/7/25/26	0/2/2/2
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/5/25/26	0/2/2/2
23	PSU	AY	39	23	-	0/7/25/26	0/2/2/2
23	MIA	CY	37	23	-	2/3/25/34	0/3/3/3
23	MIA	CW	37	23	-	3/7/29/34	0/3/3/3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C13-C14	7.28	1.53	1.32
23	AW	37	MIA	C2-S10	-7.05	1.69	1.75
23	CW	37	MIA	C2-S10	-5.97	1.70	1.75
23	CW	46	7MG	C6-C5	5.35	1.48	1.41
23	AY	46	7MG	C6-C5	5.19	1.48	1.41
24	AX	55	PSU	C5-C1'	-5.11	1.47	1.52
24	CX	32	5MC	C5-C4	4.92	1.49	1.41
23	AY	46	7MG	C5-C4	4.90	1.48	1.39
24	AX	32	5MC	C5-C4	4.78	1.48	1.41
23	CY	46	7MG	C5-C4	4.63	1.48	1.39
23	CY	39	PSU	C5-C1'	-4.43	1.48	1.52
23	AW	46	7MG	C5-C4	4.40	1.47	1.39
23	AW	46	7MG	C6-C5	4.39	1.47	1.41
23	CW	46	7MG	C5-C4	4.25	1.47	1.39
23	CY	46	7MG	C6-C5	4.20	1.47	1.41
23	AW	8	4SU	C4-S4	-4.12	1.60	1.67
23	CY	8	4SU	C4-S4	-4.08	1.60	1.67
23	AW	39	PSU	C5-C1'	-3.96	1.48	1.52
23	AY	32	PSU	C5-C1'	-3.94	1.48	1.52
23	AW	32	PSU	C5-C1'	-3.90	1.48	1.52
23	CY	55	PSU	C5-C1'	-3.88	1.48	1.52
23	CW	32	PSU	C4-C5	3.87	1.49	1.41
23	CW	8	4SU	C4-S4	-3.86	1.60	1.67
23	AY	8	4SU	C4-S4	-3.81	1.60	1.67
23	AY	55	PSU	C5-C1'	-3.79	1.49	1.52
24	CX	8	4SU	C4-S4	-3.73	1.60	1.67
24	CX	55	PSU	C4-C5	3.73	1.49	1.41
23	CY	46	7MG	C5-N7	-3.72	1.33	1.39
23	CY	32	PSU	C5-C1'	-3.72	1.49	1.52
23	AY	54	5MU	C4-C5	3.66	1.49	1.41
24	AX	8	4SU	C4-S4	-3.66	1.60	1.67
23	AW	32	PSU	C4-C5	3.65	1.49	1.41
23	CW	39	PSU	C5-C1'	-3.64	1.49	1.52
24	CX	54	5MU	C4-C5	3.62	1.49	1.41
23	AY	39	PSU	C5-C1'	-3.59	1.49	1.52
23	AY	32	PSU	C4-C5	3.57	1.49	1.41
24	AX	8	4SU	C2-N3	-3.55	1.31	1.38
23	CW	39	PSU	C4-C5	3.54	1.49	1.41
23	AW	46	7MG	C5-N7	-3.53	1.33	1.39
23	AW	55	PSU	C4-C5	3.51	1.49	1.41
23	CY	55	PSU	C4-C5	3.48	1.48	1.41
23	CY	54	5MU	C4-C5	3.47	1.48	1.41
23	CW	32	PSU	C5-C1'	-3.43	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	54	5MU	C4-C5	3.42	1.48	1.41
23	CY	32	PSU	C4-C5	3.41	1.48	1.41
23	AW	39	PSU	C4-C5	3.39	1.48	1.41
23	CW	54	5MU	C4-C5	3.38	1.48	1.41
23	CW	55	PSU	C4-C5	3.38	1.48	1.41
23	AW	55	PSU	C5-C1'	-3.32	1.49	1.52
23	AY	39	PSU	C4-C5	3.27	1.48	1.41
23	AW	54	5MU	C4-C5	3.27	1.48	1.41
23	CY	39	PSU	C4-C5	3.24	1.48	1.41
23	AY	55	PSU	C4-C5	3.23	1.48	1.41
23	CW	55	PSU	C5-C1'	-3.20	1.49	1.52
24	CX	55	PSU	C5-C1'	-3.20	1.49	1.52
23	CW	46	7MG	C5-N7	-3.15	1.34	1.39
24	CX	8	4SU	C2-N3	-3.10	1.32	1.38
24	AX	55	PSU	C4-C5	3.08	1.48	1.41
23	AY	46	7MG	C5-N7	-3.00	1.34	1.39
23	AY	37	MIA	C2-N3	2.79	1.36	1.32
23	AY	37	MIA	C5-C4	2.75	1.48	1.40
23	AW	46	7MG	C4-N9	-2.72	1.33	1.38
23	CY	37	MIA	C5-C4	2.67	1.48	1.40
23	CY	37	MIA	C2-N3	2.63	1.36	1.32
23	CW	37	MIA	C5-C4	2.53	1.47	1.40
23	AW	37	MIA	C5-C4	2.48	1.47	1.40
23	CW	37	MIA	C6-N1	2.30	1.36	1.32
23	CY	55	PSU	O4'-C1'	-2.29	1.41	1.44
23	CY	55	PSU	C2-N3	-2.29	1.33	1.38
23	CY	55	PSU	C2-N1	-2.21	1.33	1.38
23	AY	55	PSU	O4'-C1'	-2.14	1.41	1.44
23	CW	46	7MG	C4-N9	-2.12	1.34	1.38
23	AW	39	PSU	O4'-C1'	-2.11	1.41	1.44
23	AW	37	MIA	C6-N1	2.03	1.35	1.32
23	AW	55	PSU	C2-N1	-2.03	1.34	1.38
24	AX	55	PSU	O4'-C1'	-2.00	1.41	1.44

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CY	46	7MG	N3-C4-N9	10.74	140.70	126.91
24	AX	8	4SU	C2-N3-C4	9.47	128.89	115.15
23	AY	46	7MG	N3-C4-N9	9.44	139.04	126.91
23	AY	39	PSU	N1-C2-N3	-9.24	121.08	128.43
23	CW	39	PSU	N1-C2-N3	-9.17	121.14	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AW	46	7MG	N3-C4-N9	8.96	138.42	126.91
23	CW	32	PSU	N1-C2-N3	-8.88	121.37	128.43
23	CY	32	PSU	N1-C2-N3	-8.88	121.37	128.43
23	AY	32	PSU	N1-C2-N3	-8.85	121.40	128.43
23	CY	39	PSU	N1-C2-N3	-8.75	121.47	128.43
23	CW	46	7MG	N3-C4-N9	8.70	138.09	126.91
23	CW	55	PSU	N1-C2-N3	-8.68	121.53	128.43
24	CX	55	PSU	N1-C2-N3	-8.63	121.57	128.43
23	AW	39	PSU	N1-C2-N3	-8.59	121.61	128.43
24	CX	8	4SU	C2-N3-C4	8.55	127.55	115.15
24	AX	55	PSU	N1-C2-N3	-8.42	121.73	128.43
23	AW	55	PSU	N1-C2-N3	-8.35	121.80	128.43
23	AW	32	PSU	N1-C2-N3	-8.26	121.87	128.43
23	AY	55	PSU	N1-C2-N3	-8.08	122.01	128.43
23	CY	55	PSU	N1-C2-N3	-7.91	122.14	128.43
23	CW	39	PSU	C4-N3-C2	7.74	121.67	115.14
23	CW	54	5MU	C4-N3-C2	7.61	121.57	115.14
24	AX	54	5MU	C4-N3-C2	7.55	121.52	115.14
23	AW	37	MIA	C12-C13-C14	-7.51	112.52	127.14
23	AY	39	PSU	C4-N3-C2	7.46	121.44	115.14
23	CY	39	PSU	C4-N3-C2	7.05	121.10	115.14
23	CY	55	PSU	C4-N3-C2	7.05	121.09	115.14
23	AW	54	5MU	C4-N3-C2	7.01	121.06	115.14
23	AW	39	PSU	C4-N3-C2	6.99	121.05	115.14
23	AW	55	PSU	C4-N3-C2	6.99	121.04	115.14
23	AY	32	PSU	C4-N3-C2	6.97	121.03	115.14
23	CY	32	PSU	C4-N3-C2	6.88	120.95	115.14
23	CW	32	PSU	C4-N3-C2	6.86	120.94	115.14
23	AW	32	PSU	C4-N3-C2	6.73	120.83	115.14
24	AX	55	PSU	C4-N3-C2	6.73	120.82	115.14
23	CW	55	PSU	C4-N3-C2	6.70	120.80	115.14
24	CX	55	PSU	C4-N3-C2	6.33	120.49	115.14
23	CY	54	5MU	C4-N3-C2	6.31	120.47	115.14
23	AY	55	PSU	C4-N3-C2	6.28	120.45	115.14
24	CX	54	5MU	C4-N3-C2	6.14	120.33	115.14
23	CY	46	7MG	C5-C4-N3	-6.05	116.60	126.49
23	AW	55	PSU	C5-C1'-C2'	-5.87	104.85	115.32
23	CY	39	PSU	C5-C1'-C2'	-5.76	105.05	115.32
23	CY	55	PSU	C5-C4-N3	-5.74	117.96	125.36
23	AW	8	4SU	C2-N3-C4	5.73	123.45	115.15
23	AW	46	7MG	N7-C8-N9	-5.67	95.27	103.38
24	AX	55	PSU	C5-C4-N3	-5.55	118.21	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CW	46	7MG	N7-C8-N9	-5.53	95.46	103.38
23	AW	55	PSU	C5-C4-N3	-5.46	118.33	125.36
23	CY	39	PSU	C5-C4-N3	-5.44	118.35	125.36
23	AW	39	PSU	C5-C4-N3	-5.44	118.35	125.36
23	AY	54	5MU	C4-N3-C2	5.43	119.72	115.14
23	AY	32	PSU	C5-C4-N3	-5.35	118.46	125.36
23	AW	32	PSU	C5-C4-N3	-5.35	118.47	125.36
23	CW	46	7MG	C5-C4-N3	-5.34	117.77	126.49
23	CW	39	PSU	C5-C4-N3	-5.30	118.53	125.36
23	AY	55	PSU	C5-C4-N3	-5.27	118.57	125.36
23	CY	32	PSU	C5-C4-N3	-5.27	118.58	125.36
23	AW	46	7MG	C6-N1-C2	5.26	124.29	115.93
23	CW	32	PSU	C5-C4-N3	-5.20	118.66	125.36
23	AY	46	7MG	C6-N1-C2	5.18	124.16	115.93
23	AY	46	7MG	N7-C8-N9	-5.08	96.11	103.38
23	AY	39	PSU	C5-C4-N3	-5.03	118.89	125.36
23	CW	55	PSU	C5-C4-N3	-5.00	118.91	125.36
23	CY	46	7MG	C6-N1-C2	4.98	123.84	115.93
23	AY	46	7MG	C5-C4-N3	-4.96	118.39	126.49
23	CY	46	7MG	C6-C5-C4	4.84	120.40	115.20
23	CW	8	4SU	C2-N3-C4	4.75	122.04	115.15
24	CX	55	PSU	C5-C4-N3	-4.73	119.26	125.36
23	CW	55	PSU	C5-C1'-C2'	-4.73	106.89	115.32
24	CX	8	4SU	C5-C4-N3	-4.70	117.54	123.83
24	AX	8	4SU	C5-C4-N3	-4.61	117.66	123.83
23	CY	46	7MG	N7-C8-N9	-4.61	96.79	103.38
23	CW	37	MIA	C2-N3-C4	4.50	121.53	115.32
24	AX	55	PSU	C5-C6-N1	-4.50	118.91	124.44
23	AW	46	7MG	C5-C4-N3	-4.47	119.19	126.49
23	AY	8	4SU	C2-N3-C4	4.46	121.61	115.15
24	CX	55	PSU	C5-C6-N1	-4.43	119.00	124.44
24	CX	55	PSU	C6-N1-C2	4.41	122.64	115.36
23	CW	32	PSU	C6-N1-C2	4.35	122.54	115.36
23	AY	55	PSU	C5-C6-N1	-4.35	119.10	124.44
23	CY	32	PSU	C6-N1-C2	4.18	122.26	115.36
23	CW	55	PSU	C6-N1-C2	4.17	122.25	115.36
23	AY	32	PSU	C6-N1-C2	4.14	122.19	115.36
24	AX	55	PSU	C6-N1-C2	4.14	122.18	115.36
23	CY	39	PSU	C5-C6-N1	-4.13	119.36	124.44
23	CY	39	PSU	C6-N1-C2	4.10	122.12	115.36
23	CW	37	MIA	C5-C6-N1	-4.08	117.42	120.81
24	AX	55	PSU	C5-C1'-C2'	-4.08	108.05	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AW	39	PSU	C6-N1-C2	4.07	122.07	115.36
23	AY	39	PSU	C6-N1-C2	4.06	122.06	115.36
23	CW	39	PSU	C6-N1-C2	4.05	122.04	115.36
23	AW	32	PSU	C6-N1-C2	4.02	121.99	115.36
23	AW	39	PSU	C5-C6-N1	-4.00	119.53	124.44
23	AY	55	PSU	C6-N1-C2	4.00	121.95	115.36
23	AW	46	7MG	C5-C6-N1	-3.99	114.93	123.14
23	CY	55	PSU	C5-C6-N1	-3.99	119.53	124.44
23	AW	37	MIA	C5-C6-N1	-3.99	117.49	120.81
23	CY	55	PSU	C6-N1-C2	3.98	121.93	115.36
23	AW	37	MIA	C2-N3-C4	3.96	120.79	115.32
23	CW	55	PSU	C5-C6-N1	-3.96	119.57	124.44
23	AY	46	7MG	C6-C5-C4	3.96	119.44	115.20
23	CW	46	7MG	C6-N1-C2	3.95	122.21	115.93
23	CW	32	PSU	C5-C6-N1	-3.95	119.59	124.44
23	AW	55	PSU	C6-N1-C2	3.94	121.86	115.36
23	AY	32	PSU	C5-C6-N1	-3.93	119.60	124.44
23	CW	39	PSU	C5-C6-N1	-3.91	119.64	124.44
23	AW	46	7MG	C6-C5-C4	3.89	119.38	115.20
23	CY	32	PSU	C5-C6-N1	-3.87	119.68	124.44
23	AY	46	7MG	C5-C6-N1	-3.87	115.19	123.14
23	AW	32	PSU	C5-C6-N1	-3.84	119.72	124.44
23	AY	39	PSU	C5-C6-N1	-3.84	119.72	124.44
24	AX	32	5MC	C2-N3-C4	3.84	120.65	116.02
23	AW	37	MIA	C15-C14-C13	-3.83	111.58	122.65
23	CW	46	7MG	C6-C5-C4	3.76	119.23	115.20
23	AW	37	MIA	C16-C14-C13	-3.70	111.97	122.65
23	CY	46	7MG	C5-C6-N1	-3.63	115.68	123.14
24	CX	32	5MC	C2-N3-C4	3.61	120.38	116.02
23	CY	37	MIA	N3-C2-N1	-3.49	123.22	128.68
23	CY	8	4SU	C2-N3-C4	3.47	120.18	115.15
23	AW	55	PSU	C5-C6-N1	-3.43	120.22	124.44
23	CW	8	4SU	C5-C4-N3	-3.35	119.34	123.83
23	AY	37	MIA	N3-C2-N1	-3.31	123.51	128.68
23	CY	46	7MG	N2-C2-N3	3.30	122.39	117.25
23	CW	46	7MG	C5-C6-N1	-3.28	116.41	123.14
23	AY	8	4SU	C5-C4-N3	-3.23	119.51	123.83
23	AW	8	4SU	C5-C4-N3	-3.15	119.61	123.83
23	CW	37	MIA	C12-N6-C6	-3.05	120.25	122.87
23	CW	37	MIA	C4-C5-N7	-3.04	106.23	109.40
23	AY	54	5MU	C5-C6-N1	-2.94	119.02	122.19
23	AW	32	PSU	C5-C1'-C2'	-2.90	110.15	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AW	46	7MG	C5-C4-N9	-2.89	102.39	106.44
23	CW	46	7MG	C8-N7-C5	2.87	116.40	108.94
23	AW	37	MIA	C4-C5-N7	-2.85	106.43	109.40
23	CW	37	MIA	C2-N1-C6	2.84	122.26	117.19
23	AY	39	PSU	C5-C1'-C2'	-2.83	110.27	115.32
23	AY	37	MIA	C4-C5-N7	-2.82	106.46	109.40
23	AW	37	MIA	C2-N1-C6	2.82	122.23	117.19
23	AY	32	PSU	C5-C1'-C2'	-2.80	110.33	115.32
24	CX	54	5MU	C5-C6-N1	-2.79	119.18	122.19
23	CY	8	4SU	C5-C4-N3	-2.77	120.13	123.83
23	AY	46	7MG	C5-C4-N9	-2.77	102.57	106.44
23	CY	46	7MG	C5-C4-N9	-2.70	102.66	106.44
23	CY	54	5MU	C5-C6-N1	-2.63	119.36	122.19
23	AY	46	7MG	C8-N7-C5	2.61	115.73	108.94
23	AW	46	7MG	C8-N7-C5	2.56	115.59	108.94
23	CW	39	PSU	C5-C1'-C2'	-2.50	110.86	115.32
23	CW	37	MIA	N3-C2-N1	-2.49	122.39	126.98
23	CY	46	7MG	C8-N7-C5	2.46	115.35	108.94
24	CX	32	5MC	N4-C4-N3	2.45	120.49	117.03
23	AW	39	PSU	C5-C1'-C2'	-2.44	110.96	115.32
24	AX	32	5MC	N4-C4-N3	2.44	120.49	117.03
23	CW	37	MIA	N6-C6-N1	2.43	121.54	118.50
23	CW	46	7MG	C2-N3-C4	2.43	120.60	113.89
23	CY	46	7MG	C2-N3-C4	2.41	120.55	113.89
24	AX	54	5MU	C5-C6-N1	-2.28	119.73	122.19
23	AW	37	MIA	N3-C2-N1	-2.27	122.80	126.98
23	CW	32	PSU	C5-C1'-C2'	-2.25	111.30	115.32
24	CX	32	5MC	C5-C6-N1	-2.25	119.77	122.19
23	CY	55	PSU	C5-C1'-C2'	-2.20	111.39	115.32
24	AX	32	5MC	C5-C6-N1	-2.20	119.83	122.19
23	CY	32	PSU	C5-C1'-C2'	-2.19	111.41	115.32
23	AY	46	7MG	CM7-N7-C5	2.19	132.43	124.01
23	CY	46	7MG	C4-N9-C1'	2.16	131.72	126.60
23	AW	37	MIA	C12-N6-C6	-2.16	119.35	122.55
23	AY	46	7MG	C2-N3-C4	2.11	119.73	113.89
23	CY	55	PSU	O4'-C1'-C2'	2.09	108.05	104.66
23	CY	37	MIA	C4-C5-N7	-2.09	107.23	109.40
24	AX	55	PSU	O4'-C1'-C2'	2.01	107.91	104.66

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	CW	8	4SU	O4'-C1'-N1-C6
23	AY	54	5MU	O4'-C4'-C5'-O5'
23	CY	54	5MU	C3'-C4'-C5'-O5'
23	CY	54	5MU	O4'-C4'-C5'-O5'
23	CY	55	PSU	C2'-C1'-C5-C4
23	CY	55	PSU	C2'-C1'-C5-C6
23	AY	8	4SU	C2'-C1'-N1-C6
23	AW	37	MIA	C12-C13-C14-C15
23	AW	37	MIA	C12-C13-C14-C16
24	CX	54	5MU	O4'-C4'-C5'-O5'
23	AY	46	7MG	C4'-C5'-O5'-P
23	CY	37	MIA	C3'-C4'-C5'-O5'
23	CW	37	MIA	N1-C6-N6-C12
23	CW	37	MIA	N1-C2-S10-C11
23	CW	37	MIA	N3-C2-S10-C11
23	AY	54	5MU	C3'-C4'-C5'-O5'
24	CX	54	5MU	C3'-C4'-C5'-O5'
23	CY	37	MIA	O4'-C4'-C5'-O5'
23	CY	55	PSU	O4'-C1'-C5-C4
23	CY	46	7MG	C2'-C1'-N9-C8
23	AW	46	7MG	C4'-C5'-O5'-P
23	CY	46	7MG	O4'-C1'-N9-C4
23	AY	54	5MU	C4'-C5'-O5'-P
23	CY	55	PSU	O4'-C1'-C5-C6
23	CW	46	7MG	O4'-C4'-C5'-O5'
23	CW	32	PSU	C2'-C1'-C5-C6
23	CW	46	7MG	C3'-C4'-C5'-O5'
23	CY	46	7MG	C2'-C1'-N9-C4
23	CY	46	7MG	O4'-C1'-N9-C8
23	AW	37	MIA	C5-C6-N6-C12
23	CY	55	PSU	O4'-C4'-C5'-O5'
23	AY	37	MIA	C3'-C4'-C5'-O5'
23	AY	37	MIA	C4'-C5'-O5'-P
23	AW	37	MIA	N1-C6-N6-C12

There are no ring outliers.

16 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	CW	8	4SU	2	0
23	CY	8	4SU	2	0
23	AY	37	MIA	2	0
24	AX	8	4SU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	55	PSU	1	0
23	AY	55	PSU	2	0
23	AY	32	PSU	1	0
23	CY	55	PSU	6	0
23	AY	8	4SU	3	0
23	AW	46	7MG	1	0
23	CY	46	7MG	3	0
24	CX	32	5MC	3	0
23	CW	39	PSU	1	0
23	AY	46	7MG	1	0
23	CW	46	7MG	1	0
23	CY	37	MIA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2325 ligands modelled in this entry, 2321 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
57	UAM	AA	3232	56	31,31,31	1.40	2 (6%)	38,44,44	1.25	3 (7%)
58	SF4	CD	501	4	0,12,12	0.00	-	-		
57	UAM	CA	3202	-	31,31,31	1.42	2 (6%)	38,44,44	1.32	6 (15%)
58	SF4	AD	501	4	0,12,12	0.00	-	-		

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
57	UAM	AA	3232	56	-	5/28/40/40	0/2/2/2
58	SF4	CD	501	4	-	-	0/6/5/5
57	UAM	CA	3202	-	-	5/28/40/40	0/2/2/2
58	SF4	AD	501	4	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	AA	3232	UAM	CAO-CAW	-6.54	1.39	1.51
57	CA	3202	UAM	CAO-CAW	-6.30	1.39	1.51
57	CA	3202	UAM	CAX-CAU	-3.30	1.38	1.46
57	AA	3232	UAM	CAX-CAU	-2.73	1.39	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	AA	3232	UAM	CAY-CAP-CBC	-3.75	108.39	115.84
57	AA	3232	UAM	CBD-OAR-CAU	-3.60	113.28	118.92
57	CA	3202	UAM	OAR-CAU-OAG	3.34	121.32	117.60
57	CA	3202	UAM	CBD-OAR-CAU	-3.32	113.71	118.92
57	AA	3232	UAM	OAR-CAU-OAG	3.01	120.96	117.60
57	CA	3202	UAM	CAY-CAP-CBC	-2.94	109.99	115.84
57	CA	3202	UAM	CAP-CBC-CBD	-2.68	108.58	112.56
57	CA	3202	UAM	OAH-CAV-CAX	-2.43	116.59	121.14
57	CA	3202	UAM	CAZ-CAN-CAS	-2.19	109.63	112.65

There are no chirality outliers.

All (10) torsion outliers are listed below:

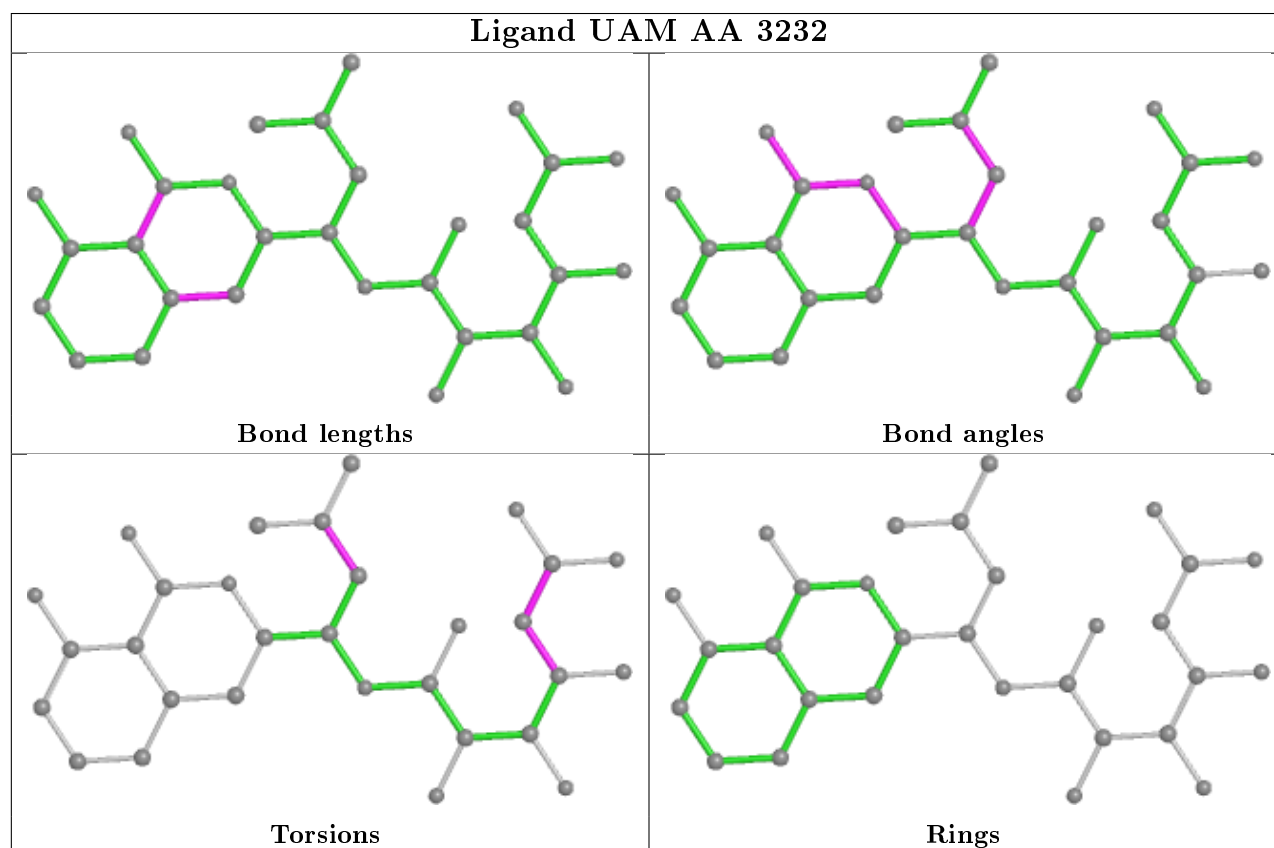
Mol	Chain	Res	Type	Atoms
57	CA	3202	UAM	CAY-CAP-CBC-CBD
57	CA	3202	UAM	CBD-CBC-NAQ-CAT
57	AA	3232	UAM	CAZ-CAN-CAS-OAE
57	AA	3232	UAM	CAZ-CAN-CAS-NAC
57	CA	3202	UAM	CAP-CBC-NAQ-CAT
57	CA	3202	UAM	CAY-CAP-CBC-NAQ
57	AA	3232	UAM	CBC-CAP-CAY-CAB
57	AA	3232	UAM	CAS-CAN-CAZ-NAD
57	AA	3232	UAM	CBC-CAP-CAY-CAA
57	CA	3202	UAM	CAT-CBA-CBB-OAJ

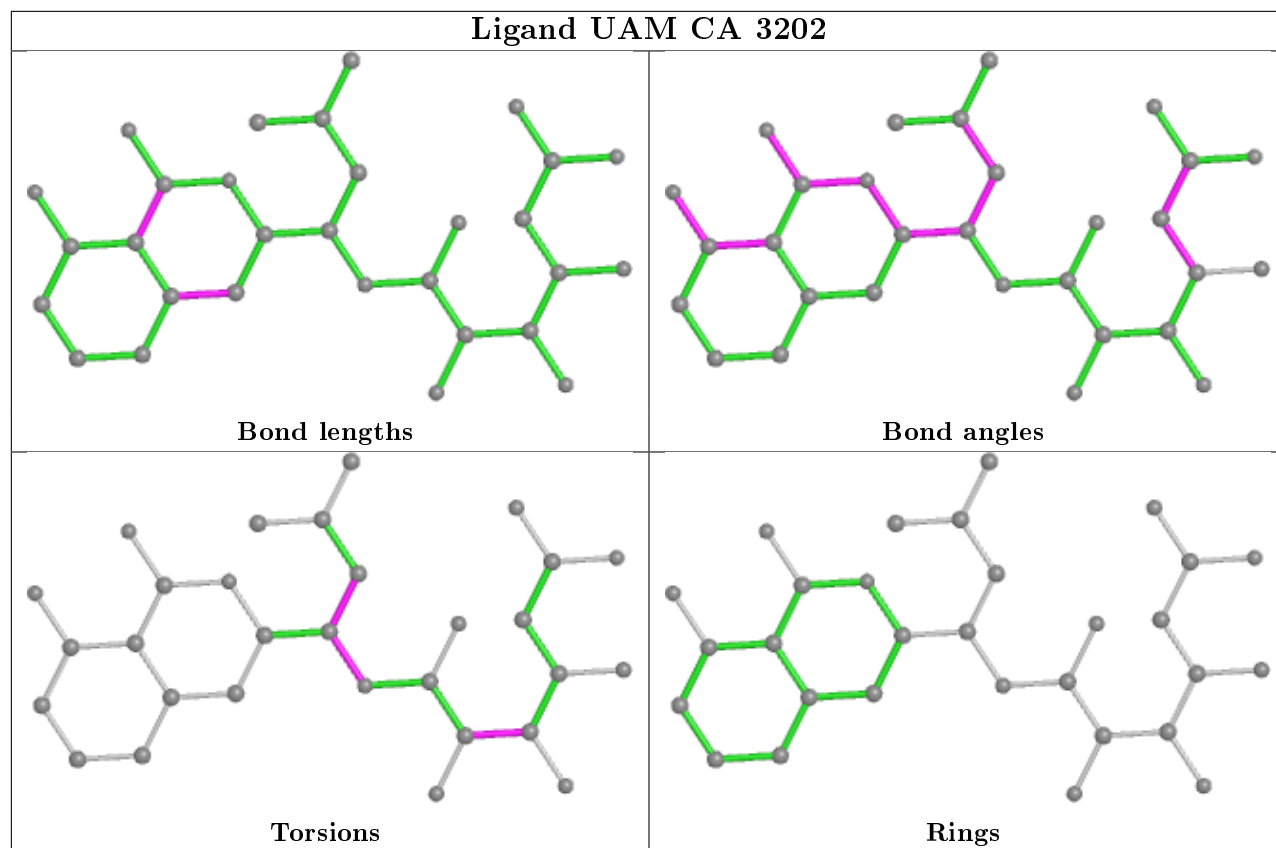
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	3232	UAM	1	0
57	CA	3202	UAM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	AA	1497/1521 (98%)	0.22	33 (2%) 62 60	36, 63, 86, 100	0
1	CA	1503/1521 (98%)	0.30	70 (4%) 31 30	38, 65, 87, 100	0
2	AB	231/256 (90%)	0.51	16 (6%) 16 15	62, 75, 84, 89	0
2	CB	231/256 (90%)	0.80	35 (15%) 2 1	64, 77, 84, 90	0
3	AC	206/239 (86%)	0.77	13 (6%) 20 18	59, 70, 80, 85	0
3	CC	206/239 (86%)	1.24	38 (18%) 1 1	61, 72, 81, 86	0
4	AD	208/209 (99%)	0.77	18 (8%) 10 9	48, 63, 72, 77	0
4	CD	208/209 (99%)	0.78	15 (7%) 15 14	49, 63, 72, 76	0
5	AE	148/162 (91%)	0.70	8 (5%) 25 24	49, 63, 73, 80	0
5	CE	148/162 (91%)	0.68	11 (7%) 14 13	49, 65, 74, 80	0
6	AF	100/101 (99%)	0.36	0 100 100	50, 60, 69, 74	0
6	CF	100/101 (99%)	0.40	3 (3%) 50 49	49, 61, 70, 75	0
7	AG	155/156 (99%)	0.55	7 (4%) 33 31	54, 66, 76, 83	0
7	CG	155/156 (99%)	1.22	32 (20%) 1 0	55, 68, 77, 85	0
8	AH	137/138 (99%)	0.53	3 (2%) 62 60	53, 64, 71, 78	0
8	CH	137/138 (99%)	0.58	8 (5%) 23 22	54, 66, 72, 78	0
9	AI	127/128 (99%)	1.04	19 (14%) 2 1	49, 72, 79, 83	0
9	CI	127/128 (99%)	2.16	71 (55%) 0 0	55, 74, 81, 84	0
10	AJ	97/105 (92%)	0.98	14 (14%) 2 2	46, 69, 84, 88	0
10	CJ	96/105 (91%)	1.51	20 (20%) 1 0	59, 78, 87, 91	0
11	AK	114/129 (88%)	0.91	13 (11%) 5 4	42, 61, 72, 76	0
11	CK	114/129 (88%)	0.97	10 (8%) 10 9	43, 63, 73, 77	0
12	AL	122/132 (92%)	0.40	3 (2%) 57 55	43, 54, 65, 72	0
12	CL	122/132 (92%)	0.79	15 (12%) 4 3	46, 56, 66, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
13	AM	123/126 (97%)	0.80	10 (8%)	12	11	51, 66, 73, 77	0
13	CM	122/126 (96%)	1.68	42 (34%)	0	0	53, 69, 74, 79	0
14	AN	60/61 (98%)	1.09	6 (10%)	7	6	60, 67, 74, 76	0
14	CN	60/61 (98%)	2.69	34 (56%)	0	0	61, 70, 76, 79	0
15	AO	88/89 (98%)	0.58	5 (5%)	23	22	41, 61, 70, 75	0
15	CO	88/89 (98%)	0.57	4 (4%)	33	31	45, 61, 71, 77	0
16	AP	82/88 (93%)	0.54	2 (2%)	59	57	53, 62, 72, 74	0
16	CP	82/88 (93%)	0.57	4 (4%)	29	28	52, 62, 71, 74	0
17	AQ	99/105 (94%)	0.64	4 (4%)	38	37	50, 62, 72, 74	0
17	CQ	99/105 (94%)	0.73	8 (8%)	12	11	50, 63, 73, 75	0
18	AR	68/88 (77%)	0.63	7 (10%)	6	6	45, 57, 70, 73	0
18	CR	68/88 (77%)	0.29	1 (1%)	73	72	51, 64, 72, 77	0
19	AS	83/93 (89%)	0.77	6 (7%)	15	14	60, 70, 78, 85	0
19	CS	83/93 (89%)	1.67	31 (37%)	0	0	64, 72, 80, 87	0
20	AT	96/106 (90%)	0.47	3 (3%)	49	47	53, 64, 75, 76	0
20	CT	96/106 (90%)	0.68	7 (7%)	15	13	53, 63, 76, 78	0
21	AU	23/27 (85%)	1.05	4 (17%)	1	1	58, 64, 67, 70	0
21	CU	23/27 (85%)	1.57	8 (34%)	0	0	60, 66, 70, 74	0
22	AV	13/24 (54%)	0.96	2 (15%)	2	1	50, 59, 78, 86	0
22	CV	13/24 (54%)	1.67	4 (30%)	0	0	54, 62, 81, 88	0
23	AW	67/76 (88%)	1.47	16 (23%)	0	0	42, 83, 94, 98	0
23	AY	67/76 (88%)	1.57	22 (32%)	0	0	36, 88, 94, 99	0
23	CW	65/76 (85%)	2.27	29 (44%)	0	0	45, 84, 94, 99	0
23	CY	66/76 (86%)	1.64	24 (36%)	0	0	39, 88, 94, 96	0
24	AX	72/77 (93%)	0.63	5 (6%)	16	15	35, 66, 80, 89	0
24	CX	72/77 (93%)	0.42	4 (5%)	24	23	38, 69, 81, 90	0
25	BA	2871/2915 (98%)	0.69	107 (3%)	41	41	19, 38, 88, 103	0
25	DA	2800/2915 (96%)	0.13	93 (3%)	46	45	24, 42, 84, 100	0
26	BB	120/121 (99%)	0.47	0	100	100	36, 56, 68, 86	0
26	DB	120/121 (99%)	0.20	5 (4%)	36	35	42, 60, 71, 88	0
27	BD	275/276 (99%)	0.64	5 (1%)	68	66	21, 36, 51, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DD	275/276 (99%)	0.56	13 (4%) 31 30	22, 38, 53, 75	0
28	BE	204/206 (99%)	0.67	3 (1%) 73 72	21, 42, 59, 72	0
28	DE	204/206 (99%)	0.28	2 (0%) 82 80	23, 45, 62, 74	0
29	BF	203/210 (96%)	0.76	3 (1%) 73 72	20, 46, 69, 82	0
29	DF	203/210 (96%)	0.38	6 (2%) 50 49	23, 52, 69, 83	0
30	BG	181/182 (99%)	0.80	9 (4%) 28 27	45, 61, 73, 84	0
30	DG	181/182 (99%)	1.64	59 (32%) 0 0	50, 63, 75, 84	0
31	BH	174/180 (96%)	0.59	1 (0%) 89 88	47, 60, 69, 77	0
31	DH	174/180 (96%)	0.87	25 (14%) 2 2	51, 65, 73, 78	0
32	BI	146/148 (98%)	0.35	4 (2%) 54 52	43, 66, 77, 81	0
32	DI	146/148 (98%)	0.33	3 (2%) 63 61	43, 67, 77, 81	0
33	BN	140/140 (100%)	0.79	1 (0%) 87 86	29, 42, 62, 72	0
33	DN	140/140 (100%)	0.21	2 (1%) 75 73	34, 47, 66, 74	0
34	BO	122/122 (100%)	0.63	0 100 100	31, 42, 59, 65	0
34	DO	122/122 (100%)	0.32	0 100 100	35, 45, 60, 67	0
35	BP	149/150 (99%)	0.56	1 (0%) 87 86	22, 51, 68, 76	0
35	DP	149/150 (99%)	0.43	7 (4%) 31 30	25, 54, 70, 77	0
36	BQ	141/141 (100%)	0.79	2 (1%) 75 73	29, 45, 62, 70	0
36	DQ	141/141 (100%)	0.84	16 (11%) 5 4	34, 50, 66, 71	0
37	BR	118/118 (100%)	0.72	0 100 100	24, 35, 46, 56	0
37	DR	118/118 (100%)	0.12	0 100 100	26, 38, 49, 58	0
38	BS	110/112 (98%)	0.73	2 (1%) 68 66	41, 54, 66, 71	0
38	DS	110/112 (98%)	1.05	15 (13%) 3 2	45, 58, 68, 73	0
39	BT	131/146 (89%)	0.56	0 100 100	34, 46, 66, 75	0
39	DT	131/146 (89%)	0.31	0 100 100	38, 50, 70, 76	0
40	BU	116/118 (98%)	0.78	1 (0%) 84 82	23, 33, 52, 64	0
40	DU	116/118 (98%)	0.33	1 (0%) 84 82	29, 39, 56, 66	0
41	BV	101/101 (100%)	0.36	0 100 100	15, 31, 49, 71	0
41	DV	101/101 (100%)	0.57	5 (4%) 28 27	40, 66, 74, 84	0
42	BW	112/113 (99%)	0.71	1 (0%) 84 82	23, 31, 50, 75	0
42	DW	112/113 (99%)	0.35	0 100 100	27, 35, 54, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
43	BX	95/96 (98%)	0.67	0	100 100	28, 40, 61, 75	0
43	DX	95/96 (98%)	0.60	5 (5%)	26 25	30, 44, 62, 75	0
44	BY	107/110 (97%)	0.67	2 (1%)	66 64	36, 52, 68, 76	0
44	DY	107/110 (97%)	0.62	7 (6%)	18 17	38, 56, 70, 76	0
45	BZ	154/206 (74%)	0.95	19 (12%)	4 3	34, 59, 80, 89	0
45	DZ	160/206 (77%)	1.69	48 (30%)	0 0	62, 77, 87, 97	0
46	B0	83/85 (97%)	0.61	1 (1%)	79 77	25, 33, 50, 61	0
46	D0	83/85 (97%)	1.13	10 (12%)	4 3	42, 61, 69, 73	0
47	B1	97/98 (98%)	0.45	1 (1%)	82 80	27, 43, 66, 70	0
47	D1	97/98 (98%)	0.50	2 (2%)	63 61	30, 44, 66, 73	0
48	B2	70/72 (97%)	0.29	0	100 100	25, 42, 57, 67	0
48	D2	70/72 (97%)	0.60	4 (5%)	23 22	51, 64, 70, 72	0
49	B3	59/60 (98%)	0.37	0	100 100	16, 29, 52, 70	0
49	D3	59/60 (98%)	0.88	5 (8%)	10 10	49, 63, 74, 78	0
50	B4	69/71 (97%)	1.18	16 (23%)	0 0	55, 71, 83, 88	0
50	D4	69/71 (97%)	2.29	33 (47%)	0 0	61, 74, 85, 89	0
51	B5	59/60 (98%)	0.74	1 (1%)	70 68	19, 32, 48, 58	0
51	D5	59/60 (98%)	0.20	0	100 100	25, 35, 52, 59	0
52	B6	53/54 (98%)	0.59	0	100 100	22, 38, 55, 57	0
52	D6	53/54 (98%)	0.49	3 (5%)	23 22	42, 56, 67, 73	0
53	B7	48/49 (97%)	0.77	3 (6%)	20 18	15, 26, 50, 64	0
53	D7	48/49 (97%)	0.87	4 (8%)	11 10	25, 37, 63, 68	0
54	B8	64/65 (98%)	0.42	0	100 100	21, 28, 35, 52	0
54	D8	64/65 (98%)	0.70	0	100 100	39, 51, 58, 64	0
55	B9	37/37 (100%)	0.67	0	100 100	26, 44, 62, 69	0
55	D9	37/37 (100%)	0.51	1 (2%)	54 52	39, 49, 64, 73	0
All	All	20920/21748 (96%)	0.59	1324 (6%)	20 18	15, 56, 82, 103	0

All (1324) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CA	1030(B)	C	11.7
50	D4	49	PHE	11.1

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Mol	Chain	Res	Type	RSRZ
23	CW	71	G	11.1
23	AW	71	G	9.7
25	BA	936	C	8.6
1	CA	1030(A)	G	8.6
25	DA	883	G	8.4
45	DZ	144	LEU	8.3
25	DA	888	C	8.2
1	AA	1030(B)	C	8.2
45	DZ	141	VAL	8.0
25	BA	942	A	7.9
25	DA	885	C	7.8
7	CG	83	ALA	7.7
14	CN	38	GLY	7.6
19	CS	80	TYR	7.6
25	DA	2802	G	7.6
14	CN	25	VAL	7.6
25	BA	943	C	7.4
1	CA	1001(A)	G	7.4
1	CA	1030(C)	G	7.4
45	DZ	155	LEU	7.3
1	CA	1033	G	7.3
25	BA	932	C	7.3
25	BA	934	A	7.2
1	AA	1030(C)	G	7.1
46	D0	3	HIS	7.0
23	CW	70	G	7.0
45	DZ	147	GLY	6.9
50	D4	50	VAL	6.8
50	D4	52	THR	6.7
45	DZ	149	SER	6.7
23	AW	70	G	6.6
50	D4	45	GLY	6.5
25	DA	887	A	6.5
9	CI	28	VAL	6.5
50	D4	63	TYR	6.5
43	DX	92	LEU	6.4
25	DA	884	C	6.4
25	DA	892	G	6.4
10	CJ	10	GLY	6.4
3	CC	155	GLY	6.3
14	CN	39	LEU	6.3
25	BA	1555	C	6.3

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Mol	Chain	Res	Type	RSRZ
25	DA	886	C	6.3
1	CA	1257	U	6.3
25	BA	2153	G	6.3
2	CB	123	ALA	6.2
14	CN	34	TYR	6.2
23	AW	72	C	6.2
30	DG	115	ARG	6.2
45	DZ	172	ALA	6.2
23	AY	20	U	6.2
14	CN	61	TRP	6.1
23	CW	72	C	6.1
25	DA	896	A	6.1
25	BA	931	C	6.1
25	BA	2181	G	6.0
10	CJ	85	LEU	6.0
7	CG	82	GLY	6.0
50	D4	59	PHE	5.9
22	CV	24	A	5.9
1	AA	1257	U	5.9
1	CA	1032	G	5.8
13	CM	87	TYR	5.8
14	CN	44	LEU	5.8
25	BA	2168	C	5.8
1	CA	1035	A	5.8
36	DQ	109	VAL	5.8
25	BA	933	C	5.8
13	CM	68	GLY	5.7
1	CA	1030	C	5.7
25	BA	935	C	5.7
25	DA	897	C	5.7
23	CY	45	U	5.5
1	CA	1036	G	5.5
1	AA	1028	C	5.5
1	AA	841	U	5.5
7	CG	156	TRP	5.5
9	CI	27	THR	5.5
45	DZ	148	ASP	5.5
25	BA	2162	C	5.4
25	DA	229	A	5.4
50	D4	54	GLY	5.4
23	CW	44	G	5.4
44	DY	1	MET	5.4

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Mol	Chain	Res	Type	RSRZ
25	DA	882	G	5.4
7	CG	147	ALA	5.4
2	CB	34	ALA	5.4
7	CG	2	ALA	5.4
1	AA	1030(A)	G	5.3
9	CI	65	VAL	5.3
25	BA	1120	G	5.3
23	CW	4	C	5.3
14	CN	55	GLY	5.3
23	CY	36	A	5.3
10	CJ	47	PHE	5.3
7	CG	81	GLY	5.3
7	AG	82	GLY	5.2
45	BZ	141	VAL	5.2
1	CA	1029	C	5.2
25	DA	889	C	5.2
25	BA	1112	U	5.2
7	CG	154	TYR	5.2
25	BA	2163	G	5.2
45	BZ	165	VAL	5.2
50	D4	53	GLU	5.2
30	DG	17	PRO	5.1
53	D7	46	VAL	5.1
25	BA	938	G	5.1
30	BG	146	TYR	5.1
25	DA	2144	U	5.1
45	BZ	147	GLY	5.1
3	CC	87	LEU	5.1
25	DA	2139	C	5.1
46	D0	5	LYS	5.0
25	DA	2146	C	5.0
1	CA	1024	G	5.0
45	DZ	170	THR	5.0
19	CS	30	LEU	5.0
1	AA	1030(D)	A	5.0
13	CM	124	PRO	5.0
45	DZ	152	ALA	5.0
23	CW	3	C	5.0
25	BA	2167	C	5.0
25	DA	2140	C	4.9
3	CC	51	GLY	4.9
1	CA	1532	U	4.9

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Mol	Chain	Res	Type	RSRZ
23	AY	35	A	4.9
1	AA	1031	G	4.9
13	CM	123	ALA	4.9
1	CA	1034	G	4.9
30	DG	85	GLY	4.9
13	AM	25	ILE	4.9
30	DG	39	ILE	4.9
3	CC	145	GLY	4.8
23	AW	73	A	4.8
12	CL	95	GLY	4.8
2	CB	127	ILE	4.8
14	AN	7	ILE	4.8
14	CN	35	ARG	4.8
23	AW	44	G	4.8
1	CA	1027	C	4.8
23	CW	31	A	4.8
9	CI	72	GLY	4.7
30	DG	61	ALA	4.7
19	CS	50	ALA	4.7
50	D4	40	HIS	4.7
13	CM	64	TRP	4.7
7	CG	117	ALA	4.7
10	CJ	72	VAL	4.7
3	AC	81	GLY	4.7
3	CC	182	ILE	4.7
30	DG	140	ILE	4.7
53	B7	48	LYS	4.6
27	DD	2	ALA	4.6
45	BZ	155	LEU	4.6
25	DA	2804	C	4.6
44	DY	65	ALA	4.6
2	CB	216	SER	4.6
45	DZ	128	VAL	4.5
14	CN	51	GLY	4.5
9	CI	114	TYR	4.5
3	CC	157	ILE	4.5
7	CG	6	ARG	4.5
50	B4	46	GLN	4.5
25	BA	2166	U	4.5
3	AC	80	GLY	4.5
2	AB	233	SER	4.5
14	CN	37	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
3	CC	193	TYR	4.5
14	CN	12	ARG	4.5
25	BA	1221	G	4.5
2	CB	31	TYR	4.5
13	CM	20	THR	4.5
1	AA	1034	G	4.5
45	BZ	169	GLU	4.5
1	CA	998	G	4.4
13	CM	100	GLY	4.4
25	DA	2801(A)	A	4.4
1	AA	1001(A)	G	4.4
9	CI	15	ALA	4.4
3	AC	87	LEU	4.4
25	DA	894	C	4.4
10	CJ	13	HIS	4.4
1	AA	1027	C	4.4
2	CB	165	VAL	4.4
45	BZ	164	ALA	4.4
1	CA	1031	G	4.4
50	D4	18	CYS	4.4
50	D4	68	ARG	4.3
2	AB	207	ALA	4.3
30	DG	151	ALA	4.3
25	BA	2806	G	4.3
9	CI	8	GLY	4.3
19	CS	63	THR	4.3
45	BZ	104	PHE	4.3
5	CE	13	ILE	4.3
19	CS	40	ILE	4.3
1	AA	1033	G	4.3
19	CS	79	THR	4.3
23	AY	36	A	4.3
47	B1	2	SER	4.3
13	CM	70	LEU	4.3
14	CN	42	ILE	4.2
45	BZ	167	PRO	4.2
23	CW	45	U	4.2
4	AD	104	VAL	4.2
45	BZ	120	ILE	4.2
1	CA	1531	A	4.2
25	BA	2816	G	4.2
18	CR	85	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
9	CI	81	ILE	4.2
25	BA	2805	G	4.2
12	CL	28	LYS	4.2
25	BA	941	U	4.2
30	DG	139	LEU	4.2
1	CA	1286	A	4.2
31	DH	44	VAL	4.2
7	CG	84	ASN	4.2
23	AY	13	C	4.2
25	DA	1509	C	4.2
9	CI	103	THR	4.2
1	AA	1032	G	4.2
23	AY	34	G	4.2
46	D0	2	ALA	4.2
1	CA	1002	G	4.1
25	BA	930	G	4.1
50	D4	44	THR	4.1
9	AI	15	ALA	4.1
38	DS	20	ARG	4.1
23	AY	24	G	4.1
30	DG	29	TRP	4.1
9	AI	117	HIS	4.1
7	CG	24	THR	4.1
13	CM	60	VAL	4.1
23	AY	19	G	4.1
25	DA	2160	G	4.1
50	B4	63	TYR	4.1
23	AY	47	U	4.1
25	DA	2154	G	4.1
1	AA	1532	U	4.1
25	BA	1220	U	4.1
21	CU	14	TRP	4.1
10	AJ	36	GLY	4.1
13	CM	88	ARG	4.1
10	CJ	65	LEU	4.0
25	DA	2155	G	4.0
1	AA	1029	C	4.0
45	DZ	106	GLY	4.0
17	CQ	9	VAL	4.0
45	DZ	139	VAL	4.0
1	AA	1030	C	4.0
25	BA	2169	G	4.0

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Mol	Chain	Res	Type	RSRZ
9	CI	123	PRO	4.0
2	CB	51	LEU	4.0
23	CW	28	G	4.0
12	CL	60	LEU	4.0
7	CG	7	ALA	4.0
45	DZ	9	TYR	4.0
49	D3	47	VAL	4.0
51	B5	60	VAL	4.0
1	AA	1036	G	4.0
45	DZ	4	ARG	4.0
45	DZ	50	GLN	4.0
23	AW	67	C	3.9
9	CI	95	LYS	3.9
25	DA	899	A	3.9
9	CI	14	VAL	3.9
9	CI	7	THR	3.9
3	CC	198	VAL	3.9
45	BZ	150	LEU	3.9
50	B4	49	PHE	3.9
9	AI	81	ILE	3.9
25	DA	2803	C	3.9
44	DY	55	TYR	3.9
13	CM	120	LYS	3.9
25	DA	1026	U	3.9
25	DA	1041	C	3.9
1	CA	1030(D)	A	3.9
23	CY	19	G	3.9
25	DA	2792	G	3.9
25	DA	2793	G	3.9
13	CM	92	HIS	3.8
1	CA	1040	U	3.8
23	AW	69	G	3.8
25	DA	2161	C	3.8
45	DZ	57	ILE	3.8
50	D4	27	THR	3.8
23	CY	44	G	3.8
45	DZ	140	ASP	3.8
12	CL	39	VAL	3.8
2	CB	236	TYR	3.8
14	CN	36	PHE	3.8
25	BA	945	A	3.8
7	AG	79	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
17	CQ	23	VAL	3.8
3	CC	159	GLY	3.8
5	CE	99	GLY	3.8
9	CI	57	GLY	3.8
3	AC	193	TYR	3.8
10	CJ	63	PHE	3.8
47	D1	2	SER	3.8
50	D4	43	TYR	3.8
1	CA	1007	C	3.8
23	AW	20	U	3.8
23	AY	22	G	3.8
23	CW	5	G	3.8
49	D3	29	ARG	3.8
1	AA	1447	A	3.8
7	CG	4	ARG	3.7
30	DG	136	ARG	3.7
1	CA	1039	C	3.7
25	DA	898	C	3.7
43	DX	95	LEU	3.7
50	B4	66	SER	3.7
25	BA	926	G	3.7
14	CN	43	CYS	3.7
25	DA	890	A	3.7
29	DF	115	ALA	3.7
9	AI	113	LYS	3.7
50	D4	32	TYR	3.7
25	BA	2807	C	3.7
9	AI	19	LEU	3.7
18	AR	24	ALA	3.7
25	BA	1123	A	3.7
3	CC	179	ARG	3.7
24	AX	67	C	3.7
2	CB	37	ASN	3.7
14	CN	30	ALA	3.7
19	CS	51	VAL	3.7
12	CL	64	TYR	3.7
25	DA	2141	G	3.7
9	AI	80	GLY	3.7
10	CJ	44	VAL	3.7
1	CA	1001	A	3.6
50	B4	68	ARG	3.6
9	CI	90	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
13	AM	2	ALA	3.6
25	DA	2805	G	3.6
9	CI	30	GLY	3.6
9	CI	115	GLY	3.6
30	BG	51	ARG	3.6
50	D4	48	ARG	3.6
13	AM	26	GLY	3.6
23	CW	15	G	3.6
50	B4	55	ARG	3.6
15	CO	4	THR	3.6
33	DN	102	ALA	3.6
25	BA	1141	A	3.6
9	CI	13	ALA	3.6
13	CM	63	THR	3.6
25	BA	2180	A	3.6
25	BA	2803	A	3.6
30	DG	7	LEU	3.6
23	CW	69	G	3.6
30	DG	57	ALA	3.6
53	D7	48	LYS	3.6
23	CY	23	A	3.5
3	CC	188	LEU	3.5
23	CW	30	G	3.5
14	CN	7	ILE	3.5
21	AU	16	GLY	3.5
23	CW	14	A	3.5
25	DA	900	A	3.5
41	DV	30	GLY	3.5
25	DA	2896	C	3.5
9	CI	86	VAL	3.5
13	CM	7	VAL	3.5
25	BA	2170	G	3.5
45	DZ	20	ARG	3.5
20	CT	55	ILE	3.5
1	CA	1021	G	3.5
50	B4	52	THR	3.5
31	DH	45	VAL	3.5
45	BZ	149	SER	3.5
25	BA	2161	C	3.5
25	BA	1124	U	3.5
14	CN	22	THR	3.5
9	CI	9	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
14	CN	31	ARG	3.5
19	CS	11	VAL	3.5
45	DZ	58	VAL	3.5
14	CN	11	LYS	3.5
13	CM	4	ILE	3.4
30	DG	138	GLN	3.4
44	BY	1	MET	3.4
38	DS	22	GLY	3.4
31	DH	35	VAL	3.4
23	AY	5	G	3.4
7	CG	32	ARG	3.4
23	CY	35	A	3.4
23	AW	3	C	3.4
2	CB	203	GLY	3.4
1	CA	1003	G	3.4
10	CJ	74	ILE	3.4
46	D0	45	PHE	3.4
25	BA	2815	C	3.4
7	CG	40	ALA	3.4
25	BA	2173	G	3.4
31	DH	93	GLY	3.4
50	B4	48	ARG	3.4
30	DG	38	VAL	3.4
45	BZ	146	ILE	3.4
23	CW	47	U	3.4
25	BA	302	A	3.4
3	CC	64	VAL	3.4
3	CC	39	ILE	3.4
9	CI	128	ARG	3.4
30	DG	62	LEU	3.4
7	AG	83	ALA	3.4
9	CI	36	TYR	3.4
14	CN	13	THR	3.4
19	CS	52	TYR	3.4
1	AA	1531	A	3.4
22	CV	12	A	3.4
1	CA	1028	C	3.4
21	CU	16	GLY	3.3
50	D4	42	PHE	3.3
13	CM	93	ARG	3.3
23	CY	66	U	3.3
25	BA	2164	C	3.3

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Mol	Chain	Res	Type	RSRZ
25	DA	2145	C	3.3
30	DG	80	PHE	3.3
31	DH	105	LEU	3.3
23	CW	29	G	3.3
53	B7	47	ARG	3.3
9	CI	109	VAL	3.3
14	CN	40	CYS	3.3
45	BZ	159	PRO	3.3
1	AA	1024	G	3.3
25	BA	1114	G	3.3
27	BD	276	LYS	3.3
9	CI	17	VAL	3.3
5	CE	8	GLU	3.3
10	CJ	59	SER	3.3
13	CM	53	VAL	3.3
27	DD	18	VAL	3.3
3	CC	160	ALA	3.3
9	CI	125	TYR	3.3
25	DA	2116	G	3.3
27	DD	113	VAL	3.3
31	DH	52	VAL	3.3
50	B4	56	VAL	3.3
5	AE	96	PRO	3.3
19	CS	48	THR	3.3
28	DE	71	GLY	3.3
13	CM	69	GLU	3.3
25	BA	1105	G	3.2
1	CA	204	U	3.2
25	BA	1111	U	3.2
23	CY	67	C	3.2
2	CB	210	SER	3.2
45	DZ	16	SER	3.2
19	CS	9	VAL	3.2
14	CN	58	LYS	3.2
1	AA	1035	A	3.2
19	CS	41	VAL	3.2
7	CG	10	ARG	3.2
30	DG	49	ASP	3.2
45	DZ	96	VAL	3.2
45	DZ	154	ASP	3.2
9	CI	63	ILE	3.2
38	DS	12	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
25	BA	937	A	3.2
35	DP	92	GLU	3.2
50	D4	57	GLU	3.2
2	AB	36	ARG	3.2
25	BA	271	U	3.2
10	AJ	93	GLY	3.2
20	CT	9	ASN	3.2
13	CM	90	LEU	3.2
30	DG	146	TYR	3.2
2	CB	29	ALA	3.2
25	DA	2173	A	3.2
30	DG	181	ARG	3.2
46	D0	7	LEU	3.2
50	B4	50	VAL	3.2
2	CB	218	ALA	3.1
13	AM	75	ALA	3.1
25	BA	2151	C	3.1
30	DG	48	GLU	3.1
38	DS	81	GLY	3.1
50	B4	54	GLY	3.1
45	DZ	156	LYS	3.1
16	CP	59	TRP	3.1
19	CS	36	ARG	3.1
16	CP	51	VAL	3.1
2	CB	207	ALA	3.1
9	CI	105	ASP	3.1
30	DG	114	ILE	3.1
30	DG	141	PHE	3.1
11	CK	17	GLY	3.1
25	BA	2171	G	3.1
25	DA	2319	G	3.1
1	CA	161	A	3.1
30	DG	11	TYR	3.1
3	CC	124	ILE	3.1
25	BA	2150	C	3.1
25	DA	2128	C	3.1
10	CJ	55	LYS	3.1
13	CM	76	ALA	3.1
30	DG	110	ALA	3.1
19	CS	65	ASN	3.1
45	DZ	153	SER	3.1
36	DQ	32	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
2	CB	223	ILE	3.1
2	AB	234	PRO	3.1
46	D0	71	ASP	3.1
25	BA	2176	G	3.1
4	AD	168	ARG	3.1
7	CG	5	ARG	3.1
25	DA	878	A	3.1
50	B4	45	GLY	3.1
25	DA	2153	G	3.1
10	CJ	11	PHE	3.1
11	CK	93	GLN	3.1
7	CG	79	ARG	3.1
25	BA	1122	C	3.1
9	CI	52	ALA	3.1
9	CI	106	ALA	3.1
3	AC	82	GLU	3.0
9	CI	49	PRO	3.0
23	CW	22	G	3.0
25	BA	1109	G	3.0
1	CA	980	C	3.0
9	CI	45	ALA	3.0
25	BA	939	C	3.0
30	DG	35	GLU	3.0
3	CC	8	ILE	3.0
10	CJ	96	ILE	3.0
23	CY	12	U	3.0
5	CE	22	GLY	3.0
23	AY	1	G	3.0
3	CC	53	ALA	3.0
5	CE	12	LEU	3.0
20	CT	38	LYS	3.0
11	CK	48	ILE	3.0
21	CU	24	ARG	3.0
9	CI	82	ALA	3.0
10	CJ	90	LEU	3.0
13	CM	75	ALA	3.0
25	DA	614(B)	G	3.0
30	DG	6	ALA	3.0
30	DG	133	LEU	3.0
8	AH	53	VAL	3.0
12	CL	55	VAL	3.0
1	AA	163	C	3.0

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Mol	Chain	Res	Type	RSRZ
25	BA	1110	C	3.0
9	CI	37	PHE	3.0
9	CI	80	GLY	3.0
15	AO	87	ILE	3.0
5	AE	94	ALA	3.0
13	CM	15	VAL	3.0
23	CW	13	C	3.0
13	CM	84	ILE	3.0
19	CS	14	HIS	3.0
17	CQ	12	SER	3.0
45	DZ	3	TYR	3.0
30	DG	51	ARG	3.0
30	BG	150	ASP	3.0
50	D4	51	ASP	3.0
8	CH	124	ALA	3.0
25	BA	218	A	3.0
9	CI	120	ARG	3.0
10	AJ	46	ARG	3.0
13	CM	26	GLY	3.0
12	CL	90	VAL	2.9
45	DZ	11	GLU	2.9
10	AJ	4	ILE	2.9
1	CA	1112	C	2.9
23	CY	57	G	2.9
25	DA	876	C	2.9
29	DF	15	SER	2.9
50	D4	38	LYS	2.9
17	CQ	95	TYR	2.9
20	AT	13	LEU	2.9
36	DQ	37	LEU	2.9
23	CW	73	A	2.9
23	CY	21	A	2.9
5	AE	10	MET	2.9
23	AW	4	C	2.9
23	CY	62	C	2.9
25	DA	2137	C	2.9
30	DG	163	ALA	2.9
31	DH	32	GLU	2.9
31	DH	106	THR	2.9
27	DD	275	LYS	2.9
10	AJ	62	HIS	2.9
46	B0	3	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
4	CD	47	ARG	2.9
4	AD	86	LYS	2.9
19	CS	12	ASP	2.9
25	BA	940	C	2.9
1	CA	1023	G	2.9
9	AI	14	VAL	2.9
11	CK	109	VAL	2.9
1	AA	1025	U	2.9
23	AY	45	U	2.9
45	DZ	104	PHE	2.9
45	DZ	171	ILE	2.9
5	AE	95	ALA	2.9
30	DG	152	LEU	2.9
45	DZ	157	LEU	2.9
17	CQ	92	ARG	2.9
25	BA	2814	C	2.9
23	CY	5	G	2.9
23	CY	14	A	2.9
25	BA	1878	A	2.9
30	BG	49	ASP	2.9
30	DG	65	GLY	2.9
36	DQ	33	GLY	2.9
4	CD	168	ARG	2.9
2	CB	33	TYR	2.9
13	CM	23	TYR	2.9
31	DH	25	LYS	2.9
19	CS	35	SER	2.9
45	DZ	93	ASP	2.9
1	AA	1003	G	2.9
25	BA	929	G	2.9
25	BA	2174	G	2.9
9	CI	93	ARG	2.9
23	CY	58	A	2.9
4	AD	165	MET	2.8
9	CI	71	SER	2.8
43	DX	94	GLY	2.8
36	DQ	5	ARG	2.8
53	D7	47	ARG	2.8
17	CQ	100	LYS	2.8
3	CC	129	ALA	2.8
9	CI	76	ALA	2.8
25	BA	2134	G	2.8

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Mol	Chain	Res	Type	RSRZ
9	CI	88	TYR	2.8
21	CU	15	ARG	2.8
31	DH	6	ARG	2.8
25	BA	697	C	2.8
10	AJ	32	ALA	2.8
36	DQ	114	ALA	2.8
22	AV	13	A	2.8
50	D4	10	VAL	2.8
1	CA	1196	U	2.8
23	CW	2	C	2.8
25	BA	2165	C	2.8
25	DA	1113	U	2.8
7	CG	16	LEU	2.8
17	CQ	22	LEU	2.8
38	DS	3	ARG	2.8
19	CS	68	GLY	2.8
30	DG	41	GLN	2.8
23	AW	65	G	2.8
23	AY	44	G	2.8
25	BA	2177	G	2.8
11	AK	75	TYR	2.8
25	DA	2167	U	2.8
2	CB	188	ALA	2.8
30	DG	116	ASP	2.8
30	DG	42	GLY	2.8
45	DZ	92	SER	2.8
14	CN	24	CYS	2.8
2	AB	15	VAL	2.8
19	AS	67	VAL	2.8
50	D4	28	LYS	2.8
14	AN	51	GLY	2.8
9	CI	116	LYS	2.8
9	CI	75	ASP	2.8
25	BA	1136	U	2.8
25	BA	2154	U	2.8
4	CD	23	GLY	2.8
25	DA	2115	G	2.8
9	CI	126	SER	2.8
23	CY	68	C	2.8
25	BA	2183	C	2.8
36	BQ	59	ARG	2.8
25	BA	1985	U	2.7

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Mol	Chain	Res	Type	RSRZ
12	CL	93	LEU	2.7
30	DG	78	SER	2.7
25	BA	944	C	2.7
4	CD	33	MET	2.7
19	CS	67	VAL	2.7
35	DP	101	VAL	2.7
41	DV	14	VAL	2.7
44	DY	80	GLY	2.7
50	D4	64	GLY	2.7
2	CB	32	ILE	2.7
7	CG	85	TYR	2.7
36	DQ	66	ILE	2.7
50	D4	39	CYS	2.7
1	CA	1008	C	2.7
1	CA	1452	C	2.7
25	DA	2157	G	2.7
12	CL	18	VAL	2.7
19	CS	81	ARG	2.7
19	CS	31	ILE	2.7
45	DZ	146	ILE	2.7
22	AV	14	A	2.7
14	CN	14	PRO	2.7
2	AB	227	GLY	2.7
1	CA	1367	C	2.7
3	CC	202	ILE	2.7
9	CI	31	GLN	2.7
13	CM	101	GLN	2.7
30	DG	3	LEU	2.7
30	DG	60	LEU	2.7
30	DG	111	LEU	2.7
30	DG	157	ILE	2.7
38	DS	58	LEU	2.7
7	CG	155	ARG	2.7
15	AO	89	GLY	2.7
22	CV	14	A	2.7
23	AY	21	A	2.7
25	BA	925	A	2.7
43	DX	93	GLU	2.7
13	CM	17	VAL	2.7
4	CD	196	LEU	2.7
30	BG	80	PHE	2.7
30	DG	12	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
50	D4	55	ARG	2.7
31	DH	13	LYS	2.7
6	CF	55	ASP	2.7
7	CG	80	VAL	2.7
10	AJ	97	GLU	2.7
25	DA	2142	C	2.7
27	DD	158	ALA	2.7
45	DZ	51	ALA	2.7
25	BA	2172	U	2.7
30	BG	43	LEU	2.7
45	DZ	124	ILE	2.7
24	AX	4	G	2.7
29	DF	16	GLY	2.7
3	AC	89	GLU	2.6
10	AJ	94	VAL	2.6
11	AK	14	VAL	2.6
25	DA	1536	C	2.6
30	BG	88	ILE	2.6
19	AS	72	GLY	2.6
9	AI	98	PRO	2.6
3	CC	206	GLU	2.6
25	DA	1170	G	2.6
10	CJ	68	HIS	2.6
26	DB	90	A	2.6
19	AS	71	LEU	2.6
19	CS	84	GLY	2.6
50	D4	7	PRO	2.6
3	CC	88	ARG	2.6
30	DG	182	LYS	2.6
1	AA	1026	G	2.6
1	CA	1220	G	2.6
25	BA	2178	G	2.6
7	CG	34	GLY	2.6
10	CJ	100	THR	2.6
15	CO	16	ALA	2.6
9	CI	4	TYR	2.6
33	BN	9	VAL	2.6
35	DP	31	ALA	2.6
48	D2	9	GLN	2.6
38	DS	5	THR	2.6
53	D7	45	ALA	2.6
1	CA	1026	G	2.6

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Mol	Chain	Res	Type	RSRZ
13	AM	90	LEU	2.6
17	AQ	98	LEU	2.6
23	CY	34	G	2.6
25	BA	2175	G	2.6
25	DA	2133	G	2.6
43	DX	68	ARG	2.6
25	DA	652(B)	A	2.6
26	DB	59	A	2.6
23	AW	2	C	2.6
25	DA	2138	C	2.6
45	DZ	121	HIS	2.6
20	AT	38	LYS	2.6
27	DD	38	LYS	2.6
11	CK	61	ALA	2.6
13	CM	80	ARG	2.6
21	AU	8	THR	2.6
21	CU	9	ARG	2.6
38	DS	54	LEU	2.6
23	CY	1	G	2.6
45	DZ	169	GLU	2.6
25	DA	2794	C	2.6
9	CI	54	ASP	2.6
3	CC	177	THR	2.6
27	BD	2	ALA	2.6
9	CI	35	GLU	2.6
30	DG	107	LEU	2.6
25	DA	2897	U	2.6
3	CC	41	GLY	2.6
25	BA	2817	G	2.6
31	DH	2	SER	2.6
31	DH	48	GLY	2.6
10	AJ	18	ALA	2.5
3	CC	207	VAL	2.5
16	AP	62	VAL	2.5
27	DD	3	VAL	2.5
3	CC	178	LEU	2.5
19	CS	70	LYS	2.5
45	DZ	70	LEU	2.5
45	DZ	150	LEU	2.5
11	CK	90	GLY	2.5
9	CI	110	GLU	2.5
22	CV	23	A	2.5

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Mol	Chain	Res	Type	RSRZ
1	CA	1385	G	2.5
20	CT	59	ALA	2.5
23	CW	10	G	2.5
25	DA	2159	G	2.5
2	AB	229	VAL	2.5
10	CJ	39	PRO	2.5
3	CC	196	LEU	2.5
9	AI	121	ARG	2.5
25	DA	895	U	2.5
2	AB	105	PHE	2.5
4	AD	158	ILE	2.5
5	AE	5	ASP	2.5
9	AI	100	GLY	2.5
28	BE	71	GLY	2.5
3	CC	180	ALA	2.5
20	CT	12	ALA	2.5
14	CN	54	PRO	2.5
1	AA	1007	C	2.5
2	CB	44	LEU	2.5
19	CS	71	LEU	2.5
27	DD	273	ARG	2.5
31	DH	17	VAL	2.5
36	DQ	59	ARG	2.5
25	BA	2155	G	2.5
25	DA	2190	G	2.5
23	CW	50	U	2.5
9	CI	6	GLY	2.5
17	AQ	36	ILE	2.5
27	DD	276	LYS	2.5
36	DQ	65	PHE	2.5
13	CM	82	MET	2.5
9	AI	52	ALA	2.5
14	AN	2	ALA	2.5
31	DH	36	PRO	2.5
9	AI	65	VAL	2.5
13	CM	96	LEU	2.5
23	CW	23	A	2.5
1	CA	1037	C	2.5
5	CE	6	PHE	2.5
25	DA	2127	G	2.5
12	CL	41	ARG	2.5
13	CM	110	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
38	DS	17	ARG	2.5
2	AB	188	ALA	2.5
17	AQ	28	PRO	2.5
32	DI	59	ALA	2.5
2	CB	220	ASP	2.5
19	CS	13	ASP	2.5
29	BF	20	LEU	2.5
30	DG	15	VAL	2.5
45	DZ	5	LEU	2.5
1	AA	840	C	2.5
2	CB	17	PHE	2.5
17	AQ	27	PHE	2.5
30	BG	48	GLU	2.5
31	DH	123	PHE	2.5
48	D2	7	ARG	2.5
25	DA	1533	G	2.5
3	CC	15	THR	2.5
4	CD	164	ALA	2.5
4	CD	94	LEU	2.5
18	AR	85	LEU	2.5
31	DH	79	VAL	2.5
38	DS	56	LEU	2.5
35	DP	94	GLU	2.5
9	CI	42	ARG	2.5
9	CI	51	ARG	2.5
25	BA	2131	U	2.5
2	CB	211	ILE	2.5
9	CI	18	PHE	2.5
44	DY	44	ILE	2.5
4	AD	167	GLY	2.5
11	AK	68	ALA	2.5
15	AO	23	GLY	2.5
23	AY	15	G	2.5
25	BA	2843	G	2.5
25	DA	1042	G	2.5
30	DG	137	GLU	2.5
3	CC	6	HIS	2.4
11	AK	78	GLN	2.4
14	AN	41	ARG	2.4
18	AR	42	ARG	2.4
14	AN	56	VAL	2.4
41	DV	72	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
25	BA	1140	U	2.4
4	AD	110	PHE	2.4
7	CG	27	ILE	2.4
14	AN	16	PHE	2.4
2	CB	48	MET	2.4
45	BZ	148	ASP	2.4
11	CK	46	GLY	2.4
8	CH	104	ARG	2.4
9	AI	31	GLN	2.4
20	CT	49	ALA	2.4
27	BD	112	GLN	2.4
35	DP	15	ARG	2.4
46	D0	4	LYS	2.4
4	CD	186	LEU	2.4
24	CX	4	G	2.4
25	BA	1137	G	2.4
25	BA	2179	G	2.4
30	DG	135	LEU	2.4
27	BD	18	VAL	2.4
4	AD	138	TYR	2.4
24	AX	47	U	2.4
25	BA	2152	U	2.4
5	CE	131	ILE	2.4
19	CS	82	GLY	2.4
36	DQ	113	GLN	2.4
2	CB	19	HIS	2.4
23	AY	56	C	2.4
3	CC	94	LEU	2.4
5	AE	34	VAL	2.4
1	CA	1190	G	2.4
50	D4	67	TYR	2.4
44	DY	5	MET	2.4
52	D6	50	ARG	2.4
44	DY	58	GLY	2.4
9	CI	61	ALA	2.4
8	CH	112	LEU	2.4
30	DG	19	LEU	2.4
10	CJ	22	LYS	2.4
49	D3	54	VAL	2.4
52	D6	52	VAL	2.4
9	CI	121	ARG	2.4
3	AC	39	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
30	DG	25	TYR	2.4
10	AJ	47	PHE	2.4
31	DH	47	GLU	2.4
6	CF	29	ALA	2.4
1	CA	1256	A	2.4
1	CA	1357	A	2.4
11	AK	98	LEU	2.4
25	BA	1113	A	2.4
25	BA	1138	C	2.4
25	BA	2812	A	2.4
30	DG	28	VAL	2.4
41	DV	47	VAL	2.4
45	DZ	47	VAL	2.4
13	AM	68	GLY	2.4
30	DG	121	ASN	2.4
50	D4	17	GLY	2.4
4	AD	70	ILE	2.4
30	DG	88	ILE	2.4
2	CB	131	PRO	2.4
9	CI	33	PHE	2.4
13	CM	41	PRO	2.4
45	BZ	152	ALA	2.4
2	CB	121	LEU	2.4
2	CB	124	SER	2.4
36	DQ	6	ARG	2.4
2	CB	212	GLN	2.4
30	DG	106	LEU	2.4
32	DI	38	LEU	2.4
1	AA	1286	A	2.4
1	CA	1115	C	2.4
4	AD	170	VAL	2.4
9	AI	26	VAL	2.4
23	CY	56	C	2.4
24	CX	72	A	2.4
25	BA	1142	A	2.4
25	DA	645	C	2.4
25	DA	2062	A	2.4
47	D1	62	VAL	2.4
4	AD	164	ALA	2.4
13	CM	66	LEU	2.4
35	DP	34	GLY	2.3
38	DS	45	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	CA	1303	C	2.3
25	BA	1118	C	2.3
25	BA	1125	C	2.3
25	DA	2113	U	2.3
2	CB	232	PRO	2.3
30	DG	87	PRO	2.3
9	CI	62	TYR	2.3
3	AC	100	ALA	2.3
14	CN	10	ALA	2.3
41	DV	71	LEU	2.3
2	AB	125	PRO	2.3
30	DG	142	PRO	2.3
25	DA	2298	A	2.3
45	DZ	145	GLU	2.3
3	AC	168	ALA	2.3
9	CI	122	ALA	2.3
11	CK	25	TYR	2.3
11	CK	74	ALA	2.3
14	CN	50	LYS	2.3
35	DP	93	GLY	2.3
45	BZ	160	GLY	2.3
9	CI	56	LEU	2.3
1	CA	1060	C	2.3
1	CA	1197	G	2.3
25	DA	2206	G	2.3
1	CA	1447	A	2.3
25	DA	2126	A	2.3
32	DI	74	ASN	2.3
7	CG	76	ARG	2.3
7	CG	94	ARG	2.3
2	CB	201	ILE	2.3
36	DQ	28	ALA	2.3
23	CY	15	G	2.3
25	DA	2148	G	2.3
9	CI	32	ASP	2.3
2	CB	81	VAL	2.3
12	CL	65	GLU	2.3
32	BI	41	GLU	2.3
11	AK	94	ALA	2.3
11	AK	107	SER	2.3
50	B4	65	ASP	2.3
45	DZ	38	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	AA	1503	A	2.3
9	CI	102	LEU	2.3
23	CY	29	G	2.3
25	DA	869	G	2.3
12	AL	43	VAL	2.3
9	CI	23	ASN	2.3
3	CC	185	GLY	2.3
2	AB	222	ILE	2.3
13	CM	78	ILE	2.3
30	DG	23	PHE	2.3
30	DG	58	GLN	2.3
30	DG	100	TRP	2.3
33	DN	8	GLN	2.3
50	D4	66	SER	2.3
2	AB	120	ALA	2.3
20	AT	40	ALA	2.3
1	CA	1362	C	2.3
8	AH	133	LEU	2.3
8	CH	133	LEU	2.3
15	AO	81	LEU	2.3
17	CQ	98	LEU	2.3
24	CX	71	C	2.3
21	CU	6	ARG	2.2
1	CA	79	G	2.2
1	CA	1224	G	2.2
24	AX	70	G	2.2
25	BA	2813	G	2.2
25	DA	880	G	2.2
26	DB	56	G	2.2
5	CE	10	MET	2.2
25	BA	2906	U	2.2
10	CJ	18	ALA	2.2
13	CM	121	LYS	2.2
15	CO	57	LEU	2.2
50	D4	62	ARG	2.2
23	AY	58	A	2.2
25	BA	1128	U	2.2
23	CY	28	G	2.2
35	BP	98	GLU	2.2
31	DH	92	ILE	2.2
13	CM	65	LYS	2.2
30	DG	180	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
38	BS	6	ALA	2.2
10	AJ	45	ARG	2.2
45	BZ	80	ARG	2.2
28	BE	195	LEU	2.2
12	AL	64	TYR	2.2
13	AM	124	PRO	2.2
21	CU	11	GLY	2.2
29	DF	131	GLY	2.2
25	BA	696	C	2.2
25	BA	2905	C	2.2
7	CG	31	MET	2.2
38	DS	50	SER	2.2
45	BZ	166	SER	2.2
25	BA	924	U	2.2
25	BA	1144	A	2.2
10	CJ	98	ILE	2.2
50	B4	59	PHE	2.2
1	AA	347	G	2.2
1	CA	1154	G	2.2
23	CW	65	G	2.2
31	DH	128	PRO	2.2
38	DS	32	LEU	2.2
45	DZ	68	PRO	2.2
9	AI	11	LYS	2.2
7	CG	91	VAL	2.2
7	CG	119	ARG	2.2
13	CM	71	ARG	2.2
23	AW	45	U	2.2
23	CY	47	U	2.2
24	AX	68	C	2.2
46	D0	77	ARG	2.2
25	DA	2218	U	2.2
7	CG	30	ILE	2.2
13	CM	103	THR	2.2
18	AR	25	THR	2.2
23	CW	36	A	2.2
13	CM	12	ASN	2.2
3	CC	194	GLY	2.2
4	CD	11	LEU	2.2
4	CD	64	LEU	2.2
18	AR	79	LEU	2.2
21	AU	2	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
23	AY	65	G	2.2
25	DA	2162	G	2.2
38	BS	90	GLY	2.2
50	B4	64	GLY	2.2
9	AI	114	TYR	2.2
36	BQ	5	ARG	2.2
1	AA	1446	U	2.2
4	AD	112	VAL	2.2
42	BW	17	VAL	2.2
23	CW	61	C	2.2
25	BA	1126	C	2.2
29	DF	127	GLU	2.2
3	AC	124	ILE	2.2
5	CE	16	THR	2.2
10	AJ	98	ILE	2.2
14	CN	17	LYS	2.2
1	CA	1248	A	2.2
5	CE	84	PHE	2.2
19	CS	10	PHE	2.2
36	DQ	89	ASN	2.2
4	AD	19	LEU	2.2
12	CL	27	LEU	2.2
12	CL	63	GLY	2.2
14	CN	6	LEU	2.2
48	D2	21	LEU	2.2
19	CS	61	TYR	2.2
23	AW	5	G	2.2
25	BA	927	G	2.2
50	B4	53	GLU	2.2
1	CA	202	U	2.2
9	CI	112	LYS	2.2
12	AL	18	VAL	2.2
28	BE	1	MET	2.2
23	AY	12	U	2.2
13	AM	107	ALA	2.2
20	CT	44	ALA	2.2
31	DH	102	ALA	2.2
50	D4	5	ILE	2.2
5	CE	14	ARG	2.2
7	AG	81	GLY	2.2
29	BF	208	GLY	2.2
8	AH	67	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	CA	162	A	2.2
1	CA	1250	A	2.2
9	CI	99	LEU	2.2
19	CS	38	SER	2.2
9	CI	117	HIS	2.1
11	AK	25	TYR	2.1
2	CB	229	VAL	2.1
15	CO	60	VAL	2.1
25	DA	1039	G	2.1
26	DB	89	G	2.1
45	DZ	126	VAL	2.1
3	AC	157	ILE	2.1
5	AE	85	GLY	2.1
29	BF	180	GLY	2.1
46	D0	11	ARG	2.1
19	AS	40	ILE	2.1
4	CD	51	PRO	2.1
25	DA	893	C	2.1
4	AD	186	LEU	2.1
9	CI	50	LEU	2.1
4	AD	184	LYS	2.1
9	CI	127	LYS	2.1
25	DA	2117	A	2.1
48	D2	4	SER	2.1
15	AO	78	TYR	2.1
2	AB	165	VAL	2.1
13	AM	123	ALA	2.1
32	BI	136	VAL	2.1
40	DU	89	GLU	2.1
45	DZ	173	ALA	2.1
50	D4	19	GLY	2.1
36	DQ	75	THR	2.1
1	CA	485	G	2.1
1	CA	1186	G	2.1
25	BA	2138	G	2.1
25	BA	2203	G	2.1
25	DA	1114	G	2.1
25	DA	1117	G	2.1
49	D3	23	LEU	2.1
23	AY	4	C	2.1
19	AS	4	SER	2.1
1	CA	1014	A	2.1

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Mol	Chain	Res	Type	RSRZ
2	CB	116	GLU	2.1
25	DA	6	A	2.1
3	CC	63	ASN	2.1
32	BI	85	GLU	2.1
9	AI	8	GLY	2.1
19	CS	26	GLY	2.1
3	AC	65	ALA	2.1
10	AJ	44	VAL	2.1
11	AK	65	ALA	2.1
53	B7	46	VAL	2.1
4	CD	160	GLN	2.1
8	CH	134	ILE	2.1
27	DD	112	GLN	2.1
45	DZ	62	PRO	2.1
9	CI	101	PHE	2.1
2	CB	215	LEU	2.1
9	CI	19	LEU	2.1
9	CI	58	HIS	2.1
11	AK	79	SER	2.1
14	CN	49	HIS	2.1
18	AR	54	ARG	2.1
25	DA	881	G	2.1
25	DA	2147	G	2.1
50	D4	37	SER	2.1
27	BD	275	LYS	2.1
1	CA	1005	A	2.1
1	CA	1349	A	2.1
25	DA	1847	A	2.1
8	CH	65	TYR	2.1
13	CM	59	TYR	2.1
14	CN	18	VAL	2.1
38	DS	92	TYR	2.1
2	AB	232	PRO	2.1
3	CC	174	PRO	2.1
8	CH	101	PRO	2.1
29	DF	14	PRO	2.1
31	DH	10	PRO	2.1
55	D9	30	PRO	2.1
4	CD	146	ILE	2.1
3	CC	140	ARG	2.1
6	CF	77	ARG	2.1
9	CI	47	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
16	CP	9	PHE	2.1
19	AS	22	LEU	2.1
21	AU	14	TRP	2.1
27	DD	171	ASP	2.1
23	CW	42	C	2.1
25	BA	2130	C	2.1
25	DA	1116	C	2.1
11	AK	93	GLN	2.1
1	CA	1004	A	2.1
3	CC	7	PRO	2.1
4	AD	198	VAL	2.1
36	DQ	117	ALA	2.1
25	BA	2135	U	2.1
7	CG	41	ARG	2.1
7	CG	78	ARG	2.1
30	DG	165	THR	2.1
45	BZ	133	ILE	2.1
4	AD	93	PHE	2.1
45	DZ	151	HIS	2.1
11	CK	117	ASN	2.1
40	BU	43	GLY	2.1
2	AB	126	GLU	2.1
11	AK	73	MET	2.1
23	CW	25	C	2.1
25	DA	1043	C	2.1
25	DA	2129	C	2.1
1	CA	1061	G	2.1
1	CA	1323	G	2.1
25	BA	2182	G	2.1
31	DH	132	ARG	2.1
1	CA	1150	U	2.1
11	AK	80	VAL	2.1
13	AM	53	VAL	2.1
19	CS	76	PRO	2.1
38	DS	37	ALA	2.1
27	DD	205	VAL	2.1
4	CD	20	TYR	2.1
25	BA	2157	A	2.1
25	DA	901	A	2.1
49	D3	53	LEU	2.1
4	AD	87	GLY	2.1
5	AE	74	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
8	CH	135	CYS	2.1
31	BH	174	GLY	2.1
46	D0	42	GLY	2.1
7	AG	32	ARG	2.1
7	AG	2	ALA	2.0
16	CP	77	ALA	2.0
25	BA	1121	C	2.0
10	AJ	24	VAL	2.0
13	CM	117	VAL	2.0
27	DD	141	VAL	2.0
32	BI	86	THR	2.0
44	BY	85	VAL	2.0
23	AW	1	G	2.0
23	CY	65	G	2.0
25	BA	2188	G	2.0
25	DA	879	G	2.0
2	CB	152	PHE	2.0
3	CC	82	GLU	2.0
30	BG	152	LEU	2.0
30	DG	123	ASN	2.0
45	DZ	133	ILE	2.0
23	AW	14	A	2.0
31	DH	98	LEU	2.0
3	AC	2	GLY	2.0
36	DQ	86	GLY	2.0
7	AG	156	TRP	2.0
2	AB	123	ALA	2.0
9	AI	119	ALA	2.0
12	CL	43	VAL	2.0
25	BA	1127	U	2.0
28	DE	59	VAL	2.0
31	DH	18	GLU	2.0
52	D6	48	VAL	2.0
9	CI	78	LYS	2.0
16	AP	50	LYS	2.0
12	CL	59	ARG	2.0
14	CN	53	LEU	2.0
1	AA	1002	G	2.0
1	AA	1023	G	2.0
1	CA	1022	G	2.0
18	AR	29	PHE	2.0
24	CX	53	G	2.0

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Mol	Chain	Res	Type	RSRZ
1	CA	968	A	2.0
25	BA	2901	A	2.0
14	CN	46	GLU	2.0
3	CC	95	THR	2.0
9	CI	87	GLN	2.0
14	CN	27	CYS	2.0
1	CA	1149	C	2.0
4	CD	69	GLY	2.0
21	CU	2	GLY	2.0
23	AY	48	C	2.0
23	CW	49	C	2.0
25	DA	2143	C	2.0
26	DB	88	C	2.0
13	CM	48	LEU	2.0
1	CA	1111	A	2.0
23	AY	23	A	2.0
25	BA	1139	G	2.0
25	DA	2156	G	2.0
25	DA	2807	G	2.0
9	AI	90	PRO	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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	7MG	CY	46	24/25	0.65	0.24	84,93,103,111	0
23	4SU	CY	8	20/21	0.69	0.19	76,90,105,117	0
23	5MU	CY	54	21/22	0.70	0.24	78,87,97,118	0
23	7MG	AY	46	24/25	0.71	0.27	76,92,102,121	0
23	PSU	CY	32	20/21	0.72	0.25	71,78,92,94	0
23	4SU	CW	8	20/21	0.72	0.30	78,89,106,119	0
23	5MU	AY	54	21/22	0.75	0.28	70,85,94,111	0
23	7MG	CW	46	24/25	0.76	0.33	81,92,99,121	0
23	4SU	AY	8	20/21	0.77	0.20	77,91,110,118	0
23	PSU	CY	55	20/21	0.77	0.27	80,91,104,111	0
23	PSU	AY	55	20/21	0.78	0.30	82,92,102,111	0
23	7MG	AW	46	24/25	0.80	0.25	66,84,103,129	0
23	MIA	CY	37	22/30	0.81	0.33	65,78,95,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	PSU	AW	55	20/21	0.82	0.22	62,70,81,83	0
23	MIA	AY	37	22/30	0.83	0.30	69,78,88,91	0
23	PSU	AY	32	20/21	0.84	0.17	71,79,89,91	0
23	PSU	CW	55	20/21	0.85	0.20	64,74,85,87	0
23	4SU	AW	8	20/21	0.85	0.18	56,80,91,93	0
24	PSU	CX	55	20/21	0.87	0.19	48,69,86,88	0
23	5MU	CW	54	21/22	0.87	0.18	65,75,84,86	0
23	PSU	AW	32	20/21	0.88	0.19	61,69,75,77	0
23	PSU	CY	39	20/21	0.89	0.23	64,74,81,84	0
24	4SU	CX	8	20/21	0.89	0.14	65,74,85,85	0
23	MIA	CW	37	25/30	0.89	0.20	36,64,70,71	0
24	5MU	CX	54	21/22	0.90	0.26	70,78,82,89	0
23	PSU	AY	39	20/21	0.92	0.20	67,73,79,81	0
24	PSU	AX	55	20/21	0.92	0.20	45,66,84,85	0
23	PSU	CW	32	20/21	0.92	0.28	66,72,78,78	0
23	PSU	CW	39	20/21	0.93	0.27	57,65,69,71	0
23	MIA	AW	37	29/30	0.93	0.18	37,49,63,66	0
24	4SU	AX	8	20/21	0.93	0.17	53,60,66,68	0
23	PSU	AW	39	20/21	0.94	0.20	55,62,65,67	0
24	5MU	AX	54	21/22	0.94	0.20	54,66,74,75	0
23	5MU	AW	54	21/22	0.94	0.16	38,59,67,72	0
24	5MC	CX	32	21/22	0.94	0.17	51,66,72,75	0
24	5MC	AX	32	21/22	0.96	0.19	43,51,61,70	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. 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3720	1/1	0.33	0.24	73,73,73,73	0
56	MG	DA	3404	1/1	0.39	0.20	49,49,49,49	0
56	MG	AA	3054	1/1	0.42	0.22	68,68,68,68	0
56	MG	DE	305	1/1	0.52	0.23	49,49,49,49	0
56	MG	BA	3372	1/1	0.52	0.13	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3449	1/1	0.55	0.13	45,45,45,45	0
56	MG	AA	3139	1/1	0.56	0.20	82,82,82,82	0
56	MG	AA	3122	1/1	0.59	0.14	61,61,61,61	0
56	MG	BA	3469	1/1	0.59	0.17	61,61,61,61	0
56	MG	BA	3640	1/1	0.59	0.16	60,60,60,60	0
56	MG	BA	3694	1/1	0.59	0.23	62,62,62,62	0
56	MG	DA	3500	1/1	0.60	0.19	67,67,67,67	0
56	MG	BA	3617	1/1	0.60	0.12	44,44,44,44	0
56	MG	BA	3793	1/1	0.60	0.17	64,64,64,64	0
56	MG	BA	3759	1/1	0.61	0.12	44,44,44,44	0
56	MG	BA	3784	1/1	0.62	0.20	49,49,49,49	0
56	MG	DA	3582	1/1	0.62	0.19	52,52,52,52	0
56	MG	CA	3058	1/1	0.62	0.21	63,63,63,63	0
56	MG	DA	3247	1/1	0.62	0.12	63,63,63,63	0
56	MG	BA	3714	1/1	0.62	0.09	58,58,58,58	0
56	MG	DA	3621	1/1	0.63	0.16	48,48,48,48	0
56	MG	DA	3383	1/1	0.65	0.17	41,41,41,41	0
56	MG	BA	3454	1/1	0.65	0.19	39,39,39,39	0
56	MG	BA	3766	1/1	0.65	0.09	48,48,48,48	0
56	MG	BA	3643	1/1	0.66	0.18	60,60,60,60	0
56	MG	AW	102	1/1	0.66	0.13	69,69,69,69	0
56	MG	DA	3524	1/1	0.67	0.14	53,53,53,53	0
56	MG	CA	3056	1/1	0.67	0.16	84,84,84,84	0
56	MG	BA	3750	1/1	0.68	0.15	54,54,54,54	0
56	MG	BA	3505	1/1	0.68	0.20	44,44,44,44	0
56	MG	BA	3361	1/1	0.68	0.21	41,41,41,41	0
56	MG	DA	3117	1/1	0.68	0.25	62,62,62,62	0
56	MG	BA	3484	1/1	0.69	0.22	42,42,42,42	0
56	MG	AA	3153	1/1	0.69	0.12	58,58,58,58	0
56	MG	BB	3021	1/1	0.69	0.26	73,73,73,73	0
56	MG	CX	3004	1/1	0.70	0.16	61,61,61,61	0
56	MG	BA	3021	1/1	0.70	0.22	53,53,53,53	0
56	MG	AA	3063	1/1	0.70	0.15	55,55,55,55	0
56	MG	BP	205	1/1	0.70	0.11	44,44,44,44	0
56	MG	DA	3276	1/1	0.70	0.19	60,60,60,60	0
56	MG	BA	3491	1/1	0.71	0.26	44,44,44,44	0
56	MG	AA	3197	1/1	0.71	0.18	65,65,65,65	0
56	MG	BA	3318	1/1	0.71	0.17	53,53,53,53	0
56	MG	AX	3013	1/1	0.71	0.14	61,61,61,61	0
56	MG	DA	3075	1/1	0.72	0.12	57,57,57,57	0
56	MG	BA	3381	1/1	0.72	0.12	56,56,56,56	0
56	MG	CA	3040	1/1	0.72	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3008	1/1	0.72	0.19	71,71,71,71	0
56	MG	BA	3209	1/1	0.72	0.25	58,58,58,58	0
56	MG	BA	3630	1/1	0.72	0.22	29,29,29,29	0
56	MG	DA	3574	1/1	0.72	0.18	48,48,48,48	0
56	MG	BA	3448	1/1	0.72	0.14	48,48,48,48	0
56	MG	DA	3292	1/1	0.72	0.15	53,53,53,53	0
56	MG	DA	3505	1/1	0.72	0.10	61,61,61,61	0
56	MG	BA	3810	1/1	0.73	0.26	46,46,46,46	0
56	MG	DA	3658	1/1	0.73	0.36	60,60,60,60	0
56	MG	DA	3472	1/1	0.73	0.12	57,57,57,57	0
56	MG	BB	3020	1/1	0.73	0.15	64,64,64,64	0
56	MG	AA	3213	1/1	0.73	0.12	64,64,64,64	0
56	MG	DA	3521	1/1	0.73	0.14	56,56,56,56	0
56	MG	BA	3492	1/1	0.73	0.08	43,43,43,43	0
56	MG	BA	3673	1/1	0.73	0.22	62,62,62,62	0
56	MG	CA	3063	1/1	0.73	0.14	53,53,53,53	0
56	MG	CA	3125	1/1	0.73	0.11	61,61,61,61	0
56	MG	BA	3638	1/1	0.74	0.11	58,58,58,58	0
56	MG	BA	3813	1/1	0.74	0.22	59,59,59,59	0
56	MG	BA	3731	1/1	0.74	0.09	64,64,64,64	0
56	MG	DA	3408	1/1	0.74	0.14	53,53,53,53	0
56	MG	CA	3077	1/1	0.74	0.16	54,54,54,54	0
56	MG	BA	3182	1/1	0.74	0.20	59,59,59,59	0
56	MG	BA	3757	1/1	0.74	0.17	49,49,49,49	0
56	MG	AN	502	1/1	0.74	0.12	45,45,45,45	0
56	MG	CA	3078	1/1	0.74	0.12	48,48,48,48	0
56	MG	DA	3181	1/1	0.74	0.18	52,52,52,52	0
56	MG	DA	3447	1/1	0.74	0.23	50,50,50,50	0
56	MG	AB	3001	1/1	0.74	0.22	73,73,73,73	0
56	MG	CA	3188	1/1	0.74	0.16	72,72,72,72	0
56	MG	BA	3466	1/1	0.75	0.21	46,46,46,46	0
56	MG	DA	3040	1/1	0.75	0.13	51,51,51,51	0
56	MG	BA	3095	1/1	0.75	0.17	43,43,43,43	0
56	MG	DA	3355	1/1	0.75	0.14	48,48,48,48	0
56	MG	AW	104	1/1	0.75	0.11	64,64,64,64	0
56	MG	CA	3190	1/1	0.75	0.10	67,67,67,67	0
56	MG	BA	3659	1/1	0.75	0.15	55,55,55,55	0
56	MG	AA	3005	1/1	0.76	0.15	66,66,66,66	0
56	MG	DA	3116	1/1	0.76	0.32	66,66,66,66	0
56	MG	BA	3671	1/1	0.76	0.18	50,50,50,50	0
56	MG	DA	3325	1/1	0.76	0.19	53,53,53,53	0
56	MG	DA	3311	1/1	0.76	0.18	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3194	1/1	0.76	0.23	37,37,37,37	0
56	MG	BA	3508	1/1	0.76	0.17	48,48,48,48	0
56	MG	BA	3580	1/1	0.76	0.17	35,35,35,35	0
56	MG	CJ	5001	1/1	0.76	0.15	70,70,70,70	0
56	MG	BW	202	1/1	0.76	0.29	49,49,49,49	0
56	MG	CA	3009	1/1	0.76	0.15	46,46,46,46	0
56	MG	DA	3106	1/1	0.76	0.13	63,63,63,63	0
56	MG	BA	3665	1/1	0.76	0.16	49,49,49,49	0
56	MG	CA	3132	1/1	0.76	0.17	64,64,64,64	0
56	MG	BA	3212	1/1	0.76	0.13	49,49,49,49	0
56	MG	BB	3011	1/1	0.76	0.15	66,66,66,66	0
56	MG	DA	3360	1/1	0.76	0.09	47,47,47,47	0
56	MG	AA	3114	1/1	0.76	0.09	65,65,65,65	0
56	MG	CA	3175	1/1	0.77	0.13	62,62,62,62	0
56	MG	DA	3134	1/1	0.77	0.22	56,56,56,56	0
56	MG	DA	3076	1/1	0.77	0.22	44,44,44,44	0
56	MG	DA	3143	1/1	0.77	0.15	56,56,56,56	0
56	MG	BA	3600	1/1	0.77	0.15	43,43,43,43	0
56	MG	DA	3504	1/1	0.77	0.10	58,58,58,58	0
56	MG	CA	3057	1/1	0.77	0.13	59,59,59,59	0
56	MG	AA	3003	1/1	0.77	0.10	62,62,62,62	0
56	MG	AA	3124	1/1	0.77	0.15	58,58,58,58	0
56	MG	DA	3035	1/1	0.77	0.13	36,36,36,36	0
56	MG	BA	3704	1/1	0.77	0.20	57,57,57,57	0
56	MG	BA	3447	1/1	0.78	0.15	46,46,46,46	0
56	MG	AA	3201	1/1	0.78	0.17	60,60,60,60	0
56	MG	DA	3079	1/1	0.78	0.19	49,49,49,49	0
56	MG	DA	3167	1/1	0.78	0.19	48,48,48,48	0
56	MG	AM	201	1/1	0.78	0.08	53,53,53,53	0
56	MG	BA	3614	1/1	0.78	0.15	53,53,53,53	0
56	MG	AX	3007	1/1	0.78	0.13	58,58,58,58	0
56	MG	BA	3541	1/1	0.78	0.15	59,59,59,59	0
56	MG	DR	5001	1/1	0.78	0.17	51,51,51,51	0
56	MG	DA	3114	1/1	0.78	0.24	55,55,55,55	0
56	MG	BA	3819	1/1	0.78	0.15	61,61,61,61	0
56	MG	DA	3542	1/1	0.78	0.11	45,45,45,45	0
56	MG	BA	3881	1/1	0.78	0.13	47,47,47,47	0
56	MG	DA	3461	1/1	0.78	0.08	48,48,48,48	0
56	MG	DA	3220	1/1	0.78	0.22	69,69,69,69	0
56	MG	AA	3147	1/1	0.78	0.17	65,65,65,65	0
56	MG	BA	3274	1/1	0.78	0.30	45,45,45,45	0
56	MG	AA	3099	1/1	0.79	0.11	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3154	1/1	0.79	0.15	44,44,44,44	0
56	MG	DA	3100	1/1	0.79	0.16	46,46,46,46	0
56	MG	DA	3349	1/1	0.79	0.15	50,50,50,50	0
56	MG	DB	3016	1/1	0.79	0.23	61,61,61,61	0
56	MG	B6	101	1/1	0.79	0.24	47,47,47,47	0
56	MG	BB	3016	1/1	0.79	0.18	49,49,49,49	0
56	MG	BA	3474	1/1	0.79	0.15	53,53,53,53	0
56	MG	CA	3152	1/1	0.79	0.12	67,67,67,67	0
56	MG	B8	102	1/1	0.79	0.27	42,42,42,42	0
56	MG	AW	101	1/1	0.79	0.12	58,58,58,58	0
56	MG	AA	3192	1/1	0.79	0.12	50,50,50,50	0
56	MG	DA	3274	1/1	0.79	0.05	47,47,47,47	0
56	MG	DA	3673	1/1	0.79	0.12	61,61,61,61	0
56	MG	DA	3511	1/1	0.79	0.11	31,31,31,31	0
56	MG	BZ	3001	1/1	0.79	0.26	69,69,69,69	0
59	ZN	D4	501	1/1	0.79	0.09	95,95,95,95	0
56	MG	BA	3565	1/1	0.79	0.15	45,45,45,45	0
56	MG	BA	3487	1/1	0.79	0.20	50,50,50,50	0
56	MG	BA	3147	1/1	0.79	0.23	39,39,39,39	0
56	MG	BA	3596	1/1	0.79	0.22	44,44,44,44	0
56	MG	AA	3137	1/1	0.79	0.10	64,64,64,64	0
56	MG	CA	3011	1/1	0.79	0.20	56,56,56,56	0
56	MG	DA	3453	1/1	0.79	0.24	51,51,51,51	0
56	MG	BA	3635	1/1	0.79	0.11	65,65,65,65	0
56	MG	BB	3026	1/1	0.79	0.24	66,66,66,66	0
56	MG	AR	101	1/1	0.79	0.27	56,56,56,56	0
56	MG	DA	3433	1/1	0.79	0.15	40,40,40,40	0
56	MG	AA	3131	1/1	0.80	0.12	56,56,56,56	0
56	MG	DA	3301	1/1	0.80	0.12	52,52,52,52	0
56	MG	BA	3628	1/1	0.80	0.13	51,51,51,51	0
56	MG	DA	3321	1/1	0.80	0.22	39,39,39,39	0
56	MG	BB	3013	1/1	0.80	0.14	52,52,52,52	0
56	MG	DA	3432	1/1	0.80	0.15	57,57,57,57	0
56	MG	BA	3611	1/1	0.80	0.12	61,61,61,61	0
56	MG	DA	3087	1/1	0.80	0.17	48,48,48,48	0
56	MG	BA	3456	1/1	0.80	0.20	41,41,41,41	0
56	MG	DA	3397	1/1	0.80	0.13	53,53,53,53	0
56	MG	DA	3160	1/1	0.80	0.43	38,38,38,38	0
56	MG	CA	3081	1/1	0.80	0.28	56,56,56,56	0
56	MG	DA	3228	1/1	0.80	0.16	38,38,38,38	0
56	MG	DA	3007	1/1	0.80	0.22	54,54,54,54	0
56	MG	DA	3370	1/1	0.80	0.19	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3805	1/1	0.80	0.17	32,32,32,32	0
56	MG	DA	3529	1/1	0.80	0.09	48,48,48,48	0
56	MG	BA	3748	1/1	0.80	0.23	58,58,58,58	0
56	MG	DF	303	1/1	0.80	0.15	42,42,42,42	0
56	MG	CA	3041	1/1	0.80	0.11	49,49,49,49	0
56	MG	DB	3002	1/1	0.80	0.14	68,68,68,68	0
56	MG	BA	3409	1/1	0.80	0.10	65,65,65,65	0
56	MG	CG	5001	1/1	0.81	0.09	64,64,64,64	0
56	MG	DA	3023	1/1	0.81	0.14	48,48,48,48	0
56	MG	DA	3034	1/1	0.81	0.12	51,51,51,51	0
56	MG	AA	3214	1/1	0.81	0.14	60,60,60,60	0
56	MG	DA	3151	1/1	0.81	0.11	59,59,59,59	0
56	MG	AA	3210	1/1	0.81	0.14	76,76,76,76	0
56	MG	AA	3223	1/1	0.81	0.11	72,72,72,72	0
56	MG	BA	3203	1/1	0.81	0.24	41,41,41,41	0
56	MG	CA	3186	1/1	0.81	0.18	62,62,62,62	0
56	MG	BA	3161	1/1	0.81	0.21	46,46,46,46	0
56	MG	BA	3133	1/1	0.81	0.17	45,45,45,45	0
56	MG	DA	3579	1/1	0.81	0.09	48,48,48,48	0
56	MG	CW	3002	1/1	0.81	0.15	60,60,60,60	0
56	MG	DA	3348	1/1	0.81	0.19	32,32,32,32	0
56	MG	BA	3719	1/1	0.81	0.17	61,61,61,61	0
56	MG	DW	3003	1/1	0.81	0.33	47,47,47,47	0
56	MG	BA	3005	1/1	0.81	0.15	49,49,49,49	0
56	MG	DA	3424	1/1	0.81	0.17	47,47,47,47	0
56	MG	AA	3047	1/1	0.81	0.15	56,56,56,56	0
56	MG	DA	3463	1/1	0.81	0.13	52,52,52,52	0
56	MG	BA	3501	1/1	0.81	0.30	50,50,50,50	0
56	MG	DA	3575	1/1	0.81	0.14	51,51,51,51	0
56	MG	DA	3668	1/1	0.81	0.16	61,61,61,61	0
56	MG	DA	3188	1/1	0.81	0.14	44,44,44,44	0
56	MG	BA	3727	1/1	0.81	0.31	64,64,64,64	0
56	MG	DA	3513	1/1	0.81	0.21	54,54,54,54	0
56	MG	AA	3120	1/1	0.81	0.10	67,67,67,67	0
56	MG	DA	3611	1/1	0.81	0.22	65,65,65,65	0
56	MG	BA	3285	1/1	0.81	0.29	48,48,48,48	0
56	MG	BA	3556	1/1	0.81	0.15	48,48,48,48	0
56	MG	AA	3023	1/1	0.81	0.15	56,56,56,56	0
56	MG	AA	3015	1/1	0.81	0.10	71,71,71,71	0
56	MG	DA	3018	1/1	0.81	0.12	45,45,45,45	0
56	MG	AA	3165	1/1	0.81	0.10	57,57,57,57	0
56	MG	BA	3566	1/1	0.81	0.16	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3426	1/1	0.82	0.25	42,42,42,42	0
56	MG	AA	3222	1/1	0.82	0.15	55,55,55,55	0
56	MG	DA	3045	1/1	0.82	0.17	52,52,52,52	0
56	MG	CA	3158	1/1	0.82	0.11	76,76,76,76	0
56	MG	BA	3111	1/1	0.82	0.10	60,60,60,60	0
56	MG	BA	3094	1/1	0.82	0.20	33,33,33,33	0
56	MG	DA	3157	1/1	0.82	0.18	54,54,54,54	0
56	MG	BA	3058	1/1	0.82	0.15	48,48,48,48	0
56	MG	AE	3001	1/1	0.82	0.12	65,65,65,65	0
56	MG	DA	3223	1/1	0.82	0.18	51,51,51,51	0
56	MG	DA	3531	1/1	0.82	0.12	56,56,56,56	0
56	MG	BA	3083	1/1	0.82	0.17	54,54,54,54	0
56	MG	AA	3096	1/1	0.82	0.12	60,60,60,60	0
56	MG	DA	3216	1/1	0.82	0.10	48,48,48,48	0
56	MG	CA	3127	1/1	0.82	0.12	57,57,57,57	0
56	MG	DA	3591	1/1	0.82	0.08	55,55,55,55	0
56	MG	DB	3013	1/1	0.82	0.12	53,53,53,53	0
56	MG	BG	204	1/1	0.82	0.11	58,58,58,58	0
56	MG	DA	3506	1/1	0.82	0.18	55,55,55,55	0
56	MG	DW	3001	1/1	0.82	0.33	44,44,44,44	0
56	MG	DA	3261	1/1	0.82	0.14	47,47,47,47	0
56	MG	DA	3322	1/1	0.82	0.15	41,41,41,41	0
56	MG	CA	3088	1/1	0.82	0.32	62,62,62,62	0
56	MG	DA	3608	1/1	0.82	0.10	55,55,55,55	0
56	MG	DA	3395	1/1	0.82	0.14	45,45,45,45	0
56	MG	BA	3581	1/1	0.82	0.18	33,33,33,33	0
56	MG	B0	103	1/1	0.82	0.18	49,49,49,49	0
56	MG	DA	3125	1/1	0.82	0.24	44,44,44,44	0
56	MG	BA	3348	1/1	0.82	0.13	65,65,65,65	0
56	MG	CA	3116	1/1	0.82	0.23	54,54,54,54	0
56	MG	BA	3639	1/1	0.82	0.15	59,59,59,59	0
56	MG	DA	3328	1/1	0.82	0.23	64,64,64,64	0
56	MG	CA	3053	1/1	0.82	0.16	61,61,61,61	0
56	MG	CA	3114	1/1	0.82	0.26	60,60,60,60	0
56	MG	BA	3066	1/1	0.82	0.16	54,54,54,54	0
56	MG	BA	3314	1/1	0.82	0.19	60,60,60,60	0
56	MG	AA	3044	1/1	0.82	0.19	54,54,54,54	0
56	MG	CA	3061	1/1	0.82	0.21	58,58,58,58	0
56	MG	DA	3288	1/1	0.83	0.17	44,44,44,44	0
56	MG	AA	3117	1/1	0.83	0.15	68,68,68,68	0
56	MG	DA	3612	1/1	0.83	0.15	52,52,52,52	0
56	MG	AA	3028	1/1	0.83	0.24	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3610	1/1	0.83	0.25	61,61,61,61	0
56	MG	AA	3060	1/1	0.83	0.21	62,62,62,62	0
56	MG	B0	101	1/1	0.83	0.22	44,44,44,44	0
56	MG	CA	3173	1/1	0.83	0.13	81,81,81,81	0
56	MG	B4	502	1/1	0.83	0.12	65,65,65,65	0
56	MG	BA	3699	1/1	0.83	0.13	45,45,45,45	0
56	MG	CA	3001	1/1	0.83	0.09	67,67,67,67	0
56	MG	AA	3071	1/1	0.83	0.26	61,61,61,61	0
56	MG	CA	3021	1/1	0.83	0.26	79,79,79,79	0
56	MG	BO	3001	1/1	0.83	0.30	62,62,62,62	0
56	MG	BA	3103	1/1	0.83	0.17	58,58,58,58	0
56	MG	CA	3193	1/1	0.83	0.09	66,66,66,66	0
56	MG	DA	3515	1/1	0.83	0.21	59,59,59,59	0
56	MG	BE	302	1/1	0.83	0.21	27,27,27,27	0
56	MG	BA	3298	1/1	0.83	0.27	51,51,51,51	0
56	MG	AA	3080	1/1	0.83	0.20	61,61,61,61	0
56	MG	BA	3351	1/1	0.83	0.21	33,33,33,33	0
56	MG	AA	3219	1/1	0.83	0.21	63,63,63,63	0
56	MG	AA	3089	1/1	0.83	0.26	66,66,66,66	0
56	MG	BA	3486	1/1	0.83	0.19	29,29,29,29	0
56	MG	BA	3502	1/1	0.83	0.12	56,56,56,56	0
56	MG	BA	3795	1/1	0.83	0.22	22,22,22,22	0
56	MG	AA	3056	1/1	0.83	0.26	60,60,60,60	0
56	MG	DA	3129	1/1	0.83	0.22	37,37,37,37	0
56	MG	CA	3015	1/1	0.83	0.23	57,57,57,57	0
56	MG	BA	3493	1/1	0.83	0.14	41,41,41,41	0
56	MG	BA	3472	1/1	0.83	0.14	31,31,31,31	0
56	MG	BA	3855	1/1	0.83	0.11	53,53,53,53	0
56	MG	DA	3393	1/1	0.83	0.11	55,55,55,55	0
56	MG	CA	3090	1/1	0.83	0.11	74,74,74,74	0
56	MG	BA	3533	1/1	0.83	0.17	47,47,47,47	0
56	MG	BA	3557	1/1	0.83	0.14	41,41,41,41	0
56	MG	DA	3161	1/1	0.83	0.12	41,41,41,41	0
56	MG	DA	3429	1/1	0.83	0.14	35,35,35,35	0
56	MG	AA	3090	1/1	0.83	0.17	51,51,51,51	0
56	MG	DA	3329	1/1	0.83	0.15	51,51,51,51	0
56	MG	CA	3023	1/1	0.83	0.20	60,60,60,60	0
56	MG	BA	3573	1/1	0.83	0.18	34,34,34,34	0
56	MG	BA	3623	1/1	0.83	0.08	48,48,48,48	0
56	MG	CW	3004	1/1	0.83	0.19	64,64,64,64	0
56	MG	CA	3084	1/1	0.83	0.23	57,57,57,57	0
56	MG	BA	3906	1/1	0.83	0.23	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CX	3005	1/1	0.83	0.31	60,60,60,60	0
56	MG	DA	3363	1/1	0.83	0.13	42,42,42,42	0
56	MG	DA	3150	1/1	0.83	0.20	42,42,42,42	0
56	MG	BA	3445	1/1	0.83	0.15	48,48,48,48	0
56	MG	BA	3754	1/1	0.83	0.16	54,54,54,54	0
56	MG	CA	3184	1/1	0.83	0.14	68,68,68,68	0
56	MG	CA	3004	1/1	0.83	0.12	66,66,66,66	0
56	MG	CA	3138	1/1	0.84	0.14	59,59,59,59	0
56	MG	BA	3322	1/1	0.84	0.29	57,57,57,57	0
56	MG	AA	3031	1/1	0.84	0.15	43,43,43,43	0
56	MG	DA	3541	1/1	0.84	0.14	59,59,59,59	0
56	MG	DA	3238	1/1	0.84	0.20	48,48,48,48	0
56	MG	DA	3074	1/1	0.84	0.10	45,45,45,45	0
56	MG	CA	3020	1/1	0.84	0.17	57,57,57,57	0
56	MG	CA	3161	1/1	0.84	0.07	61,61,61,61	0
56	MG	BQ	3003	1/1	0.84	0.19	54,54,54,54	0
56	MG	BA	3417	1/1	0.84	0.17	46,46,46,46	0
56	MG	BA	3844	1/1	0.84	0.13	49,49,49,49	0
56	MG	BA	3739	1/1	0.84	0.16	49,49,49,49	0
56	MG	DA	3446	1/1	0.84	0.14	68,68,68,68	0
56	MG	DA	3289	1/1	0.84	0.14	53,53,53,53	0
56	MG	DA	3002	1/1	0.84	0.12	60,60,60,60	0
56	MG	BN	3002	1/1	0.84	0.19	38,38,38,38	0
56	MG	DA	3362	1/1	0.84	0.14	61,61,61,61	0
57	UAM	CA	3202	30/30	0.84	0.38	45,72,83,85	0
56	MG	AD	502	1/1	0.84	0.25	55,55,55,55	0
56	MG	BA	3020	1/1	0.84	0.21	46,46,46,46	0
56	MG	BA	3204	1/1	0.84	0.14	34,34,34,34	0
56	MG	AA	3037	1/1	0.84	0.31	63,63,63,63	0
56	MG	CA	3073	1/1	0.84	0.10	64,64,64,64	0
56	MG	DB	3019	1/1	0.84	0.29	60,60,60,60	0
56	MG	AA	3009	1/1	0.84	0.11	49,49,49,49	0
56	MG	BA	3142	1/1	0.84	0.43	46,46,46,46	0
56	MG	D5	101	1/1	0.84	0.10	45,45,45,45	0
56	MG	DA	3633	1/1	0.84	0.17	50,50,50,50	0
56	MG	DA	3195	1/1	0.84	0.14	39,39,39,39	0
56	MG	BA	3356	1/1	0.84	0.10	52,52,52,52	0
56	MG	BA	3459	1/1	0.84	0.25	38,38,38,38	0
56	MG	DA	3062	1/1	0.84	0.14	49,49,49,49	0
56	MG	DA	3056	1/1	0.84	0.20	41,41,41,41	0
56	MG	BA	3552	1/1	0.84	0.17	38,38,38,38	0
56	MG	AA	3012	1/1	0.84	0.14	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3432	1/1	0.84	0.10	55,55,55,55	0
56	MG	CA	3130	1/1	0.84	0.13	62,62,62,62	0
56	MG	DA	3445	1/1	0.84	0.14	45,45,45,45	0
56	MG	CA	3091	1/1	0.84	0.15	67,67,67,67	0
56	MG	DA	3107	1/1	0.84	0.21	48,48,48,48	0
56	MG	BA	3359	1/1	0.84	0.20	58,58,58,58	0
56	MG	DA	3372	1/1	0.84	0.09	51,51,51,51	0
56	MG	BA	3214	1/1	0.84	0.20	44,44,44,44	0
56	MG	BA	3269	1/1	0.84	0.17	45,45,45,45	0
56	MG	AA	3170	1/1	0.84	0.13	67,67,67,67	0
56	MG	BA	3482	1/1	0.84	0.22	39,39,39,39	0
56	MG	AA	3187	1/1	0.84	0.17	65,65,65,65	0
56	MG	BA	3849	1/1	0.84	0.21	29,29,29,29	0
56	MG	BA	3743	1/1	0.84	0.19	50,50,50,50	0
56	MG	BA	3901	1/1	0.84	0.16	39,39,39,39	0
56	MG	BA	3610	1/1	0.84	0.15	60,60,60,60	0
56	MG	AA	3073	1/1	0.84	0.15	53,53,53,53	0
56	MG	BA	3585	1/1	0.84	0.17	36,36,36,36	0
56	MG	AA	3182	1/1	0.84	0.22	65,65,65,65	0
56	MG	DA	3588	1/1	0.84	0.15	64,64,64,64	0
56	MG	DA	3387	1/1	0.84	0.18	46,46,46,46	0
56	MG	AA	3218	1/1	0.84	0.07	75,75,75,75	0
56	MG	CA	3160	1/1	0.84	0.11	55,55,55,55	0
56	MG	BI	3001	1/1	0.84	0.08	60,60,60,60	0
56	MG	DE	301	1/1	0.84	0.17	47,47,47,47	0
56	MG	AA	3079	1/1	0.84	0.25	60,60,60,60	0
56	MG	CA	3013	1/1	0.84	0.19	62,62,62,62	0
56	MG	AA	3014	1/1	0.85	0.12	47,47,47,47	0
56	MG	BA	3512	1/1	0.85	0.16	57,57,57,57	0
56	MG	CA	3071	1/1	0.85	0.18	68,68,68,68	0
56	MG	DA	3519	1/1	0.85	0.14	46,46,46,46	0
56	MG	BA	3306	1/1	0.85	0.16	28,28,28,28	0
56	MG	BA	3168	1/1	0.85	0.17	35,35,35,35	0
56	MG	CA	3124	1/1	0.85	0.08	57,57,57,57	0
56	MG	BA	3818	1/1	0.85	0.19	58,58,58,58	0
56	MG	DA	3417	1/1	0.85	0.20	53,53,53,53	0
56	MG	BA	3261	1/1	0.85	0.26	38,38,38,38	0
56	MG	DA	3266	1/1	0.85	0.18	44,44,44,44	0
56	MG	BA	3365	1/1	0.85	0.08	44,44,44,44	0
56	MG	DA	3503	1/1	0.85	0.11	57,57,57,57	0
56	MG	BA	3471	1/1	0.85	0.12	57,57,57,57	0
56	MG	DF	302	1/1	0.85	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3104	1/1	0.85	0.13	58,58,58,58	0
56	MG	DA	3415	1/1	0.85	0.19	39,39,39,39	0
56	MG	DA	3215	1/1	0.85	0.20	60,60,60,60	0
56	MG	CX	3002	1/1	0.85	0.18	63,63,63,63	0
56	MG	CA	3007	1/1	0.85	0.15	66,66,66,66	0
56	MG	AA	3200	1/1	0.85	0.20	61,61,61,61	0
56	MG	AA	3026	1/1	0.85	0.17	50,50,50,50	0
56	MG	DA	3380	1/1	0.85	0.13	49,49,49,49	0
56	MG	DA	3211	1/1	0.85	0.09	37,37,37,37	0
56	MG	D0	3001	1/1	0.85	0.12	51,51,51,51	0
56	MG	BA	3751	1/1	0.85	0.20	51,51,51,51	0
56	MG	CA	3192	1/1	0.85	0.20	69,69,69,69	0
56	MG	DA	3509	1/1	0.85	0.18	55,55,55,55	0
56	MG	AA	3231	1/1	0.85	0.25	61,61,61,61	0
56	MG	AX	3003	1/1	0.85	0.25	50,50,50,50	0
56	MG	BA	3801	1/1	0.85	0.13	27,27,27,27	0
56	MG	BA	3877	1/1	0.85	0.16	44,44,44,44	0
56	MG	BA	3390	1/1	0.85	0.09	33,33,33,33	0
56	MG	CA	3135	1/1	0.85	0.22	57,57,57,57	0
56	MG	DA	3502	1/1	0.85	0.09	63,63,63,63	0
56	MG	DA	3402	1/1	0.85	0.17	56,56,56,56	0
56	MG	BA	3355	1/1	0.85	0.21	35,35,35,35	0
56	MG	CA	3019	1/1	0.85	0.11	44,44,44,44	0
56	MG	AA	3111	1/1	0.85	0.17	57,57,57,57	0
56	MG	CX	3006	1/1	0.85	0.11	50,50,50,50	0
56	MG	DA	3430	1/1	0.85	0.14	35,35,35,35	0
56	MG	AA	3101	1/1	0.85	0.12	45,45,45,45	0
56	MG	DA	3102	1/1	0.85	0.15	51,51,51,51	0
56	MG	DA	3566	1/1	0.85	0.08	67,67,67,67	0
56	MG	BA	3675	1/1	0.85	0.19	38,38,38,38	0
56	MG	BA	3165	1/1	0.85	0.24	32,32,32,32	0
56	MG	BA	3208	1/1	0.85	0.29	62,62,62,62	0
56	MG	BA	3782	1/1	0.85	0.21	46,46,46,46	0
56	MG	BA	3527	1/1	0.85	0.13	57,57,57,57	0
56	MG	DA	3296	1/1	0.85	0.10	56,56,56,56	0
56	MG	DA	3366	1/1	0.85	0.19	53,53,53,53	0
56	MG	CL	202	1/1	0.85	0.19	50,50,50,50	0
56	MG	DB	3007	1/1	0.85	0.17	64,64,64,64	0
56	MG	BF	307	1/1	0.85	0.17	31,31,31,31	0
56	MG	BA	3691	1/1	0.85	0.19	55,55,55,55	0
56	MG	DA	3270	1/1	0.85	0.17	33,33,33,33	0
56	MG	DA	3050	1/1	0.85	0.16	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3039	1/1	0.85	0.14	55,55,55,55	0
56	MG	DU	3004	1/1	0.85	0.15	48,48,48,48	0
56	MG	AA	3084	1/1	0.85	0.16	53,53,53,53	0
56	MG	DA	3555	1/1	0.85	0.14	30,30,30,30	0
56	MG	DA	3225	1/1	0.86	0.16	38,38,38,38	0
56	MG	AA	3091	1/1	0.86	0.15	50,50,50,50	0
56	MG	DA	3092	1/1	0.86	0.14	50,50,50,50	0
56	MG	BA	3715	1/1	0.86	0.11	53,53,53,53	0
56	MG	BA	3097	1/1	0.86	0.17	48,48,48,48	0
56	MG	CA	3086	1/1	0.86	0.18	62,62,62,62	0
56	MG	DA	3490	1/1	0.86	0.09	51,51,51,51	0
56	MG	DA	3400	1/1	0.86	0.15	36,36,36,36	0
56	MG	AA	3158	1/1	0.86	0.24	54,54,54,54	0
56	MG	BB	3012	1/1	0.86	0.07	61,61,61,61	0
57	UAM	AA	3232	30/30	0.86	0.31	44,65,77,80	0
56	MG	DA	3303	1/1	0.86	0.10	30,30,30,30	0
56	MG	CA	3064	1/1	0.86	0.10	53,53,53,53	0
56	MG	BA	3481	1/1	0.86	0.13	31,31,31,31	0
56	MG	AA	3149	1/1	0.86	0.11	51,51,51,51	0
56	MG	BA	3271	1/1	0.86	0.17	54,54,54,54	0
56	MG	BA	3567	1/1	0.86	0.14	46,46,46,46	0
56	MG	BA	3051	1/1	0.86	0.21	51,51,51,51	0
56	MG	BA	3470	1/1	0.86	0.17	46,46,46,46	0
56	MG	AA	3177	1/1	0.86	0.10	57,57,57,57	0
56	MG	BA	3399	1/1	0.86	0.12	57,57,57,57	0
56	MG	BA	3603	1/1	0.86	0.09	42,42,42,42	0
56	MG	BA	3518	1/1	0.86	0.09	57,57,57,57	0
56	MG	BA	3716	1/1	0.86	0.08	47,47,47,47	0
56	MG	BA	3729	1/1	0.86	0.23	56,56,56,56	0
56	MG	DA	3458	1/1	0.86	0.09	55,55,55,55	0
56	MG	BA	3540	1/1	0.86	0.10	50,50,50,50	0
56	MG	BA	3425	1/1	0.86	0.09	60,60,60,60	0
56	MG	DA	3414	1/1	0.86	0.20	56,56,56,56	0
56	MG	DB	3001	1/1	0.86	0.17	71,71,71,71	0
56	MG	DA	3438	1/1	0.86	0.16	42,42,42,42	0
56	MG	DA	3128	1/1	0.86	0.20	45,45,45,45	0
56	MG	AA	3027	1/1	0.86	0.26	60,60,60,60	0
56	MG	CA	3170	1/1	0.86	0.09	61,61,61,61	0
56	MG	BA	3579	1/1	0.86	0.21	42,42,42,42	0
56	MG	BA	3575	1/1	0.86	0.24	27,27,27,27	0
56	MG	CA	3049	1/1	0.86	0.45	67,67,67,67	0
56	MG	AA	3189	1/1	0.86	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3446	1/1	0.86	0.17	63,63,63,63	0
56	MG	BA	3607	1/1	0.86	0.05	57,57,57,57	0
56	MG	DA	3252	1/1	0.86	0.08	57,57,57,57	0
56	MG	DG	3001	1/1	0.86	0.20	53,53,53,53	0
56	MG	BA	3571	1/1	0.86	0.21	23,23,23,23	0
56	MG	AA	3085	1/1	0.86	0.15	47,47,47,47	0
56	MG	CF	3002	1/1	0.86	0.17	59,59,59,59	0
56	MG	DA	3625	1/1	0.86	0.09	50,50,50,50	0
56	MG	DA	3244	1/1	0.86	0.09	47,47,47,47	0
56	MG	CA	3183	1/1	0.86	0.18	69,69,69,69	0
56	MG	BA	3262	1/1	0.86	0.29	48,48,48,48	0
56	MG	BB	3028	1/1	0.86	0.17	42,42,42,42	0
56	MG	CA	3169	1/1	0.86	0.11	60,60,60,60	0
56	MG	AA	3018	1/1	0.87	0.14	73,73,73,73	0
56	MG	AA	3050	1/1	0.87	0.25	67,67,67,67	0
56	MG	DA	3314	1/1	0.87	0.14	38,38,38,38	0
56	MG	DA	3607	1/1	0.87	0.14	35,35,35,35	0
56	MG	DA	3385	1/1	0.87	0.17	47,47,47,47	0
56	MG	BG	203	1/1	0.87	0.20	51,51,51,51	0
56	MG	DA	3632	1/1	0.87	0.15	57,57,57,57	0
56	MG	BA	3763	1/1	0.87	0.14	58,58,58,58	0
56	MG	BA	3796	1/1	0.87	0.15	29,29,29,29	0
56	MG	BA	3102	1/1	0.87	0.24	44,44,44,44	0
56	MG	DA	3121	1/1	0.87	0.20	41,41,41,41	0
56	MG	AA	3025	1/1	0.87	0.12	50,50,50,50	0
56	MG	AA	3181	1/1	0.87	0.14	70,70,70,70	0
56	MG	BA	3320	1/1	0.87	0.22	50,50,50,50	0
56	MG	BA	3263	1/1	0.87	0.23	42,42,42,42	0
56	MG	DA	3618	1/1	0.87	0.14	49,49,49,49	0
56	MG	AA	3207	1/1	0.87	0.12	53,53,53,53	0
56	MG	CA	3085	1/1	0.87	0.15	53,53,53,53	0
56	MG	BE	309	1/1	0.87	0.19	31,31,31,31	0
56	MG	CA	3050	1/1	0.87	0.09	72,72,72,72	0
56	MG	BA	3672	1/1	0.87	0.18	24,24,24,24	0
56	MG	CA	3103	1/1	0.87	0.12	63,63,63,63	0
56	MG	CA	3157	1/1	0.87	0.16	72,72,72,72	0
56	MG	BA	3831	1/1	0.87	0.18	53,53,53,53	0
56	MG	BA	3871	1/1	0.87	0.15	55,55,55,55	0
56	MG	CA	3140	1/1	0.87	0.13	56,56,56,56	0
56	MG	DA	3444	1/1	0.87	0.16	40,40,40,40	0
56	MG	BA	3100	1/1	0.87	0.28	33,33,33,33	0
56	MG	BA	3002	1/1	0.87	0.18	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3570	1/1	0.87	0.11	28,28,28,28	0
56	MG	DA	3580	1/1	0.87	0.14	40,40,40,40	0
56	MG	AA	3082	1/1	0.87	0.21	34,34,34,34	0
56	MG	AA	3107	1/1	0.87	0.17	53,53,53,53	0
56	MG	BA	3836	1/1	0.87	0.23	59,59,59,59	0
56	MG	BE	306	1/1	0.87	0.19	34,34,34,34	0
56	MG	BA	3619	1/1	0.87	0.09	68,68,68,68	0
56	MG	CA	3089	1/1	0.87	0.24	65,65,65,65	0
56	MG	DA	3015	1/1	0.87	0.18	37,37,37,37	0
56	MG	DA	3077	1/1	0.87	0.12	44,44,44,44	0
56	MG	AA	3126	1/1	0.87	0.29	54,54,54,54	0
56	MG	CA	3195	1/1	0.87	0.12	69,69,69,69	0
56	MG	BA	3107	1/1	0.87	0.26	50,50,50,50	0
56	MG	AA	3019	1/1	0.87	0.18	54,54,54,54	0
56	MG	CA	3069	1/1	0.87	0.13	57,57,57,57	0
56	MG	AA	3109	1/1	0.87	0.14	60,60,60,60	0
56	MG	DA	3551	1/1	0.87	0.10	53,53,53,53	0
56	MG	BA	3621	1/1	0.87	0.19	50,50,50,50	0
56	MG	BA	3842	1/1	0.87	0.18	43,43,43,43	0
56	MG	BA	3707	1/1	0.87	0.24	53,53,53,53	0
56	MG	DA	3617	1/1	0.87	0.09	49,49,49,49	0
56	MG	DA	3585	1/1	0.87	0.10	51,51,51,51	0
56	MG	BA	3415	1/1	0.87	0.17	33,33,33,33	0
56	MG	AX	3011	1/1	0.87	0.19	53,53,53,53	0
56	MG	BA	3663	1/1	0.87	0.13	39,39,39,39	0
56	MG	DA	3536	1/1	0.87	0.15	51,51,51,51	0
56	MG	CA	3002	1/1	0.87	0.13	55,55,55,55	0
56	MG	CP	101	1/1	0.87	0.19	57,57,57,57	0
56	MG	DA	3597	1/1	0.87	0.16	54,54,54,54	0
56	MG	DA	3054	1/1	0.87	0.26	52,52,52,52	0
56	MG	BA	3898	1/1	0.87	0.15	44,44,44,44	0
56	MG	CA	3172	1/1	0.87	0.14	54,54,54,54	0
56	MG	BG	202	1/1	0.87	0.17	36,36,36,36	0
56	MG	DA	3654	1/1	0.87	0.09	53,53,53,53	0
56	MG	DA	3664	1/1	0.87	0.13	71,71,71,71	0
56	MG	BA	3130	1/1	0.87	0.20	43,43,43,43	0
56	MG	DA	3191	1/1	0.87	0.09	52,52,52,52	0
56	MG	BA	3465	1/1	0.87	0.27	43,43,43,43	0
56	MG	CA	3102	1/1	0.88	0.17	52,52,52,52	0
56	MG	BA	3488	1/1	0.88	0.22	31,31,31,31	0
56	MG	BA	3882	1/1	0.88	0.25	53,53,53,53	0
56	MG	CA	3162	1/1	0.88	0.15	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3840	1/1	0.88	0.17	50,50,50,50	0
56	MG	DA	3662	1/1	0.88	0.35	52,52,52,52	0
56	MG	BA	3424	1/1	0.88	0.11	50,50,50,50	0
56	MG	CA	3072	1/1	0.88	0.10	55,55,55,55	0
56	MG	BA	3389	1/1	0.88	0.20	21,21,21,21	0
56	MG	BA	3838	1/1	0.88	0.15	47,47,47,47	0
56	MG	BA	3833	1/1	0.88	0.20	57,57,57,57	0
56	MG	AA	3045	1/1	0.88	0.28	47,47,47,47	0
56	MG	DA	3653	1/1	0.88	0.15	46,46,46,46	0
56	MG	DA	3482	1/1	0.88	0.20	53,53,53,53	0
56	MG	DA	3265	1/1	0.88	0.16	39,39,39,39	0
56	MG	DA	3218	1/1	0.88	0.19	62,62,62,62	0
56	MG	BA	3589	1/1	0.88	0.27	42,42,42,42	0
56	MG	BA	3752	1/1	0.88	0.14	54,54,54,54	0
56	MG	AA	3040	1/1	0.88	0.18	68,68,68,68	0
56	MG	AA	3061	1/1	0.88	0.31	51,51,51,51	0
56	MG	BA	3173	1/1	0.88	0.20	35,35,35,35	0
56	MG	BA	3028	1/1	0.88	0.10	45,45,45,45	0
56	MG	DA	3426	1/1	0.88	0.15	41,41,41,41	0
56	MG	BA	3048	1/1	0.88	0.24	36,36,36,36	0
56	MG	BA	3545	1/1	0.88	0.12	43,43,43,43	0
56	MG	AX	3006	1/1	0.88	0.15	46,46,46,46	0
56	MG	CA	3017	1/1	0.88	0.21	56,56,56,56	0
56	MG	AA	3194	1/1	0.88	0.14	58,58,58,58	0
56	MG	BA	3451	1/1	0.88	0.15	38,38,38,38	0
56	MG	BA	3476	1/1	0.88	0.22	54,54,54,54	0
56	MG	BA	3830	1/1	0.88	0.18	56,56,56,56	0
56	MG	DA	3550	1/1	0.88	0.09	63,63,63,63	0
56	MG	DA	3650	1/1	0.88	0.13	53,53,53,53	0
56	MG	DA	3624	1/1	0.88	0.12	32,32,32,32	0
56	MG	CA	3164	1/1	0.88	0.07	63,63,63,63	0
56	MG	BA	3865	1/1	0.88	0.18	36,36,36,36	0
56	MG	CA	3046	1/1	0.88	0.16	42,42,42,42	0
56	MG	BA	3730	1/1	0.88	0.27	45,45,45,45	0
56	MG	BA	3144	1/1	0.88	0.27	53,53,53,53	0
56	MG	DA	3338	1/1	0.88	0.10	43,43,43,43	0
56	MG	AA	3036	1/1	0.88	0.18	46,46,46,46	0
56	MG	BQ	3001	1/1	0.88	0.29	41,41,41,41	0
56	MG	DA	3577	1/1	0.88	0.10	54,54,54,54	0
56	MG	BA	3211	1/1	0.88	0.35	63,63,63,63	0
56	MG	BG	205	1/1	0.88	0.13	40,40,40,40	0
56	MG	CA	3191	1/1	0.88	0.14	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3155	1/1	0.88	0.19	72,72,72,72	0
56	MG	DA	3176	1/1	0.88	0.21	36,36,36,36	0
56	MG	BA	3867	1/1	0.88	0.12	58,58,58,58	0
56	MG	AA	3221	1/1	0.88	0.13	55,55,55,55	0
56	MG	DA	3471	1/1	0.88	0.12	49,49,49,49	0
56	MG	BA	3294	1/1	0.88	0.22	38,38,38,38	0
56	MG	BA	3649	1/1	0.88	0.15	24,24,24,24	0
56	MG	DA	3158	1/1	0.88	0.09	49,49,49,49	0
56	MG	DA	3229	1/1	0.88	0.22	43,43,43,43	0
56	MG	DA	3622	1/1	0.88	0.18	51,51,51,51	0
56	MG	DA	3568	1/1	0.88	0.18	30,30,30,30	0
56	MG	BA	3515	1/1	0.88	0.18	64,64,64,64	0
56	MG	CA	3108	1/1	0.88	0.23	57,57,57,57	0
56	MG	DA	3237	1/1	0.88	0.18	47,47,47,47	0
56	MG	BX	3005	1/1	0.88	0.21	42,42,42,42	0
56	MG	DA	3409	1/1	0.88	0.08	36,36,36,36	0
56	MG	BA	3873	1/1	0.88	0.28	26,26,26,26	0
56	MG	AA	3174	1/1	0.88	0.16	58,58,58,58	0
56	MG	DA	3368	1/1	0.88	0.10	47,47,47,47	0
56	MG	BA	3815	1/1	0.88	0.22	51,51,51,51	0
56	MG	BA	3450	1/1	0.88	0.17	35,35,35,35	0
56	MG	AA	3067	1/1	0.88	0.23	56,56,56,56	0
56	MG	BA	3420	1/1	0.88	0.19	47,47,47,47	0
56	MG	AA	3125	1/1	0.88	0.07	52,52,52,52	0
56	MG	DA	3306	1/1	0.88	0.16	33,33,33,33	0
56	MG	AA	3176	1/1	0.88	0.22	47,47,47,47	0
56	MG	BA	3019	1/1	0.88	0.18	34,34,34,34	0
56	MG	DA	3665	1/1	0.88	0.19	34,34,34,34	0
56	MG	DA	3227	1/1	0.88	0.23	39,39,39,39	0
56	MG	BA	3631	1/1	0.89	0.24	38,38,38,38	0
56	MG	BA	3695	1/1	0.89	0.19	56,56,56,56	0
56	MG	DA	3231	1/1	0.89	0.13	49,49,49,49	0
56	MG	BA	3655	1/1	0.89	0.14	44,44,44,44	0
56	MG	DA	3571	1/1	0.89	0.23	43,43,43,43	0
56	MG	CW	3003	1/1	0.89	0.09	58,58,58,58	0
56	MG	BA	3698	1/1	0.89	0.17	55,55,55,55	0
56	MG	DA	3088	1/1	0.89	0.18	47,47,47,47	0
56	MG	DA	3375	1/1	0.89	0.14	37,37,37,37	0
56	MG	BA	3468	1/1	0.89	0.23	36,36,36,36	0
56	MG	BA	3086	1/1	0.89	0.21	57,57,57,57	0
56	MG	AA	3035	1/1	0.89	0.13	41,41,41,41	0
56	MG	DA	3170	1/1	0.89	0.17	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3427	1/1	0.89	0.16	57,57,57,57	0
56	MG	AA	3055	1/1	0.89	0.14	61,61,61,61	0
56	MG	BB	3024	1/1	0.89	0.10	60,60,60,60	0
56	MG	BA	3666	1/1	0.89	0.30	74,74,74,74	0
56	MG	DA	3171	1/1	0.89	0.16	45,45,45,45	0
56	MG	AA	3180	1/1	0.89	0.08	57,57,57,57	0
56	MG	BA	3436	1/1	0.89	0.18	54,54,54,54	0
56	MG	DA	3214	1/1	0.89	0.22	53,53,53,53	0
56	MG	BE	310	1/1	0.89	0.16	80,80,80,80	0
56	MG	CA	3065	1/1	0.89	0.24	58,58,58,58	0
56	MG	AA	3086	1/1	0.89	0.14	45,45,45,45	0
56	MG	BA	3313	1/1	0.89	0.09	60,60,60,60	0
56	MG	BA	3176	1/1	0.89	0.16	53,53,53,53	0
56	MG	BB	3004	1/1	0.89	0.26	59,59,59,59	0
56	MG	DA	3514	1/1	0.89	0.14	45,45,45,45	0
56	MG	BA	3498	1/1	0.89	0.23	26,26,26,26	0
56	MG	AA	3004	1/1	0.89	0.09	68,68,68,68	0
56	MG	AA	3058	1/1	0.89	0.15	54,54,54,54	0
56	MG	BA	3017	1/1	0.89	0.15	52,52,52,52	0
56	MG	BA	3870	1/1	0.89	0.17	24,24,24,24	0
56	MG	DA	3560	1/1	0.89	0.14	50,50,50,50	0
56	MG	DA	3354	1/1	0.89	0.14	34,34,34,34	0
56	MG	DA	3031	1/1	0.89	0.19	44,44,44,44	0
56	MG	DB	3021	1/1	0.89	0.06	67,67,67,67	0
56	MG	DA	3401	1/1	0.89	0.14	37,37,37,37	0
56	MG	DA	3086	1/1	0.89	0.20	59,59,59,59	0
56	MG	AA	3188	1/1	0.89	0.18	67,67,67,67	0
56	MG	BA	3310	1/1	0.89	0.28	44,44,44,44	0
56	MG	DA	3396	1/1	0.89	0.12	41,41,41,41	0
56	MG	BA	3305	1/1	0.89	0.22	46,46,46,46	0
56	MG	DA	3573	1/1	0.89	0.13	46,46,46,46	0
56	MG	DA	3175	1/1	0.89	0.10	50,50,50,50	0
56	MG	BA	3385	1/1	0.89	0.11	32,32,32,32	0
56	MG	AX	3004	1/1	0.89	0.19	53,53,53,53	0
56	MG	DA	3593	1/1	0.89	0.12	60,60,60,60	0
56	MG	BA	3861	1/1	0.89	0.26	34,34,34,34	0
56	MG	CA	3126	1/1	0.89	0.17	68,68,68,68	0
56	MG	DA	3263	1/1	0.89	0.16	40,40,40,40	0
56	MG	DA	3549	1/1	0.89	0.14	49,49,49,49	0
56	MG	BA	3781	1/1	0.89	0.19	47,47,47,47	0
56	MG	DA	3070	1/1	0.89	0.16	39,39,39,39	0
56	MG	DB	3014	1/1	0.89	0.17	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3065	1/1	0.89	0.18	51,51,51,51	0
56	MG	BA	3170	1/1	0.89	0.12	40,40,40,40	0
56	MG	BB	3025	1/1	0.89	0.20	71,71,71,71	0
56	MG	BA	3522	1/1	0.89	0.14	50,50,50,50	0
56	MG	CA	3151	1/1	0.89	0.17	60,60,60,60	0
56	MG	BA	3654	1/1	0.89	0.14	54,54,54,54	0
56	MG	CA	3167	1/1	0.89	0.15	65,65,65,65	0
56	MG	CA	3182	1/1	0.89	0.23	58,58,58,58	0
56	MG	DB	3018	1/1	0.89	0.23	62,62,62,62	0
56	MG	DA	3267	1/1	0.89	0.07	53,53,53,53	0
56	MG	DA	3177	1/1	0.89	0.23	44,44,44,44	0
56	MG	DA	3264	1/1	0.89	0.12	48,48,48,48	0
56	MG	DA	3026	1/1	0.89	0.29	41,41,41,41	0
56	MG	CA	3008	1/1	0.89	0.15	49,49,49,49	0
56	MG	BA	3087	1/1	0.89	0.23	45,45,45,45	0
56	MG	AA	3208	1/1	0.89	0.11	48,48,48,48	0
56	MG	CA	3133	1/1	0.89	0.12	53,53,53,53	0
56	MG	BA	3809	1/1	0.89	0.25	58,58,58,58	0
56	MG	DA	3657	1/1	0.89	0.12	44,44,44,44	0
56	MG	DA	3327	1/1	0.89	0.15	48,48,48,48	0
56	MG	DA	3073	1/1	0.89	0.12	45,45,45,45	0
56	MG	B5	105	1/1	0.89	0.07	52,52,52,52	0
56	MG	BA	3526	1/1	0.89	0.09	43,43,43,43	0
56	MG	DA	3183	1/1	0.89	0.27	44,44,44,44	0
56	MG	BF	312	1/1	0.89	0.27	49,49,49,49	0
56	MG	BA	3455	1/1	0.89	0.14	31,31,31,31	0
56	MG	BA	3116	1/1	0.89	0.12	56,56,56,56	0
56	MG	BA	3808	1/1	0.89	0.24	40,40,40,40	0
56	MG	DA	3552	1/1	0.89	0.12	55,55,55,55	0
56	MG	BA	3059	1/1	0.89	0.23	36,36,36,36	0
56	MG	BA	3680	1/1	0.89	0.14	32,32,32,32	0
56	MG	BA	3485	1/1	0.89	0.18	29,29,29,29	0
56	MG	DA	3295	1/1	0.89	0.21	38,38,38,38	0
56	MG	CA	3179	1/1	0.89	0.13	49,49,49,49	0
56	MG	AA	3007	1/1	0.89	0.19	50,50,50,50	0
56	MG	DA	3341	1/1	0.89	0.25	43,43,43,43	0
56	MG	CA	3036	1/1	0.89	0.08	64,64,64,64	0
56	MG	DA	3532	1/1	0.89	0.13	61,61,61,61	0
56	MG	BA	3275	1/1	0.89	0.18	62,62,62,62	0
56	MG	BQ	3006	1/1	0.89	0.15	53,53,53,53	0
56	MG	DA	3061	1/1	0.90	0.18	43,43,43,43	0
56	MG	AA	3087	1/1	0.90	0.15	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3706	1/1	0.90	0.14	54,54,54,54	0
56	MG	CA	3128	1/1	0.90	0.17	49,49,49,49	0
56	MG	AA	3038	1/1	0.90	0.27	55,55,55,55	0
56	MG	AA	3141	1/1	0.90	0.24	70,70,70,70	0
56	MG	DA	3659	1/1	0.90	0.27	53,53,53,53	0
56	MG	DA	3562	1/1	0.90	0.24	49,49,49,49	0
56	MG	BA	3561	1/1	0.90	0.21	54,54,54,54	0
56	MG	CA	3100	1/1	0.90	0.16	65,65,65,65	0
56	MG	AH	201	1/1	0.90	0.14	67,67,67,67	0
56	MG	DA	3072	1/1	0.90	0.13	45,45,45,45	0
56	MG	DA	3133	1/1	0.90	0.21	50,50,50,50	0
56	MG	BA	3293	1/1	0.90	0.25	42,42,42,42	0
56	MG	DA	3122	1/1	0.90	0.17	51,51,51,51	0
56	MG	DA	3326	1/1	0.90	0.19	34,34,34,34	0
56	MG	BA	3490	1/1	0.90	0.26	31,31,31,31	0
56	MG	AA	3161	1/1	0.90	0.18	35,35,35,35	0
56	MG	DA	3309	1/1	0.90	0.15	43,43,43,43	0
56	MG	BA	3374	1/1	0.90	0.15	54,54,54,54	0
56	MG	DA	3162	1/1	0.90	0.09	48,48,48,48	0
56	MG	DA	3379	1/1	0.90	0.18	46,46,46,46	0
56	MG	BA	3652	1/1	0.90	0.24	46,46,46,46	0
56	MG	BZ	3003	1/1	0.90	0.19	51,51,51,51	0
56	MG	BA	3398	1/1	0.90	0.14	58,58,58,58	0
56	MG	DU	3003	1/1	0.90	0.14	45,45,45,45	0
56	MG	AA	3166	1/1	0.90	0.16	81,81,81,81	0
56	MG	DA	3091	1/1	0.90	0.20	32,32,32,32	0
56	MG	DA	3278	1/1	0.90	0.16	49,49,49,49	0
56	MG	BA	3890	1/1	0.90	0.19	34,34,34,34	0
56	MG	BA	3112	1/1	0.90	0.27	49,49,49,49	0
56	MG	BA	3875	1/1	0.90	0.19	51,51,51,51	0
56	MG	BA	3769	1/1	0.90	0.15	46,46,46,46	0
56	MG	BA	3323	1/1	0.90	0.29	48,48,48,48	0
56	MG	BA	3578	1/1	0.90	0.20	23,23,23,23	0
56	MG	BA	3253	1/1	0.90	0.19	29,29,29,29	0
56	MG	DA	3488	1/1	0.90	0.10	55,55,55,55	0
56	MG	CA	3189	1/1	0.90	0.14	57,57,57,57	0
56	MG	DA	3561	1/1	0.90	0.07	51,51,51,51	0
56	MG	D8	102	1/1	0.90	0.22	52,52,52,52	0
56	MG	AA	3144	1/1	0.90	0.12	47,47,47,47	0
56	MG	BA	3226	1/1	0.90	0.09	52,52,52,52	0
56	MG	DA	3285	1/1	0.90	0.23	42,42,42,42	0
56	MG	BA	3220	1/1	0.90	0.16	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3814	1/1	0.90	0.10	43,43,43,43	0
56	MG	DA	3149	1/1	0.90	0.23	59,59,59,59	0
56	MG	BA	3570	1/1	0.90	0.28	51,51,51,51	0
56	MG	BA	3444	1/1	0.90	0.14	39,39,39,39	0
56	MG	AA	3102	1/1	0.90	0.18	44,44,44,44	0
56	MG	BA	3866	1/1	0.90	0.18	54,54,54,54	0
56	MG	AA	3010	1/1	0.90	0.16	52,52,52,52	0
56	MG	CA	3187	1/1	0.90	0.14	51,51,51,51	0
56	MG	DA	3016	1/1	0.90	0.14	59,59,59,59	0
56	MG	AA	3190	1/1	0.90	0.12	54,54,54,54	0
56	MG	DA	3620	1/1	0.90	0.16	49,49,49,49	0
56	MG	CA	3137	1/1	0.90	0.22	66,66,66,66	0
56	MG	BA	3696	1/1	0.90	0.15	46,46,46,46	0
56	MG	AA	3169	1/1	0.90	0.16	62,62,62,62	0
56	MG	AA	3104	1/1	0.90	0.15	64,64,64,64	0
56	MG	DA	3164	1/1	0.90	0.12	61,61,61,61	0
56	MG	BA	3108	1/1	0.90	0.15	45,45,45,45	0
56	MG	DA	3544	1/1	0.90	0.13	44,44,44,44	0
56	MG	CA	3200	1/1	0.90	0.23	62,62,62,62	0
56	MG	DA	3130	1/1	0.90	0.14	49,49,49,49	0
56	MG	BA	3824	1/1	0.90	0.14	30,30,30,30	0
56	MG	BU	204	1/1	0.90	0.18	48,48,48,48	0
56	MG	BA	3852	1/1	0.90	0.14	33,33,33,33	0
56	MG	CA	3098	1/1	0.90	0.10	57,57,57,57	0
56	MG	DA	3553	1/1	0.90	0.04	58,58,58,58	0
56	MG	CA	3153	1/1	0.90	0.17	60,60,60,60	0
56	MG	DA	3606	1/1	0.90	0.07	61,61,61,61	0
56	MG	AL	5001	1/1	0.90	0.20	52,52,52,52	0
56	MG	DA	3399	1/1	0.90	0.10	47,47,47,47	0
56	MG	BA	3056	1/1	0.90	0.31	47,47,47,47	0
56	MG	BA	3302	1/1	0.90	0.22	43,43,43,43	0
56	MG	CA	3059	1/1	0.90	0.13	58,58,58,58	0
56	MG	DA	3193	1/1	0.90	0.14	59,59,59,59	0
56	MG	BA	3858	1/1	0.90	0.13	61,61,61,61	0
56	MG	CA	3177	1/1	0.90	0.15	64,64,64,64	0
56	MG	BA	3648	1/1	0.90	0.18	56,56,56,56	0
56	MG	BA	3588	1/1	0.90	0.19	30,30,30,30	0
56	MG	CA	3024	1/1	0.90	0.22	55,55,55,55	0
56	MG	CA	3131	1/1	0.90	0.10	76,76,76,76	0
56	MG	CA	3180	1/1	0.90	0.21	55,55,55,55	0
56	MG	BA	3897	1/1	0.90	0.15	49,49,49,49	0
56	MG	BA	3776	1/1	0.90	0.16	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3249	1/1	0.90	0.20	37,37,37,37	0
56	MG	DA	3639	1/1	0.90	0.26	57,57,57,57	0
56	MG	DA	3011	1/1	0.90	0.17	34,34,34,34	0
56	MG	BA	3006	1/1	0.90	0.15	43,43,43,43	0
56	MG	BB	3009	1/1	0.90	0.11	52,52,52,52	0
56	MG	AA	3030	1/1	0.90	0.22	49,49,49,49	0
56	MG	BA	3821	1/1	0.90	0.17	42,42,42,42	0
56	MG	DA	3572	1/1	0.90	0.11	45,45,45,45	0
56	MG	DA	3628	1/1	0.90	0.14	47,47,47,47	0
56	MG	CR	3001	1/1	0.90	0.13	64,64,64,64	0
56	MG	BA	3463	1/1	0.90	0.22	23,23,23,23	0
56	MG	DA	3394	1/1	0.90	0.16	55,55,55,55	0
56	MG	DA	3517	1/1	0.90	0.13	48,48,48,48	0
56	MG	BA	3067	1/1	0.90	0.20	62,62,62,62	0
56	MG	DA	3205	1/1	0.90	0.11	37,37,37,37	0
56	MG	BA	3645	1/1	0.90	0.15	57,57,57,57	0
56	MG	BA	3550	1/1	0.90	0.27	29,29,29,29	0
56	MG	DA	3584	1/1	0.90	0.06	57,57,57,57	0
56	MG	DA	3619	1/1	0.90	0.09	65,65,65,65	0
56	MG	DA	3427	1/1	0.90	0.12	35,35,35,35	0
56	MG	BA	3740	1/1	0.90	0.08	41,41,41,41	0
56	MG	BA	3590	1/1	0.90	0.17	23,23,23,23	0
56	MG	DA	3320	1/1	0.90	0.16	48,48,48,48	0
56	MG	DA	3001	1/1	0.90	0.17	55,55,55,55	0
56	MG	AA	3106	1/1	0.90	0.18	54,54,54,54	0
56	MG	DA	3331	1/1	0.90	0.12	30,30,30,30	0
56	MG	BA	3770	1/1	0.90	0.31	54,54,54,54	0
56	MG	BA	3756	1/1	0.90	0.10	53,53,53,53	0
56	MG	DA	3146	1/1	0.90	0.09	40,40,40,40	0
56	MG	AA	3094	1/1	0.91	0.30	49,49,49,49	0
56	MG	CA	3006	1/1	0.91	0.09	62,62,62,62	0
56	MG	DA	3200	1/1	0.91	0.16	46,46,46,46	0
56	MG	BA	3295	1/1	0.91	0.22	37,37,37,37	0
56	MG	BA	3244	1/1	0.91	0.14	39,39,39,39	0
56	MG	DA	3279	1/1	0.91	0.13	56,56,56,56	0
56	MG	BA	3027	1/1	0.91	0.15	37,37,37,37	0
56	MG	AA	3150	1/1	0.91	0.18	66,66,66,66	0
56	MG	AA	3209	1/1	0.91	0.16	61,61,61,61	0
56	MG	DA	3576	1/1	0.91	0.08	49,49,49,49	0
56	MG	CD	503	1/1	0.91	0.27	53,53,53,53	0
56	MG	BA	3438	1/1	0.91	0.23	27,27,27,27	0
56	MG	BA	3721	1/1	0.91	0.32	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3081	1/1	0.91	0.15	33,33,33,33	0
56	MG	BA	3442	1/1	0.91	0.16	37,37,37,37	0
56	MG	BA	3273	1/1	0.91	0.13	50,50,50,50	0
56	MG	DA	3557	1/1	0.91	0.10	54,54,54,54	0
56	MG	BA	3316	1/1	0.91	0.17	43,43,43,43	0
56	MG	DX	3001	1/1	0.91	0.21	44,44,44,44	0
56	MG	DA	3032	1/1	0.91	0.16	44,44,44,44	0
56	MG	BB	3014	1/1	0.91	0.20	43,43,43,43	0
56	MG	DP	201	1/1	0.91	0.13	57,57,57,57	0
56	MG	BA	3551	1/1	0.91	0.14	37,37,37,37	0
56	MG	BA	3449	1/1	0.91	0.23	39,39,39,39	0
56	MG	AA	3225	1/1	0.91	0.30	48,48,48,48	0
56	MG	CA	3082	1/1	0.91	0.06	58,58,58,58	0
56	MG	AA	3006	1/1	0.91	0.13	50,50,50,50	0
56	MG	BA	3101	1/1	0.91	0.29	42,42,42,42	0
56	MG	CT	3001	1/1	0.91	0.22	46,46,46,46	0
56	MG	AA	3171	1/1	0.91	0.12	46,46,46,46	0
56	MG	BW	203	1/1	0.91	0.26	47,47,47,47	0
56	MG	BB	3030	1/1	0.91	0.12	39,39,39,39	0
56	MG	DA	3596	1/1	0.91	0.13	62,62,62,62	0
56	MG	DA	3667	1/1	0.91	0.18	36,36,36,36	0
56	MG	DA	3545	1/1	0.91	0.07	52,52,52,52	0
56	MG	DA	3454	1/1	0.91	0.21	44,44,44,44	0
56	MG	BB	3007	1/1	0.91	0.23	56,56,56,56	0
56	MG	BA	3612	1/1	0.91	0.19	53,53,53,53	0
56	MG	DA	3156	1/1	0.91	0.12	33,33,33,33	0
56	MG	DA	3422	1/1	0.91	0.12	52,52,52,52	0
56	MG	DA	3147	1/1	0.91	0.07	53,53,53,53	0
56	MG	BA	3668	1/1	0.91	0.21	48,48,48,48	0
56	MG	DA	3184	1/1	0.91	0.26	37,37,37,37	0
56	MG	DA	3067	1/1	0.91	0.17	54,54,54,54	0
56	MG	DA	3304	1/1	0.91	0.11	40,40,40,40	0
56	MG	BA	3210	1/1	0.91	0.19	53,53,53,53	0
56	MG	AA	3041	1/1	0.91	0.10	53,53,53,53	0
56	MG	B0	106	1/1	0.91	0.15	66,66,66,66	0
56	MG	DA	3496	1/1	0.91	0.15	53,53,53,53	0
56	MG	CA	3045	1/1	0.91	0.07	47,47,47,47	0
56	MG	BA	3400	1/1	0.91	0.23	32,32,32,32	0
56	MG	BA	3872	1/1	0.91	0.09	42,42,42,42	0
56	MG	BA	3510	1/1	0.91	0.28	49,49,49,49	0
56	MG	DA	3145	1/1	0.91	0.21	47,47,47,47	0
56	MG	DA	3043	1/1	0.91	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3595	1/1	0.91	0.12	45,45,45,45	0
56	MG	DA	3487	1/1	0.91	0.16	48,48,48,48	0
56	MG	DA	3269	1/1	0.91	0.13	54,54,54,54	0
56	MG	CA	3003	1/1	0.91	0.17	63,63,63,63	0
56	MG	DA	3307	1/1	0.91	0.13	41,41,41,41	0
56	MG	BA	3412	1/1	0.91	0.18	42,42,42,42	0
56	MG	DA	3365	1/1	0.91	0.10	38,38,38,38	0
56	MG	BA	3243	1/1	0.91	0.17	39,39,39,39	0
56	MG	BA	3479	1/1	0.91	0.15	41,41,41,41	0
56	MG	CA	3075	1/1	0.91	0.07	52,52,52,52	0
59	ZN	B4	501	1/1	0.91	0.15	75,75,75,75	0
56	MG	DA	3275	1/1	0.91	0.11	33,33,33,33	0
56	MG	BB	3023	1/1	0.91	0.13	71,71,71,71	0
56	MG	BA	3300	1/1	0.91	0.14	58,58,58,58	0
56	MG	DB	3004	1/1	0.91	0.22	57,57,57,57	0
56	MG	BA	3542	1/1	0.91	0.12	43,43,43,43	0
56	MG	DA	3154	1/1	0.91	0.25	57,57,57,57	0
56	MG	DA	3462	1/1	0.91	0.10	42,42,42,42	0
56	MG	AY	3002	1/1	0.91	0.10	66,66,66,66	0
56	MG	BA	3239	1/1	0.91	0.17	38,38,38,38	0
56	MG	DA	3323	1/1	0.91	0.15	34,34,34,34	0
56	MG	BA	3191	1/1	0.91	0.15	31,31,31,31	0
56	MG	BA	3800	1/1	0.91	0.23	29,29,29,29	0
56	MG	DA	3272	1/1	0.91	0.10	52,52,52,52	0
56	MG	DA	3337	1/1	0.91	0.13	44,44,44,44	0
56	MG	DA	3381	1/1	0.91	0.17	47,47,47,47	0
56	MG	DA	3670	1/1	0.91	0.11	51,51,51,51	0
56	MG	DA	3206	1/1	0.91	0.15	33,33,33,33	0
56	MG	DA	3153	1/1	0.91	0.17	43,43,43,43	0
56	MG	BA	3113	1/1	0.91	0.16	66,66,66,66	0
56	MG	DA	3280	1/1	0.91	0.08	57,57,57,57	0
56	MG	DA	3212	1/1	0.91	0.14	52,52,52,52	0
56	MG	DA	3298	1/1	0.91	0.14	50,50,50,50	0
56	MG	BA	3396	1/1	0.91	0.15	42,42,42,42	0
56	MG	CA	3174	1/1	0.91	0.21	57,57,57,57	0
56	MG	BB	3018	1/1	0.91	0.25	32,32,32,32	0
56	MG	DA	3068	1/1	0.91	0.26	58,58,58,58	0
56	MG	DA	3594	1/1	0.91	0.12	56,56,56,56	0
56	MG	BE	303	1/1	0.91	0.20	35,35,35,35	0
56	MG	DE	307	1/1	0.91	0.14	53,53,53,53	0
56	MG	BA	3495	1/1	0.91	0.22	40,40,40,40	0
56	MG	BA	3171	1/1	0.91	0.17	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3220	1/1	0.91	0.16	57,57,57,57	0
56	MG	CA	3005	1/1	0.91	0.11	55,55,55,55	0
56	MG	BA	3423	1/1	0.91	0.09	34,34,34,34	0
56	MG	DB	3003	1/1	0.91	0.14	62,62,62,62	0
56	MG	CA	3035	1/1	0.91	0.17	49,49,49,49	0
56	MG	BA	3228	1/1	0.91	0.18	35,35,35,35	0
56	MG	BA	3546	1/1	0.91	0.17	47,47,47,47	0
56	MG	BA	3264	1/1	0.91	0.15	38,38,38,38	0
56	MG	DA	3569	1/1	0.91	0.24	47,47,47,47	0
56	MG	CA	3028	1/1	0.91	0.19	58,58,58,58	0
56	MG	BA	3637	1/1	0.91	0.28	32,32,32,32	0
56	MG	DA	3132	1/1	0.91	0.22	50,50,50,50	0
56	MG	AA	3081	1/1	0.91	0.12	48,48,48,48	0
56	MG	CA	3048	1/1	0.91	0.18	53,53,53,53	0
56	MG	BA	3004	1/1	0.91	0.23	33,33,33,33	0
56	MG	CA	3067	1/1	0.91	0.21	55,55,55,55	0
56	MG	BZ	3002	1/1	0.91	0.12	50,50,50,50	0
56	MG	BA	3124	1/1	0.91	0.20	26,26,26,26	0
56	MG	BA	3880	1/1	0.91	0.09	35,35,35,35	0
56	MG	DA	3405	1/1	0.91	0.12	44,44,44,44	0
56	MG	CW	3001	1/1	0.91	0.47	57,57,57,57	0
56	MG	BA	3791	1/1	0.91	0.09	47,47,47,47	0
56	MG	CA	3099	1/1	0.91	0.21	72,72,72,72	0
56	MG	DA	3174	1/1	0.91	0.27	49,49,49,49	0
56	MG	BA	3562	1/1	0.91	0.20	41,41,41,41	0
56	MG	DA	3005	1/1	0.91	0.22	52,52,52,52	0
56	MG	DA	3099	1/1	0.91	0.18	44,44,44,44	0
56	MG	DA	3049	1/1	0.91	0.19	43,43,43,43	0
56	MG	CA	3097	1/1	0.91	0.10	43,43,43,43	0
56	MG	DA	3661	1/1	0.91	0.10	39,39,39,39	0
56	MG	DA	3587	1/1	0.91	0.09	64,64,64,64	0
56	MG	AA	3024	1/1	0.91	0.18	39,39,39,39	0
56	MG	BA	3418	1/1	0.91	0.14	60,60,60,60	0
56	MG	CA	3147	1/1	0.91	0.13	64,64,64,64	0
56	MG	CA	3112	1/1	0.91	0.17	65,65,65,65	0
56	MG	CA	3156	1/1	0.91	0.15	59,59,59,59	0
56	MG	CA	3070	1/1	0.91	0.09	59,59,59,59	0
56	MG	DA	3538	1/1	0.91	0.17	57,57,57,57	0
56	MG	BB	3006	1/1	0.91	0.23	40,40,40,40	0
56	MG	BA	3718	1/1	0.91	0.17	47,47,47,47	0
56	MG	BA	3079	1/1	0.91	0.28	40,40,40,40	0
56	MG	DA	3127	1/1	0.91	0.18	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BB	3017	1/1	0.91	0.26	37,37,37,37	0
56	MG	BA	3308	1/1	0.91	0.21	40,40,40,40	0
56	MG	DA	3374	1/1	0.91	0.08	36,36,36,36	0
56	MG	BA	3787	1/1	0.91	0.18	24,24,24,24	0
56	MG	BQ	3005	1/1	0.91	0.13	37,37,37,37	0
56	MG	BD	305	1/1	0.91	0.16	35,35,35,35	0
56	MG	BA	3267	1/1	0.92	0.14	51,51,51,51	0
56	MG	AA	3098	1/1	0.92	0.12	60,60,60,60	0
56	MG	CA	3038	1/1	0.92	0.11	51,51,51,51	0
56	MG	BA	3291	1/1	0.92	0.28	49,49,49,49	0
56	MG	BA	3015	1/1	0.92	0.14	33,33,33,33	0
56	MG	DA	3642	1/1	0.92	0.13	40,40,40,40	0
56	MG	BF	301	1/1	0.92	0.28	41,41,41,41	0
56	MG	CA	3196	1/1	0.92	0.14	53,53,53,53	0
56	MG	BA	3864	1/1	0.92	0.17	26,26,26,26	0
56	MG	BA	3854	1/1	0.92	0.13	51,51,51,51	0
56	MG	DA	3510	1/1	0.92	0.12	46,46,46,46	0
56	MG	BA	3894	1/1	0.92	0.27	44,44,44,44	0
56	MG	BA	3352	1/1	0.92	0.17	42,42,42,42	0
56	MG	BA	3126	1/1	0.92	0.13	38,38,38,38	0
56	MG	BA	3335	1/1	0.92	0.22	33,33,33,33	0
56	MG	DA	3131	1/1	0.92	0.26	48,48,48,48	0
56	MG	BD	304	1/1	0.92	0.53	49,49,49,49	0
56	MG	BA	3473	1/1	0.92	0.21	59,59,59,59	0
56	MG	BA	3188	1/1	0.92	0.29	55,55,55,55	0
56	MG	BA	3159	1/1	0.92	0.13	50,50,50,50	0
56	MG	DA	3095	1/1	0.92	0.14	46,46,46,46	0
56	MG	DA	3004	1/1	0.92	0.21	36,36,36,36	0
56	MG	DA	3382	1/1	0.92	0.23	40,40,40,40	0
56	MG	BH	3001	1/1	0.92	0.33	40,40,40,40	0
56	MG	DA	3460	1/1	0.92	0.23	51,51,51,51	0
56	MG	BA	3700	1/1	0.92	0.16	51,51,51,51	0
56	MG	BA	3548	1/1	0.92	0.10	49,49,49,49	0
56	MG	BA	3156	1/1	0.92	0.15	46,46,46,46	0
56	MG	DA	3421	1/1	0.92	0.19	44,44,44,44	0
56	MG	BA	3847	1/1	0.92	0.11	52,52,52,52	0
56	MG	DV	201	1/1	0.92	0.38	51,51,51,51	0
56	MG	BA	3384	1/1	0.92	0.14	48,48,48,48	0
56	MG	DA	3305	1/1	0.92	0.12	42,42,42,42	0
56	MG	DA	3232	1/1	0.92	0.11	44,44,44,44	0
56	MG	BA	3679	1/1	0.92	0.18	33,33,33,33	0
56	MG	BA	3062	1/1	0.92	0.21	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3084	1/1	0.92	0.25	42,42,42,42	0
56	MG	AA	3172	1/1	0.92	0.07	43,43,43,43	0
56	MG	BA	3070	1/1	0.92	0.34	47,47,47,47	0
56	MG	DA	3448	1/1	0.92	0.19	36,36,36,36	0
56	MG	CA	3120	1/1	0.92	0.14	62,62,62,62	0
56	MG	DA	3403	1/1	0.92	0.14	46,46,46,46	0
56	MG	BA	3633	1/1	0.92	0.10	42,42,42,42	0
56	MG	BX	3002	1/1	0.92	0.18	37,37,37,37	0
56	MG	BA	3461	1/1	0.92	0.22	23,23,23,23	0
56	MG	BE	304	1/1	0.92	0.30	56,56,56,56	0
56	MG	BU	206	1/1	0.92	0.20	38,38,38,38	0
56	MG	BA	3554	1/1	0.92	0.20	48,48,48,48	0
56	MG	DA	3636	1/1	0.92	0.18	55,55,55,55	0
56	MG	DA	3085	1/1	0.92	0.10	39,39,39,39	0
56	MG	BA	3169	1/1	0.92	0.30	40,40,40,40	0
56	MG	BA	3032	1/1	0.92	0.16	29,29,29,29	0
56	MG	DA	3246	1/1	0.92	0.07	59,59,59,59	0
56	MG	DF	301	1/1	0.92	0.15	36,36,36,36	0
56	MG	DA	3630	1/1	0.92	0.17	45,45,45,45	0
56	MG	BA	3016	1/1	0.92	0.27	51,51,51,51	0
56	MG	BE	307	1/1	0.92	0.18	37,37,37,37	0
56	MG	BA	3163	1/1	0.92	0.24	46,46,46,46	0
56	MG	AA	3074	1/1	0.92	0.13	57,57,57,57	0
56	MG	BA	3798	1/1	0.92	0.27	55,55,55,55	0
56	MG	DA	3605	1/1	0.92	0.22	51,51,51,51	0
56	MG	CA	3129	1/1	0.92	0.13	69,69,69,69	0
56	MG	DA	3342	1/1	0.92	0.16	44,44,44,44	0
56	MG	BA	3145	1/1	0.92	0.19	41,41,41,41	0
56	MG	BA	3734	1/1	0.92	0.25	32,32,32,32	0
56	MG	CA	3029	1/1	0.92	0.13	60,60,60,60	0
56	MG	BA	3009	1/1	0.92	0.17	23,23,23,23	0
56	MG	DA	3535	1/1	0.92	0.13	41,41,41,41	0
56	MG	BA	3789	1/1	0.92	0.23	23,23,23,23	0
56	MG	BA	3594	1/1	0.92	0.14	22,22,22,22	0
56	MG	DA	3353	1/1	0.92	0.15	34,34,34,34	0
56	MG	BA	3001	1/1	0.92	0.19	45,45,45,45	0
56	MG	DA	3313	1/1	0.92	0.13	42,42,42,42	0
56	MG	DA	3112	1/1	0.92	0.13	42,42,42,42	0
56	MG	BA	3783	1/1	0.92	0.18	33,33,33,33	0
56	MG	BA	3022	1/1	0.92	0.12	40,40,40,40	0
56	MG	AA	3020	1/1	0.92	0.19	45,45,45,45	0
56	MG	BA	3179	1/1	0.92	0.16	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3512	1/1	0.92	0.19	54,54,54,54	0
56	MG	BA	3693	1/1	0.92	0.23	39,39,39,39	0
56	MG	BX	3001	1/1	0.92	0.33	37,37,37,37	0
56	MG	AA	3016	1/1	0.92	0.18	57,57,57,57	0
56	MG	BR	202	1/1	0.92	0.28	38,38,38,38	0
56	MG	BA	3279	1/1	0.92	0.18	32,32,32,32	0
56	MG	DA	3060	1/1	0.92	0.15	53,53,53,53	0
56	MG	BA	3205	1/1	0.92	0.15	50,50,50,50	0
56	MG	DD	302	1/1	0.92	0.11	42,42,42,42	0
56	MG	DA	3371	1/1	0.92	0.10	42,42,42,42	0
56	MG	BA	3137	1/1	0.92	0.16	35,35,35,35	0
56	MG	B0	105	1/1	0.92	0.21	52,52,52,52	0
56	MG	BA	3347	1/1	0.92	0.11	41,41,41,41	0
56	MG	BA	3434	1/1	0.92	0.22	41,41,41,41	0
56	MG	DA	3644	1/1	0.92	0.10	60,60,60,60	0
56	MG	AW	103	1/1	0.92	0.22	45,45,45,45	0
56	MG	BA	3676	1/1	0.92	0.14	50,50,50,50	0
56	MG	BA	3602	1/1	0.92	0.15	20,20,20,20	0
56	MG	BA	3139	1/1	0.92	0.22	45,45,45,45	0
56	MG	BA	3710	1/1	0.92	0.22	49,49,49,49	0
56	MG	DA	3547	1/1	0.92	0.17	52,52,52,52	0
56	MG	DA	3110	1/1	0.92	0.32	38,38,38,38	0
56	MG	BA	3152	1/1	0.92	0.15	48,48,48,48	0
56	MG	DB	3005	1/1	0.92	0.17	61,61,61,61	0
56	MG	BA	3193	1/1	0.92	0.17	50,50,50,50	0
56	MG	BA	3345	1/1	0.92	0.19	47,47,47,47	0
56	MG	BA	3206	1/1	0.92	0.15	59,59,59,59	0
56	MG	DA	3197	1/1	0.92	0.15	32,32,32,32	0
56	MG	BA	3071	1/1	0.92	0.23	32,32,32,32	0
56	MG	DA	3217	1/1	0.92	0.15	63,63,63,63	0
56	MG	BU	202	1/1	0.92	0.12	31,31,31,31	0
56	MG	BA	3141	1/1	0.92	0.20	32,32,32,32	0
56	MG	AA	3134	1/1	0.92	0.18	47,47,47,47	0
59	ZN	CN	501	1/1	0.92	0.06	83,83,83,83	0
56	MG	DA	3631	1/1	0.92	0.11	52,52,52,52	0
56	MG	AA	3198	1/1	0.92	0.18	58,58,58,58	0
56	MG	BA	3764	1/1	0.92	0.27	32,32,32,32	0
56	MG	BA	3703	1/1	0.92	0.16	55,55,55,55	0
56	MG	B7	101	1/1	0.92	0.17	41,41,41,41	0
56	MG	BA	3073	1/1	0.92	0.18	49,49,49,49	0
56	MG	CA	3026	1/1	0.92	0.26	56,56,56,56	0
56	MG	AA	3065	1/1	0.92	0.26	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3248	1/1	0.92	0.19	50,50,50,50	0
56	MG	DF	306	1/1	0.92	0.36	46,46,46,46	0
56	MG	DA	3343	1/1	0.92	0.08	39,39,39,39	0
56	MG	BA	3146	1/1	0.92	0.11	62,62,62,62	0
56	MG	AE	3002	1/1	0.92	0.21	57,57,57,57	0
56	MG	DQ	3003	1/1	0.92	0.23	57,57,57,57	0
56	MG	BA	3096	1/1	0.92	0.28	42,42,42,42	0
56	MG	BA	3669	1/1	0.92	0.26	44,44,44,44	0
56	MG	CQ	3002	1/1	0.92	0.18	65,65,65,65	0
56	MG	BA	3288	1/1	0.92	0.30	51,51,51,51	0
56	MG	BA	3689	1/1	0.92	0.21	44,44,44,44	0
56	MG	BA	3896	1/1	0.92	0.17	41,41,41,41	0
56	MG	BA	3530	1/1	0.92	0.18	43,43,43,43	0
56	MG	AX	3009	1/1	0.92	0.15	32,32,32,32	0
56	MG	CA	3111	1/1	0.92	0.24	53,53,53,53	0
56	MG	BA	3622	1/1	0.92	0.09	56,56,56,56	0
56	MG	DA	3390	1/1	0.92	0.17	42,42,42,42	0
56	MG	CA	3016	1/1	0.92	0.11	45,45,45,45	0
56	MG	DA	3467	1/1	0.92	0.13	40,40,40,40	0
56	MG	B9	502	1/1	0.92	0.28	47,47,47,47	0
56	MG	BA	3199	1/1	0.92	0.13	31,31,31,31	0
56	MG	BA	3807	1/1	0.92	0.21	46,46,46,46	0
56	MG	DZ	5001	1/1	0.92	0.11	73,73,73,73	0
56	MG	BA	3746	1/1	0.92	0.18	57,57,57,57	0
56	MG	AY	3001	1/1	0.92	0.34	76,76,76,76	0
56	MG	BA	3118	1/1	0.92	0.16	38,38,38,38	0
56	MG	BA	3895	1/1	0.92	0.17	30,30,30,30	0
56	MG	DA	3233	1/1	0.92	0.13	36,36,36,36	0
56	MG	BA	3117	1/1	0.92	0.15	29,29,29,29	0
56	MG	BA	3902	1/1	0.92	0.28	55,55,55,55	0
56	MG	CA	3079	1/1	0.92	0.16	58,58,58,58	0
56	MG	AA	3059	1/1	0.92	0.18	60,60,60,60	0
56	MG	BA	3061	1/1	0.93	0.25	19,19,19,19	0
56	MG	CA	3143	1/1	0.93	0.23	65,65,65,65	0
56	MG	AA	3046	1/1	0.93	0.15	43,43,43,43	0
56	MG	BA	3804	1/1	0.93	0.14	37,37,37,37	0
56	MG	DA	3310	1/1	0.93	0.16	54,54,54,54	0
56	MG	CA	3185	1/1	0.93	0.18	59,59,59,59	0
56	MG	DA	3104	1/1	0.93	0.11	45,45,45,45	0
56	MG	DA	3089	1/1	0.93	0.27	46,46,46,46	0
56	MG	BA	3286	1/1	0.93	0.22	52,52,52,52	0
56	MG	DA	3556	1/1	0.93	0.09	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3083	1/1	0.93	0.14	34,34,34,34	0
56	MG	DA	3111	1/1	0.93	0.16	40,40,40,40	0
56	MG	BA	3832	1/1	0.93	0.15	38,38,38,38	0
56	MG	AA	3052	1/1	0.93	0.20	58,58,58,58	0
56	MG	AA	3110	1/1	0.93	0.24	51,51,51,51	0
56	MG	CA	3030	1/1	0.93	0.19	61,61,61,61	0
56	MG	CA	3163	1/1	0.93	0.21	47,47,47,47	0
56	MG	BA	3722	1/1	0.93	0.14	52,52,52,52	0
56	MG	AA	3216	1/1	0.93	0.12	68,68,68,68	0
56	MG	CA	3165	1/1	0.93	0.08	36,36,36,36	0
56	MG	AA	3206	1/1	0.93	0.11	53,53,53,53	0
56	MG	DA	3235	1/1	0.93	0.08	52,52,52,52	0
56	MG	DA	3581	1/1	0.93	0.15	55,55,55,55	0
56	MG	BA	3616	1/1	0.93	0.28	43,43,43,43	0
56	MG	B7	103	1/1	0.93	0.13	44,44,44,44	0
56	MG	BA	3601	1/1	0.93	0.13	33,33,33,33	0
56	MG	BA	3303	1/1	0.93	0.13	27,27,27,27	0
56	MG	DA	3256	1/1	0.93	0.10	47,47,47,47	0
56	MG	DA	3388	1/1	0.93	0.08	32,32,32,32	0
56	MG	DA	3559	1/1	0.93	0.12	64,64,64,64	0
56	MG	DA	3501	1/1	0.93	0.20	33,33,33,33	0
56	MG	BU	201	1/1	0.93	0.18	39,39,39,39	0
56	MG	BA	3827	1/1	0.93	0.14	41,41,41,41	0
56	MG	DB	3017	1/1	0.93	0.13	58,58,58,58	0
56	MG	DA	3373	1/1	0.93	0.11	60,60,60,60	0
56	MG	BB	3005	1/1	0.93	0.10	52,52,52,52	0
56	MG	DA	3221	1/1	0.93	0.22	46,46,46,46	0
56	MG	DB	3011	1/1	0.93	0.19	60,60,60,60	0
56	MG	AA	3116	1/1	0.93	0.20	58,58,58,58	0
56	MG	AX	3002	1/1	0.93	0.23	49,49,49,49	0
56	MG	CA	3052	1/1	0.93	0.30	53,53,53,53	0
56	MG	DD	303	1/1	0.93	0.38	46,46,46,46	0
56	MG	BA	3593	1/1	0.93	0.10	44,44,44,44	0
56	MG	BV	204	1/1	0.93	0.22	44,44,44,44	0
56	MG	BA	3595	1/1	0.93	0.18	36,36,36,36	0
56	MG	DA	3344	1/1	0.93	0.07	54,54,54,54	0
56	MG	BA	3428	1/1	0.93	0.21	40,40,40,40	0
56	MG	DA	3240	1/1	0.93	0.15	45,45,45,45	0
56	MG	AA	3160	1/1	0.93	0.11	38,38,38,38	0
56	MG	BA	3047	1/1	0.93	0.23	31,31,31,31	0
56	MG	DA	3109	1/1	0.93	0.24	34,34,34,34	0
56	MG	DA	3126	1/1	0.93	0.14	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3029	1/1	0.93	0.19	48,48,48,48	0
56	MG	DA	3613	1/1	0.93	0.16	44,44,44,44	0
56	MG	AA	3032	1/1	0.93	0.10	60,60,60,60	0
56	MG	BA	3845	1/1	0.93	0.19	28,28,28,28	0
56	MG	DA	3014	1/1	0.93	0.12	33,33,33,33	0
56	MG	DA	3523	1/1	0.93	0.10	46,46,46,46	0
56	MG	BA	3324	1/1	0.93	0.17	36,36,36,36	0
56	MG	BA	3702	1/1	0.93	0.09	39,39,39,39	0
56	MG	BA	3331	1/1	0.93	0.20	32,32,32,32	0
56	MG	AA	3162	1/1	0.93	0.22	67,67,67,67	0
56	MG	DA	3308	1/1	0.93	0.14	45,45,45,45	0
56	MG	BD	303	1/1	0.93	0.19	40,40,40,40	0
56	MG	AX	3014	1/1	0.93	0.11	51,51,51,51	0
56	MG	CA	3117	1/1	0.93	0.10	58,58,58,58	0
56	MG	AA	3132	1/1	0.93	0.08	42,42,42,42	0
56	MG	DA	3230	1/1	0.93	0.27	54,54,54,54	0
56	MG	BA	3537	1/1	0.93	0.17	31,31,31,31	0
56	MG	AA	3230	1/1	0.93	0.22	56,56,56,56	0
56	MG	BA	3069	1/1	0.93	0.24	32,32,32,32	0
56	MG	AA	3178	1/1	0.93	0.10	49,49,49,49	0
56	MG	BA	3843	1/1	0.93	0.17	34,34,34,34	0
56	MG	BA	3232	1/1	0.93	0.17	33,33,33,33	0
56	MG	CA	3171	1/1	0.93	0.10	52,52,52,52	0
56	MG	BA	3464	1/1	0.93	0.21	25,25,25,25	0
56	MG	BA	3268	1/1	0.93	0.15	46,46,46,46	0
56	MG	DA	3251	1/1	0.93	0.10	43,43,43,43	0
56	MG	CA	3198	1/1	0.93	0.14	39,39,39,39	0
56	MG	DA	3634	1/1	0.93	0.12	62,62,62,62	0
56	MG	DA	3507	1/1	0.93	0.06	63,63,63,63	0
56	MG	CA	3027	1/1	0.93	0.16	49,49,49,49	0
56	MG	DA	3312	1/1	0.93	0.15	36,36,36,36	0
56	MG	DA	3477	1/1	0.93	0.18	51,51,51,51	0
56	MG	CA	3148	1/1	0.93	0.14	50,50,50,50	0
56	MG	BA	3219	1/1	0.93	0.15	28,28,28,28	0
56	MG	BA	3629	1/1	0.93	0.13	25,25,25,25	0
56	MG	AA	3088	1/1	0.93	0.20	46,46,46,46	0
56	MG	DA	3359	1/1	0.93	0.29	47,47,47,47	0
56	MG	AA	3064	1/1	0.93	0.33	54,54,54,54	0
56	MG	AA	3156	1/1	0.93	0.23	62,62,62,62	0
56	MG	BA	3686	1/1	0.93	0.09	52,52,52,52	0
56	MG	DA	3209	1/1	0.93	0.27	45,45,45,45	0
56	MG	BA	3080	1/1	0.93	0.20	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3863	1/1	0.93	0.20	44,44,44,44	0
56	MG	BA	3549	1/1	0.93	0.15	38,38,38,38	0
56	MG	AA	3127	1/1	0.93	0.12	33,33,33,33	0
56	MG	BA	3592	1/1	0.93	0.26	27,27,27,27	0
56	MG	DA	3097	1/1	0.93	0.20	44,44,44,44	0
56	MG	BA	3829	1/1	0.93	0.15	51,51,51,51	0
56	MG	DA	3627	1/1	0.93	0.11	42,42,42,42	0
56	MG	BA	3606	1/1	0.93	0.20	29,29,29,29	0
56	MG	DA	3044	1/1	0.93	0.17	48,48,48,48	0
56	MG	DB	3006	1/1	0.93	0.14	40,40,40,40	0
56	MG	DA	3589	1/1	0.93	0.08	50,50,50,50	0
56	MG	CA	3014	1/1	0.93	0.18	51,51,51,51	0
56	MG	DA	3663	1/1	0.93	0.16	46,46,46,46	0
56	MG	DA	3065	1/1	0.93	0.12	50,50,50,50	0
56	MG	CA	3066	1/1	0.93	0.21	44,44,44,44	0
56	MG	BA	3247	1/1	0.93	0.14	35,35,35,35	0
56	MG	BA	3745	1/1	0.93	0.22	45,45,45,45	0
56	MG	DA	3260	1/1	0.93	0.12	39,39,39,39	0
56	MG	BA	3555	1/1	0.93	0.19	64,64,64,64	0
56	MG	DA	3437	1/1	0.93	0.09	53,53,53,53	0
56	MG	BA	3658	1/1	0.93	0.24	44,44,44,44	0
56	MG	DA	3412	1/1	0.93	0.20	50,50,50,50	0
56	MG	AT	3001	1/1	0.93	0.12	54,54,54,54	0
56	MG	BA	3569	1/1	0.93	0.24	48,48,48,48	0
56	MG	BB	3015	1/1	0.93	0.16	51,51,51,51	0
56	MG	BA	3350	1/1	0.93	0.15	29,29,29,29	0
56	MG	BA	3089	1/1	0.93	0.21	47,47,47,47	0
56	MG	BA	3713	1/1	0.93	0.15	59,59,59,59	0
56	MG	BA	3382	1/1	0.93	0.25	26,26,26,26	0
56	MG	AA	3184	1/1	0.93	0.10	60,60,60,60	0
56	MG	BA	3516	1/1	0.93	0.09	49,49,49,49	0
56	MG	DA	3564	1/1	0.93	0.17	43,43,43,43	0
56	MG	BA	3129	1/1	0.93	0.18	37,37,37,37	0
56	MG	BA	3098	1/1	0.93	0.20	43,43,43,43	0
56	MG	CA	3018	1/1	0.93	0.21	46,46,46,46	0
56	MG	DA	3476	1/1	0.93	0.13	42,42,42,42	0
56	MG	CA	3096	1/1	0.93	0.13	39,39,39,39	0
56	MG	BA	3319	1/1	0.93	0.12	36,36,36,36	0
56	MG	DA	3450	1/1	0.93	0.15	35,35,35,35	0
56	MG	BA	3167	1/1	0.93	0.18	33,33,33,33	0
56	MG	CA	3104	1/1	0.93	0.05	53,53,53,53	0
56	MG	BA	3825	1/1	0.93	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3202	1/1	0.93	0.08	46,46,46,46	0
56	MG	DA	3626	1/1	0.93	0.39	41,41,41,41	0
56	MG	BF	306	1/1	0.93	0.16	34,34,34,34	0
56	MG	BA	3509	1/1	0.93	0.10	48,48,48,48	0
56	MG	CJ	5002	1/1	0.93	0.07	65,65,65,65	0
56	MG	BA	3181	1/1	0.93	0.22	38,38,38,38	0
56	MG	BA	3114	1/1	0.93	0.39	55,55,55,55	0
56	MG	BA	3099	1/1	0.93	0.14	49,49,49,49	0
56	MG	AA	3062	1/1	0.93	0.19	61,61,61,61	0
56	MG	DA	3407	1/1	0.93	0.16	67,67,67,67	0
56	MG	CA	3093	1/1	0.93	0.08	65,65,65,65	0
56	MG	CA	3094	1/1	0.93	0.10	47,47,47,47	0
56	MG	DA	3142	1/1	0.93	0.14	50,50,50,50	0
56	MG	BA	3217	1/1	0.93	0.28	49,49,49,49	0
56	MG	CA	3194	1/1	0.93	0.21	66,66,66,66	0
56	MG	BA	3670	1/1	0.93	0.24	57,57,57,57	0
56	MG	BA	3806	1/1	0.93	0.11	44,44,44,44	0
56	MG	BA	3234	1/1	0.93	0.20	43,43,43,43	0
56	MG	DA	3066	1/1	0.93	0.20	49,49,49,49	0
56	MG	BA	3543	1/1	0.93	0.15	48,48,48,48	0
56	MG	DA	3459	1/1	0.93	0.25	50,50,50,50	0
56	MG	AA	3076	1/1	0.93	0.30	58,58,58,58	0
56	MG	BA	3312	1/1	0.93	0.24	54,54,54,54	0
56	MG	BA	3136	1/1	0.93	0.42	49,49,49,49	0
56	MG	DA	3115	1/1	0.93	0.20	44,44,44,44	0
56	MG	AA	3097	1/1	0.93	0.14	54,54,54,54	0
56	MG	AA	3212	1/1	0.93	0.22	59,59,59,59	0
56	MG	BA	3717	1/1	0.93	0.11	57,57,57,57	0
56	MG	DA	3135	1/1	0.93	0.25	47,47,47,47	0
56	MG	CA	3149	1/1	0.93	0.20	71,71,71,71	0
56	MG	BA	3839	1/1	0.93	0.10	47,47,47,47	0
56	MG	BA	3192	1/1	0.93	0.18	41,41,41,41	0
56	MG	DA	3024	1/1	0.93	0.12	46,46,46,46	0
56	MG	BA	3251	1/1	0.93	0.27	45,45,45,45	0
56	MG	BA	3187	1/1	0.93	0.18	41,41,41,41	0
56	MG	CA	3025	1/1	0.93	0.17	51,51,51,51	0
56	MG	DA	3443	1/1	0.93	0.11	50,50,50,50	0
56	MG	BA	3309	1/1	0.93	0.31	50,50,50,50	0
56	MG	AA	3133	1/1	0.93	0.13	32,32,32,32	0
56	MG	DA	3210	1/1	0.93	0.22	30,30,30,30	0
56	MG	AA	3042	1/1	0.93	0.29	47,47,47,47	0
56	MG	BA	3627	1/1	0.93	0.16	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BT	5002	1/1	0.93	0.10	49,49,49,49	0
56	MG	BA	3646	1/1	0.93	0.14	46,46,46,46	0
56	MG	BA	3862	1/1	0.94	0.12	29,29,29,29	0
56	MG	DA	3033	1/1	0.94	0.14	40,40,40,40	0
56	MG	AA	3043	1/1	0.94	0.11	56,56,56,56	0
56	MG	AA	3103	1/1	0.94	0.17	50,50,50,50	0
56	MG	DT	3001	1/1	0.94	0.29	54,54,54,54	0
56	MG	BA	3011	1/1	0.94	0.17	37,37,37,37	0
56	MG	DA	3498	1/1	0.94	0.09	42,42,42,42	0
56	MG	BA	3311	1/1	0.94	0.18	43,43,43,43	0
56	MG	DA	3010	1/1	0.94	0.19	36,36,36,36	0
56	MG	CA	3095	1/1	0.94	0.24	46,46,46,46	0
56	MG	DA	3196	1/1	0.94	0.18	46,46,46,46	0
56	MG	DA	3290	1/1	0.94	0.14	52,52,52,52	0
56	MG	DA	3273	1/1	0.94	0.14	30,30,30,30	0
56	MG	BA	3414	1/1	0.94	0.15	32,32,32,32	0
56	MG	DA	3219	1/1	0.94	0.15	55,55,55,55	0
56	MG	BA	3859	1/1	0.94	0.18	34,34,34,34	0
56	MG	DA	3119	1/1	0.94	0.22	36,36,36,36	0
56	MG	BA	3364	1/1	0.94	0.22	57,57,57,57	0
56	MG	AA	3092	1/1	0.94	0.18	52,52,52,52	0
56	MG	DA	3526	1/1	0.94	0.20	42,42,42,42	0
56	MG	AA	3152	1/1	0.94	0.15	54,54,54,54	0
56	MG	AA	3033	1/1	0.94	0.13	55,55,55,55	0
56	MG	AA	3093	1/1	0.94	0.20	53,53,53,53	0
56	MG	BA	3307	1/1	0.94	0.17	36,36,36,36	0
56	MG	BA	3705	1/1	0.94	0.12	56,56,56,56	0
56	MG	BA	3249	1/1	0.94	0.26	41,41,41,41	0
56	MG	DA	3609	1/1	0.94	0.05	53,53,53,53	0
56	MG	BA	3519	1/1	0.94	0.20	46,46,46,46	0
56	MG	BA	3507	1/1	0.94	0.16	33,33,33,33	0
56	MG	DA	3052	1/1	0.94	0.13	38,38,38,38	0
56	MG	BA	3088	1/1	0.94	0.18	28,28,28,28	0
56	MG	DB	3008	1/1	0.94	0.16	55,55,55,55	0
59	ZN	D9	501	1/1	0.94	0.11	63,63,63,63	0
56	MG	BA	3332	1/1	0.94	0.16	43,43,43,43	0
56	MG	BO	3003	1/1	0.94	0.17	42,42,42,42	0
56	MG	BA	3405	1/1	0.94	0.16	42,42,42,42	0
56	MG	BA	3724	1/1	0.94	0.13	37,37,37,37	0
56	MG	BA	3230	1/1	0.94	0.17	35,35,35,35	0
56	MG	DA	3546	1/1	0.94	0.13	53,53,53,53	0
56	MG	BW	201	1/1	0.94	0.08	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3182	1/1	0.94	0.18	33,33,33,33	0
56	MG	CA	3166	1/1	0.94	0.20	53,53,53,53	0
56	MG	AA	3068	1/1	0.94	0.32	55,55,55,55	0
56	MG	DW	3002	1/1	0.94	0.16	44,44,44,44	0
56	MG	BA	3195	1/1	0.94	0.16	37,37,37,37	0
56	MG	AA	3142	1/1	0.94	0.13	44,44,44,44	0
56	MG	CA	3068	1/1	0.94	0.27	53,53,53,53	0
56	MG	BA	3539	1/1	0.94	0.24	38,38,38,38	0
56	MG	BA	3583	1/1	0.94	0.29	35,35,35,35	0
56	MG	CA	3010	1/1	0.94	0.26	52,52,52,52	0
59	ZN	D6	501	1/1	0.94	0.17	58,58,58,58	0
56	MG	DA	3428	1/1	0.94	0.18	42,42,42,42	0
56	MG	BA	3252	1/1	0.94	0.14	38,38,38,38	0
56	MG	AA	3049	1/1	0.94	0.25	62,62,62,62	0
56	MG	CA	3092	1/1	0.94	0.21	63,63,63,63	0
56	MG	CA	3054	1/1	0.94	0.15	53,53,53,53	0
56	MG	BA	3779	1/1	0.94	0.14	30,30,30,30	0
56	MG	BA	3197	1/1	0.94	0.11	27,27,27,27	0
56	MG	CA	3106	1/1	0.94	0.12	67,67,67,67	0
56	MG	AA	3130	1/1	0.94	0.11	62,62,62,62	0
56	MG	CA	3060	1/1	0.94	0.25	55,55,55,55	0
56	MG	CA	3119	1/1	0.94	0.22	48,48,48,48	0
56	MG	DA	3163	1/1	0.94	0.21	52,52,52,52	0
56	MG	AA	3233	1/1	0.94	0.27	52,52,52,52	0
56	MG	DF	304	1/1	0.94	0.21	38,38,38,38	0
56	MG	CA	3136	1/1	0.94	0.05	59,59,59,59	0
56	MG	DB	3009	1/1	0.94	0.17	59,59,59,59	0
56	MG	DA	3241	1/1	0.94	0.10	60,60,60,60	0
56	MG	BA	3524	1/1	0.94	0.16	24,24,24,24	0
56	MG	BA	3768	1/1	0.94	0.21	29,29,29,29	0
56	MG	DA	3069	1/1	0.94	0.21	58,58,58,58	0
56	MG	BA	3082	1/1	0.94	0.19	23,23,23,23	0
56	MG	AA	3002	1/1	0.94	0.12	55,55,55,55	0
56	MG	BA	3202	1/1	0.94	0.19	30,30,30,30	0
56	MG	DA	3528	1/1	0.94	0.11	67,67,67,67	0
56	MG	BA	3140	1/1	0.94	0.23	49,49,49,49	0
56	MG	DA	3224	1/1	0.94	0.20	32,32,32,32	0
56	MG	BA	3856	1/1	0.94	0.11	40,40,40,40	0
56	MG	AA	3145	1/1	0.94	0.09	35,35,35,35	0
56	MG	DE	304	1/1	0.94	0.15	43,43,43,43	0
56	MG	BA	3480	1/1	0.94	0.15	54,54,54,54	0
56	MG	DA	3645	1/1	0.94	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3884	1/1	0.94	0.17	27,27,27,27	0
56	MG	BA	3026	1/1	0.94	0.15	42,42,42,42	0
56	MG	DA	3441	1/1	0.94	0.08	44,44,44,44	0
56	MG	DA	3598	1/1	0.94	0.14	63,63,63,63	0
56	MG	BA	3281	1/1	0.94	0.23	38,38,38,38	0
56	MG	BA	3517	1/1	0.94	0.10	31,31,31,31	0
56	MG	CX	3007	1/1	0.94	0.15	57,57,57,57	0
56	MG	CA	3115	1/1	0.94	0.14	60,60,60,60	0
56	MG	BA	3780	1/1	0.94	0.15	45,45,45,45	0
56	MG	BA	3166	1/1	0.94	0.23	31,31,31,31	0
56	MG	BA	3742	1/1	0.94	0.15	43,43,43,43	0
56	MG	BA	3620	1/1	0.94	0.20	39,39,39,39	0
56	MG	BA	3853	1/1	0.94	0.16	41,41,41,41	0
56	MG	DA	3615	1/1	0.94	0.12	50,50,50,50	0
56	MG	DA	3096	1/1	0.94	0.12	44,44,44,44	0
56	MG	BA	3375	1/1	0.94	0.18	30,30,30,30	0
56	MG	BA	3876	1/1	0.94	0.27	62,62,62,62	0
56	MG	BA	3651	1/1	0.94	0.17	52,52,52,52	0
56	MG	DA	3420	1/1	0.94	0.09	45,45,45,45	0
56	MG	B0	104	1/1	0.94	0.13	35,35,35,35	0
56	MG	B1	102	1/1	0.94	0.09	59,59,59,59	0
56	MG	BA	3503	1/1	0.94	0.19	44,44,44,44	0
56	MG	DA	3053	1/1	0.94	0.22	43,43,43,43	0
56	MG	BA	3007	1/1	0.94	0.12	43,43,43,43	0
56	MG	DA	3466	1/1	0.94	0.17	50,50,50,50	0
56	MG	BA	3222	1/1	0.94	0.28	42,42,42,42	0
56	MG	BA	3260	1/1	0.94	0.17	40,40,40,40	0
56	MG	BA	3349	1/1	0.94	0.19	42,42,42,42	0
56	MG	BX	3006	1/1	0.94	0.20	35,35,35,35	0
56	MG	DA	3318	1/1	0.94	0.11	59,59,59,59	0
56	MG	DA	3319	1/1	0.94	0.09	43,43,43,43	0
56	MG	BA	3528	1/1	0.94	0.09	58,58,58,58	0
56	MG	BA	3582	1/1	0.94	0.22	34,34,34,34	0
56	MG	BA	3266	1/1	0.94	0.14	28,28,28,28	0
56	MG	CA	3139	1/1	0.94	0.18	61,61,61,61	0
56	MG	AF	3001	1/1	0.94	0.21	31,31,31,31	0
56	MG	BA	3437	1/1	0.94	0.23	31,31,31,31	0
56	MG	BA	3560	1/1	0.94	0.20	28,28,28,28	0
56	MG	BA	3301	1/1	0.94	0.17	47,47,47,47	0
56	MG	DA	3484	1/1	0.94	0.08	39,39,39,39	0
56	MG	BA	3826	1/1	0.94	0.19	42,42,42,42	0
56	MG	BA	3778	1/1	0.94	0.30	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3660	1/1	0.94	0.11	34,34,34,34	0
56	MG	BA	3883	1/1	0.94	0.26	45,45,45,45	0
56	MG	BF	311	1/1	0.94	0.20	40,40,40,40	0
56	MG	BA	3105	1/1	0.94	0.23	44,44,44,44	0
56	MG	BA	3797	1/1	0.94	0.22	52,52,52,52	0
56	MG	BA	3333	1/1	0.94	0.28	55,55,55,55	0
56	MG	DA	3592	1/1	0.94	0.13	54,54,54,54	0
56	MG	BX	3003	1/1	0.94	0.15	36,36,36,36	0
56	MG	BA	3367	1/1	0.94	0.17	49,49,49,49	0
56	MG	BB	3027	1/1	0.94	0.17	58,58,58,58	0
56	MG	BA	3238	1/1	0.94	0.23	42,42,42,42	0
56	MG	DA	3136	1/1	0.94	0.16	41,41,41,41	0
56	MG	BA	3357	1/1	0.94	0.20	40,40,40,40	0
56	MG	CA	3144	1/1	0.94	0.21	69,69,69,69	0
56	MG	BA	3732	1/1	0.94	0.18	24,24,24,24	0
56	MG	DA	3324	1/1	0.94	0.21	47,47,47,47	0
56	MG	CA	3076	1/1	0.94	0.22	42,42,42,42	0
56	MG	BA	3257	1/1	0.94	0.20	45,45,45,45	0
56	MG	BA	3609	1/1	0.94	0.17	30,30,30,30	0
56	MG	BA	3259	1/1	0.94	0.21	33,33,33,33	0
56	MG	BF	314	1/1	0.94	0.11	46,46,46,46	0
56	MG	AA	3175	1/1	0.94	0.13	62,62,62,62	0
56	MG	DA	3199	1/1	0.94	0.20	51,51,51,51	0
56	MG	BA	3586	1/1	0.94	0.21	40,40,40,40	0
59	ZN	DY	501	1/1	0.94	0.11	81,81,81,81	0
56	MG	BA	3240	1/1	0.94	0.18	39,39,39,39	0
56	MG	AA	3070	1/1	0.94	0.21	51,51,51,51	0
56	MG	BA	3299	1/1	0.94	0.32	51,51,51,51	0
56	MG	BA	3499	1/1	0.94	0.16	35,35,35,35	0
56	MG	BA	3885	1/1	0.94	0.27	55,55,55,55	0
56	MG	DA	3155	1/1	0.94	0.13	41,41,41,41	0
56	MG	CA	3141	1/1	0.94	0.13	65,65,65,65	0
56	MG	BA	3457	1/1	0.94	0.16	25,25,25,25	0
56	MG	DA	3623	1/1	0.94	0.17	54,54,54,54	0
56	MG	DA	3452	1/1	0.94	0.18	49,49,49,49	0
56	MG	BA	3591	1/1	0.94	0.22	31,31,31,31	0
56	MG	DA	3039	1/1	0.94	0.10	29,29,29,29	0
56	MG	B8	101	1/1	0.94	0.30	47,47,47,47	0
56	MG	BA	3598	1/1	0.94	0.11	40,40,40,40	0
56	MG	BA	3023	1/1	0.94	0.19	20,20,20,20	0
56	MG	AA	3048	1/1	0.94	0.26	46,46,46,46	0
56	MG	DA	3604	1/1	0.94	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3204	1/1	0.94	0.18	53,53,53,53	0
56	MG	B2	3002	1/1	0.94	0.21	43,43,43,43	0
56	MG	AA	3164	1/1	0.94	0.17	62,62,62,62	0
56	MG	DA	3242	1/1	0.94	0.15	40,40,40,40	0
56	MG	DA	3548	1/1	0.94	0.10	55,55,55,55	0
56	MG	CA	3043	1/1	0.94	0.27	57,57,57,57	0
56	MG	BA	3828	1/1	0.94	0.11	46,46,46,46	0
56	MG	DA	3058	1/1	0.94	0.14	56,56,56,56	0
56	MG	BA	3326	1/1	0.94	0.17	38,38,38,38	0
56	MG	AA	3183	1/1	0.94	0.12	59,59,59,59	0
56	MG	CA	3062	1/1	0.94	0.25	64,64,64,64	0
56	MG	DA	3616	1/1	0.94	0.15	54,54,54,54	0
56	MG	BA	3119	1/1	0.94	0.21	40,40,40,40	0
56	MG	AA	3112	1/1	0.94	0.17	40,40,40,40	0
56	MG	BO	3002	1/1	0.94	0.16	50,50,50,50	0
56	MG	BA	3564	1/1	0.94	0.09	39,39,39,39	0
56	MG	DA	3025	1/1	0.94	0.43	48,48,48,48	0
56	MG	BE	311	1/1	0.94	0.10	37,37,37,37	0
56	MG	BA	3216	1/1	0.94	0.27	35,35,35,35	0
56	MG	BA	3584	1/1	0.94	0.23	40,40,40,40	0
56	MG	BA	3376	1/1	0.94	0.20	32,32,32,32	0
56	MG	BA	3330	1/1	0.94	0.25	41,41,41,41	0
56	MG	BA	3613	1/1	0.94	0.15	54,54,54,54	0
56	MG	BA	3068	1/1	0.94	0.23	44,44,44,44	0
56	MG	DA	3599	1/1	0.94	0.10	51,51,51,51	0
56	MG	BA	3287	1/1	0.94	0.23	48,48,48,48	0
56	MG	BA	3031	1/1	0.94	0.17	40,40,40,40	0
56	MG	CA	3146	1/1	0.94	0.17	43,43,43,43	0
56	MG	DA	3469	1/1	0.94	0.07	45,45,45,45	0
56	MG	DA	3451	1/1	0.94	0.10	34,34,34,34	0
56	MG	DA	3483	1/1	0.94	0.09	45,45,45,45	0
56	MG	DA	3567	1/1	0.94	0.09	44,44,44,44	0
56	MG	DA	3120	1/1	0.94	0.18	47,47,47,47	0
56	MG	CA	3118	1/1	0.94	0.11	63,63,63,63	0
56	MG	DA	3351	1/1	0.94	0.13	36,36,36,36	0
56	MG	DA	3340	1/1	0.94	0.13	45,45,45,45	0
56	MG	AA	3205	1/1	0.94	0.21	56,56,56,56	0
56	MG	DA	3180	1/1	0.94	0.25	57,57,57,57	0
56	MG	BA	3128	1/1	0.94	0.26	35,35,35,35	0
56	MG	DA	3317	1/1	0.94	0.12	56,56,56,56	0
56	MG	BN	3001	1/1	0.94	0.19	41,41,41,41	0
56	MG	DA	3243	1/1	0.94	0.13	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3179	1/1	0.94	0.21	66,66,66,66	0
56	MG	CA	3142	1/1	0.94	0.07	61,61,61,61	0
56	MG	BA	3758	1/1	0.94	0.20	48,48,48,48	0
56	MG	BA	3774	1/1	0.94	0.25	47,47,47,47	0
56	MG	AA	3017	1/1	0.94	0.21	48,48,48,48	0
56	MG	AA	3119	1/1	0.94	0.12	60,60,60,60	0
56	MG	CA	3047	1/1	0.94	0.24	53,53,53,53	0
56	MG	BA	3289	1/1	0.94	0.18	30,30,30,30	0
56	MG	DE	302	1/1	0.94	0.14	52,52,52,52	0
56	MG	DA	3082	1/1	0.94	0.14	48,48,48,48	0
56	MG	DA	3666	1/1	0.94	0.12	55,55,55,55	0
56	MG	DA	3330	1/1	0.94	0.21	47,47,47,47	0
56	MG	BA	3525	1/1	0.94	0.06	59,59,59,59	0
56	MG	B2	3001	1/1	0.94	0.14	44,44,44,44	0
56	MG	BA	3738	1/1	0.95	0.21	46,46,46,46	0
56	MG	DA	3391	1/1	0.95	0.18	50,50,50,50	0
56	MG	BA	3074	1/1	0.95	0.26	33,33,33,33	0
56	MG	AA	3135	1/1	0.95	0.15	54,54,54,54	0
56	MG	BA	3799	1/1	0.95	0.20	22,22,22,22	0
56	MG	AA	3163	1/1	0.95	0.23	53,53,53,53	0
56	MG	CA	3034	1/1	0.95	0.15	52,52,52,52	0
56	MG	DQ	3002	1/1	0.95	0.18	35,35,35,35	0
56	MG	BA	3236	1/1	0.95	0.17	30,30,30,30	0
56	MG	AA	3039	1/1	0.95	0.29	51,51,51,51	0
56	MG	BA	3536	1/1	0.95	0.21	34,34,34,34	0
56	MG	DA	3537	1/1	0.95	0.07	38,38,38,38	0
56	MG	BA	3760	1/1	0.95	0.16	36,36,36,36	0
56	MG	BA	3803	1/1	0.95	0.14	67,67,67,67	0
56	MG	BA	3605	1/1	0.95	0.15	49,49,49,49	0
56	MG	CQ	3001	1/1	0.95	0.11	56,56,56,56	0
56	MG	DV	202	1/1	0.95	0.21	49,49,49,49	0
56	MG	BA	3221	1/1	0.95	0.19	49,49,49,49	0
56	MG	BA	3343	1/1	0.95	0.17	45,45,45,45	0
56	MG	DA	3392	1/1	0.95	0.12	39,39,39,39	0
56	MG	BA	3431	1/1	0.95	0.17	54,54,54,54	0
56	MG	DA	3416	1/1	0.95	0.13	47,47,47,47	0
56	MG	BA	3653	1/1	0.95	0.15	45,45,45,45	0
56	MG	AA	3167	1/1	0.95	0.17	53,53,53,53	0
56	MG	DA	3046	1/1	0.95	0.15	40,40,40,40	0
56	MG	BB	3029	1/1	0.95	0.15	21,21,21,21	0
56	MG	BA	3060	1/1	0.95	0.18	39,39,39,39	0
56	MG	BA	3256	1/1	0.95	0.21	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3837	1/1	0.95	0.20	52,52,52,52	0
56	MG	DA	3006	1/1	0.95	0.19	41,41,41,41	0
56	MG	BA	3395	1/1	0.95	0.21	44,44,44,44	0
56	MG	DA	3234	1/1	0.95	0.15	47,47,47,47	0
56	MG	DA	3413	1/1	0.95	0.21	42,42,42,42	0
56	MG	CA	3074	1/1	0.95	0.43	73,73,73,73	0
56	MG	BA	3851	1/1	0.95	0.16	33,33,33,33	0
56	MG	AA	3211	1/1	0.95	0.17	56,56,56,56	0
56	MG	BA	3063	1/1	0.95	0.31	41,41,41,41	0
56	MG	BA	3338	1/1	0.95	0.20	44,44,44,44	0
56	MG	DA	3516	1/1	0.95	0.12	56,56,56,56	0
56	MG	CX	3003	1/1	0.95	0.20	59,59,59,59	0
56	MG	BA	3122	1/1	0.95	0.20	22,22,22,22	0
56	MG	BA	3538	1/1	0.95	0.17	25,25,25,25	0
56	MG	AA	3227	1/1	0.95	0.13	25,25,25,25	0
56	MG	BA	3677	1/1	0.95	0.14	29,29,29,29	0
56	MG	AA	3095	1/1	0.95	0.27	58,58,58,58	0
56	MG	BA	3334	1/1	0.95	0.21	35,35,35,35	0
56	MG	DA	3141	1/1	0.95	0.14	42,42,42,42	0
56	MG	BA	3175	1/1	0.95	0.15	39,39,39,39	0
56	MG	DA	3213	1/1	0.95	0.16	44,44,44,44	0
56	MG	BA	3572	1/1	0.95	0.18	48,48,48,48	0
56	MG	BA	3200	1/1	0.95	0.22	35,35,35,35	0
56	MG	BA	3811	1/1	0.95	0.14	40,40,40,40	0
56	MG	DA	3457	1/1	0.95	0.16	30,30,30,30	0
60	K	AX	3001	1/1	0.95	0.16	45,45,45,45	0
56	MG	BA	3386	1/1	0.95	0.18	47,47,47,47	0
56	MG	BA	3110	1/1	0.95	0.26	17,17,17,17	0
56	MG	BA	3762	1/1	0.95	0.12	60,60,60,60	0
56	MG	BA	3368	1/1	0.95	0.19	37,37,37,37	0
56	MG	BA	3014	1/1	0.95	0.20	21,21,21,21	0
56	MG	BP	203	1/1	0.95	0.21	28,28,28,28	0
56	MG	DA	3435	1/1	0.95	0.20	39,39,39,39	0
56	MG	BA	3317	1/1	0.95	0.17	47,47,47,47	0
56	MG	DA	3071	1/1	0.95	0.12	41,41,41,41	0
56	MG	BA	3383	1/1	0.95	0.12	42,42,42,42	0
56	MG	BA	3053	1/1	0.95	0.17	28,28,28,28	0
56	MG	BA	3453	1/1	0.95	0.18	17,17,17,17	0
56	MG	DA	3291	1/1	0.95	0.20	52,52,52,52	0
56	MG	DA	3480	1/1	0.95	0.12	43,43,43,43	0
56	MG	DA	3629	1/1	0.95	0.10	36,36,36,36	0
56	MG	DA	3297	1/1	0.95	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3282	1/1	0.95	0.24	32,32,32,32	0
56	MG	BA	3360	1/1	0.95	0.12	49,49,49,49	0
56	MG	BQ	3002	1/1	0.95	0.27	24,24,24,24	0
56	MG	CA	3044	1/1	0.95	0.23	52,52,52,52	0
56	MG	DA	3475	1/1	0.95	0.13	42,42,42,42	0
56	MG	DA	3456	1/1	0.95	0.26	55,55,55,55	0
56	MG	DA	3442	1/1	0.95	0.10	46,46,46,46	0
56	MG	CA	3145	1/1	0.95	0.30	46,46,46,46	0
56	MG	DA	3036	1/1	0.95	0.12	34,34,34,34	0
56	MG	BA	3711	1/1	0.95	0.26	53,53,53,53	0
56	MG	AA	3069	1/1	0.95	0.16	44,44,44,44	0
56	MG	BP	206	1/1	0.95	0.18	31,31,31,31	0
56	MG	BE	301	1/1	0.95	0.17	36,36,36,36	0
56	MG	AA	3191	1/1	0.95	0.15	40,40,40,40	0
56	MG	BA	3406	1/1	0.95	0.18	28,28,28,28	0
56	MG	CA	3154	1/1	0.95	0.24	56,56,56,56	0
56	MG	DA	3525	1/1	0.95	0.19	46,46,46,46	0
56	MG	BA	3342	1/1	0.95	0.20	41,41,41,41	0
56	MG	BA	3667	1/1	0.95	0.14	43,43,43,43	0
56	MG	BA	3577	1/1	0.95	0.17	40,40,40,40	0
56	MG	BA	3160	1/1	0.95	0.18	44,44,44,44	0
56	MG	BA	3404	1/1	0.95	0.19	38,38,38,38	0
56	MG	BA	3177	1/1	0.95	0.22	40,40,40,40	0
56	MG	BA	3246	1/1	0.95	0.15	30,30,30,30	0
56	MG	DA	3138	1/1	0.95	0.13	55,55,55,55	0
56	MG	DB	3020	1/1	0.95	0.17	52,52,52,52	0
56	MG	AA	3029	1/1	0.95	0.34	56,56,56,56	0
56	MG	DA	3101	1/1	0.95	0.11	46,46,46,46	0
56	MG	DA	3583	1/1	0.95	0.13	54,54,54,54	0
56	MG	BA	3520	1/1	0.95	0.12	42,42,42,42	0
56	MG	BF	313	1/1	0.95	0.18	49,49,49,49	0
56	MG	BA	3773	1/1	0.95	0.21	29,29,29,29	0
56	MG	CA	3199	1/1	0.95	0.27	51,51,51,51	0
56	MG	CA	3087	1/1	0.95	0.24	60,60,60,60	0
56	MG	BA	3358	1/1	0.95	0.21	28,28,28,28	0
56	MG	DA	3059	1/1	0.95	0.13	39,39,39,39	0
56	MG	BA	3370	1/1	0.95	0.20	34,34,34,34	0
56	MG	DB	3015	1/1	0.95	0.24	44,44,44,44	0
56	MG	DA	3017	1/1	0.95	0.21	42,42,42,42	0
56	MG	BA	3081	1/1	0.95	0.18	21,21,21,21	0
56	MG	DA	3486	1/1	0.95	0.25	38,38,38,38	0
56	MG	AA	3129	1/1	0.95	0.09	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3903	1/1	0.95	0.19	42,42,42,42	0
56	MG	DA	3671	1/1	0.95	0.22	36,36,36,36	0
56	MG	DA	3367	1/1	0.95	0.10	57,57,57,57	0
56	MG	BA	3802	1/1	0.95	0.16	27,27,27,27	0
56	MG	B3	3002	1/1	0.95	0.29	39,39,39,39	0
56	MG	BA	3272	1/1	0.95	0.20	40,40,40,40	0
56	MG	BA	3513	1/1	0.95	0.20	51,51,51,51	0
56	MG	DA	3190	1/1	0.95	0.18	47,47,47,47	0
56	MG	DA	3539	1/1	0.95	0.10	56,56,56,56	0
56	MG	CL	201	1/1	0.95	0.12	55,55,55,55	0
56	MG	D3	3001	1/1	0.95	0.12	62,62,62,62	0
56	MG	BA	3632	1/1	0.95	0.18	41,41,41,41	0
56	MG	BA	3377	1/1	0.95	0.22	35,35,35,35	0
56	MG	BA	3131	1/1	0.95	0.19	37,37,37,37	0
56	MG	BA	3248	1/1	0.95	0.12	47,47,47,47	0
56	MG	BA	3625	1/1	0.95	0.20	20,20,20,20	0
56	MG	BF	302	1/1	0.95	0.17	37,37,37,37	0
56	MG	BA	3558	1/1	0.95	0.20	46,46,46,46	0
56	MG	BA	3547	1/1	0.95	0.11	48,48,48,48	0
60	K	CX	3001	1/1	0.95	0.08	62,62,62,62	0
56	MG	AA	3100	1/1	0.95	0.17	41,41,41,41	0
56	MG	BA	3344	1/1	0.95	0.25	33,33,33,33	0
56	MG	BF	305	1/1	0.95	0.17	28,28,28,28	0
56	MG	BA	3741	1/1	0.95	0.19	63,63,63,63	0
56	MG	DA	3201	1/1	0.95	0.11	52,52,52,52	0
56	MG	DA	3189	1/1	0.95	0.14	39,39,39,39	0
56	MG	DA	3578	1/1	0.95	0.07	46,46,46,46	0
56	MG	DA	3186	1/1	0.95	0.22	54,54,54,54	0
56	MG	DA	3603	1/1	0.95	0.15	52,52,52,52	0
56	MG	DA	3108	1/1	0.95	0.16	38,38,38,38	0
56	MG	BA	3336	1/1	0.95	0.21	43,43,43,43	0
56	MG	AA	3066	1/1	0.95	0.16	30,30,30,30	0
56	MG	BA	3057	1/1	0.95	0.14	39,39,39,39	0
56	MG	BA	3599	1/1	0.95	0.06	60,60,60,60	0
56	MG	BA	3904	1/1	0.95	0.15	46,46,46,46	0
56	MG	BA	3237	1/1	0.95	0.20	57,57,57,57	0
56	MG	CA	3037	1/1	0.95	0.10	50,50,50,50	0
56	MG	BA	3184	1/1	0.95	0.22	41,41,41,41	0
56	MG	BA	3419	1/1	0.95	0.14	38,38,38,38	0
56	MG	AA	3199	1/1	0.95	0.21	54,54,54,54	0
56	MG	BA	3363	1/1	0.95	0.17	45,45,45,45	0
56	MG	CA	3122	1/1	0.95	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3222	1/1	0.95	0.10	50,50,50,50	0
56	MG	BA	3043	1/1	0.95	0.18	43,43,43,43	0
56	MG	DA	3464	1/1	0.95	0.21	31,31,31,31	0
56	MG	BA	3393	1/1	0.95	0.17	23,23,23,23	0
56	MG	BA	3475	1/1	0.95	0.20	28,28,28,28	0
56	MG	AA	3001	1/1	0.95	0.19	35,35,35,35	0
56	MG	BA	3692	1/1	0.95	0.18	47,47,47,47	0
56	MG	BA	3529	1/1	0.95	0.14	53,53,53,53	0
56	MG	BA	3725	1/1	0.95	0.22	42,42,42,42	0
56	MG	BA	3189	1/1	0.95	0.21	30,30,30,30	0
56	MG	BA	3411	1/1	0.95	0.19	44,44,44,44	0
56	MG	BA	3723	1/1	0.95	0.22	27,27,27,27	0
56	MG	DA	3083	1/1	0.95	0.17	31,31,31,31	0
56	MG	DA	3334	1/1	0.95	0.09	44,44,44,44	0
56	MG	BA	3401	1/1	0.95	0.24	10,10,10,10	0
56	MG	BO	3004	1/1	0.95	0.19	53,53,53,53	0
56	MG	BA	3155	1/1	0.95	0.18	39,39,39,39	0
56	MG	BA	3737	1/1	0.95	0.23	29,29,29,29	0
56	MG	BA	3280	1/1	0.95	0.18	23,23,23,23	0
56	MG	BB	3002	1/1	0.95	0.28	43,43,43,43	0
56	MG	DA	3179	1/1	0.95	0.25	42,42,42,42	0
56	MG	DA	3098	1/1	0.95	0.18	36,36,36,36	0
56	MG	BA	3785	1/1	0.95	0.17	39,39,39,39	0
56	MG	DA	3470	1/1	0.95	0.13	46,46,46,46	0
56	MG	AA	3118	1/1	0.95	0.21	45,45,45,45	0
56	MG	DA	3406	1/1	0.95	0.10	39,39,39,39	0
56	MG	BA	3366	1/1	0.95	0.18	25,25,25,25	0
56	MG	DD	306	1/1	0.95	0.21	46,46,46,46	0
56	MG	BA	3683	1/1	0.95	0.22	37,37,37,37	0
56	MG	BG	206	1/1	0.95	0.11	59,59,59,59	0
56	MG	DA	3051	1/1	0.95	0.17	45,45,45,45	0
56	MG	DA	3020	1/1	0.95	0.16	48,48,48,48	0
56	MG	BA	3186	1/1	0.96	0.23	37,37,37,37	0
56	MG	DD	301	1/1	0.96	0.23	38,38,38,38	0
56	MG	DA	3169	1/1	0.96	0.10	44,44,44,44	0
56	MG	DA	3376	1/1	0.96	0.10	27,27,27,27	0
56	MG	DA	3640	1/1	0.96	0.07	56,56,56,56	0
56	MG	BA	3392	1/1	0.96	0.23	48,48,48,48	0
56	MG	DA	3302	1/1	0.96	0.13	57,57,57,57	0
56	MG	DA	3643	1/1	0.96	0.12	51,51,51,51	0
56	MG	CA	3033	1/1	0.96	0.07	65,65,65,65	0
56	MG	BA	3439	1/1	0.96	0.22	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3078	1/1	0.96	0.24	47,47,47,47	0
56	MG	CA	3051	1/1	0.96	0.21	32,32,32,32	0
56	MG	AA	3228	1/1	0.96	0.33	58,58,58,58	0
56	MG	BD	310	1/1	0.96	0.15	46,46,46,46	0
56	MG	BY	502	1/1	0.96	0.22	45,45,45,45	0
56	MG	DA	3669	1/1	0.96	0.16	46,46,46,46	0
56	MG	BA	3325	1/1	0.96	0.13	33,33,33,33	0
56	MG	BA	3321	1/1	0.96	0.13	43,43,43,43	0
56	MG	DA	3254	1/1	0.96	0.17	37,37,37,37	0
56	MG	AA	3053	1/1	0.96	0.20	42,42,42,42	0
56	MG	AA	3011	1/1	0.96	0.28	46,46,46,46	0
56	MG	BA	3850	1/1	0.96	0.20	47,47,47,47	0
56	MG	BA	3429	1/1	0.96	0.17	51,51,51,51	0
56	MG	DA	3271	1/1	0.96	0.07	48,48,48,48	0
56	MG	BA	3276	1/1	0.96	0.24	42,42,42,42	0
56	MG	BA	3792	1/1	0.96	0.12	47,47,47,47	0
56	MG	BA	3297	1/1	0.96	0.13	45,45,45,45	0
56	MG	BA	3077	1/1	0.96	0.22	27,27,27,27	0
56	MG	DA	3064	1/1	0.96	0.12	44,44,44,44	0
56	MG	DA	3185	1/1	0.96	0.17	39,39,39,39	0
56	MG	DA	3078	1/1	0.96	0.10	39,39,39,39	0
56	MG	BA	3823	1/1	0.96	0.13	57,57,57,57	0
56	MG	BW	204	1/1	0.96	0.20	23,23,23,23	0
56	MG	AA	3138	1/1	0.96	0.17	57,57,57,57	0
56	MG	BA	3777	1/1	0.96	0.26	52,52,52,52	0
56	MG	DA	3207	1/1	0.96	0.22	52,52,52,52	0
56	MG	BA	3353	1/1	0.96	0.29	49,49,49,49	0
56	MG	DA	3520	1/1	0.96	0.14	38,38,38,38	0
56	MG	BA	3233	1/1	0.96	0.18	26,26,26,26	0
56	MG	BA	3132	1/1	0.96	0.21	57,57,57,57	0
56	MG	AA	3136	1/1	0.96	0.15	52,52,52,52	0
56	MG	DA	3590	1/1	0.96	0.07	37,37,37,37	0
56	MG	DA	3333	1/1	0.96	0.18	31,31,31,31	0
56	MG	BA	3893	1/1	0.96	0.12	26,26,26,26	0
56	MG	BU	208	1/1	0.96	0.16	34,34,34,34	0
56	MG	BA	3008	1/1	0.96	0.26	24,24,24,24	0
56	MG	DA	3478	1/1	0.96	0.12	50,50,50,50	0
56	MG	DA	3499	1/1	0.96	0.20	44,44,44,44	0
56	MG	BA	3042	1/1	0.96	0.26	43,43,43,43	0
56	MG	BA	3012	1/1	0.96	0.15	31,31,31,31	0
56	MG	DA	3137	1/1	0.96	0.13	45,45,45,45	0
56	MG	DA	3649	1/1	0.96	0.20	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3115	1/1	0.96	0.09	44,44,44,44	0
56	MG	DA	3600	1/1	0.96	0.06	48,48,48,48	0
56	MG	DA	3614	1/1	0.96	0.06	47,47,47,47	0
56	MG	BB	3022	1/1	0.96	0.24	46,46,46,46	0
56	MG	BA	3391	1/1	0.96	0.17	24,24,24,24	0
56	MG	BA	3416	1/1	0.96	0.20	29,29,29,29	0
56	MG	CA	3197	1/1	0.96	0.19	43,43,43,43	0
56	MG	DA	3236	1/1	0.96	0.15	36,36,36,36	0
56	MG	DA	3440	1/1	0.96	0.14	34,34,34,34	0
56	MG	BA	3422	1/1	0.96	0.20	24,24,24,24	0
56	MG	BA	3076	1/1	0.96	0.28	17,17,17,17	0
56	MG	CA	3201	1/1	0.96	0.06	51,51,51,51	0
56	MG	BF	303	1/1	0.96	0.20	31,31,31,31	0
56	MG	DA	3389	1/1	0.96	0.13	54,54,54,54	0
56	MG	CA	3123	1/1	0.96	0.10	51,51,51,51	0
56	MG	DA	3495	1/1	0.96	0.12	48,48,48,48	0
56	MG	BB	3019	1/1	0.96	0.20	49,49,49,49	0
56	MG	DA	3094	1/1	0.96	0.09	41,41,41,41	0
56	MG	DA	3377	1/1	0.96	0.15	43,43,43,43	0
56	MG	BA	3378	1/1	0.96	0.18	43,43,43,43	0
56	MG	AA	3193	1/1	0.96	0.21	51,51,51,51	0
56	MG	DA	3431	1/1	0.96	0.14	34,34,34,34	0
56	MG	BY	503	1/1	0.96	0.14	47,47,47,47	0
56	MG	BA	3121	1/1	0.96	0.21	33,33,33,33	0
56	MG	BA	3380	1/1	0.96	0.23	45,45,45,45	0
56	MG	BU	207	1/1	0.96	0.15	37,37,37,37	0
56	MG	DA	3345	1/1	0.96	0.16	36,36,36,36	0
56	MG	BA	3559	1/1	0.96	0.13	37,37,37,37	0
56	MG	DA	3652	1/1	0.96	0.15	53,53,53,53	0
56	MG	DA	3534	1/1	0.96	0.11	39,39,39,39	0
56	MG	DA	3335	1/1	0.96	0.17	28,28,28,28	0
56	MG	BA	3568	1/1	0.96	0.23	56,56,56,56	0
56	MG	BA	3874	1/1	0.96	0.20	31,31,31,31	0
56	MG	BA	3687	1/1	0.96	0.23	49,49,49,49	0
56	MG	CA	3031	1/1	0.96	0.09	51,51,51,51	0
56	MG	AA	3057	1/1	0.96	0.12	32,32,32,32	0
56	MG	BA	3157	1/1	0.96	0.24	41,41,41,41	0
56	MG	BA	3494	1/1	0.96	0.18	32,32,32,32	0
56	MG	AA	3185	1/1	0.96	0.24	52,52,52,52	0
56	MG	DA	3009	1/1	0.96	0.22	39,39,39,39	0
56	MG	BA	3134	1/1	0.96	0.28	29,29,29,29	0
56	MG	DA	3300	1/1	0.96	0.14	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3586	1/1	0.96	0.20	31,31,31,31	0
56	MG	D1	101	1/1	0.96	0.14	44,44,44,44	0
56	MG	AA	3146	1/1	0.96	0.14	42,42,42,42	0
56	MG	BN	3004	1/1	0.96	0.13	37,37,37,37	0
56	MG	DA	3105	1/1	0.96	0.06	56,56,56,56	0
56	MG	DA	3346	1/1	0.96	0.10	31,31,31,31	0
56	MG	BA	3534	1/1	0.96	0.09	54,54,54,54	0
56	MG	BA	3618	1/1	0.96	0.20	19,19,19,19	0
56	MG	BA	3817	1/1	0.96	0.18	50,50,50,50	0
56	MG	BA	3647	1/1	0.96	0.23	47,47,47,47	0
56	MG	BQ	3007	1/1	0.96	0.16	44,44,44,44	0
56	MG	BA	3604	1/1	0.96	0.21	52,52,52,52	0
56	MG	BA	3489	1/1	0.96	0.07	60,60,60,60	0
56	MG	BA	3886	1/1	0.96	0.10	37,37,37,37	0
56	MG	BA	3218	1/1	0.96	0.29	33,33,33,33	0
56	MG	AX	3012	1/1	0.96	0.06	60,60,60,60	0
56	MG	DA	3084	1/1	0.96	0.14	35,35,35,35	0
56	MG	DA	3259	1/1	0.96	0.18	41,41,41,41	0
56	MG	BA	3033	1/1	0.96	0.23	37,37,37,37	0
56	MG	BA	3339	1/1	0.96	0.20	30,30,30,30	0
56	MG	AA	3143	1/1	0.96	0.10	38,38,38,38	0
56	MG	BA	3151	1/1	0.96	0.23	41,41,41,41	0
56	MG	DA	3194	1/1	0.96	0.15	40,40,40,40	0
56	MG	BA	3497	1/1	0.96	0.22	49,49,49,49	0
56	MG	DF	307	1/1	0.96	0.07	48,48,48,48	0
56	MG	B1	101	1/1	0.96	0.33	40,40,40,40	0
56	MG	DA	3063	1/1	0.96	0.12	34,34,34,34	0
56	MG	BA	3223	1/1	0.96	0.40	36,36,36,36	0
56	MG	AA	3151	1/1	0.96	0.12	48,48,48,48	0
56	MG	AX	3005	1/1	0.96	0.12	60,60,60,60	0
56	MG	DA	3113	1/1	0.96	0.06	39,39,39,39	0
56	MG	CA	3134	1/1	0.96	0.20	53,53,53,53	0
56	MG	BA	3397	1/1	0.96	0.16	46,46,46,46	0
56	MG	BA	3050	1/1	0.96	0.16	15,15,15,15	0
56	MG	BA	3045	1/1	0.96	0.15	35,35,35,35	0
56	MG	DA	3152	1/1	0.96	0.27	39,39,39,39	0
56	MG	BA	3346	1/1	0.96	0.14	38,38,38,38	0
56	MG	DA	3638	1/1	0.96	0.13	50,50,50,50	0
56	MG	BA	3553	1/1	0.96	0.19	19,19,19,19	0
56	MG	BA	3090	1/1	0.96	0.21	28,28,28,28	0
56	MG	BA	3511	1/1	0.96	0.14	38,38,38,38	0
56	MG	BA	3452	1/1	0.96	0.18	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3204	1/1	0.96	0.06	42,42,42,42	0
56	MG	DA	3369	1/1	0.96	0.19	58,58,58,58	0
56	MG	DA	3019	1/1	0.96	0.28	30,30,30,30	0
56	MG	DE	303	1/1	0.96	0.10	38,38,38,38	0
56	MG	BB	3003	1/1	0.96	0.19	31,31,31,31	0
56	MG	DA	3436	1/1	0.96	0.11	38,38,38,38	0
56	MG	DA	3386	1/1	0.96	0.24	46,46,46,46	0
56	MG	CA	3107	1/1	0.96	0.09	54,54,54,54	0
56	MG	BA	3283	1/1	0.96	0.11	43,43,43,43	0
56	MG	CA	3032	1/1	0.96	0.17	56,56,56,56	0
56	MG	B8	103	1/1	0.96	0.17	31,31,31,31	0
56	MG	BA	3443	1/1	0.96	0.18	22,22,22,22	0
56	MG	DA	3479	1/1	0.96	0.13	43,43,43,43	0
56	MG	AA	3203	1/1	0.96	0.21	59,59,59,59	0
56	MG	D8	101	1/1	0.96	0.19	50,50,50,50	0
56	MG	BA	3215	1/1	0.96	0.24	38,38,38,38	0
56	MG	BA	3841	1/1	0.96	0.17	56,56,56,56	0
56	MG	BX	3004	1/1	0.96	0.67	48,48,48,48	0
56	MG	DA	3672	1/1	0.96	0.17	43,43,43,43	0
56	MG	BA	3149	1/1	0.96	0.11	35,35,35,35	0
56	MG	BA	3435	1/1	0.96	0.15	60,60,60,60	0
56	MG	BA	3018	1/1	0.96	0.20	32,32,32,32	0
56	MG	AA	3224	1/1	0.96	0.24	51,51,51,51	0
56	MG	DA	3563	1/1	0.96	0.14	60,60,60,60	0
56	MG	BU	209	1/1	0.96	0.13	24,24,24,24	0
56	MG	AA	3108	1/1	0.96	0.09	65,65,65,65	0
56	MG	BA	3458	1/1	0.96	0.17	25,25,25,25	0
56	MG	BA	3661	1/1	0.96	0.08	47,47,47,47	0
56	MG	BV	203	1/1	0.96	0.12	23,23,23,23	0
56	MG	BS	3002	1/1	0.96	0.11	39,39,39,39	0
56	MG	AA	3051	1/1	0.96	0.25	22,22,22,22	0
56	MG	BR	201	1/1	0.96	0.13	35,35,35,35	0
56	MG	BU	203	1/1	0.96	0.29	44,44,44,44	0
56	MG	DA	3635	1/1	0.96	0.18	44,44,44,44	0
56	MG	DA	3540	1/1	0.96	0.09	51,51,51,51	0
56	MG	BA	3678	1/1	0.96	0.15	25,25,25,25	0
56	MG	BA	3093	1/1	0.96	0.41	41,41,41,41	0
56	MG	DA	3352	1/1	0.96	0.20	35,35,35,35	0
56	MG	DF	305	1/1	0.96	0.16	39,39,39,39	0
56	MG	BA	3701	1/1	0.96	0.22	44,44,44,44	0
56	MG	BA	3013	1/1	0.96	0.14	25,25,25,25	0
56	MG	DA	3202	1/1	0.96	0.33	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3657	1/1	0.96	0.16	65,65,65,65	0
56	MG	DA	3192	1/1	0.96	0.21	38,38,38,38	0
56	MG	BA	3761	1/1	0.96	0.16	52,52,52,52	0
56	MG	BA	3587	1/1	0.96	0.21	32,32,32,32	0
56	MG	BA	3402	1/1	0.96	0.12	39,39,39,39	0
56	MG	DA	3173	1/1	0.96	0.17	41,41,41,41	0
56	MG	BA	3085	1/1	0.96	0.26	27,27,27,27	0
56	MG	CA	3121	1/1	0.96	0.21	52,52,52,52	0
56	MG	CA	3176	1/1	0.96	0.17	62,62,62,62	0
56	MG	AA	3021	1/1	0.96	0.14	41,41,41,41	0
56	MG	DA	3294	1/1	0.96	0.11	39,39,39,39	0
56	MG	DA	3647	1/1	0.96	0.19	39,39,39,39	0
56	MG	DA	3165	1/1	0.96	0.12	27,27,27,27	0
56	MG	BA	3052	1/1	0.96	0.22	15,15,15,15	0
56	MG	BA	3148	1/1	0.96	0.17	36,36,36,36	0
56	MG	DA	3008	1/1	0.96	0.12	33,33,33,33	0
56	MG	DA	3037	1/1	0.96	0.23	32,32,32,32	0
56	MG	BP	201	1/1	0.96	0.16	29,29,29,29	0
56	MG	BA	3158	1/1	0.96	0.23	12,12,12,12	0
56	MG	DA	3090	1/1	0.96	0.22	53,53,53,53	0
56	MG	DA	3648	1/1	0.96	0.14	39,39,39,39	0
56	MG	AA	3121	1/1	0.96	0.18	49,49,49,49	0
56	MG	DA	3250	1/1	0.96	0.11	50,50,50,50	0
56	MG	BA	3626	1/1	0.96	0.20	22,22,22,22	0
56	MG	BA	3328	1/1	0.96	0.18	36,36,36,36	0
56	MG	DA	3410	1/1	0.96	0.20	55,55,55,55	0
56	MG	DA	3641	1/1	0.96	0.08	62,62,62,62	0
56	MG	BA	3284	1/1	0.96	0.11	39,39,39,39	0
56	MG	BA	3270	1/1	0.96	0.19	28,28,28,28	0
56	MG	DA	3047	1/1	0.96	0.27	38,38,38,38	0
56	MG	BA	3708	1/1	0.96	0.16	40,40,40,40	0
56	MG	AA	3157	1/1	0.96	0.26	39,39,39,39	0
56	MG	BA	3767	1/1	0.96	0.17	34,34,34,34	0
56	MG	B5	104	1/1	0.96	0.11	27,27,27,27	0
56	MG	BW	205	1/1	0.96	0.15	34,34,34,34	0
56	MG	DA	3315	1/1	0.96	0.12	27,27,27,27	0
56	MG	DA	3139	1/1	0.96	0.15	35,35,35,35	0
56	MG	BA	3857	1/1	0.96	0.20	46,46,46,46	0
56	MG	BA	3736	1/1	0.96	0.22	45,45,45,45	0
56	MG	BA	3681	1/1	0.97	0.16	39,39,39,39	0
56	MG	BA	3185	1/1	0.97	0.23	23,23,23,23	0
56	MG	BA	3597	1/1	0.97	0.17	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3371	1/1	0.97	0.29	34,34,34,34	0
56	MG	BA	3624	1/1	0.97	0.19	40,40,40,40	0
56	MG	DA	3347	1/1	0.97	0.09	38,38,38,38	0
56	MG	DE	306	1/1	0.97	0.13	43,43,43,43	0
56	MG	BA	3812	1/1	0.97	0.21	22,22,22,22	0
56	MG	AA	3113	1/1	0.97	0.30	55,55,55,55	0
56	MG	CA	3159	1/1	0.97	0.13	61,61,61,61	0
56	MG	DA	3527	1/1	0.97	0.14	22,22,22,22	0
56	MG	DA	3187	1/1	0.97	0.27	44,44,44,44	0
56	MG	DA	3281	1/1	0.97	0.22	42,42,42,42	0
56	MG	BA	3153	1/1	0.97	0.18	31,31,31,31	0
56	MG	CA	3080	1/1	0.97	0.34	55,55,55,55	0
56	MG	AA	3234	1/1	0.97	0.13	40,40,40,40	0
56	MG	BA	3304	1/1	0.97	0.12	43,43,43,43	0
56	MG	BA	3337	1/1	0.97	0.12	24,24,24,24	0
56	MG	DA	3533	1/1	0.97	0.14	59,59,59,59	0
56	MG	BG	201	1/1	0.97	0.06	58,58,58,58	0
56	MG	BA	3650	1/1	0.97	0.19	33,33,33,33	0
56	MG	AX	3008	1/1	0.97	0.13	54,54,54,54	0
56	MG	BA	3135	1/1	0.97	0.21	37,37,37,37	0
56	MG	BA	3120	1/1	0.97	0.15	50,50,50,50	0
56	MG	BA	3660	1/1	0.97	0.29	46,46,46,46	0
56	MG	BA	3615	1/1	0.97	0.10	28,28,28,28	0
56	MG	BA	3642	1/1	0.97	0.19	27,27,27,27	0
56	MG	BA	3728	1/1	0.97	0.18	36,36,36,36	0
56	MG	DA	3178	1/1	0.97	0.16	31,31,31,31	0
56	MG	BA	3241	1/1	0.97	0.20	48,48,48,48	0
56	MG	BA	3477	1/1	0.97	0.32	41,41,41,41	0
56	MG	BA	3753	1/1	0.97	0.07	39,39,39,39	0
56	MG	DA	3282	1/1	0.97	0.21	32,32,32,32	0
56	MG	BA	3662	1/1	0.97	0.16	23,23,23,23	0
56	MG	BA	3467	1/1	0.97	0.20	27,27,27,27	0
56	MG	BA	3054	1/1	0.97	0.20	20,20,20,20	0
56	MG	DA	3497	1/1	0.97	0.11	50,50,50,50	0
56	MG	DA	3277	1/1	0.97	0.17	41,41,41,41	0
56	MG	DA	3030	1/1	0.97	0.40	43,43,43,43	0
56	MG	DA	3055	1/1	0.97	0.12	33,33,33,33	0
56	MG	BB	3001	1/1	0.97	0.21	41,41,41,41	0
56	MG	BA	3196	1/1	0.97	0.12	26,26,26,26	0
56	MG	DA	3543	1/1	0.97	0.09	47,47,47,47	0
56	MG	DA	3041	1/1	0.97	0.16	30,30,30,30	0
56	MG	DA	3093	1/1	0.97	0.20	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3173	1/1	0.97	0.11	43,43,43,43	0
56	MG	BA	3072	1/1	0.97	0.24	27,27,27,27	0
56	MG	DA	3637	1/1	0.97	0.09	48,48,48,48	0
56	MG	DA	3655	1/1	0.97	0.28	57,57,57,57	0
56	MG	DA	3293	1/1	0.97	0.10	34,34,34,34	0
56	MG	BA	3786	1/1	0.97	0.16	20,20,20,20	0
56	MG	BA	3277	1/1	0.97	0.15	21,21,21,21	0
56	MG	BA	3403	1/1	0.97	0.27	52,52,52,52	0
56	MG	BA	3744	1/1	0.97	0.12	41,41,41,41	0
56	MG	DA	3168	1/1	0.97	0.14	28,28,28,28	0
56	MG	BB	3008	1/1	0.97	0.29	50,50,50,50	0
56	MG	DQ	3001	1/1	0.97	0.16	42,42,42,42	0
56	MG	DA	3103	1/1	0.97	0.16	45,45,45,45	0
56	MG	AA	3115	1/1	0.97	0.18	54,54,54,54	0
56	MG	BA	3387	1/1	0.97	0.12	60,60,60,60	0
56	MG	AA	3022	1/1	0.97	0.08	35,35,35,35	0
56	MG	BA	3684	1/1	0.97	0.13	55,55,55,55	0
56	MG	BA	3656	1/1	0.97	0.19	32,32,32,32	0
56	MG	DD	305	1/1	0.97	0.38	38,38,38,38	0
56	MG	BA	3462	1/1	0.97	0.13	30,30,30,30	0
56	MG	BA	3075	1/1	0.97	0.28	22,22,22,22	0
56	MG	B5	101	1/1	0.97	0.17	32,32,32,32	0
56	MG	DA	3339	1/1	0.97	0.14	57,57,57,57	0
56	MG	BA	3373	1/1	0.97	0.24	28,28,28,28	0
56	MG	DA	3048	1/1	0.97	0.13	46,46,46,46	0
56	MG	DB	3012	1/1	0.97	0.12	50,50,50,50	0
56	MG	DA	3356	1/1	0.97	0.22	44,44,44,44	0
56	MG	BA	3788	1/1	0.97	0.17	25,25,25,25	0
56	MG	BA	3726	1/1	0.97	0.22	39,39,39,39	0
56	MG	DA	3284	1/1	0.97	0.09	36,36,36,36	0
56	MG	BA	3245	1/1	0.97	0.24	26,26,26,26	0
56	MG	DA	3226	1/1	0.97	0.27	54,54,54,54	0
56	MG	CF	3001	1/1	0.97	0.19	31,31,31,31	0
56	MG	BA	3574	1/1	0.97	0.28	42,42,42,42	0
56	MG	DA	3159	1/1	0.97	0.14	45,45,45,45	0
56	MG	DA	3518	1/1	0.97	0.08	34,34,34,34	0
56	MG	BA	3532	1/1	0.97	0.14	50,50,50,50	0
56	MG	AA	3140	1/1	0.97	0.12	45,45,45,45	0
56	MG	CA	3113	1/1	0.97	0.15	37,37,37,37	0
56	MG	AA	3077	1/1	0.97	0.29	60,60,60,60	0
56	MG	AA	3105	1/1	0.97	0.13	48,48,48,48	0
56	MG	DA	3602	1/1	0.97	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3128	1/1	0.97	0.20	27,27,27,27	0
56	MG	BA	3460	1/1	0.97	0.15	20,20,20,20	0
56	MG	BA	3440	1/1	0.97	0.22	32,32,32,32	0
56	MG	BA	3329	1/1	0.97	0.15	32,32,32,32	0
56	MG	BA	3905	1/1	0.97	0.14	47,47,47,47	0
56	MG	BA	3049	1/1	0.97	0.19	32,32,32,32	0
59	ZN	BY	501	1/1	0.97	0.17	63,63,63,63	0
56	MG	BA	3634	1/1	0.97	0.24	23,23,23,23	0
56	MG	AA	3155	1/1	0.97	0.14	42,42,42,42	0
56	MG	DU	3001	1/1	0.97	0.18	43,43,43,43	0
56	MG	BF	309	1/1	0.97	0.17	30,30,30,30	0
56	MG	AA	3186	1/1	0.97	0.20	43,43,43,43	0
56	MG	BA	3690	1/1	0.97	0.20	53,53,53,53	0
56	MG	CA	3042	1/1	0.97	0.17	48,48,48,48	0
56	MG	BA	3037	1/1	0.97	0.13	35,35,35,35	0
56	MG	AA	3072	1/1	0.97	0.19	40,40,40,40	0
56	MG	B6	103	1/1	0.97	0.23	44,44,44,44	0
56	MG	BA	3735	1/1	0.97	0.23	30,30,30,30	0
56	MG	DA	3258	1/1	0.97	0.19	39,39,39,39	0
56	MG	B5	102	1/1	0.97	0.20	36,36,36,36	0
56	MG	DA	3208	1/1	0.97	0.25	46,46,46,46	0
56	MG	DA	3493	1/1	0.97	0.11	38,38,38,38	0
56	MG	BA	3041	1/1	0.97	0.21	31,31,31,31	0
56	MG	DA	3350	1/1	0.97	0.20	29,29,29,29	0
56	MG	AA	3229	1/1	0.97	0.17	50,50,50,50	0
56	MG	AA	3075	1/1	0.97	0.22	44,44,44,44	0
56	MG	DA	3118	1/1	0.97	0.16	47,47,47,47	0
56	MG	BA	3878	1/1	0.97	0.20	15,15,15,15	0
56	MG	AB	3002	1/1	0.97	0.15	70,70,70,70	0
56	MG	DU	3002	1/1	0.97	0.28	52,52,52,52	0
56	MG	BA	3064	1/1	0.97	0.15	40,40,40,40	0
56	MG	BF	315	1/1	0.97	0.20	47,47,47,47	0
56	MG	BA	3154	1/1	0.97	0.24	31,31,31,31	0
56	MG	BA	3820	1/1	0.97	0.12	30,30,30,30	0
56	MG	BA	3733	1/1	0.97	0.19	42,42,42,42	0
56	MG	BD	311	1/1	0.97	0.21	40,40,40,40	0
56	MG	DA	3286	1/1	0.97	0.18	29,29,29,29	0
56	MG	DA	3481	1/1	0.97	0.11	41,41,41,41	0
56	MG	BA	3408	1/1	0.97	0.19	41,41,41,41	0
56	MG	DA	3418	1/1	0.97	0.26	44,44,44,44	0
56	MG	AA	3226	1/1	0.97	0.20	34,34,34,34	0
56	MG	BA	3044	1/1	0.97	0.18	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3195	1/1	0.97	0.20	38,38,38,38	0
56	MG	BA	3608	1/1	0.97	0.23	58,58,58,58	0
56	MG	CA	3105	1/1	0.97	0.11	53,53,53,53	0
56	MG	AA	3196	1/1	0.97	0.16	42,42,42,42	0
56	MG	BA	3544	1/1	0.97	0.13	40,40,40,40	0
56	MG	DA	3491	1/1	0.97	0.22	53,53,53,53	0
56	MG	BA	3092	1/1	0.97	0.31	31,31,31,31	0
56	MG	DA	3489	1/1	0.97	0.08	40,40,40,40	0
56	MG	CA	3181	1/1	0.97	0.07	55,55,55,55	0
56	MG	BA	3258	1/1	0.97	0.24	38,38,38,38	0
56	MG	DA	3003	1/1	0.97	0.20	24,24,24,24	0
56	MG	AA	3215	1/1	0.97	0.17	47,47,47,47	0
56	MG	DA	3554	1/1	0.97	0.18	48,48,48,48	0
56	MG	DA	3384	1/1	0.97	0.12	55,55,55,55	0
56	MG	BF	304	1/1	0.97	0.17	34,34,34,34	0
56	MG	BA	3198	1/1	0.97	0.19	34,34,34,34	0
56	MG	DA	3198	1/1	0.97	0.19	45,45,45,45	0
56	MG	BA	3846	1/1	0.97	0.17	30,30,30,30	0
56	MG	BA	3535	1/1	0.97	0.12	46,46,46,46	0
56	MG	BA	3010	1/1	0.97	0.28	26,26,26,26	0
56	MG	DA	3299	1/1	0.97	0.15	37,37,37,37	0
56	MG	BA	3172	1/1	0.97	0.27	32,32,32,32	0
56	MG	DA	3123	1/1	0.97	0.16	38,38,38,38	0
56	MG	BA	3003	1/1	0.97	0.22	24,24,24,24	0
56	MG	BA	3765	1/1	0.97	0.16	33,33,33,33	0
56	MG	DD	304	1/1	0.97	0.19	26,26,26,26	0
56	MG	CA	3168	1/1	0.97	0.10	65,65,65,65	0
56	MG	B0	102	1/1	0.97	0.14	47,47,47,47	0
56	MG	DA	3332	1/1	0.97	0.20	53,53,53,53	0
56	MG	DA	3148	1/1	0.97	0.18	50,50,50,50	0
56	MG	DA	3262	1/1	0.97	0.12	36,36,36,36	0
56	MG	B0	107	1/1	0.97	0.11	46,46,46,46	0
56	MG	DA	3022	1/1	0.97	0.26	34,34,34,34	0
56	MG	DA	3492	1/1	0.97	0.19	51,51,51,51	0
56	MG	DA	3425	1/1	0.97	0.08	53,53,53,53	0
56	MG	BA	3433	1/1	0.97	0.14	34,34,34,34	0
56	MG	BA	3887	1/1	0.97	0.13	35,35,35,35	0
56	MG	BA	3224	1/1	0.97	0.16	30,30,30,30	0
56	MG	BA	3747	1/1	0.97	0.14	57,57,57,57	0
56	MG	BA	3174	1/1	0.97	0.20	34,34,34,34	0
56	MG	DA	3203	1/1	0.97	0.20	46,46,46,46	0
56	MG	BA	3421	1/1	0.97	0.17	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3140	1/1	0.97	0.19	43,43,43,43	0
56	MG	DA	3423	1/1	0.97	0.11	56,56,56,56	0
56	MG	BA	3362	1/1	0.97	0.17	37,37,37,37	0
56	MG	DA	3455	1/1	0.97	0.13	35,35,35,35	0
56	MG	B7	102	1/1	0.97	0.15	27,27,27,27	0
56	MG	BA	3231	1/1	0.97	0.21	21,21,21,21	0
56	MG	D5	102	1/1	0.97	0.14	38,38,38,38	0
56	MG	BA	3183	1/1	0.97	0.16	35,35,35,35	0
56	MG	BD	312	1/1	0.97	0.20	27,27,27,27	0
56	MG	DA	3027	1/1	0.97	0.17	42,42,42,42	0
56	MG	DA	3245	1/1	0.97	0.10	48,48,48,48	0
56	MG	BA	3822	1/1	0.97	0.26	18,18,18,18	0
56	MG	BA	3869	1/1	0.97	0.27	20,20,20,20	0
56	MG	BA	3207	1/1	0.97	0.23	52,52,52,52	0
56	MG	BA	3478	1/1	0.97	0.17	27,27,27,27	0
56	MG	BA	3254	1/1	0.97	0.16	41,41,41,41	0
56	MG	DA	3013	1/1	0.97	0.23	39,39,39,39	0
56	MG	BA	3900	1/1	0.97	0.29	40,40,40,40	0
58	SF4	CD	501	8/8	0.97	0.09	50,59,70,75	0
56	MG	BA	3688	1/1	0.97	0.14	41,41,41,41	0
56	MG	DA	3411	1/1	0.97	0.14	44,44,44,44	0
56	MG	AA	3123	1/1	0.97	0.25	46,46,46,46	0
56	MG	BA	3315	1/1	0.97	0.17	39,39,39,39	0
56	MG	DA	3124	1/1	0.97	0.21	35,35,35,35	0
56	MG	BN	3003	1/1	0.97	0.22	41,41,41,41	0
56	MG	BA	3899	1/1	0.97	0.17	40,40,40,40	0
56	MG	DA	3378	1/1	0.97	0.10	43,43,43,43	0
56	MG	BA	3506	1/1	0.97	0.23	34,34,34,34	0
56	MG	BA	3709	1/1	0.97	0.11	34,34,34,34	0
56	MG	BA	3834	1/1	0.97	0.15	35,35,35,35	0
56	MG	AA	3034	1/1	0.98	0.12	52,52,52,52	0
56	MG	BP	204	1/1	0.98	0.18	19,19,19,19	0
56	MG	BA	3039	1/1	0.98	0.22	17,17,17,17	0
56	MG	BA	3213	1/1	0.98	0.35	48,48,48,48	0
58	SF4	AD	501	8/8	0.98	0.11	50,60,65,68	0
56	MG	DA	3166	1/1	0.98	0.16	39,39,39,39	0
56	MG	B3	3001	1/1	0.98	0.19	23,23,23,23	0
56	MG	BA	3242	1/1	0.98	0.18	60,60,60,60	0
56	MG	DA	3530	1/1	0.98	0.15	30,30,30,30	0
56	MG	DA	3057	1/1	0.98	0.15	20,20,20,20	0
56	MG	BA	3106	1/1	0.98	0.17	27,27,27,27	0
56	MG	BA	3091	1/1	0.98	0.17	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3035	1/1	0.98	0.22	27,27,27,27	0
56	MG	DA	3255	1/1	0.98	0.20	23,23,23,23	0
56	MG	BV	201	1/1	0.98	0.20	32,32,32,32	0
56	MG	DA	3419	1/1	0.98	0.17	42,42,42,42	0
56	MG	DA	3361	1/1	0.98	0.14	44,44,44,44	0
56	MG	DA	3253	1/1	0.98	0.13	41,41,41,41	0
56	MG	BA	3296	1/1	0.98	0.25	40,40,40,40	0
56	MG	DA	3508	1/1	0.98	0.23	39,39,39,39	0
56	MG	CD	502	1/1	0.98	0.12	51,51,51,51	0
56	MG	AA	3159	1/1	0.98	0.15	32,32,32,32	0
56	MG	DA	3468	1/1	0.98	0.12	49,49,49,49	0
56	MG	BA	3523	1/1	0.98	0.14	49,49,49,49	0
56	MG	BS	3001	1/1	0.98	0.18	39,39,39,39	0
56	MG	DA	3080	1/1	0.98	0.21	33,33,33,33	0
56	MG	BA	3664	1/1	0.98	0.24	46,46,46,46	0
56	MG	BA	3636	1/1	0.98	0.21	28,28,28,28	0
56	MG	CA	3012	1/1	0.98	0.21	57,57,57,57	0
56	MG	BA	3794	1/1	0.98	0.07	48,48,48,48	0
56	MG	AA	3148	1/1	0.98	0.17	43,43,43,43	0
56	MG	BA	3891	1/1	0.98	0.21	33,33,33,33	0
56	MG	BA	3190	1/1	0.98	0.23	38,38,38,38	0
56	MG	DA	3268	1/1	0.98	0.08	36,36,36,36	0
56	MG	BA	3441	1/1	0.98	0.20	26,26,26,26	0
56	MG	BQ	3004	1/1	0.98	0.31	46,46,46,46	0
56	MG	BA	3040	1/1	0.98	0.18	25,25,25,25	0
56	MG	BA	3034	1/1	0.98	0.20	20,20,20,20	0
56	MG	DA	3439	1/1	0.98	0.19	50,50,50,50	0
56	MG	BD	306	1/1	0.98	0.20	25,25,25,25	0
56	MG	CV	101	1/1	0.98	0.20	51,51,51,51	0
56	MG	BA	3109	1/1	0.98	0.22	20,20,20,20	0
56	MG	DA	3364	1/1	0.98	0.17	58,58,58,58	0
56	MG	DA	3601	1/1	0.98	0.08	38,38,38,38	0
56	MG	BD	302	1/1	0.98	0.34	39,39,39,39	0
56	MG	BA	3038	1/1	0.98	0.17	42,42,42,42	0
56	MG	BA	3327	1/1	0.98	0.20	20,20,20,20	0
56	MG	BA	3046	1/1	0.98	0.16	30,30,30,30	0
56	MG	BA	3055	1/1	0.98	0.28	25,25,25,25	0
56	MG	BA	3162	1/1	0.98	0.18	26,26,26,26	0
56	MG	AA	3168	1/1	0.98	0.14	53,53,53,53	0
56	MG	DA	3651	1/1	0.98	0.13	50,50,50,50	0
56	MG	DA	3144	1/1	0.98	0.22	49,49,49,49	0
56	MG	DA	3336	1/1	0.98	0.15	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3239	1/1	0.98	0.13	44,44,44,44	0
56	MG	DA	3012	1/1	0.98	0.21	42,42,42,42	0
56	MG	DA	3465	1/1	0.98	0.14	38,38,38,38	0
56	MG	DA	3474	1/1	0.98	0.21	35,35,35,35	0
56	MG	DA	3565	1/1	0.98	0.12	27,27,27,27	0
56	MG	BA	3514	1/1	0.98	0.19	9,9,9,9	0
56	MG	BA	3341	1/1	0.98	0.17	28,28,28,28	0
56	MG	BT	5001	1/1	0.98	0.14	56,56,56,56	0
56	MG	DA	3316	1/1	0.98	0.16	29,29,29,29	0
56	MG	BA	3407	1/1	0.98	0.17	13,13,13,13	0
56	MG	DA	3358	1/1	0.98	0.14	45,45,45,45	0
56	MG	DA	3485	1/1	0.98	0.13	31,31,31,31	0
56	MG	BS	3003	1/1	0.98	0.08	48,48,48,48	0
56	MG	BA	3848	1/1	0.98	0.23	45,45,45,45	0
56	MG	BA	3500	1/1	0.98	0.17	15,15,15,15	0
56	MG	DA	3434	1/1	0.98	0.18	47,47,47,47	0
56	MG	BA	3229	1/1	0.98	0.21	33,33,33,33	0
56	MG	DA	3028	1/1	0.98	0.18	40,40,40,40	0
56	MG	DA	3398	1/1	0.98	0.21	42,42,42,42	0
56	MG	BE	308	1/1	0.98	0.19	25,25,25,25	0
56	MG	DB	3010	1/1	0.98	0.28	45,45,45,45	0
56	MG	BO	3005	1/1	0.98	0.17	61,61,61,61	0
56	MG	DY	502	1/1	0.98	0.18	44,44,44,44	0
56	MG	BA	3292	1/1	0.98	0.25	42,42,42,42	0
56	MG	CA	3110	1/1	0.98	0.10	51,51,51,51	0
56	MG	BA	3430	1/1	0.98	0.18	44,44,44,44	0
56	MG	BR	203	1/1	0.98	0.21	29,29,29,29	0
56	MG	BE	312	1/1	0.98	0.25	56,56,56,56	0
56	MG	CK	3001	1/1	0.98	0.12	46,46,46,46	0
56	MG	BD	309	1/1	0.98	0.17	32,32,32,32	0
56	MG	BA	3250	1/1	0.98	0.19	38,38,38,38	0
56	MG	BA	3278	1/1	0.98	0.14	42,42,42,42	0
56	MG	BA	3712	1/1	0.98	0.28	32,32,32,32	0
56	MG	DA	3029	1/1	0.98	0.17	36,36,36,36	0
56	MG	DA	3038	1/1	0.98	0.18	34,34,34,34	0
56	MG	BA	3125	1/1	0.98	0.21	29,29,29,29	0
56	MG	DA	3042	1/1	0.98	0.19	27,27,27,27	0
56	MG	BA	3255	1/1	0.98	0.16	42,42,42,42	0
56	MG	BA	3749	1/1	0.98	0.23	24,24,24,24	0
56	MG	BA	3413	1/1	0.98	0.17	30,30,30,30	0
56	MG	BA	3036	1/1	0.98	0.31	34,34,34,34	0
56	MG	BA	3388	1/1	0.98	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3101	1/1	0.98	0.15	60,60,60,60	0
56	MG	BB	3010	1/1	0.98	0.17	38,38,38,38	0
56	MG	CA	3083	1/1	0.98	0.21	52,52,52,52	0
56	MG	DA	3283	1/1	0.98	0.04	44,44,44,44	0
56	MG	BA	3290	1/1	0.98	0.32	54,54,54,54	0
56	MG	BA	3201	1/1	0.98	0.25	17,17,17,17	0
56	MG	DA	3357	1/1	0.98	0.16	24,24,24,24	0
56	MG	BA	3644	1/1	0.98	0.20	18,18,18,18	0
56	MG	DA	3473	1/1	0.98	0.13	43,43,43,43	0
56	MG	BA	3641	1/1	0.98	0.19	22,22,22,22	0
56	MG	BA	3576	1/1	0.98	0.28	39,39,39,39	0
56	MG	BA	3682	1/1	0.98	0.18	39,39,39,39	0
56	MG	AK	3001	1/1	0.98	0.17	41,41,41,41	0
56	MG	BA	3889	1/1	0.98	0.11	29,29,29,29	0
56	MG	CA	3109	1/1	0.98	0.16	45,45,45,45	0
56	MG	DO	5001	1/1	0.98	0.18	51,51,51,51	0
56	MG	AA	3217	1/1	0.98	0.14	48,48,48,48	0
56	MG	BA	3755	1/1	0.98	0.18	45,45,45,45	0
56	MG	BD	308	1/1	0.98	0.23	41,41,41,41	0
56	MG	BA	3354	1/1	0.98	0.22	53,53,53,53	0
56	MG	BA	3674	1/1	0.98	0.19	31,31,31,31	0
56	MG	CA	3150	1/1	0.98	0.23	58,58,58,58	0
56	MG	AA	3013	1/1	0.98	0.23	21,21,21,21	0
56	MG	DA	3558	1/1	0.98	0.19	47,47,47,47	0
56	MG	BA	3521	1/1	0.98	0.22	38,38,38,38	0
56	MG	CA	3055	1/1	0.98	0.14	57,57,57,57	0
56	MG	BE	305	1/1	0.98	0.16	21,21,21,21	0
56	MG	BA	3265	1/1	0.98	0.12	23,23,23,23	0
56	MG	BA	3227	1/1	0.98	0.18	33,33,33,33	0
56	MG	BA	3816	1/1	0.98	0.22	35,35,35,35	0
56	MG	BA	3685	1/1	0.98	0.17	29,29,29,29	0
56	MG	DA	3646	1/1	0.98	0.16	27,27,27,27	0
56	MG	BA	3178	1/1	0.98	0.18	29,29,29,29	0
56	MG	BA	3775	1/1	0.98	0.19	35,35,35,35	0
56	MG	DA	3494	1/1	0.98	0.10	39,39,39,39	0
56	MG	BD	313	1/1	0.98	0.20	39,39,39,39	0
56	MG	BF	310	1/1	0.98	0.32	37,37,37,37	0
56	MG	BA	3892	1/1	0.98	0.20	28,28,28,28	0
56	MG	BA	3138	1/1	0.98	0.24	40,40,40,40	0
56	MG	BA	3772	1/1	0.98	0.21	26,26,26,26	0
56	MG	BA	3860	1/1	0.98	0.22	37,37,37,37	0
56	MG	BA	3379	1/1	0.98	0.17	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BU	205	1/1	0.98	0.23	42,42,42,42	0
56	MG	DA	3021	1/1	0.98	0.21	29,29,29,29	0
56	MG	BA	3879	1/1	0.98	0.27	28,28,28,28	0
56	MG	BD	301	1/1	0.98	0.20	31,31,31,31	0
56	MG	BA	3697	1/1	0.98	0.09	35,35,35,35	0
56	MG	CA	3178	1/1	0.99	0.06	52,52,52,52	0
59	ZN	B5	103	1/1	0.99	0.18	40,40,40,40	0
56	MG	BD	307	1/1	0.99	0.22	30,30,30,30	0
56	MG	BA	3868	1/1	0.99	0.22	8,8,8,8	0
56	MG	BF	308	1/1	0.99	0.15	33,33,33,33	0
56	MG	AX	3010	1/1	0.99	0.10	53,53,53,53	0
56	MG	BA	3123	1/1	0.99	0.24	28,28,28,28	0
56	MG	BA	3024	1/1	0.99	0.18	40,40,40,40	0
56	MG	BA	3143	1/1	0.99	0.24	37,37,37,37	0
56	MG	BA	3504	1/1	0.99	0.19	31,31,31,31	0
56	MG	BA	3340	1/1	0.99	0.24	34,34,34,34	0
56	MG	DA	3287	1/1	0.99	0.22	33,33,33,33	0
56	MG	CA	3022	1/1	0.99	0.14	33,33,33,33	0
56	MG	BA	3164	1/1	0.99	0.29	33,33,33,33	0
56	MG	BA	3127	1/1	0.99	0.14	33,33,33,33	0
56	MG	BA	3483	1/1	0.99	0.13	30,30,30,30	0
56	MG	DA	3257	1/1	0.99	0.17	53,53,53,53	0
56	MG	BA	3496	1/1	0.99	0.25	22,22,22,22	0
59	ZN	AN	501	1/1	0.99	0.16	62,62,62,62	0
56	MG	DA	3172	1/1	0.99	0.25	38,38,38,38	0
56	MG	BA	3235	1/1	0.99	0.23	17,17,17,17	0
56	MG	BA	3835	1/1	0.99	0.19	34,34,34,34	0
56	MG	BA	3531	1/1	0.99	0.21	46,46,46,46	0
56	MG	BV	202	1/1	0.99	0.23	23,23,23,23	0
56	MG	BA	3563	1/1	0.99	0.17	43,43,43,43	0
56	MG	BP	202	1/1	0.99	0.16	27,27,27,27	0
56	MG	BA	3790	1/1	0.99	0.15	21,21,21,21	0
56	MG	BA	3369	1/1	0.99	0.23	12,12,12,12	0
56	MG	BA	3180	1/1	0.99	0.22	31,31,31,31	0
59	ZN	D5	103	1/1	0.99	0.19	51,51,51,51	0
56	MG	BA	3771	1/1	0.99	0.22	29,29,29,29	0
56	MG	BY	504	1/1	0.99	0.24	39,39,39,39	0
56	MG	CE	3001	1/1	0.99	0.06	67,67,67,67	0
56	MG	BA	3150	1/1	0.99	0.17	42,42,42,42	0
56	MG	DA	3656	1/1	0.99	0.14	56,56,56,56	0
56	MG	BU	210	1/1	0.99	0.22	28,28,28,28	0
56	MG	BA	3225	1/1	0.99	0.23	32,32,32,32	0

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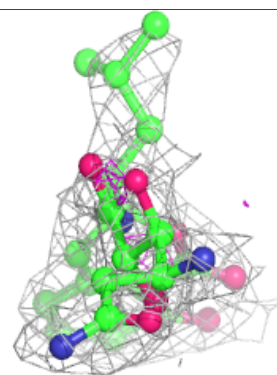
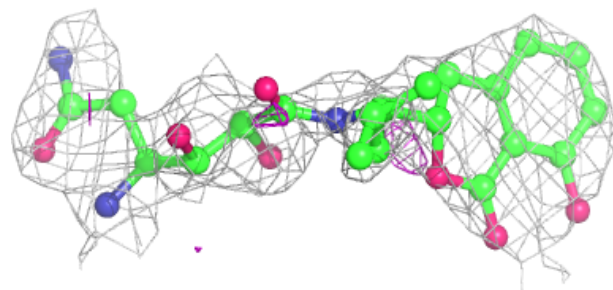
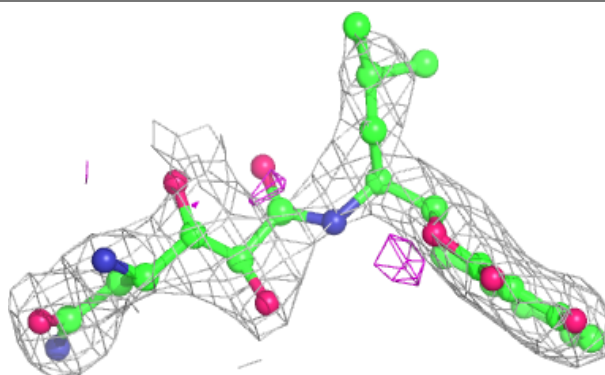
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3078	1/1	0.99	0.21	11,11,11,11	0
56	MG	DA	3522	1/1	0.99	0.18	35,35,35,35	0
56	MG	BV	205	1/1	0.99	0.17	46,46,46,46	0
56	MG	BA	3394	1/1	0.99	0.20	20,20,20,20	0
56	MG	BA	3030	1/1	0.99	0.18	28,28,28,28	0
56	MG	BA	3410	1/1	0.99	0.23	19,19,19,19	0
56	MG	BA	3888	1/1	0.99	0.13	26,26,26,26	0
56	MG	BA	3025	1/1	0.99	0.20	23,23,23,23	0
59	ZN	B9	501	1/1	1.00	0.20	38,38,38,38	0
59	ZN	B6	102	1/1	1.00	0.23	39,39,39,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

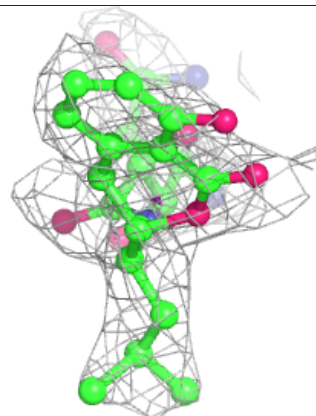
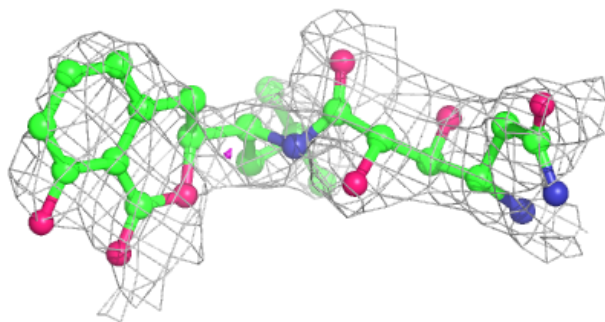
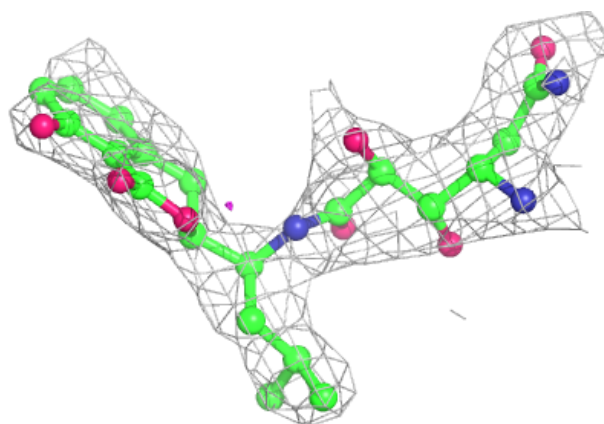
Electron density around UAM CA 3202:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UAM AA 3232:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.