Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 02:00 PM EDT

PDB ID	:	4W2G / pdb_00004w2g
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with pactamycin (soaked), 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.; Kusochek, 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	:	2.55 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

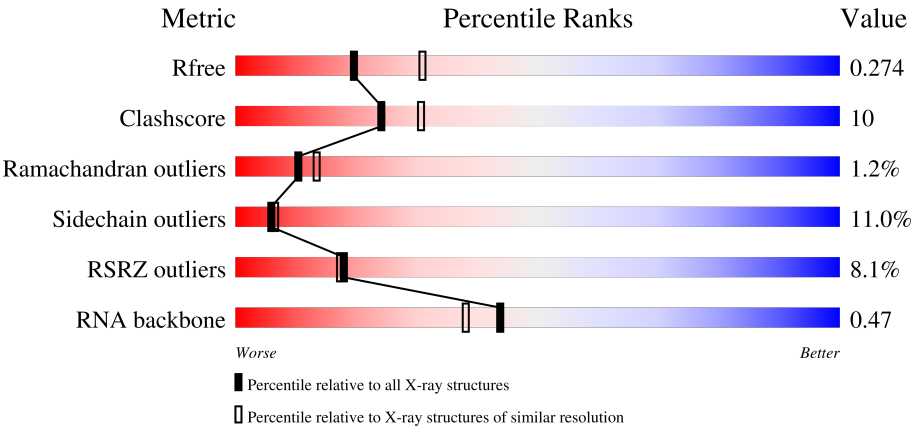
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12

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 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)
RNA backbone	3983	1112 (2.80-2.28)

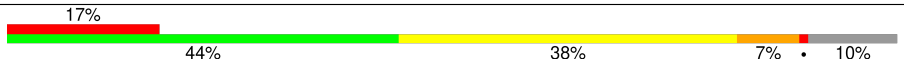
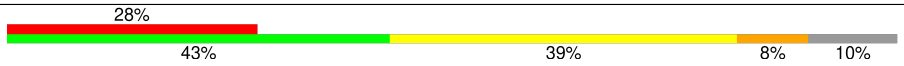
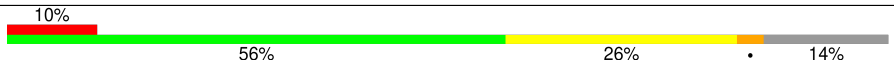
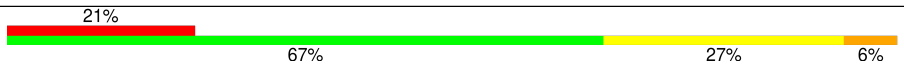
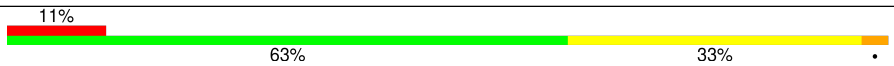
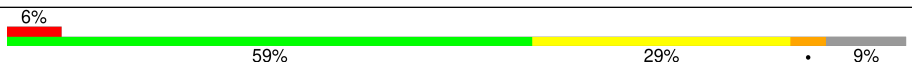
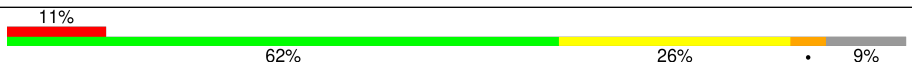
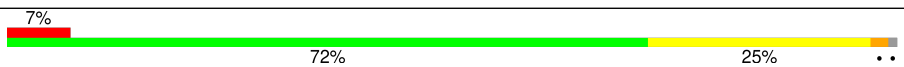
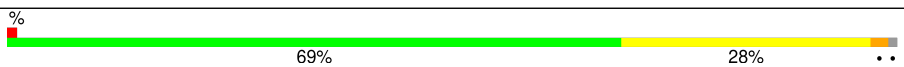
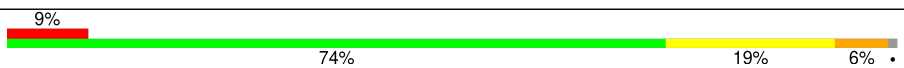
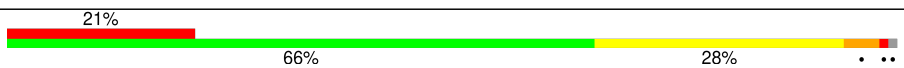
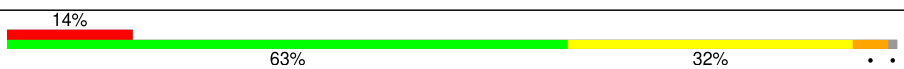
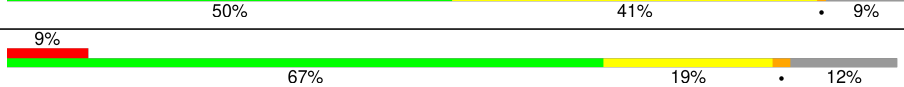
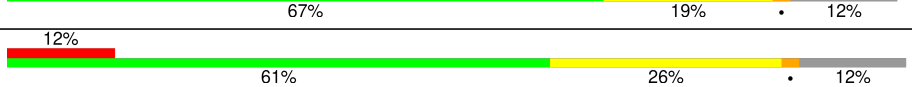
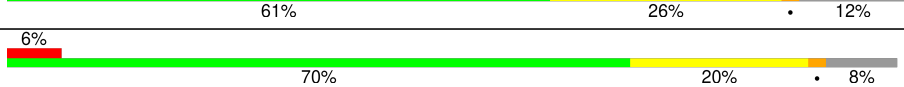
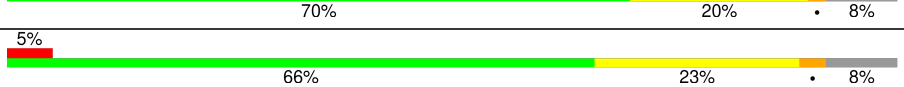
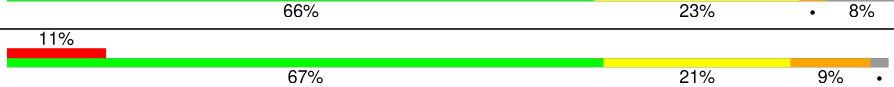
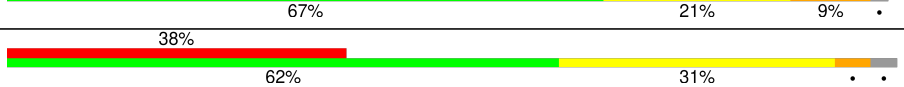
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	3% 56% 32% 11%

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Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
1	CA	1521	
2	AB	256	
2	CB	256	
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	

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Mol	Chain	Length	Quality of chain
14	AN	61	16% 61% 31% 7%
14	CN	61	54% 61% 31% 7%
15	AO	89	11% 64% 29% 6%
15	CO	89	7% 56% 35% 7%
16	AP	88	30% 58% 31% 5% 7%
16	CP	88	9% 59% 33% 7%
17	AQ	105	5% 73% 21% 6%
17	CQ	105	8% 66% 26% 6%
18	AR	88	3% 52% 24% 23%
18	CR	88	3% 47% 28% 23%
19	AS	93	13% 55% 31% 11%
19	CS	93	30% 43% 38% 6% 11%
20	AT	106	8% 54% 30% 7% 9%
20	CT	106	15% 58% 27% 5% 9%
21	AU	27	19% 63% 15% 7% 15%
21	CU	27	26% 44% 37% 15%
22	AV	24	8% 42% 8% 46%
22	CV	24	12% 42% 8% 46%
23	AW	76	9% 28% 53% 16%
23	AY	76	24% 21% 39% 36%
23	CW	76	14% 17% 51% 24% 5%
23	CY	76	30% 28% 37% 26% 5%
24	AX	77	6% 62% 30% 6%
24	CX	77	3% 45% 36% 17%
25	BA	2915	4% 62% 28% 6%

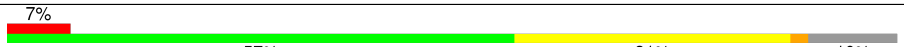
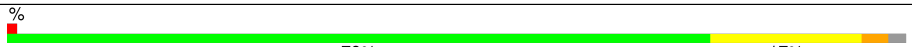
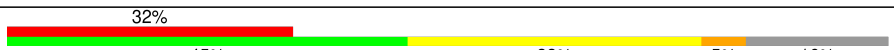
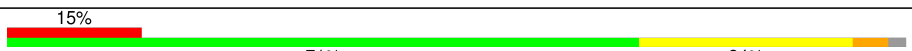
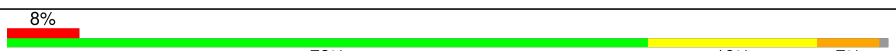
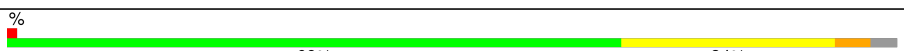
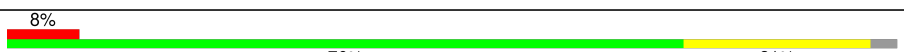
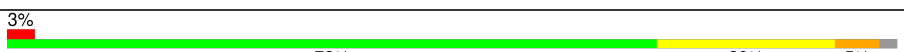
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Mol	Chain	Length	Quality of chain
25	DA	2915	3% 52% 36% 8%
26	BB	121	75% 21%
26	DB	121	2% 55% 37% 7%
27	BD	276	3% 70% 26%
27	DD	276	4% 73% 23%
28	BE	206	2% 69% 24% 6%
28	DE	206	4% 69% 23% 6%
29	BF	210	3% 69% 23% 5%
29	DF	210	4% 53% 39%
30	BG	182	15% 72% 23%
30	DG	182	13% 62% 28% 8%
31	BH	180	17% 69% 26%
31	DH	180	15% 49% 40% 7%
32	BI	148	8% 64% 26% 9%
32	DI	148	9% 70% 26%
33	BN	140	3% 76% 19% 5%
33	DN	140	2% 73% 24%
34	BO	122	2% 74% 25%
34	DO	122	2% 75% 25%
35	BP	150	5% 71% 24%
35	DP	150	5% 60% 31% 8%
36	BQ	141	72% 25%
36	DQ	141	6% 63% 33%
37	BR	118	65% 29% 6%
37	DR	118	2% 64% 29% 7%

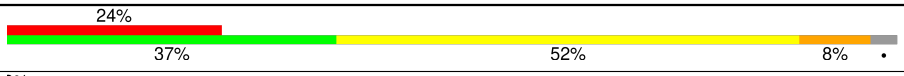
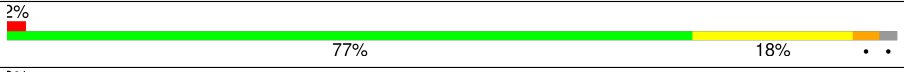
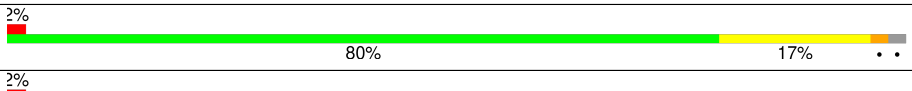
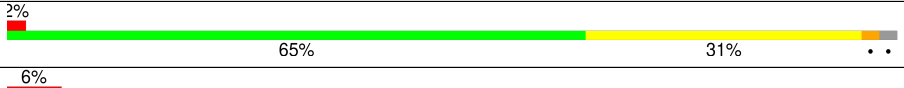
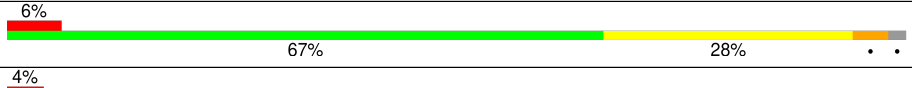
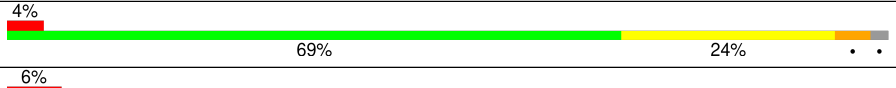
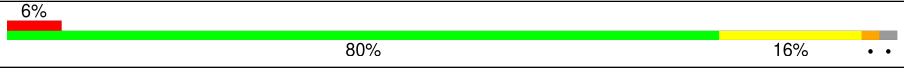
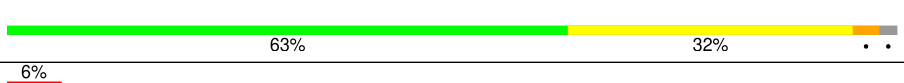
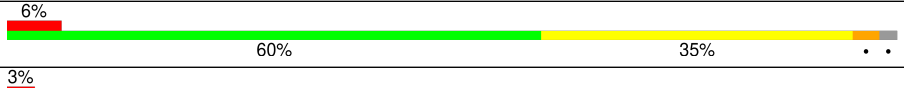
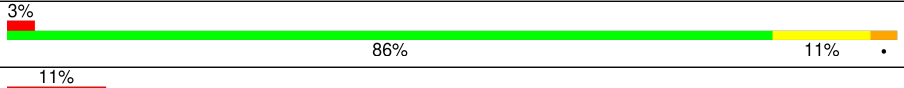
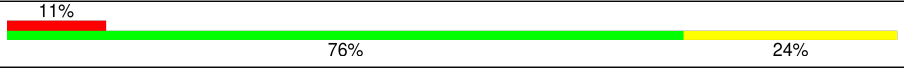
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Mol	Chain	Length	Quality of chain
38	BS	112	
38	DS	112	
39	BT	146	
39	DT	146	
40	BU	118	
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	

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Mol	Chain	Length	Quality of chain
50	D4	71	
51	B5	60	
51	D5	60	
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 (i)

There are 61 unique types of molecules in this entry. The entry contains 297273 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	1498	Total	C	N	O	P	0	0	0
			32205	14333	5970	10404	1498			
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
			1552	976	302	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
			1659	1040	326	286	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
			806	511	143	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	0	0	0
			714	445	138	131			

- 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	0	0	0
			829	516	155	155	3			
11	CK	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- 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	0	0	0
			930	585	185	159	1			
12	CL	122	Total	C	N	O	S	0	0	0
			930	585	185	159	1			

- 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	0	0	0
			958	592	198	166	2			
13	CM	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

- 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	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- 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	0	0	0
			728	456	144	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- 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
			1588	713	285	515	73	2			
23	AY	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			
23	CW	72	Total	C	N	O	P	S	0	0	0
			1541	688	278	502	72	1			
23	CY	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	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	2819	Total	C	N	O	P	0	0	0
			60729	27026	11370	19515	2818			
25	DA	2800	Total	C	N	O	P	0	0	0
			60311	26840	11284	19388	2799			

- 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
			2573	1146	476	832	119			
26	DB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- 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
			1425	914	256	251	4			
30	DG	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	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
			1085	693	189	202	1			
32	DI	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	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
			877	553	175	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	171	Total	C	N	O	S	0	0	0
			1349	862	243	242	2			
45	DZ	174	Total	C	N	O	S	0	0	0
			1360	870	243	245	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
			558	352	102	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
			511	328	99	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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	230	Total	Mg	0	0
			230	230		
56	AD	1	Total	Mg	0	0
			1	1		
56	AE	1	Total	Mg	0	0
			1	1		
56	AF	1	Total	Mg	0	0
			1	1		
56	AK	2	Total	Mg	0	0
			2	2		
56	AM	1	Total	Mg	0	0
			1	1		
56	AN	1	Total	Mg	0	0
			1	1		
56	AV	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AW	7	Total Mg 7 7	0	0
56	AX	12	Total Mg 12 12	0	0
56	AY	3	Total Mg 3 3	0	0
56	BA	839	Total Mg 839 839	0	0
56	BB	23	Total Mg 23 23	0	0
56	BD	11	Total Mg 11 11	0	0
56	BE	8	Total Mg 8 8	0	0
56	BF	12	Total Mg 12 12	0	0
56	BG	3	Total Mg 3 3	0	0
56	BN	5	Total Mg 5 5	0	0
56	BO	1	Total Mg 1 1	0	0
56	BP	3	Total Mg 3 3	0	0
56	BQ	5	Total Mg 5 5	0	0
56	BR	5	Total Mg 5 5	0	0
56	BU	9	Total Mg 9 9	0	0
56	BV	5	Total Mg 5 5	0	0
56	BW	3	Total Mg 3 3	0	0
56	BX	2	Total Mg 2 2	0	0
56	BY	1	Total Mg 1 1	0	0
56	BZ	1	Total Mg 1 1	0	0
56	B0	3	Total Mg 3 3	0	0

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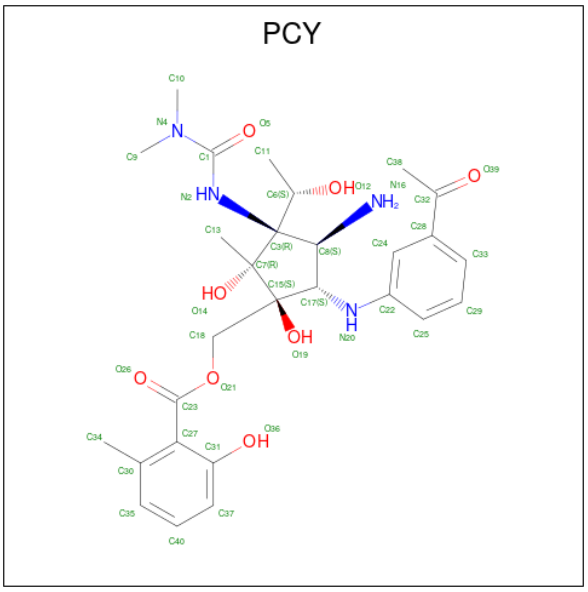
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56	B2	1	Total Mg 1 1	0	0
56	B3	3	Total Mg 3 3	0	0
56	B4	1	Total Mg 1 1	0	0
56	B5	4	Total Mg 4 4	0	0
56	B6	2	Total Mg 2 2	0	0
56	B7	2	Total Mg 2 2	0	0
56	B8	3	Total Mg 3 3	0	0
56	B9	1	Total Mg 1 1	0	0
56	CA	177	Total Mg 177 177	0	0
56	CE	2	Total Mg 2 2	0	0
56	CF	1	Total Mg 1 1	0	0
56	CJ	1	Total Mg 1 1	0	0
56	CT	1	Total Mg 1 1	0	0
56	CV	1	Total Mg 1 1	0	0
56	CW	2	Total Mg 2 2	0	0
56	CX	5	Total Mg 5 5	0	0
56	CY	1	Total Mg 1 1	0	0
56	DA	675	Total Mg 675 675	0	0
56	DB	11	Total Mg 11 11	0	0
56	DD	7	Total Mg 7 7	0	0

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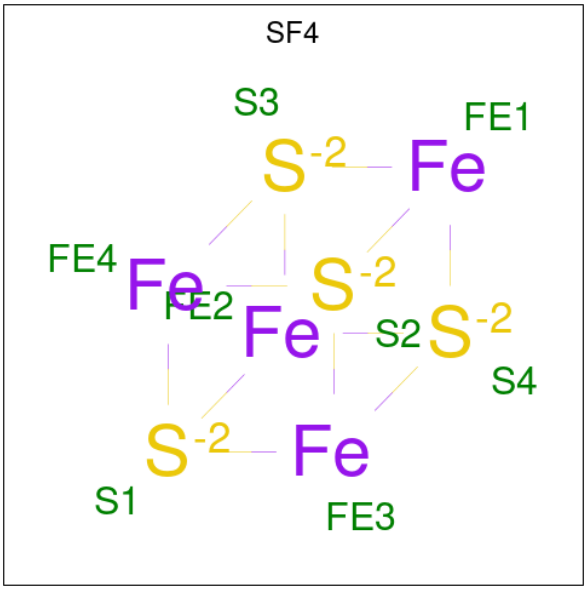
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DE	4	Total Mg 4 4	0	0
56	DF	5	Total Mg 5 5	0	0
56	DG	1	Total Mg 1 1	0	0
56	DN	1	Total Mg 1 1	0	0
56	DO	1	Total Mg 1 1	0	0
56	DQ	4	Total Mg 4 4	0	0
56	DR	1	Total Mg 1 1	0	0
56	DU	2	Total Mg 2 2	0	0
56	DV	3	Total Mg 3 3	0	0
56	DW	3	Total Mg 3 3	0	0
56	DY	1	Total Mg 1 1	0	0
56	D0	2	Total Mg 2 2	0	0
56	D3	1	Total Mg 1 1	0	0
56	D7	2	Total Mg 2 2	0	0
56	D8	1	Total Mg 1 1	0	0

- Molecule 57 is Pactamycin (CCD ID: PCY) (formula: $C_{28}H_{38}N_4O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	AA	1	Total	C	N	O	0	0
			40	28	4	8		
57	CA	1	Total	C	N	O	0	0
			40	28	4	8		

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: 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 (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AN	1	Total Zn 1 1	0	0
59	BY	1	Total Zn 1 1	0	0
59	B4	1	Total Zn 1 1	0	0
59	B5	1	Total Zn 1 1	0	0
59	B6	1	Total Zn 1 1	0	0
59	B9	1	Total Zn 1 1	0	0
59	CN	1	Total Zn 1 1	0	0
59	DY	1	Total Zn 1 1	0	0
59	D4	1	Total Zn 1 1	0	0
59	D5	1	Total Zn 1 1	0	0
59	D6	1	Total Zn 1 1	0	0
59	D9	1	Total Zn 1 1	0	0

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AA	226	Total O 226 226	0	0
61	AE	3	Total O 3 3	0	0
61	AJ	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AL	4	Total O 4 4	0	0
61	AM	1	Total O 1 1	0	0
61	AV	4	Total O 4 4	0	0
61	AW	6	Total O 6 6	0	0
61	AX	8	Total O 8 8	0	0
61	AY	3	Total O 3 3	0	0
61	BA	1411	Total O 1411 1411	0	0
61	BB	36	Total O 36 36	0	0
61	BD	16	Total O 16 16	0	0
61	BE	13	Total O 13 13	0	0
61	BF	7	Total O 7 7	0	0
61	BG	3	Total O 3 3	0	0
61	BI	1	Total O 1 1	0	0
61	BN	2	Total O 2 2	0	0
61	BO	3	Total O 3 3	0	0
61	BP	17	Total O 17 17	0	0
61	BQ	2	Total O 2 2	0	0
61	BR	2	Total O 2 2	0	0
61	BT	1	Total O 1 1	0	0
61	BU	6	Total O 6 6	0	0
61	BV	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	BW	4	Total O 4 4	0	0
61	BX	1	Total O 1 1	0	0
61	B0	4	Total O 4 4	0	0
61	B1	2	Total O 2 2	0	0
61	B3	2	Total O 2 2	0	0
61	B5	5	Total O 5 5	0	0
61	B6	1	Total O 1 1	0	0
61	B7	3	Total O 3 3	0	0
61	B8	11	Total O 11 11	0	0
61	CA	173	Total O 173 173	0	0
61	CJ	2	Total O 2 2	0	0
61	CL	1	Total O 1 1	0	0
61	CV	2	Total O 2 2	0	0
61	CW	1	Total O 1 1	0	0
61	CX	4	Total O 4 4	0	0
61	DA	1002	Total O 1002 1002	0	0
61	DB	10	Total O 10 10	0	0
61	DD	17	Total O 17 17	0	0
61	DE	11	Total O 11 11	0	0
61	DF	5	Total O 5 5	0	0
61	DN	2	Total O 2 2	0	0

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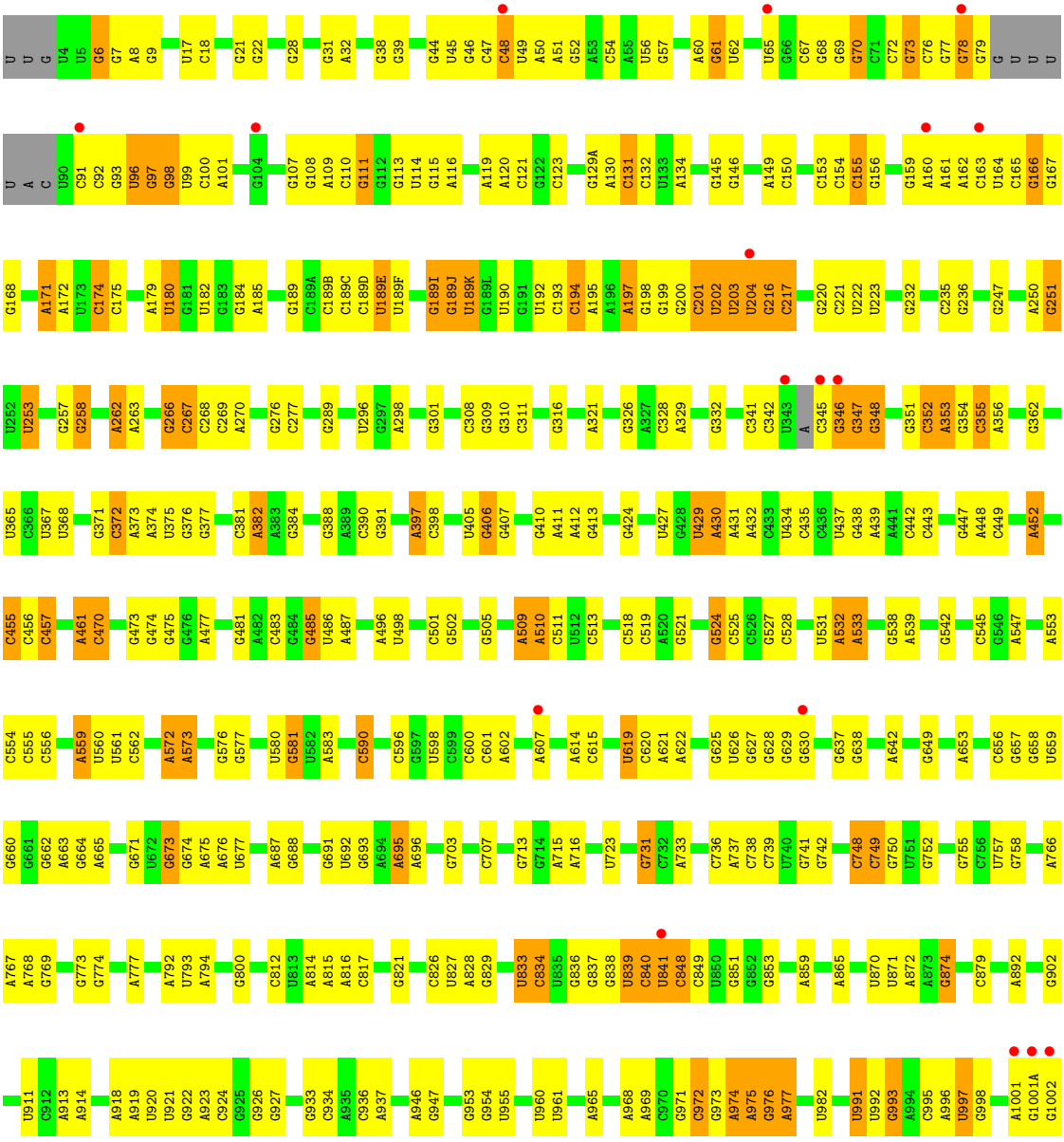
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	DO	2	Total O 2 2	0	0
61	DP	8	Total O 8 8	0	0
61	DQ	1	Total O 1 1	0	0
61	DR	1	Total O 1 1	0	0
61	DU	2	Total O 2 2	0	0
61	DW	1	Total O 1 1	0	0
61	DY	1	Total O 1 1	0	0
61	D0	5	Total O 5 5	0	0
61	D3	1	Total O 1 1	0	0
61	D7	3	Total O 3 3	0	0
61	D8	4	Total O 4 4	0	0

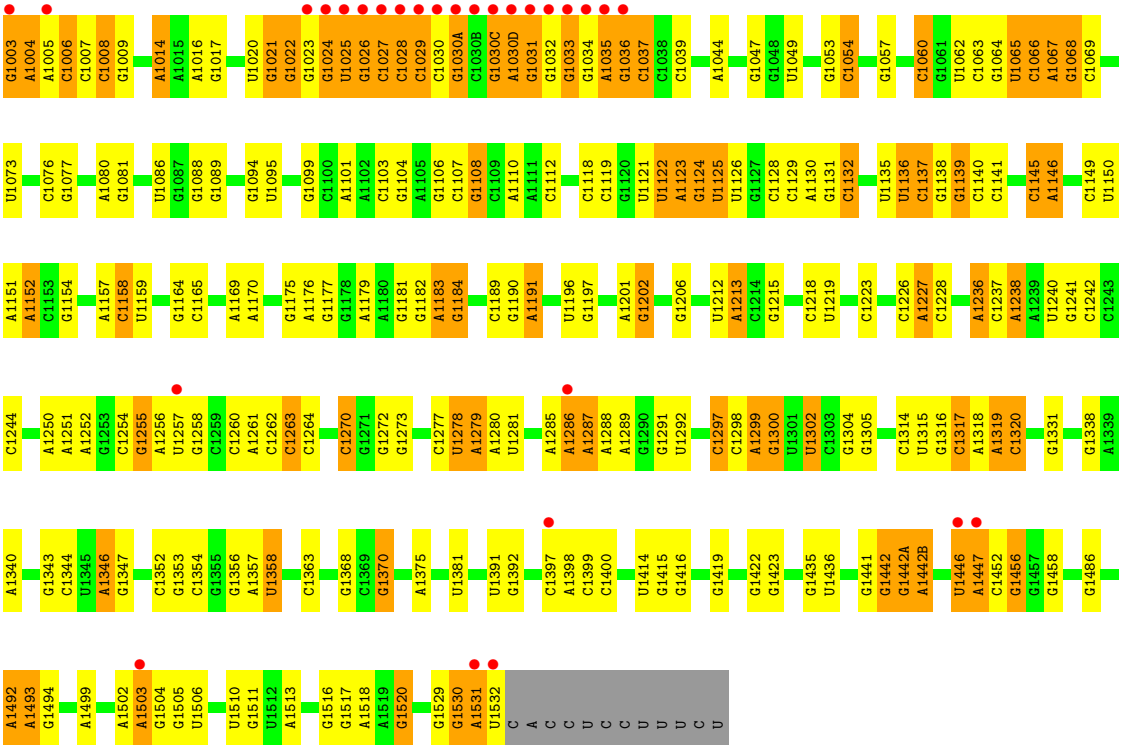
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

Chain AA: 

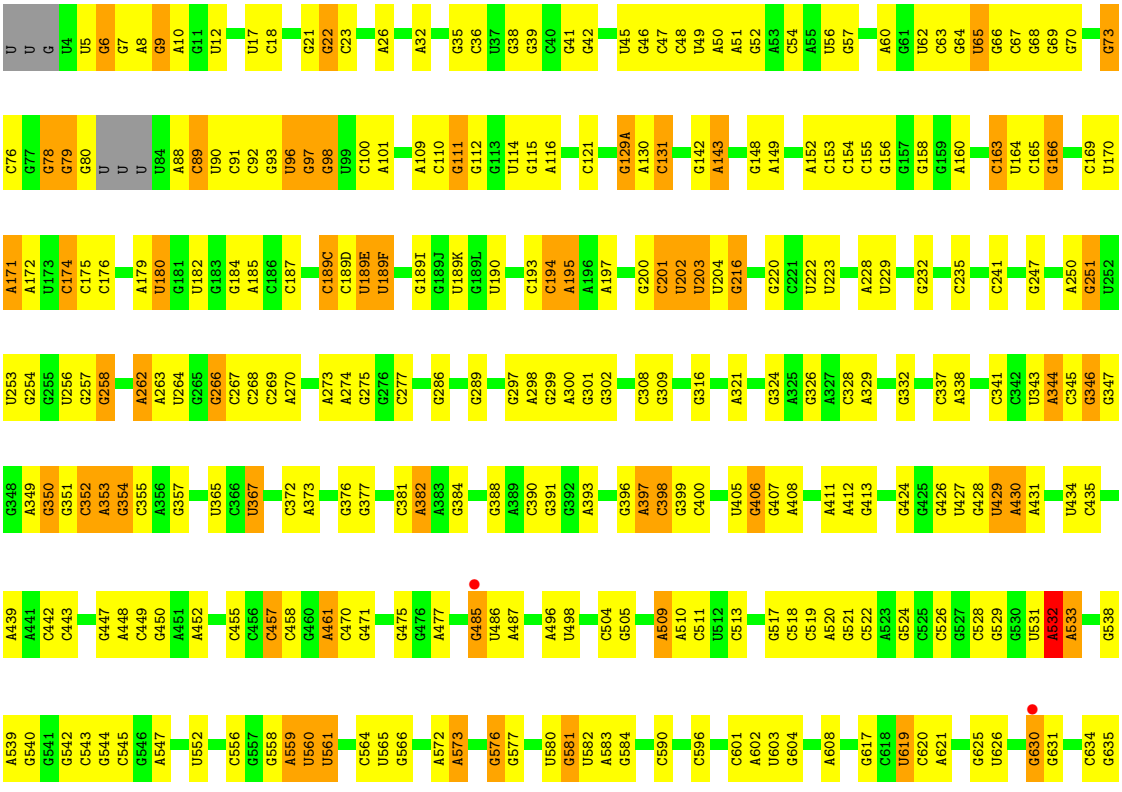


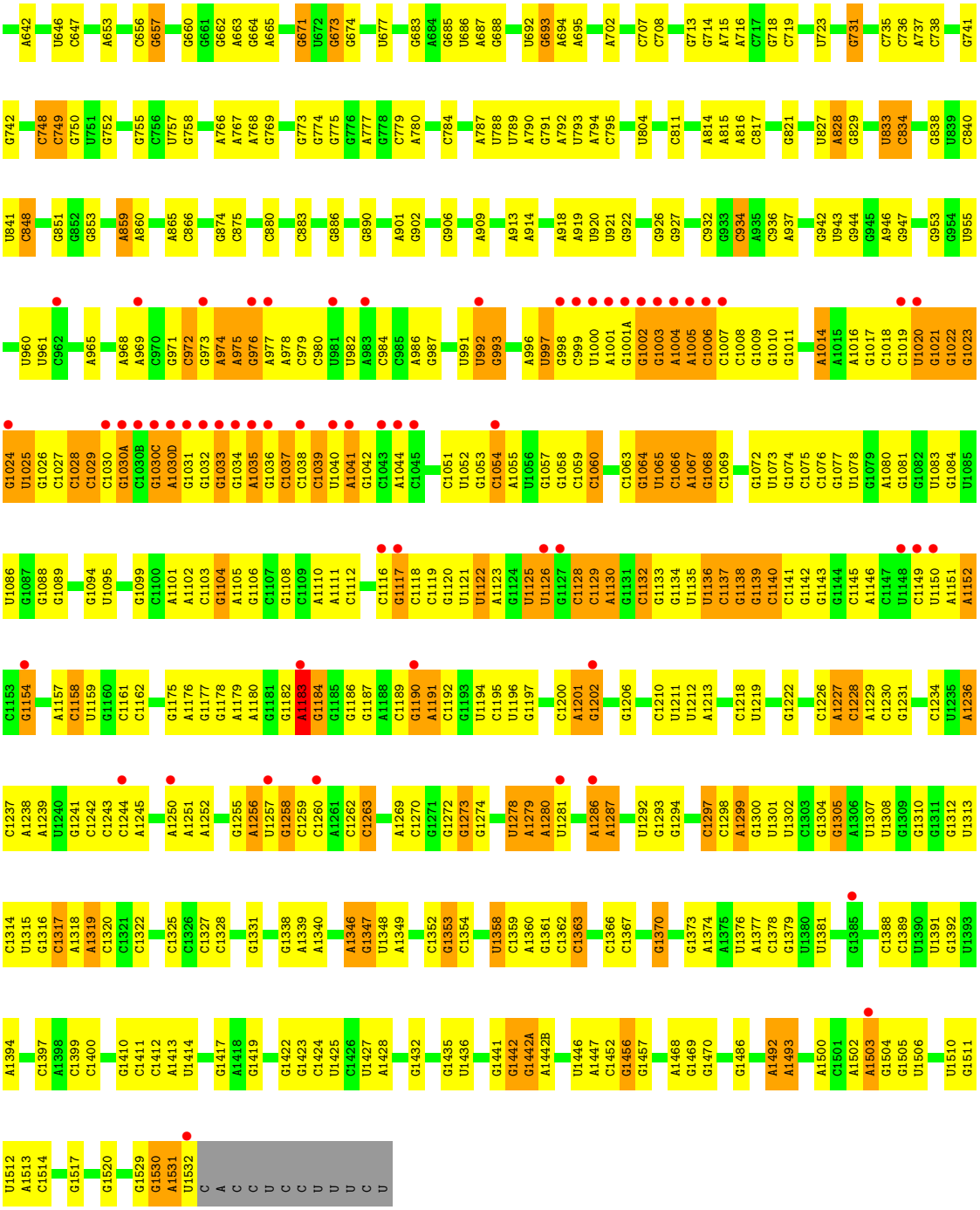


• Molecule 1: 16S Ribosomal RNA

Chain CA:

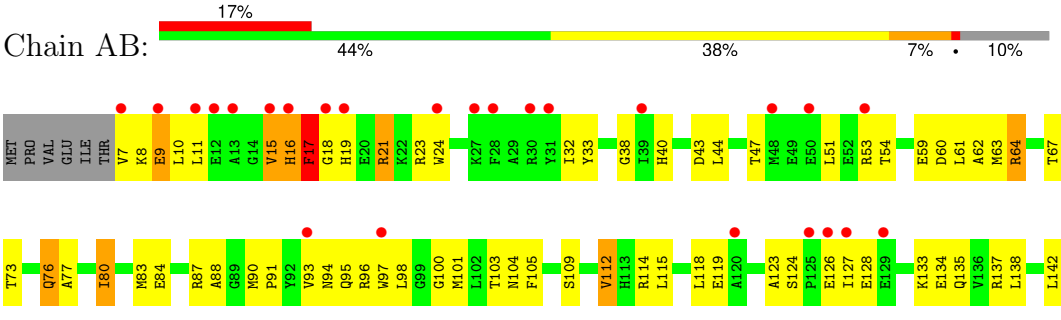


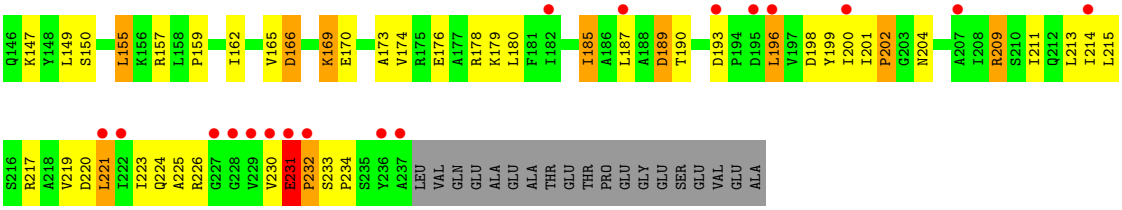




• Molecule 2: 30S Ribosomal Protein S2

Chain AB:

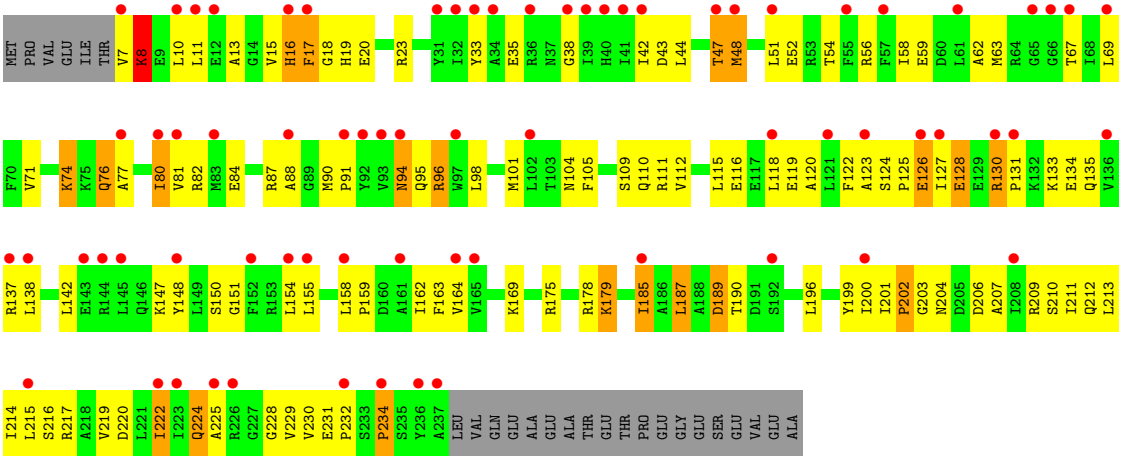




• Molecule 2: 30S Ribosomal Protein S2

Chain CB:

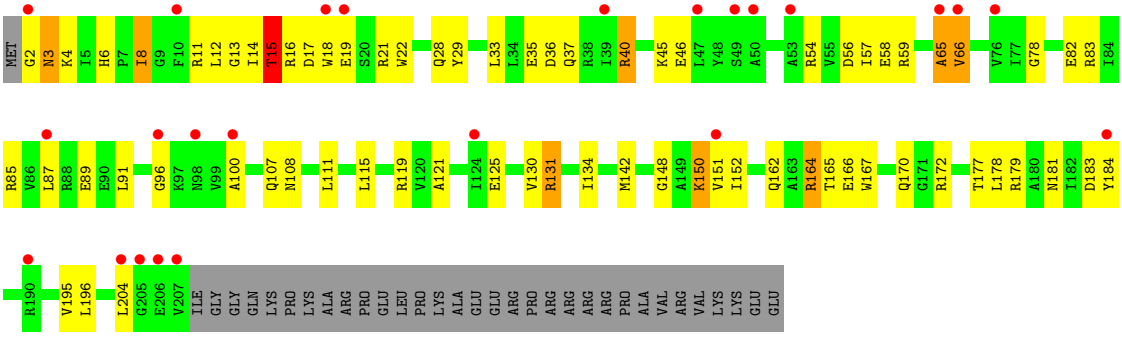




• Molecule 3: 30S Ribosomal Protein S3

Chain AC:

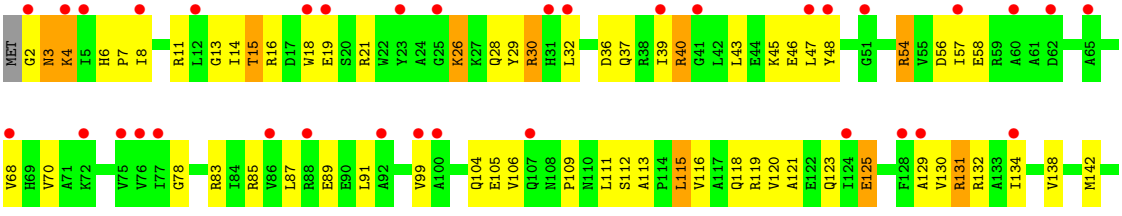


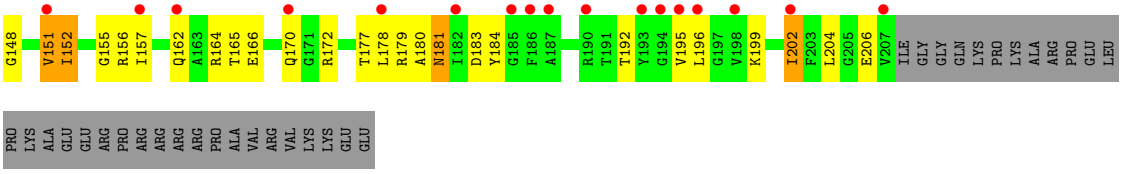


• Molecule 3: 30S Ribosomal Protein S3

Chain CC:



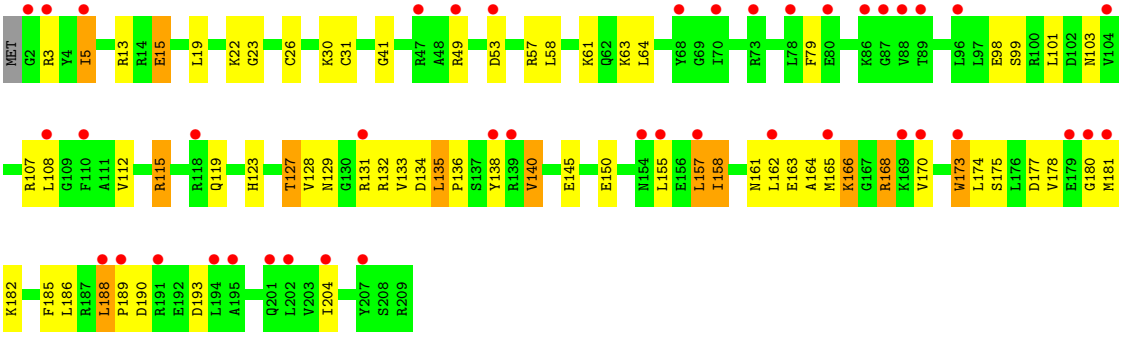




• Molecule 4: 30S Ribosomal Protein S4

Chain AD:

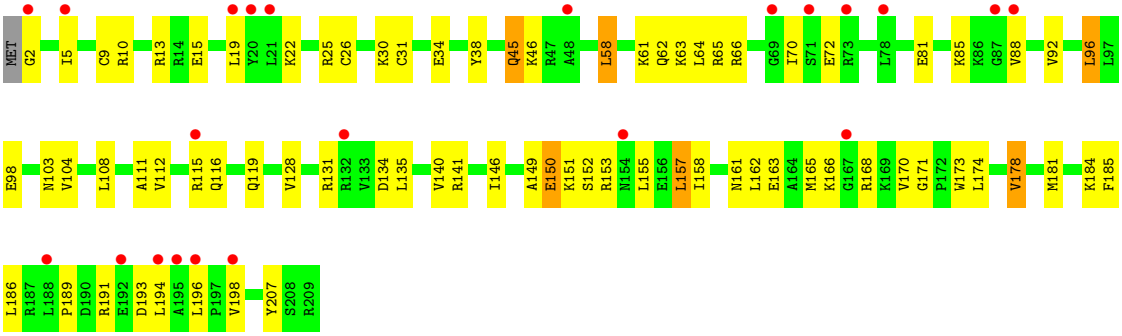




• Molecule 4: 30S Ribosomal Protein S4

Chain CD:

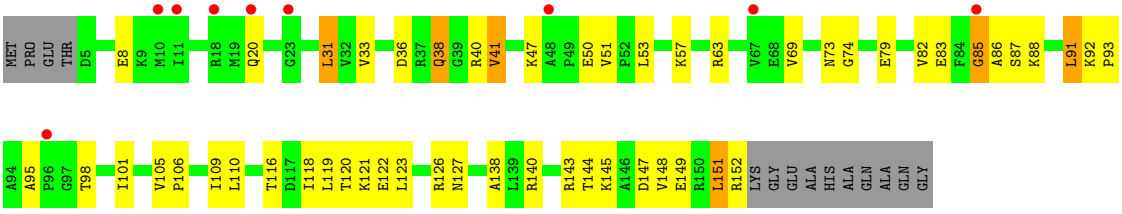




• Molecule 5: 30S Ribosomal Protein S5

Chain AE:

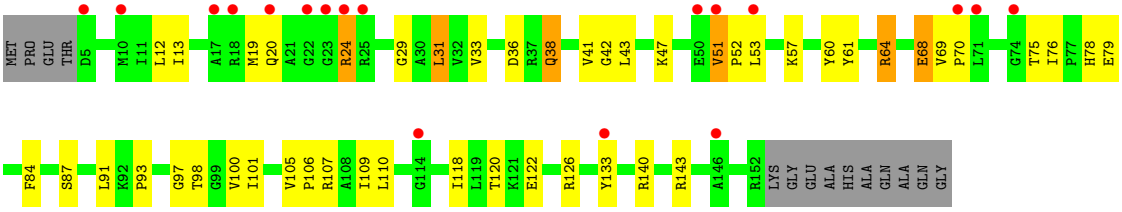




• Molecule 5: 30S Ribosomal Protein S5

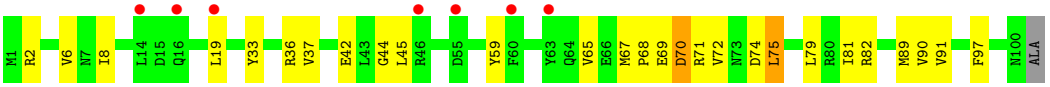
Chain CE:





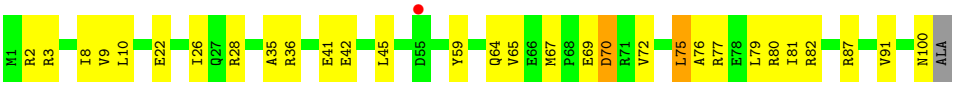
• Molecule 6: 30S Ribosomal Protein S6



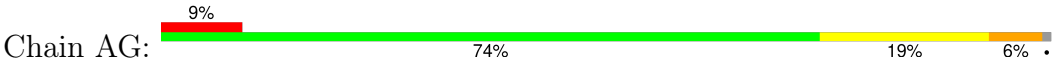


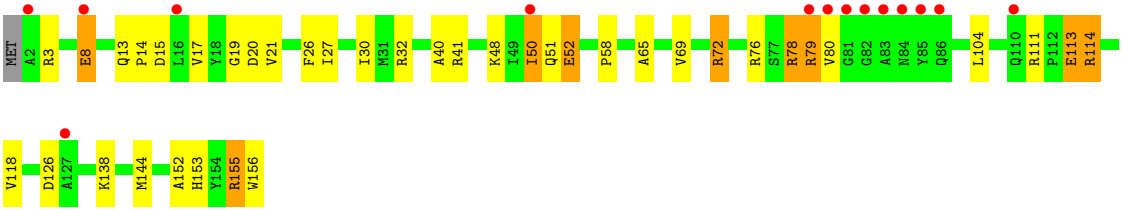
• Molecule 6: 30S Ribosomal Protein S6





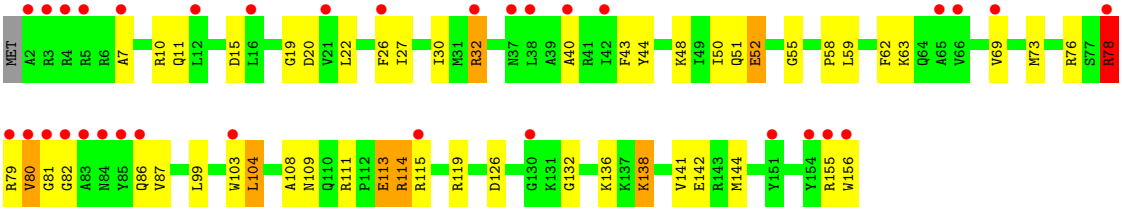
• Molecule 7: 30S Ribosomal Protein S7





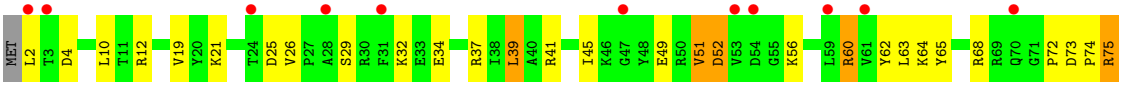
• Molecule 7: 30S Ribosomal Protein S7

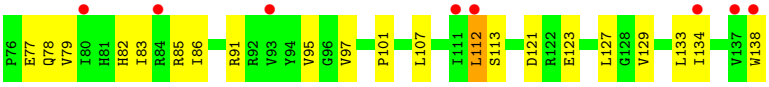




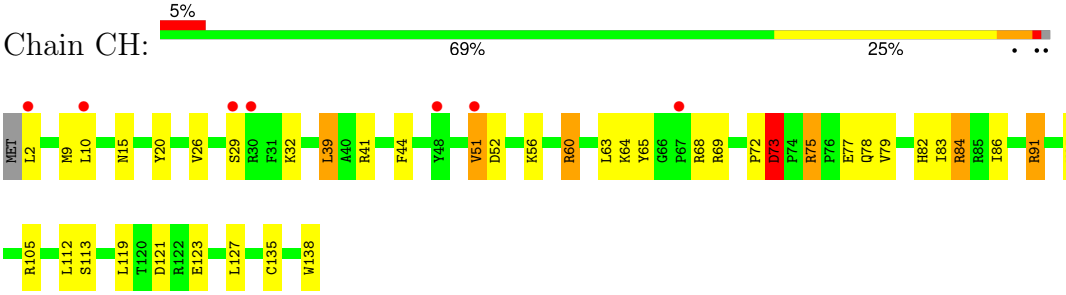
• Molecule 8: 30S Ribosomal Protein S8



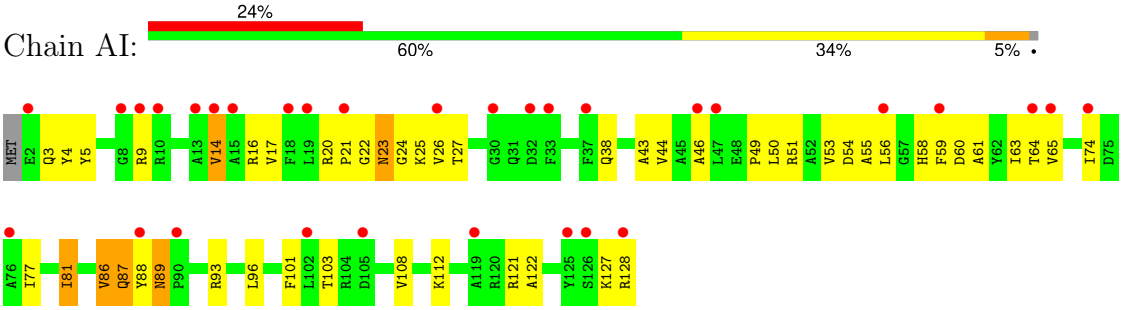




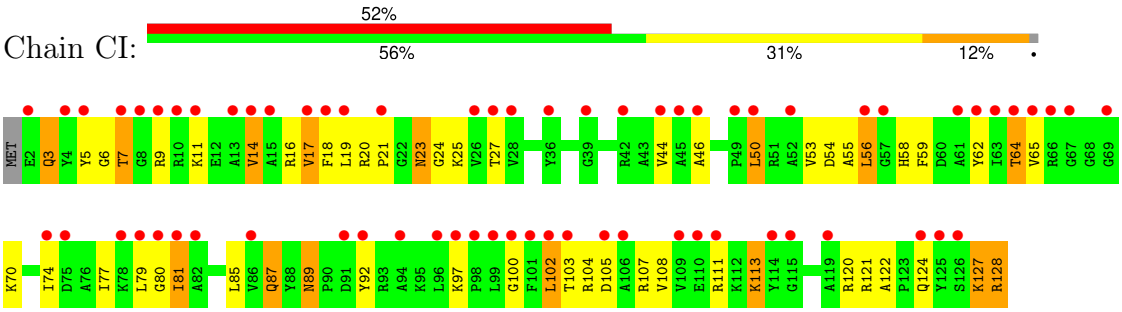
• Molecule 8: 30S Ribosomal Protein S8



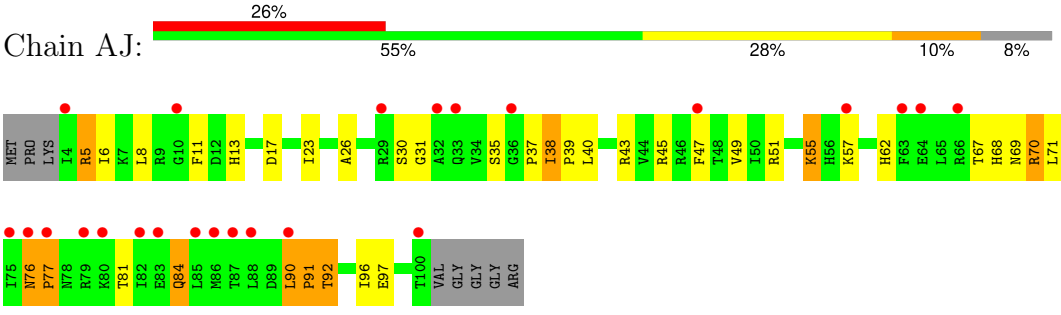
• Molecule 9: 30S Ribosomal Protein S9



• Molecule 9: 30S Ribosomal Protein S9

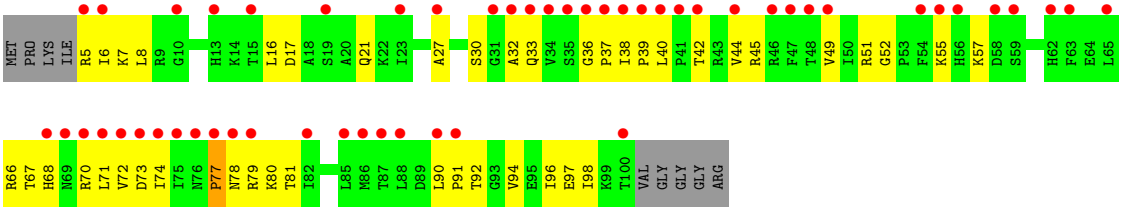


• Molecule 10: 30S Ribosomal Protein S10



• Molecule 10: 30S Ribosomal Protein S10

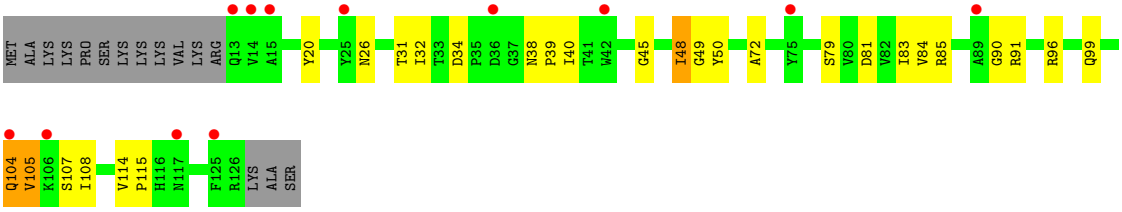




• Molecule 11: 30S Ribosomal Protein S11

Chain AK:

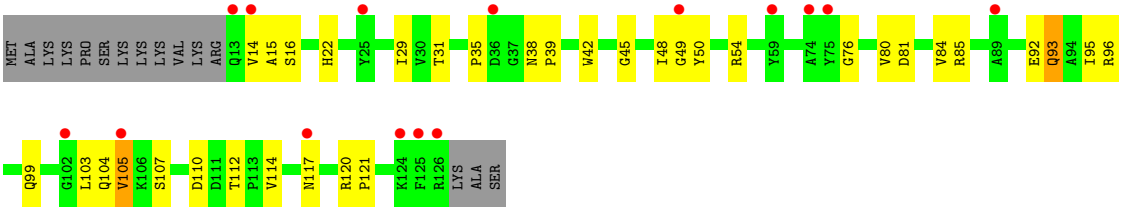




• Molecule 11: 30S Ribosomal Protein S11

Chain CK:

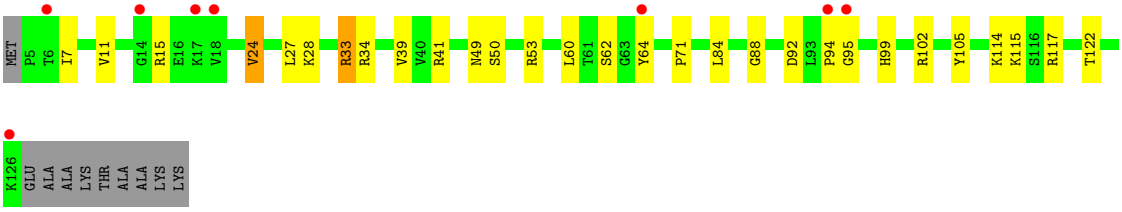




• Molecule 12: 30S Ribosomal Protein S12

Chain AL:

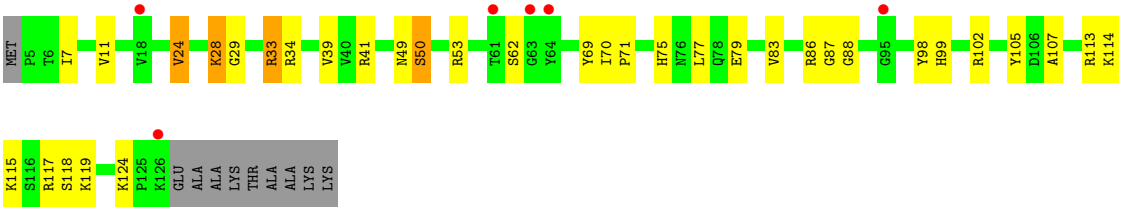




• Molecule 12: 30S Ribosomal Protein S12

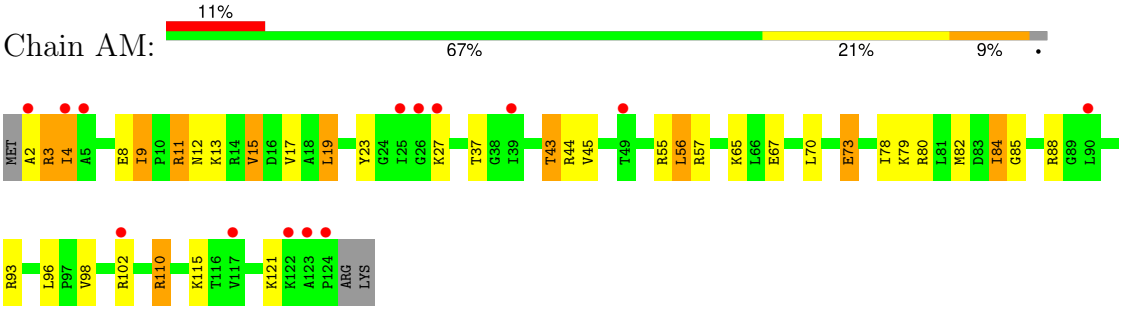
Chain CL:





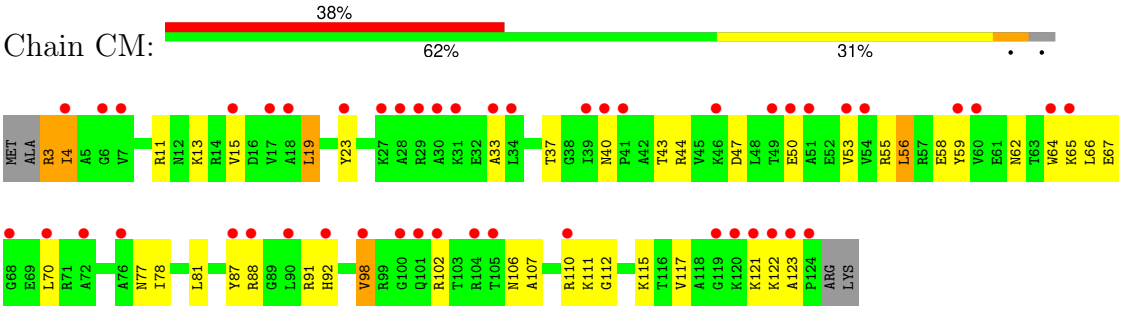
• Molecule 13: 30S Ribosomal Protein S13

Chain AM:



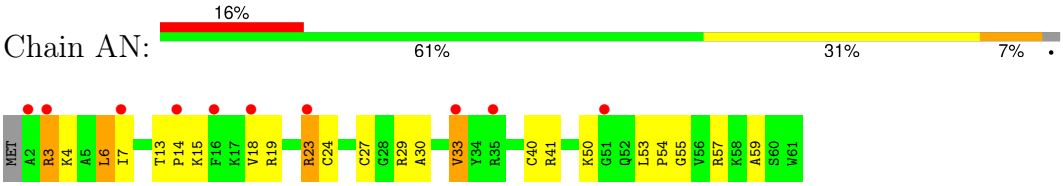
• Molecule 13: 30S Ribosomal Protein S13

Chain CM:



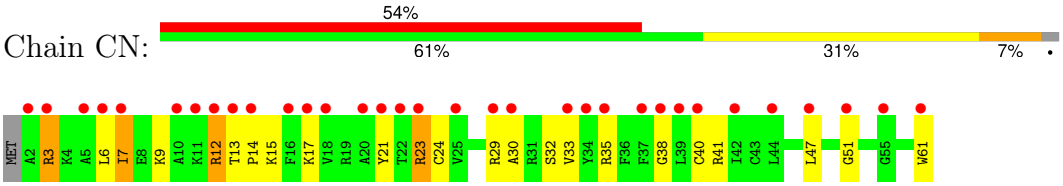
• Molecule 14: 30S Ribosomal Protein S14

Chain AN:



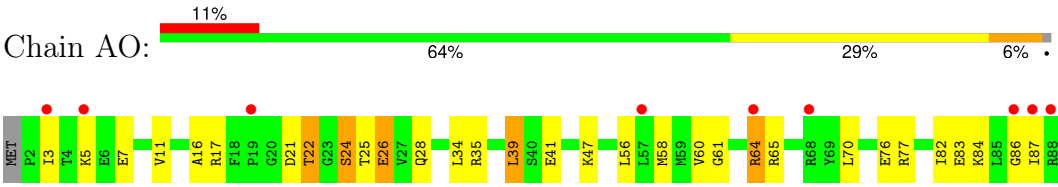
• Molecule 14: 30S Ribosomal Protein S14

Chain CN:



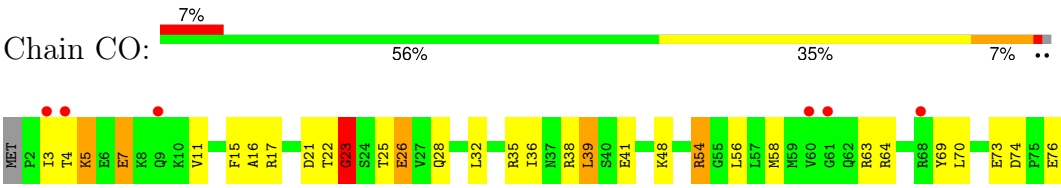
• Molecule 15: 30S Ribosomal Protein S15

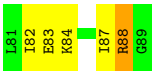
Chain AO:



• Molecule 15: 30S Ribosomal Protein S15

Chain CO:

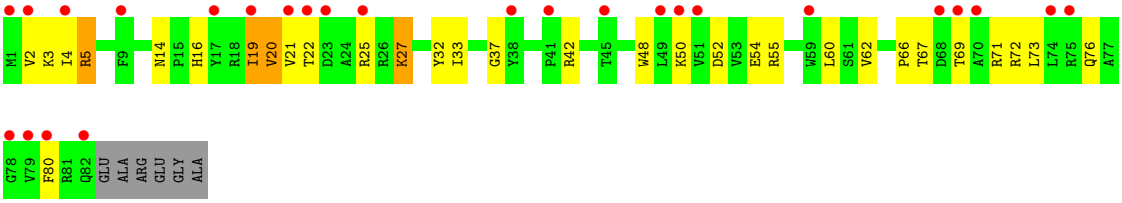




• Molecule 16: 30S Ribosomal Protein S16

Chain AP:

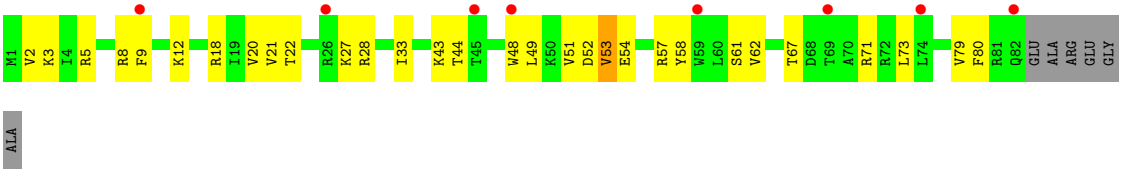




• Molecule 16: 30S Ribosomal Protein S16

Chain CP:

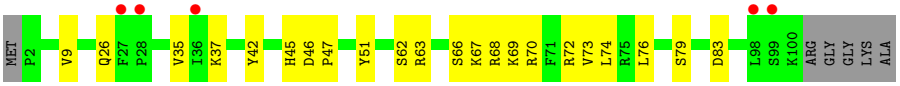




• Molecule 17: 30S Ribosomal Protein S17

Chain AQ:





• Molecule 17: 30S Ribosomal Protein S17

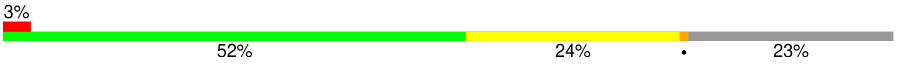
Chain CQ:

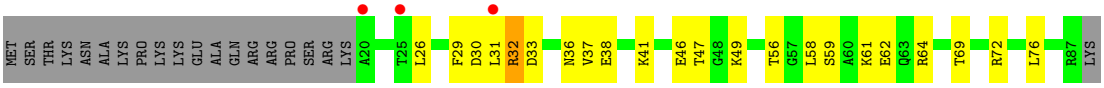




• Molecule 18: 30S Ribosomal Protein S18

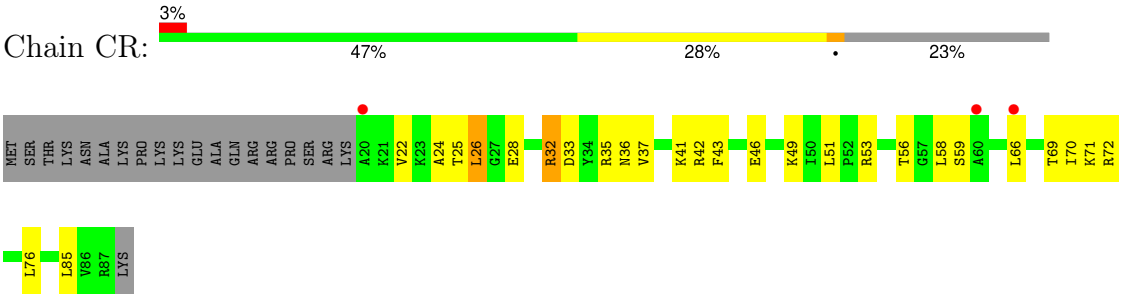
Chain AR:





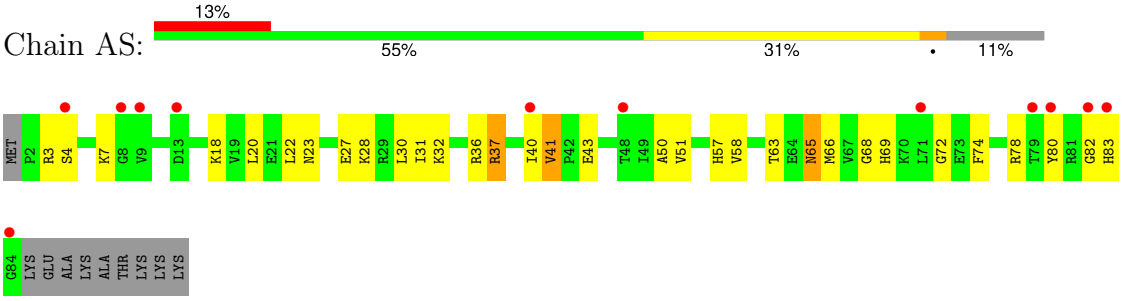
• Molecule 18: 30S Ribosomal Protein S18

Chain CR:



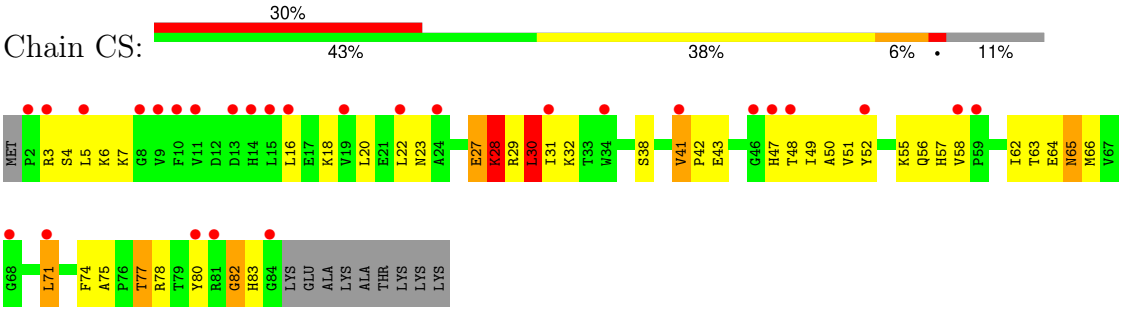
• Molecule 19: 30S Ribosomal Protein S19

Chain AS:



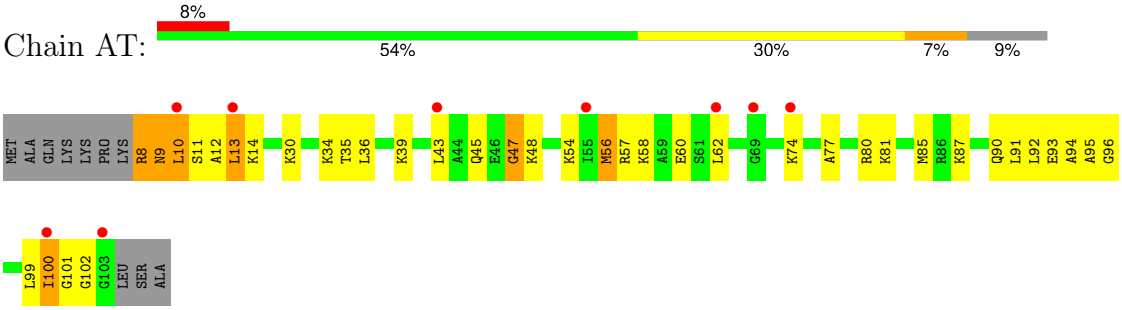
• Molecule 19: 30S Ribosomal Protein S19

Chain CS:



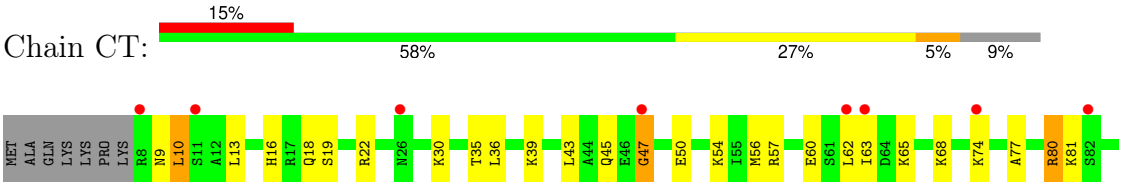
• Molecule 20: 30S Ribosomal Protein S20

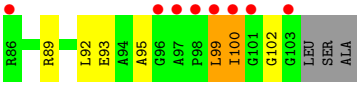
Chain AT:



• Molecule 20: 30S Ribosomal Protein S20

Chain CT:

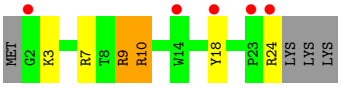




• Molecule 21: 30S Ribosomal Protein THX

Chain AU:





• Molecule 21: 30S Ribosomal Protein THX

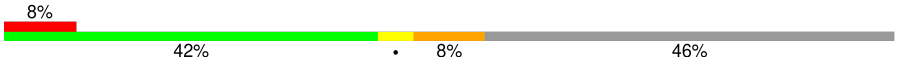
Chain CU:





• Molecule 22: mRNA

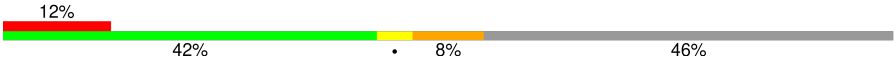
Chain AV:





• Molecule 22: mRNA

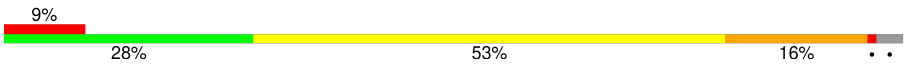
Chain CV:

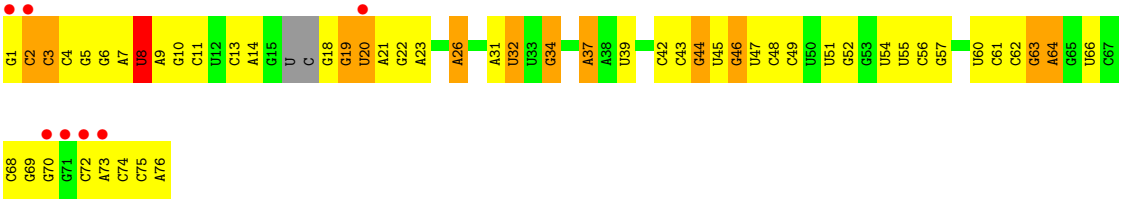




• Molecule 23: A/P-site tRNA

Chain AW:

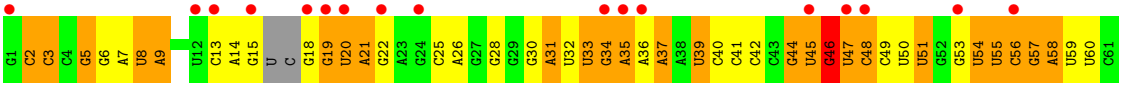


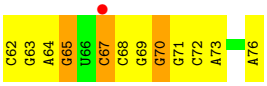


• Molecule 23: A/P-site tRNA

Chain AY:



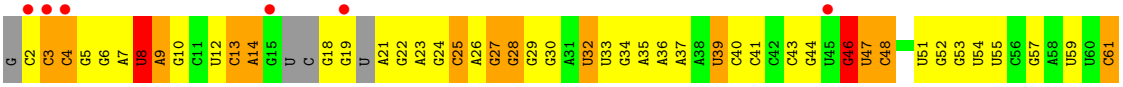


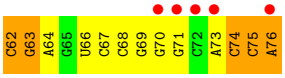


• Molecule 23: A/P-site tRNA

Chain CW:

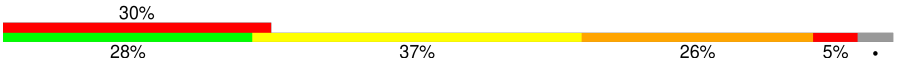


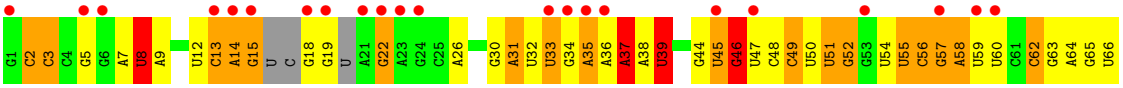


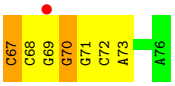


• Molecule 23: A/P-site tRNA

Chain CY:



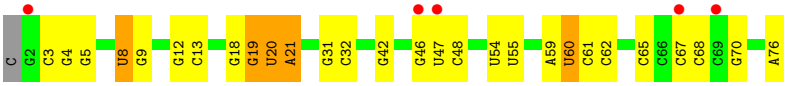




• Molecule 24: E-site tRNA

Chain AX:

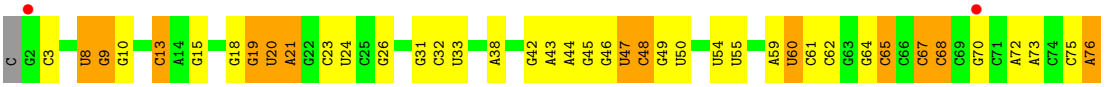




• Molecule 24: E-site tRNA

Chain CX:

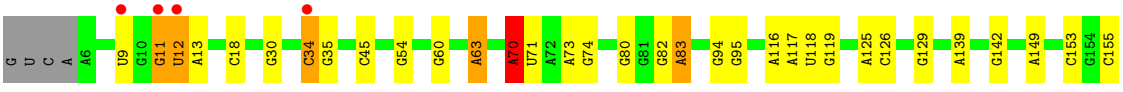


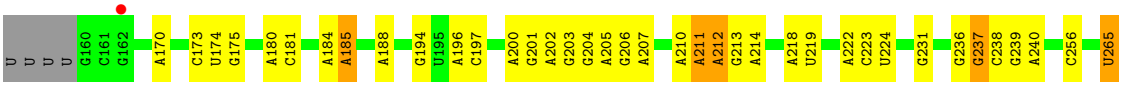


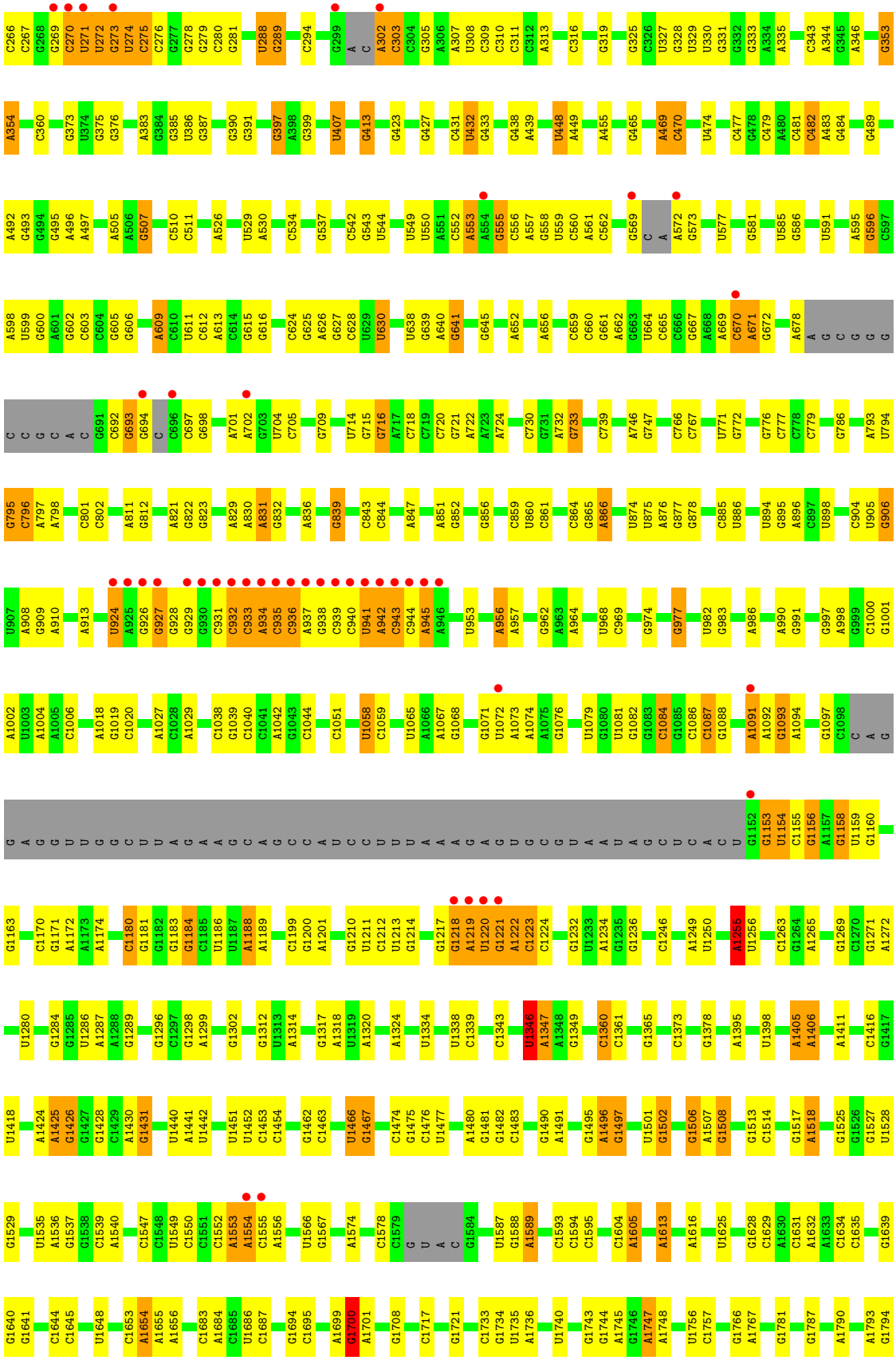
• Molecule 25: 23S Ribosomal RNA

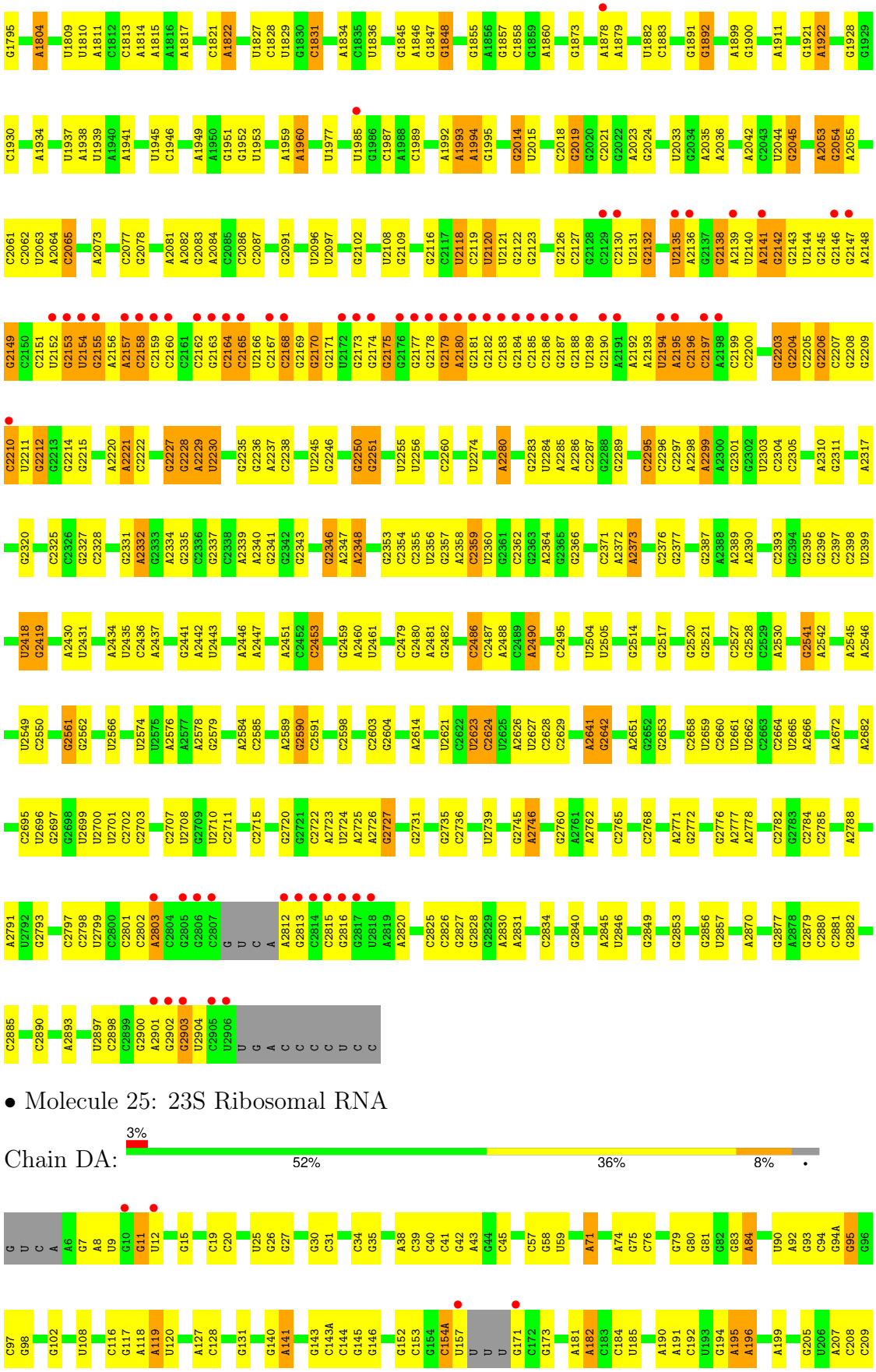
Chain BA:





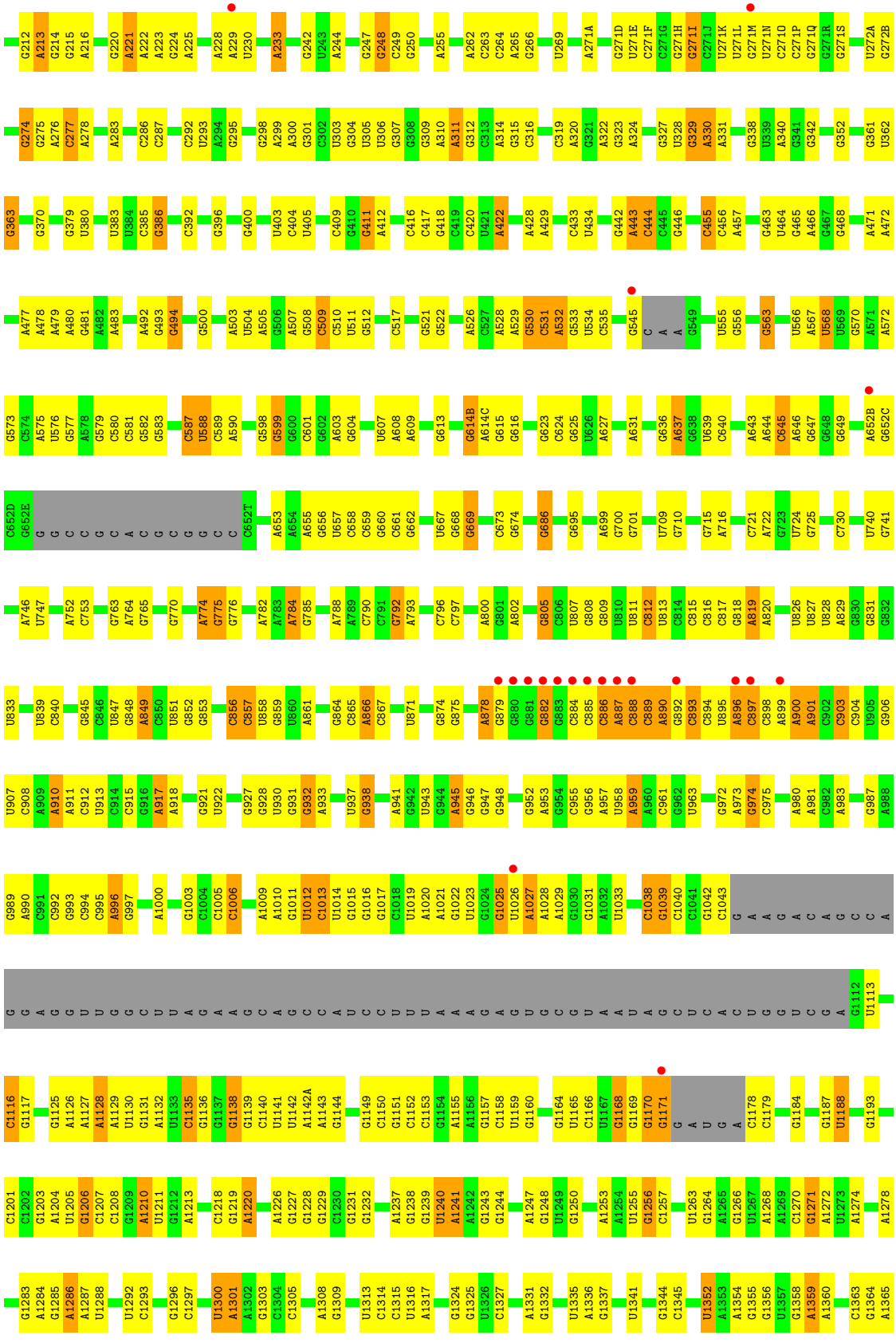


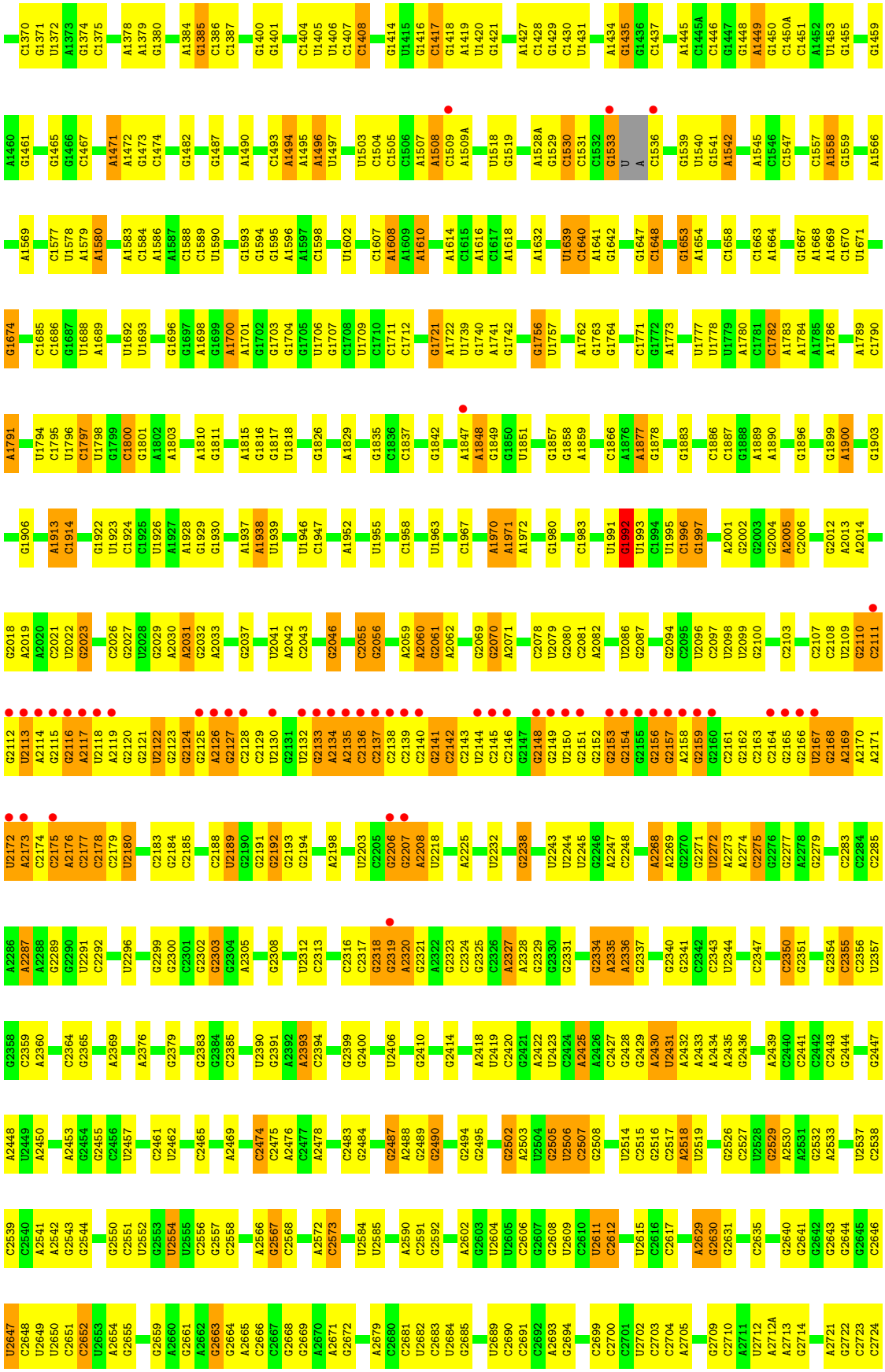

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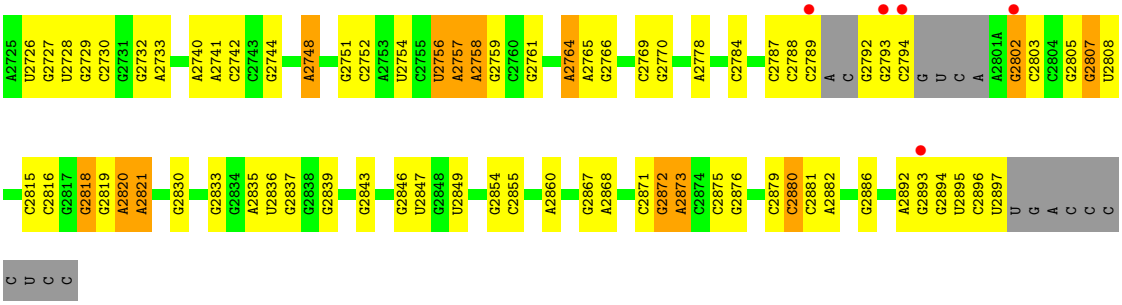


• Molecule 25: 23S Ribosomal RNA

Chain DA:


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G247 G248 C249 G250
A255
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U269
A271A
G271D U271E C271F C271G G271H G271I C271J U271K U271L G271M U271N C271O C271P C271Q G271R G271S
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A283
C286 C287
C292 U293 A294 G295
G298 A299 A300 G301
C302 U303 G304 U305 U306 G307
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G352
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G363
G370
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C392
G396
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G695
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U2647 C2648 U2649 U2650 C2651 C2652 U2653 A2654 G2655 G2659 A2660 G2661 A2662 G2663 G2664 A2665 C2666 C2667 G2668 G2669 A2670 A2671 G2672 A2679 C2680 C2681 U2682 C2683 U2684 G2685 U2689 C2690 C2691 C2692 A2693 G2694 C2699 C2700 C2701 U2702 C2703 C2704 A2705 G2709 C2710 A2711 U2712 A2712A A2713 G2714 A2721 G2722 C2723 C2724



• Molecule 26: 5S Ribosomal RNA

Chain BB:

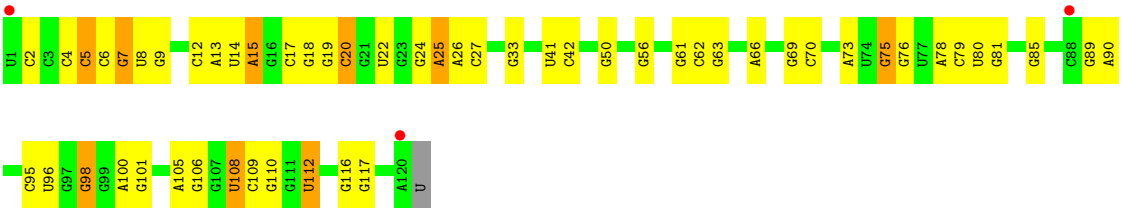




• Molecule 26: 5S Ribosomal RNA

Chain DB:

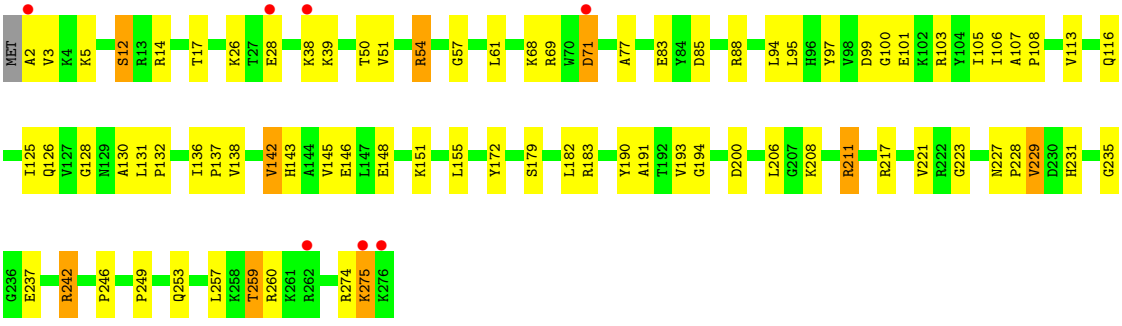




• Molecule 27: 50S Ribosomal Protein L2

Chain BD:

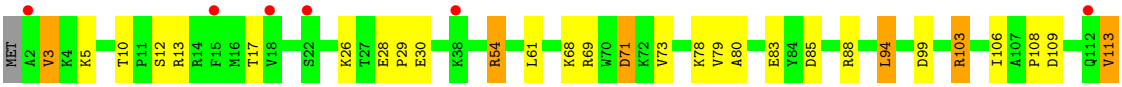


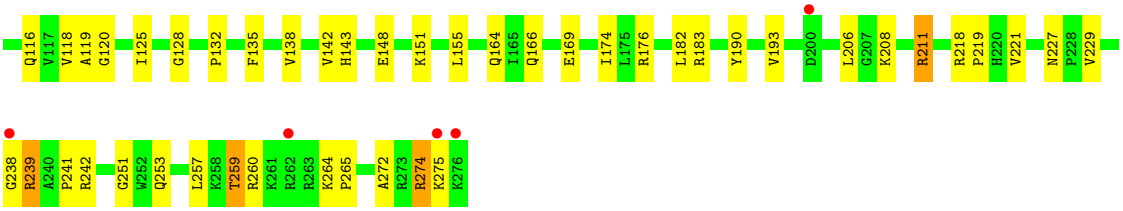


• Molecule 27: 50S Ribosomal Protein L2

Chain DD:



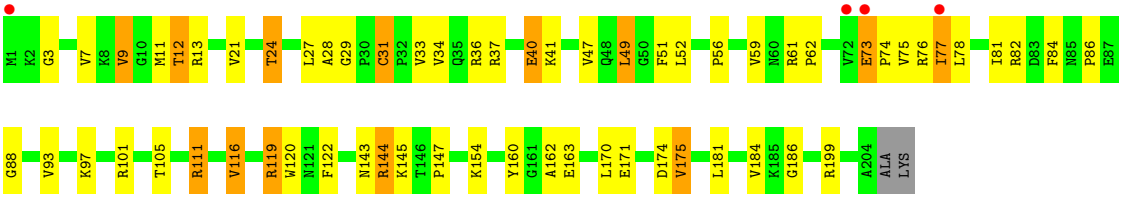




• Molecule 28: 50S Ribosomal Protein L3

Chain BE:

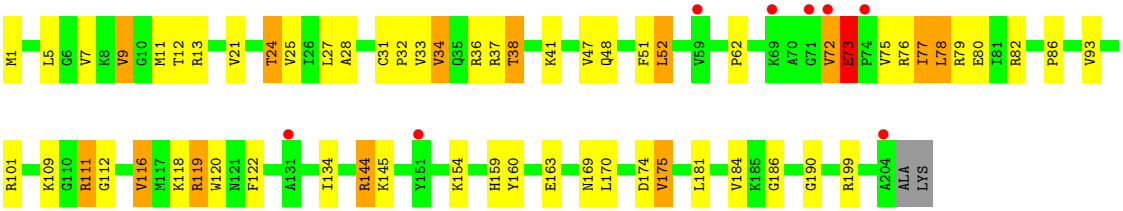




• Molecule 28: 50S Ribosomal Protein L3

Chain DE:

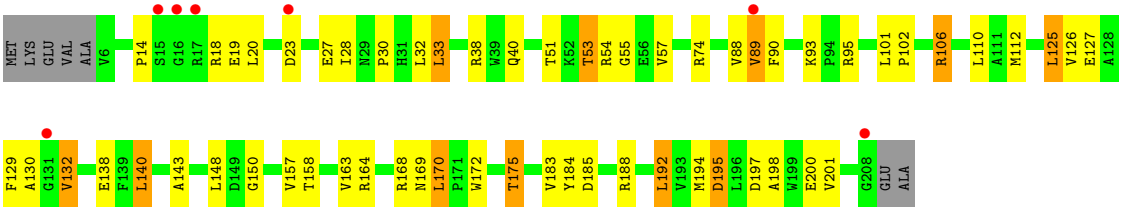




• Molecule 29: 50S Ribosomal Protein L4

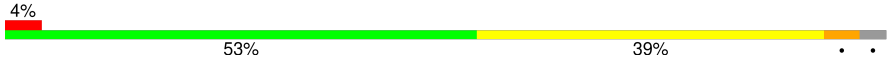
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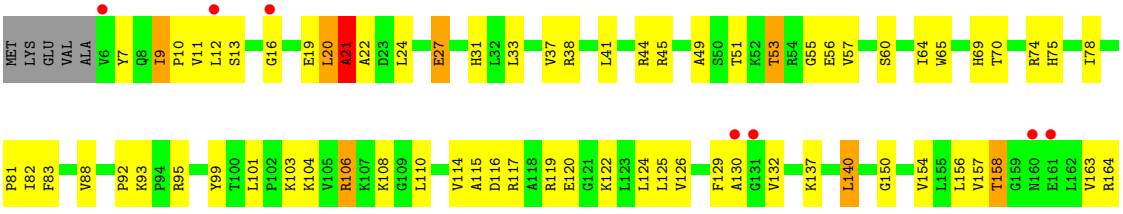


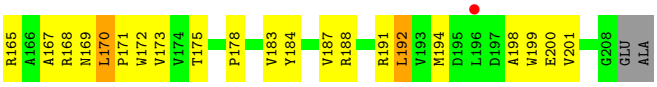


• Molecule 29: 50S Ribosomal Protein L4

Chain DF:



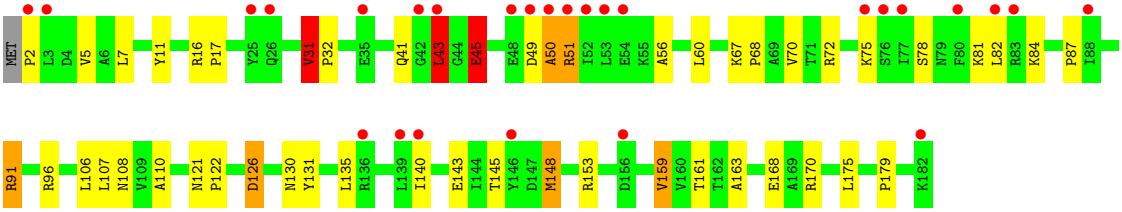




• Molecule 30: 50S Ribosomal Protein L5

Chain BG:

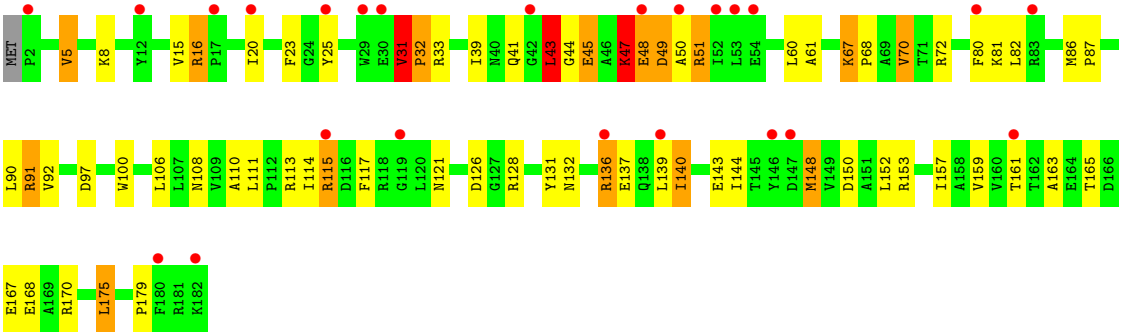




• Molecule 30: 50S Ribosomal Protein L5

Chain DG:

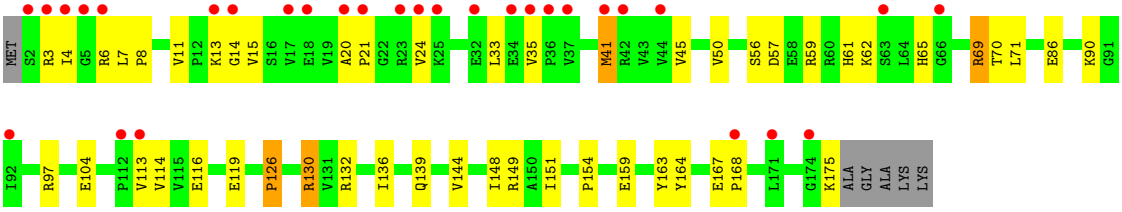




• Molecule 31: 50S Ribosomal Protein L6

Chain BH:

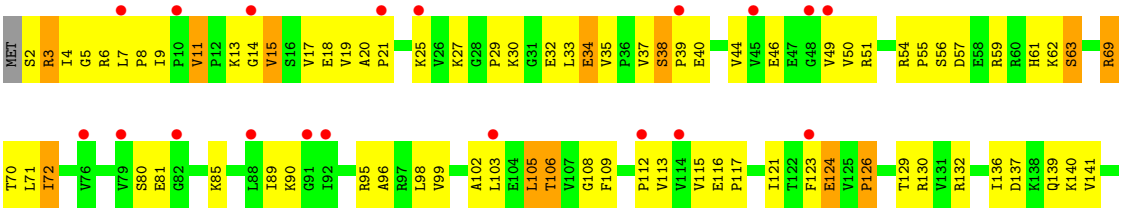


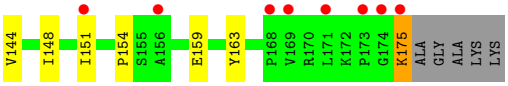


• Molecule 31: 50S Ribosomal Protein L6

Chain DH:



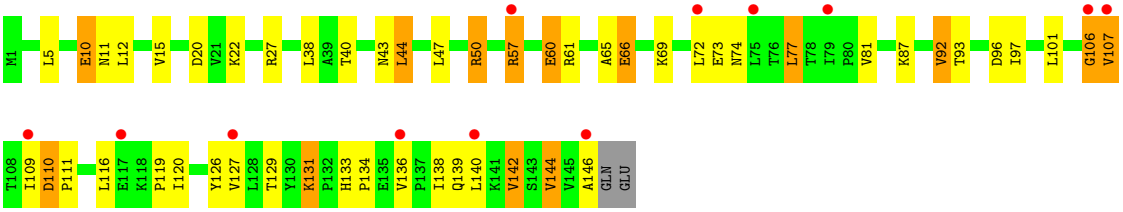




• Molecule 32: 50S Ribosomal Protein L9

Chain BI:

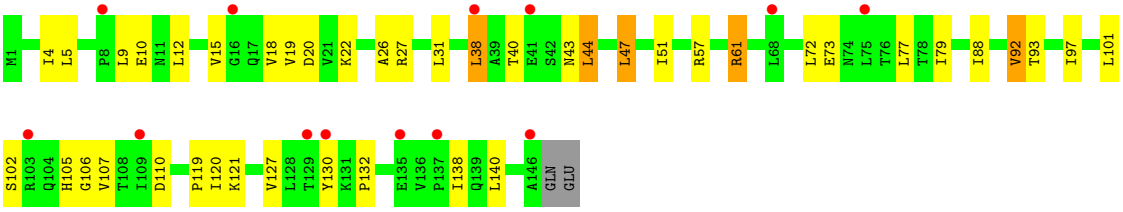




• Molecule 32: 50S Ribosomal Protein L9

Chain DI:

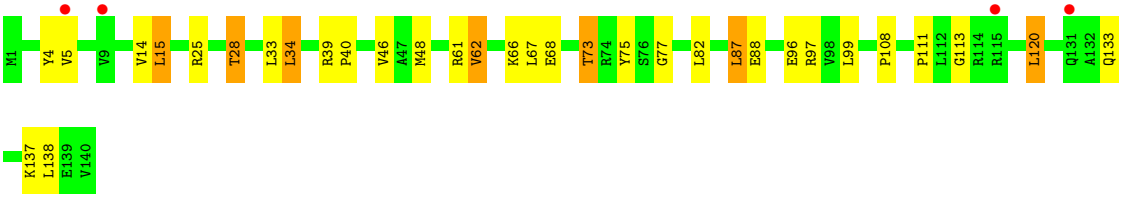




• Molecule 33: 50S Ribosomal Protein L13

Chain BN:

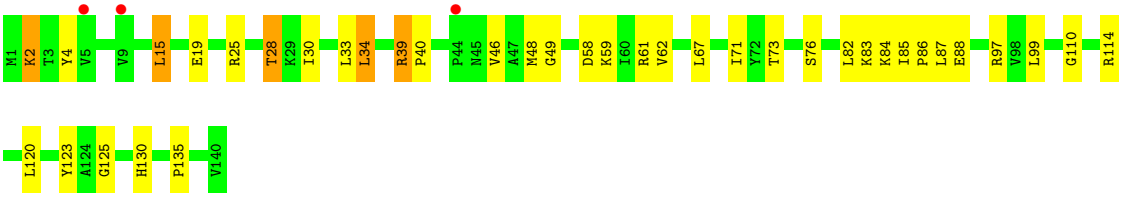




• Molecule 33: 50S Ribosomal Protein L13

Chain DN:

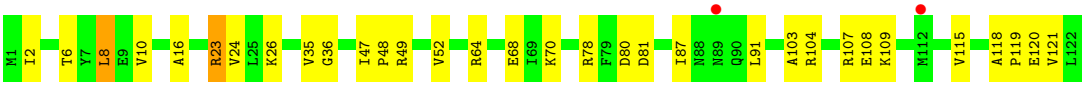




• Molecule 34: 50S Ribosomal Protein L14

Chain BO:

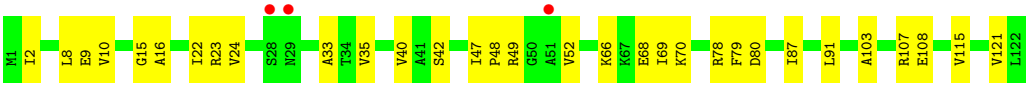




• Molecule 34: 50S Ribosomal Protein L14

Chain DO:

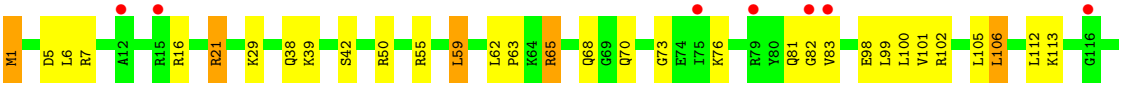


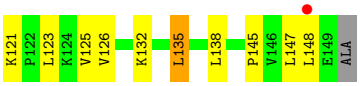


• Molecule 35: 50S Ribosomal Protein L15

Chain BP:



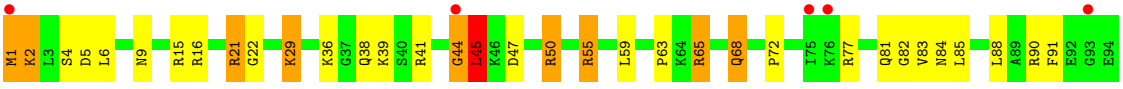


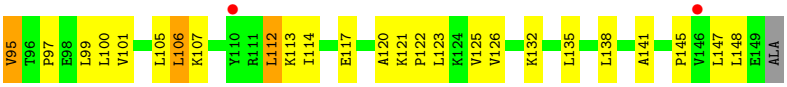


• Molecule 35: 50S Ribosomal Protein L15

Chain DP:



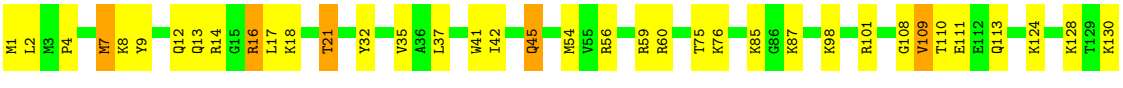




• Molecule 36: 50S Ribosomal Protein L16

Chain BQ:



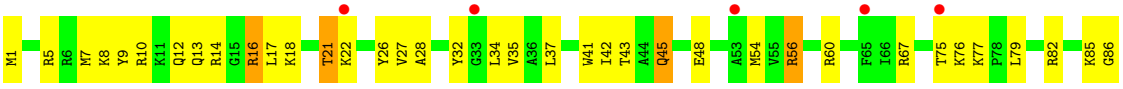


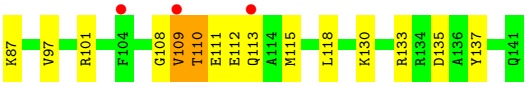


• Molecule 36: 50S Ribosomal Protein L16

Chain DQ:



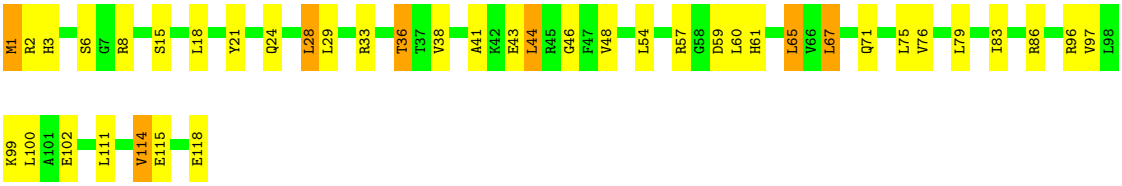




• Molecule 37: 50S Ribosomal Protein L17

Chain BR:

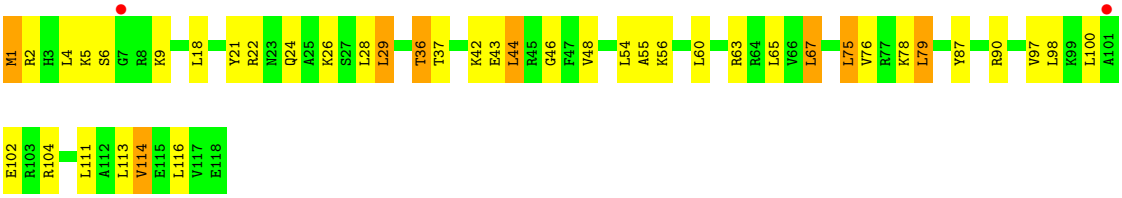




• Molecule 37: 50S Ribosomal Protein L17

Chain DR:

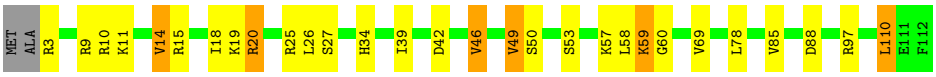




• Molecule 38: 50S Ribosomal Protein L18

Chain BS:

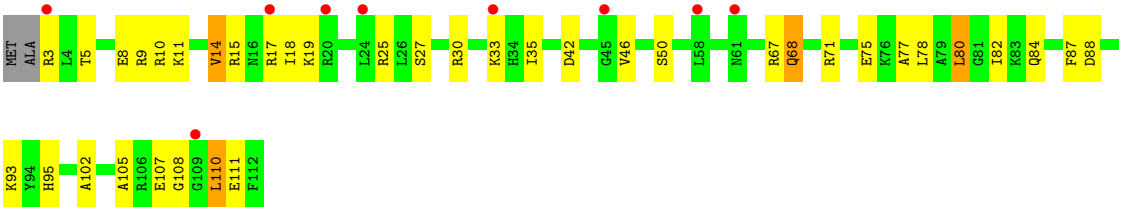




• Molecule 38: 50S Ribosomal Protein L18

Chain DS:

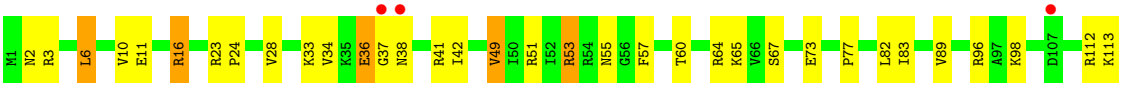


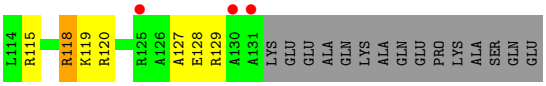


• Molecule 39: 50S Ribosomal Protein L19

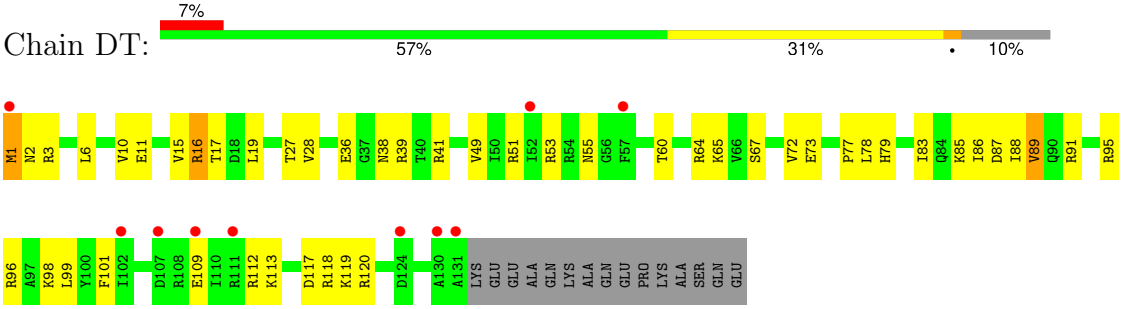
Chain BT:



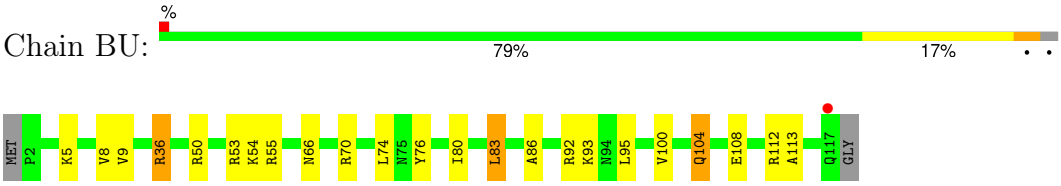




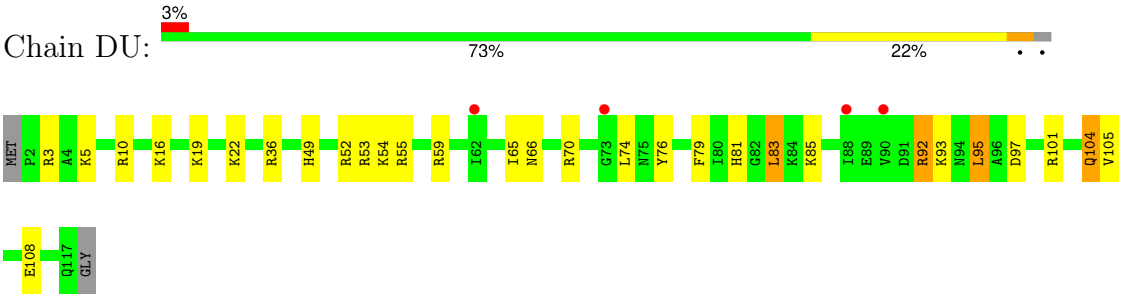
• Molecule 39: 50S Ribosomal Protein L19



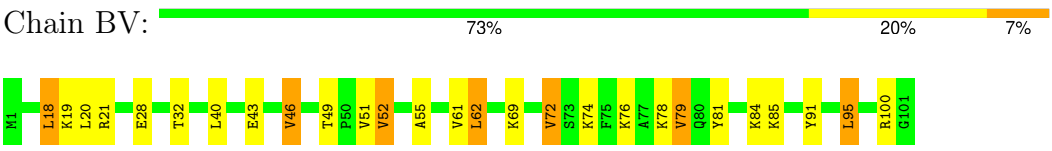
• Molecule 40: 50S Ribosomal Protein L20



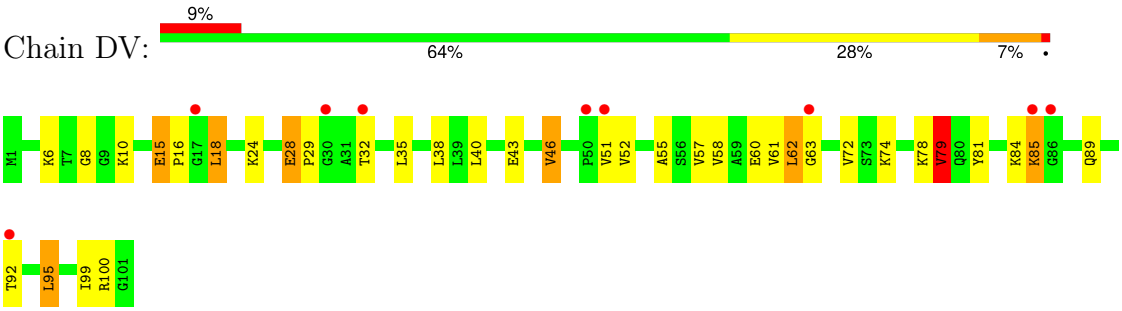
• Molecule 40: 50S Ribosomal Protein L20



• Molecule 41: 50S Ribosomal Protein L21

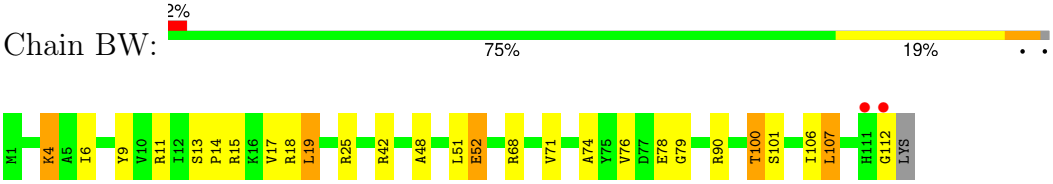


• Molecule 41: 50S Ribosomal Protein L21



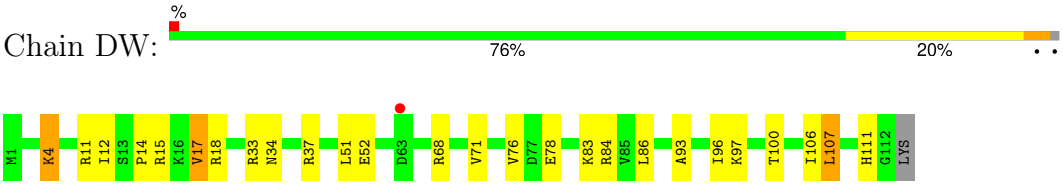
• Molecule 42: 50S Ribosomal Protein L22

Chain BW:



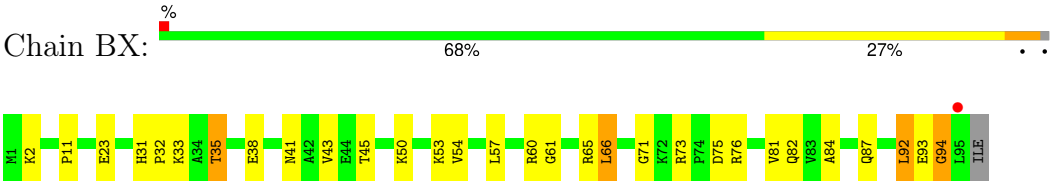
• Molecule 42: 50S Ribosomal Protein L22

Chain DW:



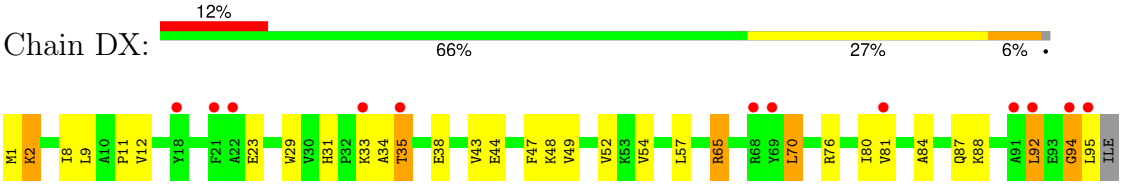
• Molecule 43: 50S Ribosomal Protein L23

Chain BX:



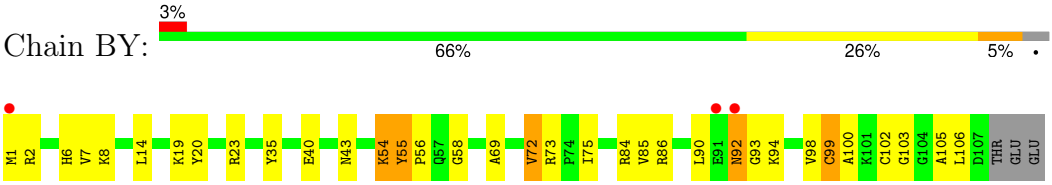
• Molecule 43: 50S Ribosomal Protein L23

Chain DX:



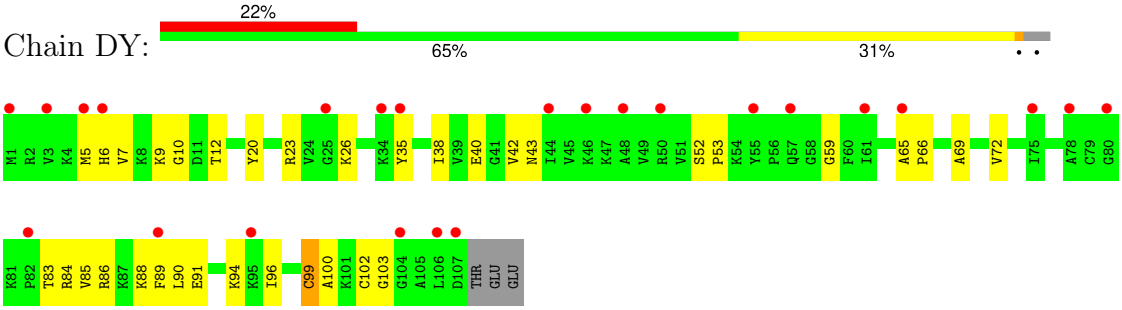
• Molecule 44: 50S Ribosomal Protein L24

Chain BY:



• Molecule 44: 50S Ribosomal Protein L24

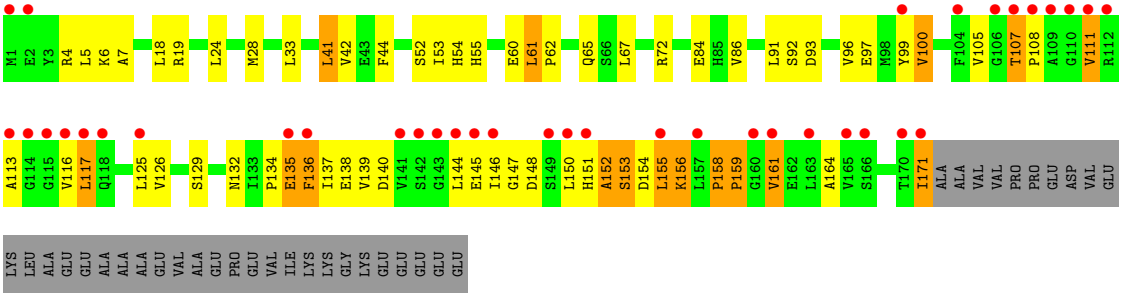
Chain DY:



• Molecule 45: 50S Ribosomal Protein L25

Chain BZ:

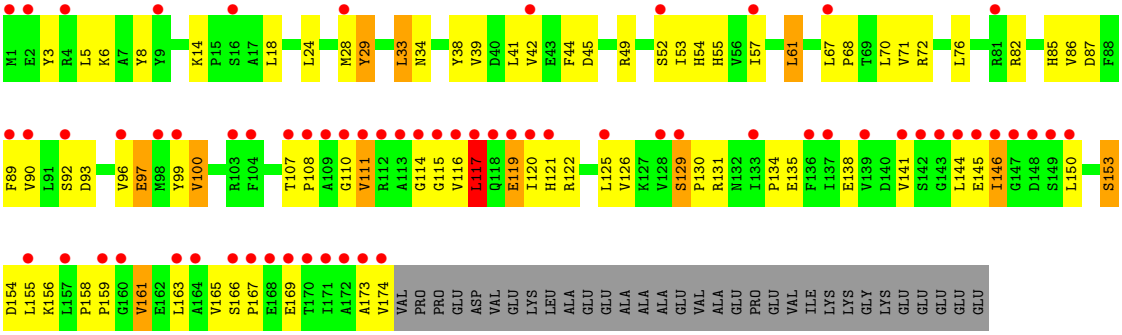




• Molecule 45: 50S Ribosomal Protein L25

Chain DZ:

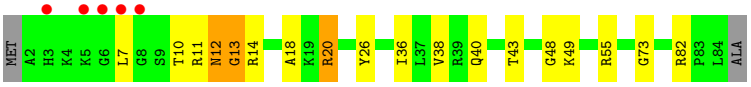




• Molecule 46: 50S Ribosomal Protein L27

Chain B0:

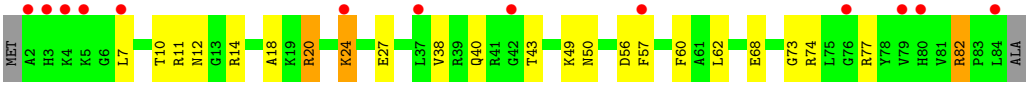




• Molecule 46: 50S Ribosomal Protein L27

Chain D0:





• Molecule 47: 50S Ribosomal Protein L28

Chain B1:

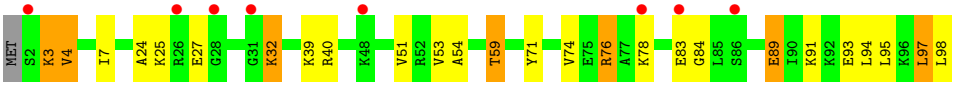




• Molecule 47: 50S Ribosomal Protein L28

Chain D1:

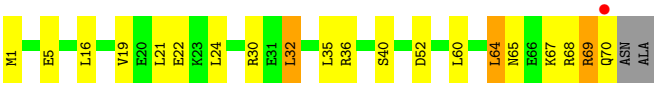




• Molecule 48: 50S Ribosomal Protein L29

Chain B2:

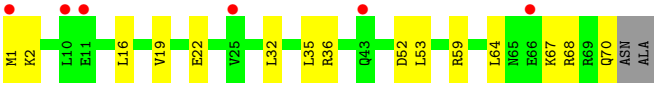




• Molecule 48: 50S Ribosomal Protein L29

Chain D2:

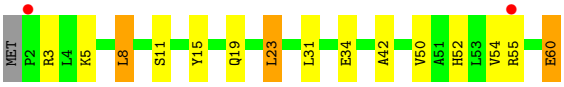




• Molecule 49: 50S Ribosomal Protein L30

Chain B3:

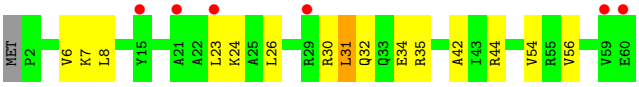




• Molecule 49: 50S Ribosomal Protein L30

Chain D3:

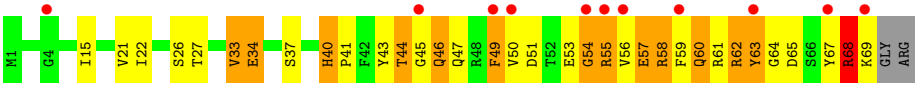




• Molecule 50: 50S Ribosomal Protein L31

Chain B4:

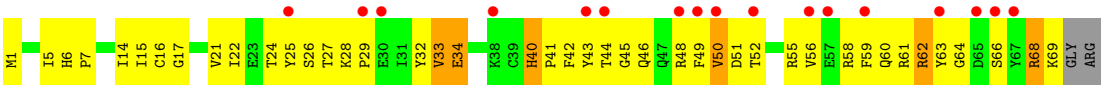




• Molecule 50: 50S Ribosomal Protein L31

Chain D4:





• Molecule 51: 50S Ribosomal Protein L32

Chain B5:

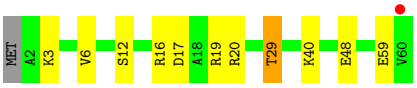




• Molecule 51: 50S Ribosomal Protein L32

Chain D5:





• Molecule 52: 50S Ribosomal Protein L33

Chain B6:

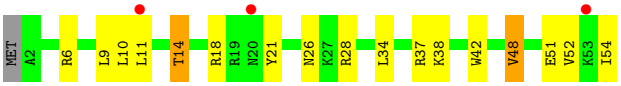




• Molecule 52: 50S Ribosomal Protein L33

Chain D6:

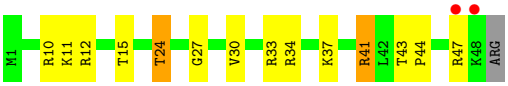




• Molecule 53: 50S Ribosomal Protein L34

Chain B7:

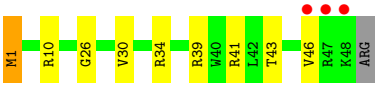




• Molecule 53: 50S Ribosomal Protein L34

Chain D7:

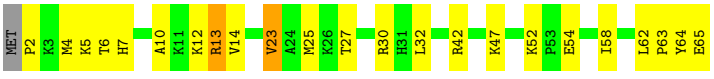




• Molecule 54: 50S Ribosomal Protein L35

Chain B8:

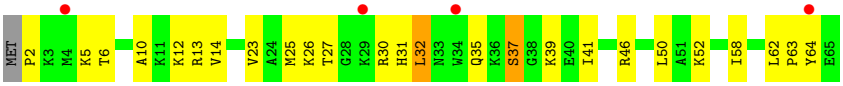




• Molecule 54: 50S Ribosomal Protein L35

Chain D8:

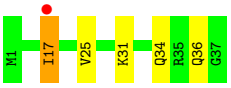




• Molecule 55: 50S Ribosomal Protein L36

Chain B9:

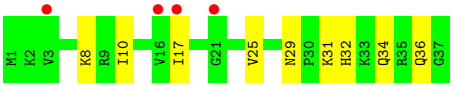




• Molecule 55: 50S Ribosomal Protein L36

Chain D9:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.35Å 449.01Å 621.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.52 – 2.55 145.52 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.0 (145.52-2.55) 99.0 (145.52-2.55)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.225 , 0.273 0.229 , 0.274	Depositor DCC
R_{free} test set	93275 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	48.2	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 59.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	297273	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, SF4, 4SU, 5MC, K, 5MU, PCY, PSU, ZN, 7MG, MIA

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	0.25	0/36049	0.45	1/56261 (0.0%)
1	CA	0.23	0/36170	0.45	2/56452 (0.0%)
2	AB	0.42	0/1881	1.00	10/2542 (0.4%)
2	CB	0.41	0/1860	0.96	5/2518 (0.2%)
3	AC	0.42	0/1576	0.89	3/2130 (0.1%)
3	CC	0.41	0/1566	0.96	6/2119 (0.3%)
4	AD	0.41	0/1689	0.87	2/2267 (0.1%)
4	CD	0.40	0/1704	0.93	3/2284 (0.1%)
5	AE	0.44	0/1145	0.94	5/1543 (0.3%)
5	CE	0.44	0/1149	1.02	6/1548 (0.4%)
6	AF	0.41	0/819	0.77	0/1111
6	CF	0.38	0/829	0.80	1/1123 (0.1%)
7	AG	0.41	0/1250	0.86	1/1679 (0.1%)
7	CG	0.38	0/1254	0.90	2/1683 (0.1%)
8	AH	0.40	0/1108	0.87	0/1494
8	CH	0.38	0/1108	0.91	2/1494 (0.1%)
9	AI	0.41	0/1002	0.92	3/1346 (0.2%)
9	CI	0.42	0/997	0.90	0/1343
10	AJ	0.42	0/722	1.05	6/982 (0.6%)
10	CJ	0.44	0/727	1.02	2/988 (0.2%)
11	AK	0.43	0/844	0.88	1/1145 (0.1%)
11	CK	0.41	0/848	0.90	0/1149
12	AL	0.43	0/946	0.79	0/1274
12	CL	0.42	0/946	0.87	2/1274 (0.2%)
13	AM	0.42	0/969	0.94	3/1302 (0.2%)
13	CM	0.37	0/961	0.90	2/1291 (0.2%)
14	AN	0.40	0/501	0.80	0/664
14	CN	0.40	0/501	0.84	0/664
15	AO	0.40	0/739	0.91	2/985 (0.2%)
15	CO	0.38	0/739	0.82	1/985 (0.1%)
16	AP	0.42	0/697	0.85	1/939 (0.1%)
16	CP	0.42	0/693	0.76	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.38	0/836	0.79	0/1117
17	CQ	0.36	0/836	0.82	0/1117
18	AR	0.39	0/560	0.85	0/746
18	CR	0.35	0/560	0.75	0/746
19	AS	0.40	0/667	0.85	0/900
19	CS	0.47	0/661	0.99	2/893 (0.2%)
20	AT	0.40	0/730	0.89	0/965
20	CT	0.41	0/729	0.87	0/965
21	AU	0.36	0/203	0.82	0/266
21	CU	0.41	0/203	0.82	0/266
22	AV	0.25	0/310	0.42	0/480
22	CV	0.25	0/310	0.41	0/480
23	AW	0.29	1/1602 (0.1%)	0.45	0/2493
23	AY	0.30	1/1602 (0.1%)	0.48	0/2493
23	CW	0.31	1/1556 (0.1%)	0.46	0/2418
23	CY	0.31	1/1579 (0.1%)	0.48	0/2455
24	AX	0.30	0/1725	0.45	0/2689
24	CX	0.29	0/1725	0.46	0/2689
25	BA	0.33	0/68013	0.50	7/106165 (0.0%)
25	DA	0.27	0/67542	0.47	1/105428 (0.0%)
26	BB	0.28	0/2878	0.45	0/4490
26	DB	0.27	0/2878	0.46	0/4490
27	BD	0.54	0/2186	0.92	1/2944 (0.0%)
27	DD	0.49	0/2186	0.92	2/2944 (0.1%)
28	BE	0.56	0/1592	0.92	2/2149 (0.1%)
28	DE	0.47	0/1592	0.95	4/2149 (0.2%)
29	BF	0.53	0/1619	0.89	1/2193 (0.0%)
29	DF	0.43	0/1615	0.93	3/2188 (0.1%)
30	BG	0.45	0/1450	0.90	4/1959 (0.2%)
30	DG	0.41	0/1449	0.97	8/1958 (0.4%)
31	BH	0.46	0/1356	0.85	0/1834
31	DH	0.44	0/1356	0.93	4/1834 (0.2%)
32	BI	0.41	0/1100	0.92	2/1501 (0.1%)
32	DI	0.39	0/1076	0.95	6/1471 (0.4%)
33	BN	0.53	0/1144	0.85	0/1543
33	DN	0.43	0/1144	0.97	4/1543 (0.3%)
34	BO	0.55	0/943	0.90	2/1269 (0.2%)
34	DO	0.42	0/943	0.82	0/1269
35	BP	0.52	0/1152	0.85	0/1533
35	DP	0.42	0/1152	0.95	4/1533 (0.3%)
36	BQ	0.52	0/1143	0.82	0/1527
36	DQ	0.43	0/1143	0.83	0/1527
37	BR	0.56	0/982	0.92	2/1312 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	DR	0.43	0/982	0.81	0/1312
38	BS	0.45	0/887	0.85	0/1180
38	DS	0.40	0/880	0.88	0/1172
39	BT	0.50	0/1105	0.84	0/1477
39	DT	0.39	0/1097	0.82	0/1468
40	BU	0.57	0/977	0.83	1/1301 (0.1%)
40	DU	0.41	0/977	0.86	0/1301
41	BV	0.55	0/782	0.86	0/1049
41	DV	0.40	0/782	0.81	0/1049
42	BW	0.57	0/897	0.94	3/1205 (0.2%)
42	DW	0.44	0/897	0.82	0/1205
43	BX	0.54	0/764	0.91	0/1025
43	DX	0.44	0/764	0.89	1/1025 (0.1%)
44	BY	0.52	0/819	0.97	1/1095 (0.1%)
44	DY	0.39	0/819	0.83	1/1095 (0.1%)
45	BZ	0.46	0/1379	1.01	7/1873 (0.4%)
45	DZ	0.44	0/1390	0.98	9/1890 (0.5%)
46	B0	0.50	0/662	0.91	2/881 (0.2%)
46	D0	0.39	0/662	0.88	2/881 (0.2%)
47	B1	0.50	0/762	0.90	2/1014 (0.2%)
47	D1	0.43	0/762	0.87	0/1014
48	B2	0.49	0/590	0.94	1/781 (0.1%)
48	D2	0.37	0/590	0.78	0/781
49	B3	0.55	0/474	0.97	2/635 (0.3%)
49	D3	0.37	0/469	0.89	0/630
50	B4	0.45	0/571	1.07	8/768 (1.0%)
50	D4	0.42	0/545	1.00	2/737 (0.3%)
51	B5	0.53	0/469	0.79	0/635
51	D5	0.45	0/469	0.85	0/635
52	B6	0.52	0/460	0.78	0/613
52	D6	0.42	0/456	0.67	0/608
53	B7	0.58	0/426	0.90	0/561
53	D7	0.51	0/426	0.86	0/561
54	B8	0.53	0/519	0.93	2/684 (0.3%)
54	D8	0.42	0/525	0.82	0/691
55	B9	0.52	0/310	0.85	0/407
55	D9	0.42	0/310	0.84	0/407
All	All	0.34	4/316672 (0.0%)	0.61	175/474091 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	1
7	AG	0	1
7	CG	0	1
19	CS	0	1
27	DD	0	1
38	BS	0	1
44	BY	0	1
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CW	8	4SU	O3'-P	5.55	1.61	1.56
23	AY	8	4SU	O3'-P	5.47	1.61	1.56
23	CY	8	4SU	O3'-P	5.36	1.61	1.56
23	AW	8	4SU	O3'-P	5.20	1.61	1.56

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BZ	158	PRO	CA-C-N	9.89	132.20	119.84
45	BZ	158	PRO	C-N-CA	9.89	132.20	119.84
46	B0	12	ASN	N-CA-C	9.36	124.90	113.38
8	CH	73	ASP	CA-C-N	9.18	129.95	120.04
8	CH	73	ASP	C-N-CA	9.18	129.95	120.04
27	DD	275	LYS	N-CA-C	-8.46	96.87	109.81
2	AB	38	GLY	N-CA-C	-8.23	103.14	115.32
3	AC	29	TYR	N-CA-C	-7.94	102.62	113.18
45	DZ	14	LYS	CA-C-N	7.93	128.36	119.32
45	DZ	14	LYS	C-N-CA	7.93	128.36	119.32
35	DP	22	GLY	CA-C-N	7.87	127.79	119.05
35	DP	22	GLY	C-N-CA	7.87	127.79	119.05
28	DE	72	VAL	CA-C-N	7.80	135.74	121.70
28	DE	72	VAL	C-N-CA	7.80	135.74	121.70
46	D0	82	ARG	CA-C-N	7.66	128.12	119.92
46	D0	82	ARG	C-N-CA	7.66	128.12	119.92
43	DX	94	GLY	N-CA-C	7.64	121.36	112.50
27	BD	274	ARG	N-CA-C	7.48	120.23	110.43
32	DI	110	ASP	CA-C-N	7.45	126.98	119.24
32	DI	110	ASP	C-N-CA	7.45	126.98	119.24
25	BA	2014	G	C2'-C3'-O3'	7.43	120.64	109.50
4	CD	171	GLY	CA-C-N	7.34	129.01	119.84
4	CD	171	GLY	C-N-CA	7.34	129.01	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	AJ	90	LEU	CA-C-N	7.23	128.87	119.84
10	AJ	90	LEU	C-N-CA	7.23	128.87	119.84
35	DP	44	GLY	CA-C-N	7.20	134.65	121.70
35	DP	44	GLY	C-N-CA	7.20	134.65	121.70
2	AB	23	ARG	N-CA-C	-7.12	105.42	112.97
10	AJ	76	ASN	CA-C-N	7.11	128.73	119.84
10	AJ	76	ASN	C-N-CA	7.11	128.73	119.84
44	BY	92	ASN	N-CA-C	7.04	119.85	111.33
47	B1	67	ILE	CA-C-N	-7.00	112.35	120.12
47	B1	67	ILE	C-N-CA	-7.00	112.35	120.12
2	AB	9	GLU	N-CA-C	6.95	125.60	110.80
50	B4	40	HIS	CA-C-N	6.86	128.41	119.84
50	B4	40	HIS	C-N-CA	6.86	128.41	119.84
5	CE	105	VAL	CA-C-N	-6.68	112.11	119.19
5	CE	105	VAL	C-N-CA	-6.68	112.11	119.19
42	BW	13	SER	CA-C-N	6.67	126.18	119.24
42	BW	13	SER	C-N-CA	6.67	126.18	119.24
32	BI	110	ASP	CA-C-N	6.59	126.83	119.32
32	BI	110	ASP	C-N-CA	6.59	126.83	119.32
10	CJ	90	LEU	CA-C-N	6.49	127.95	119.84
10	CJ	90	LEU	C-N-CA	6.49	127.95	119.84
12	CL	28	LYS	N-CA-C	6.44	120.54	111.52
5	CE	68	GLU	N-CA-C	6.38	118.77	111.11
7	AG	78	ARG	N-CA-C	6.35	117.99	107.20
30	BG	31	VAL	CA-C-N	6.34	127.77	119.84
30	BG	31	VAL	C-N-CA	6.34	127.77	119.84
30	DG	31	VAL	CA-C-N	6.22	127.62	119.84
30	DG	31	VAL	C-N-CA	6.22	127.62	119.84
5	AE	98	THR	N-CA-C	6.18	117.69	111.07
45	BZ	107	THR	CA-C-N	6.17	127.11	120.13
45	BZ	107	THR	C-N-CA	6.17	127.11	120.13
33	DN	39	ARG	CA-C-N	6.14	125.84	119.82
33	DN	39	ARG	C-N-CA	6.14	125.84	119.82
50	B4	65	ASP	N-CA-C	-6.09	104.35	112.94
29	BF	89	VAL	N-CA-C	6.08	116.72	110.82
32	DI	72	LEU	N-CA-C	6.04	117.67	111.14
3	CC	99	VAL	N-CA-C	6.01	115.27	106.55
4	AD	188	LEU	CA-C-N	6.01	126.02	119.89
4	AD	188	LEU	C-N-CA	6.01	126.02	119.89
2	CB	228	GLY	N-CA-C	5.97	119.22	110.80
25	BA	2014	G	P-O3'-C3'	5.92	129.08	120.20
13	AM	9	ILE	CA-C-N	5.91	126.25	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	AM	9	ILE	C-N-CA	5.91	126.25	119.93
28	DE	190	GLY	CA-C-N	5.89	126.35	120.52
28	DE	190	GLY	C-N-CA	5.89	126.35	120.52
12	CL	119	LYS	N-CA-C	-5.88	102.76	110.53
50	B4	60	GLN	N-CA-C	-5.86	106.76	112.97
30	DG	45	GLU	N-CA-C	-5.83	106.02	113.01
31	DH	38	SER	CA-C-N	5.82	125.50	119.56
31	DH	38	SER	C-N-CA	5.82	125.50	119.56
2	AB	17	PHE	N-CA-C	5.81	123.17	110.80
49	B3	11	SER	CA-C-N	5.79	125.40	119.56
49	B3	11	SER	C-N-CA	5.79	125.40	119.56
2	AB	193	ASP	CA-C-N	5.78	125.91	119.32
2	AB	193	ASP	C-N-CA	5.78	125.91	119.32
30	BG	45	GLU	N-CA-C	-5.76	106.10	113.01
19	CS	30	LEU	N-CA-C	5.75	118.57	110.23
45	DZ	129	SER	CA-C-N	5.74	125.42	119.05
45	DZ	129	SER	C-N-CA	5.74	125.42	119.05
3	AC	96	GLY	N-CA-C	-5.72	107.30	115.64
29	DF	21	ALA	CA-C-N	5.70	131.96	121.70
29	DF	21	ALA	C-N-CA	5.70	131.96	121.70
28	BE	31	CYS	CA-C-N	5.69	125.87	119.90
28	BE	31	CYS	C-N-CA	5.69	125.87	119.90
44	DY	91	GLU	N-CA-C	-5.69	105.60	112.54
50	D4	40	HIS	CA-C-N	5.65	126.91	119.84
50	D4	40	HIS	C-N-CA	5.65	126.91	119.84
29	DF	9	ILE	N-CA-C	5.61	114.05	107.77
30	DG	48	GLU	N-CA-C	-5.60	105.49	112.93
13	AM	84	ILE	N-CA-C	5.58	121.47	113.16
16	AP	5	ARG	N-CA-C	5.57	117.26	108.96
1	CA	532	A	C2'-C3'-O3'	5.55	117.82	109.50
40	BU	9	VAL	N-CA-C	5.53	116.18	110.82
3	CC	125	GLU	N-CA-C	-5.47	105.47	111.82
15	AO	87	ILE	N-CA-C	5.46	118.42	112.96
50	B4	54	GLY	CA-C-N	5.45	131.95	121.54
50	B4	54	GLY	C-N-CA	5.45	131.95	121.54
25	DA	1992	G	C2'-C3'-O3'	5.45	117.67	109.50
45	BZ	156	LYS	N-CA-C	5.44	117.96	111.71
3	CC	43	LEU	N-CA-C	5.43	116.89	110.97
10	AJ	38	ILE	CA-C-N	5.42	126.62	119.84
10	AJ	38	ILE	C-N-CA	5.42	126.62	119.84
32	DI	79	ILE	CA-C-N	5.42	126.25	120.13
32	DI	79	ILE	C-N-CA	5.42	126.25	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	BO	47	ILE	CA-C-N	5.41	125.42	119.90
34	BO	47	ILE	C-N-CA	5.41	125.42	119.90
4	CD	178	VAL	N-CA-C	5.41	115.61	110.42
48	B2	69	ARG	N-CA-C	5.40	116.86	110.97
2	CB	124	SER	CA-C-N	-5.39	113.72	120.51
2	CB	124	SER	C-N-CA	-5.39	113.72	120.51
5	AE	95	ALA	CA-C-N	5.39	126.58	119.84
5	AE	95	ALA	C-N-CA	5.39	126.58	119.84
6	CF	65	VAL	N-CA-C	5.39	115.39	108.82
15	AO	83	GLU	N-CA-C	-5.39	105.49	111.36
25	BA	1700	G	C2'-C3'-O3'	5.38	117.58	109.50
25	BA	70	A	C4'-C3'-O3'	5.37	117.46	109.40
50	B4	51	ASP	N-CA-C	5.35	117.90	109.39
30	BG	96	ARG	CB-CA-C	-5.35	110.39	116.54
11	AK	90	GLY	N-CA-C	-5.34	106.51	115.80
1	AA	991	U	P-O3'-C3'	5.34	128.21	120.20
2	AB	232	PRO	N-CA-C	5.33	119.58	111.11
30	DG	67	LYS	CA-C-N	5.32	125.78	120.14
30	DG	67	LYS	C-N-CA	5.32	125.78	120.14
30	DG	121	ASN	CA-C-N	5.31	125.12	119.28
30	DG	121	ASN	C-N-CA	5.31	125.12	119.28
7	CG	87	VAL	N-CA-C	5.31	113.12	107.76
2	AB	166	ASP	CA-C-N	5.27	124.90	119.05
2	AB	166	ASP	C-N-CA	5.27	124.90	119.05
2	AB	123	ALA	N-CA-C	-5.24	106.47	112.92
42	BW	101	SER	N-CA-C	5.24	118.10	109.72
50	B4	62	ARG	CB-CA-C	-5.24	110.52	116.54
3	CC	4	LYS	N-CA-C	5.23	117.67	110.35
45	DZ	115	GLY	N-CA-C	5.20	120.62	111.57
45	BZ	129	SER	CA-C-N	5.20	124.82	119.05
45	BZ	129	SER	C-N-CA	5.20	124.82	119.05
9	AI	51	ARG	N-CA-C	-5.20	106.09	112.90
54	B8	52	LYS	CA-C-N	-5.19	113.58	118.97
54	B8	52	LYS	C-N-CA	-5.19	113.58	118.97
3	AC	15	THR	N-CA-C	-5.18	107.98	114.56
25	BA	1346	U	P-O3'-C3'	5.16	127.94	120.20
25	BA	1346	U	C4'-C3'-O3'	5.15	117.13	109.40
15	CO	23	GLY	N-CA-C	5.15	125.39	113.18
3	CC	29	TYR	N-CA-C	-5.14	106.35	113.18
9	AI	89	ASN	CA-C-N	5.13	125.43	119.47
9	AI	89	ASN	C-N-CA	5.13	125.43	119.47
5	AE	127	ASN	CA-C-N	5.10	124.55	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AE	127	ASN	C-N-CA	5.10	124.55	119.24
25	BA	1255	A	C4'-C3'-O3'	5.10	117.05	109.40
2	CB	130	ARG	N-CA-C	5.09	117.11	110.08
27	DD	251	GLY	N-CA-C	5.09	120.75	114.69
19	CS	82	GLY	N-CA-C	5.08	117.30	110.43
3	CC	48	TYR	N-CA-C	-5.08	105.74	111.28
5	CE	76	ILE	CA-C-N	5.08	124.74	119.56
5	CE	76	ILE	C-N-CA	5.08	124.74	119.56
46	B0	13	GLY	N-CA-C	5.06	125.18	113.18
45	DZ	29	TYR	N-CA-C	5.06	115.99	108.60
5	CE	98	THR	N-CA-C	5.06	116.48	111.07
13	CM	112	GLY	CA-C-N	5.05	125.04	119.89
13	CM	112	GLY	C-N-CA	5.05	125.04	119.89
32	DI	132	PRO	N-CA-C	-5.05	108.92	114.92
31	DH	11	VAL	CA-C-N	5.04	125.02	120.03
31	DH	11	VAL	C-N-CA	5.04	125.02	120.03
1	CA	1183	A	P-O3'-C3'	5.04	127.76	120.20
37	BR	38	VAL	CA-C-N	-5.03	113.86	119.19
37	BR	38	VAL	C-N-CA	-5.03	113.86	119.19
2	CB	119	GLU	N-CA-C	-5.02	106.66	112.89
45	DZ	122	ARG	N-CA-C	-5.02	105.70	111.07
33	DN	125	GLY	CA-C-N	5.01	125.45	120.04
33	DN	125	GLY	C-N-CA	5.01	125.45	120.04
7	CG	78	ARG	N-CA-C	5.00	116.04	107.28
45	DZ	82	ARG	CA-C-N	5.00	124.91	119.76
45	DZ	82	ARG	C-N-CA	5.00	124.91	119.76

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide
7	AG	78	ARG	Peptide
38	BS	58	LEU	Peptide
44	BY	54	LYS	Peptide
7	CG	78	ARG	Peptide
19	CS	28	LYS	Peptide
27	DD	274	ARG	Peptide

5.2 Too-close contacts (i)

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	32205	0	16255	437	0
1	CA	32312	0	16307	559	0
2	AB	1846	0	1867	74	0
2	CB	1825	0	1828	94	0
3	AC	1552	0	1546	45	0
3	CC	1542	0	1517	57	0
4	AD	1659	0	1676	55	0
4	CD	1674	0	1714	55	0
5	AE	1129	0	1185	34	0
5	CE	1133	0	1191	31	0
6	AF	806	0	793	21	0
6	CF	816	0	808	19	0
7	AG	1231	0	1238	23	0
7	CG	1235	0	1249	32	0
8	AH	1088	0	1126	34	0
8	CH	1088	0	1126	31	0
9	AI	983	0	986	28	0
9	CI	978	0	966	45	0
10	AJ	709	0	650	33	0
10	CJ	714	0	672	37	0
11	AK	829	0	825	15	0
11	CK	833	0	836	22	0
12	AL	930	0	980	18	0
12	CL	930	0	980	23	0
13	AM	958	0	1002	26	0
13	CM	950	0	988	25	0
14	AN	492	0	529	20	0
14	CN	492	0	529	17	0
15	AO	728	0	760	19	0
15	CO	728	0	760	32	0
16	AP	681	0	697	21	0
16	CP	677	0	686	18	0
17	AQ	823	0	891	17	0
17	CQ	823	0	891	20	0
18	AR	555	0	618	13	0
18	CR	555	0	618	14	0
19	AS	652	0	662	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	646	0	644	36	0
20	AT	728	0	798	22	0
20	CT	727	0	796	21	0
21	AU	199	0	208	5	0
21	CU	199	0	208	8	0
22	AV	277	0	140	2	0
22	CV	277	0	140	2	0
23	AW	1588	0	820	29	0
23	AY	1581	0	805	60	0
23	CW	1541	0	784	51	0
23	CY	1561	0	796	48	0
24	AX	1625	0	828	11	0
24	CX	1625	0	828	28	0
25	BA	60729	0	30622	617	0
25	DA	60311	0	30414	875	0
26	BB	2573	0	1306	18	0
26	DB	2573	0	1306	38	0
27	BD	2136	0	2218	53	0
27	DD	2136	0	2218	52	0
28	BE	1559	0	1618	37	0
28	DE	1559	0	1618	41	0
29	BF	1584	0	1625	36	0
29	DF	1580	0	1619	66	0
30	BG	1425	0	1443	25	0
30	DG	1424	0	1434	49	0
31	BH	1330	0	1407	27	0
31	DH	1330	0	1407	61	0
32	BI	1085	0	1114	26	0
32	DI	1061	0	1080	19	0
33	BN	1117	0	1184	16	0
33	DN	1117	0	1184	24	0
34	BO	933	0	996	22	0
34	DO	933	0	996	19	0
35	BP	1135	0	1212	29	0
35	DP	1135	0	1212	50	0
36	BQ	1122	0	1179	26	0
36	DQ	1122	0	1179	39	0
37	BR	968	0	1033	25	0
37	DR	968	0	1033	26	0
38	BS	877	0	938	26	0
38	DS	870	0	923	24	0
39	BT	1091	0	1151	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	DT	1083	0	1136	29	0
40	BU	959	0	1019	15	0
40	DU	959	0	1019	27	0
41	BV	771	0	830	18	0
41	DV	771	0	830	22	0
42	BW	886	0	940	15	0
42	DW	886	0	940	13	0
43	BX	750	0	814	24	0
43	DX	750	0	814	23	0
44	BY	806	0	881	23	0
44	DY	806	0	881	20	0
45	BZ	1349	0	1355	42	0
45	DZ	1360	0	1363	63	0
46	B0	653	0	674	16	0
46	D0	653	0	674	24	0
47	B1	755	0	826	17	0
47	D1	755	0	826	16	0
48	B2	588	0	643	9	0
48	D2	588	0	643	8	0
49	B3	469	0	518	9	0
49	D3	464	0	514	9	0
50	B4	558	0	544	38	0
50	D4	532	0	503	28	0
51	B5	455	0	465	11	0
51	D5	455	0	465	9	0
52	B6	453	0	473	7	0
52	D6	449	0	469	8	0
53	B7	418	0	467	11	0
53	D7	418	0	467	6	0
54	B8	511	0	571	19	0
54	D8	517	0	582	21	0
55	B9	307	0	335	4	0
55	D9	307	0	335	7	0
56	AA	230	0	0	0	0
56	AD	1	0	0	0	0
56	AE	1	0	0	0	0
56	AF	1	0	0	0	0
56	AK	2	0	0	0	0
56	AM	1	0	0	0	0
56	AN	1	0	0	0	0
56	AV	1	0	0	0	0
56	AW	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	AX	12	0	0	0	0
56	AY	3	0	0	0	0
56	B0	3	0	0	0	0
56	B1	2	0	0	0	0
56	B2	1	0	0	0	0
56	B3	3	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	2	0	0	0	0
56	B8	3	0	0	0	0
56	B9	1	0	0	0	0
56	BA	839	0	0	0	0
56	BB	23	0	0	0	0
56	BD	11	0	0	0	0
56	BE	8	0	0	0	0
56	BF	12	0	0	0	0
56	BG	3	0	0	0	0
56	BN	5	0	0	0	0
56	BO	1	0	0	0	0
56	BP	3	0	0	0	0
56	BQ	5	0	0	0	0
56	BR	5	0	0	0	0
56	BU	9	0	0	0	0
56	BV	5	0	0	0	0
56	BW	3	0	0	0	0
56	BX	2	0	0	0	0
56	BY	1	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	177	0	0	0	0
56	CE	2	0	0	0	0
56	CF	1	0	0	0	0
56	CJ	1	0	0	0	0
56	CT	1	0	0	0	0
56	CV	1	0	0	0	0
56	CW	2	0	0	0	0
56	CX	5	0	0	0	0
56	CY	1	0	0	0	0
56	D0	2	0	0	0	0
56	D3	1	0	0	0	0
56	D7	2	0	0	0	0
56	D8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DA	675	0	0	0	0
56	DB	11	0	0	0	0
56	DD	7	0	0	0	0
56	DE	4	0	0	0	0
56	DF	5	0	0	0	0
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	1	0	0	0	0
56	DQ	4	0	0	0	0
56	DR	1	0	0	0	0
56	DU	2	0	0	0	0
56	DV	3	0	0	0	0
56	DW	3	0	0	0	0
56	DY	1	0	0	0	0
57	AA	40	0	37	7	0
57	CA	40	0	37	9	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	226	0	0	17	0
61	AE	3	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	4	0	0	1	0
61	AM	1	0	0	0	0
61	AV	4	0	0	0	0
61	AW	6	0	0	0	0
61	AX	8	0	0	0	0
61	AY	3	0	0	0	0
61	B0	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B1	2	0	0	0	0
61	B3	2	0	0	0	0
61	B5	5	0	0	1	0
61	B6	1	0	0	0	0
61	B7	3	0	0	1	0
61	B8	11	0	0	1	0
61	BA	1411	0	0	69	0
61	BB	36	0	0	1	0
61	BD	16	0	0	2	0
61	BE	13	0	0	2	0
61	BF	7	0	0	0	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BN	2	0	0	0	0
61	BO	3	0	0	0	0
61	BP	17	0	0	1	0
61	BQ	2	0	0	0	0
61	BR	2	0	0	0	0
61	BT	1	0	0	0	0
61	BU	6	0	0	0	0
61	BV	2	0	0	0	0
61	BW	4	0	0	0	0
61	BX	1	0	0	0	0
61	CA	173	0	0	15	0
61	CJ	2	0	0	2	0
61	CL	1	0	0	0	0
61	CV	2	0	0	0	0
61	CW	1	0	0	0	0
61	CX	4	0	0	2	0
61	D0	5	0	0	0	0
61	D3	1	0	0	0	0
61	D7	3	0	0	1	0
61	D8	4	0	0	0	0
61	DA	1002	0	0	68	0
61	DB	10	0	0	0	0
61	DD	17	0	0	1	0
61	DE	11	0	0	0	0
61	DF	5	0	0	0	0
61	DN	2	0	0	0	0
61	DO	2	0	0	0	0
61	DP	8	0	0	1	0
61	DQ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DR	1	0	0	0	0
61	DU	2	0	0	0	0
61	DW	1	0	0	0	0
61	DY	1	0	0	0	0
All	All	297273	0	196306	4735	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 10.

All (4735) 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:CA:1256:A:H61	1:CA:1278:U:H1'	1.25	1.02
1:CA:999:C:N4	1:CA:1042:G:H1	1.59	1.00
1:AA:1025:U:O2	1:AA:1036:G:O6	1.82	0.98
23:CW:27:G:H1	23:CW:43:C:N4	1.62	0.97
1:CA:1029:C:N4	1:CA:1032:G:C6	2.33	0.97
23:CW:27:G:H1	23:CW:43:C:H42	1.01	0.97
23:CY:7:A:H61	23:CY:66:U:H3	1.12	0.97
25:BA:2158:C:H42	25:BA:2177:G:H1	0.98	0.96
25:BA:2145:G:H1	25:BA:2197:C:N4	1.63	0.96
25:DA:83:G:H1	25:DA:102:G:HO2'	1.11	0.95
23:CY:15:G:H22	23:CY:48:C:H42	1.11	0.94
23:AY:2:C:H42	23:AY:71:G:H1	1.15	0.94
23:AY:51:U:H3	23:AY:63:G:H1	0.97	0.93
23:CY:50:U:H3	23:CY:64:A:H61	1.14	0.92
25:DA:1798:U:H5'	27:DD:259:THR:HG22	1.49	0.92
25:DA:826:U:OP1	61:DA:4666:HOH:O	1.88	0.91
25:BA:1736:A:H62	25:BA:1745:A:H2	1.19	0.91
25:BA:591:U:O4	61:BA:4279:HOH:O	1.89	0.90
1:CA:1502:A:H2	1:CA:1505:G:H1	1.20	0.90
23:AY:19:G:N2	23:AY:56:C:N3	2.20	0.90
6:CF:81:ILE:HD11	27:DD:125:ILE:HB	1.53	0.90
23:AY:26:A:H61	23:AY:44:G:H1	0.96	0.89
2:AB:16:HIS:HB2	2:AB:204:ASN:HB3	1.54	0.89
23:AY:26:A:N6	23:AY:44:G:H1	1.69	0.89
25:BA:2145:G:H1	25:BA:2197:C:H42	0.90	0.89
7:AG:50:ILE:HD11	7:AG:58:PRO:HA	1.55	0.89
1:AA:266:G:H5"	1:AA:268:C:H41	1.37	0.88
1:AA:376:G:H5"	16:AP:5:ARG:HG2	1.54	0.88
1:CA:532:A:O2'	1:CA:533:A:OP1	1.90	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1502:A:H2	1:AA:1505:G:H1	1.19	0.88
25:BA:656:A:OP1	35:BP:65:ARG:NH1	2.07	0.88
53:B7:24:THR:HG22	53:B7:27:GLY:H	1.37	0.88
1:CA:999:C:H42	1:CA:1042:G:H1	0.88	0.88
25:DA:323:G:HO2'	25:DA:1205:U:H3	1.21	0.87
25:BA:786:G:OP1	61:BA:5273:HOH:O	1.92	0.87
29:DF:53:THR:HG22	29:DF:56:GLU:HG3	1.56	0.87
40:DU:76:TYR:OH	40:DU:92:ARG:NH1	2.06	0.87
25:DA:1315:C:OP2	61:DA:4468:HOH:O	1.91	0.87
39:BT:16:ARG:NH2	39:BT:83:ILE:O	2.08	0.86
25:BA:2118:U:H3	25:BA:2215:G:H1	1.24	0.86
46:B0:10:THR:HG22	46:B0:12:ASN:H	1.39	0.86
46:B0:11:ARG:O	46:B0:14:ARG:NH2	2.08	0.86
25:DA:740:U:OP2	61:DA:4516:HOH:O	1.92	0.86
25:BA:2158:C:N4	25:BA:2177:G:H1	1.72	0.86
30:BG:161:THR:HG22	30:BG:163:ALA:H	1.39	0.86
26:DB:66:A:H61	26:DB:109:C:H5'	1.39	0.86
25:BA:2299:A:H62	25:BA:2356:U:H3	1.22	0.85
1:AA:1025:U:H3	1:AA:1036:G:H1	1.24	0.85
2:CB:18:GLY:HA2	2:CB:42:ILE:HG13	1.57	0.85
1:CA:1189:C:OP1	10:CJ:51:ARG:NH2	2.10	0.85
23:CY:15:G:N2	23:CY:48:C:H42	1.75	0.85
25:BA:1829:U:H5'	27:BD:259:THR:HG22	1.59	0.84
13:CM:23:TYR:HB3	13:CM:67:GLU:HA	1.59	0.84
25:DA:1689:A:H62	25:DA:1698:A:H2	1.25	0.84
33:DN:123:TYR:HH	33:DN:130:HIS:HE2	1.13	0.84
23:CY:56:C:H2'	23:CY:57:G:H8	1.42	0.84
1:CA:1024:G:H2'	1:CA:1025:U:H5"	1.59	0.84
1:CA:1422:G:H5"	34:DO:48:PRO:HB3	1.60	0.83
25:DA:301:G:OP2	44:DY:84:ARG:NH2	2.11	0.83
19:AS:20:LEU:HD23	19:AS:23:ASN:HD22	1.43	0.83
1:CA:1029:C:N3	1:CA:1032:G:C2	2.46	0.82
1:CA:390:C:O3'	16:CP:28:ARG:NH2	2.12	0.82
25:DA:2427:C:OP1	61:DA:4666:HOH:O	1.95	0.82
45:DZ:153:SER:HB3	45:DZ:167:PRO:HB3	1.62	0.82
35:BP:126:VAL:HG12	35:BP:148:LEU:HD22	1.59	0.82
1:AA:1086:U:H3	1:AA:1099:G:H22	1.23	0.82
30:DG:161:THR:HG22	30:DG:163:ALA:H	1.45	0.82
23:AY:2:C:N4	23:AY:71:G:H1	1.78	0.81
23:CY:15:G:H22	23:CY:48:C:N4	1.78	0.81
29:DF:53:THR:HG23	29:DF:55:GLY:H	1.42	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1004:A:N7	1:AA:1036:G:N2	2.28	0.81
1:AA:1158:C:H5	1:AA:1181:G:H1	1.28	0.81
23:CY:50:U:H3	23:CY:64:A:N6	1.78	0.81
25:BA:1094:A:OP2	25:BA:1155:C:N4	2.11	0.81
1:AA:1314:C:OP2	19:AS:4:SER:OG	1.97	0.81
25:DA:882:G:N2	25:DA:894:C:O2	2.14	0.81
1:CA:1029:C:C4	1:CA:1032:G:N1	2.48	0.81
25:DA:1648:C:OP1	61:DA:4508:HOH:O	1.97	0.81
1:CA:972:C:OP1	61:CA:4155:HOH:O	1.97	0.81
2:CB:128:GLU:HG3	2:CB:135:GLN:HE22	1.45	0.81
23:CW:27:G:N2	23:CW:43:C:N3	2.28	0.81
25:BA:2443:U:OP2	61:BA:4398:HOH:O	1.98	0.81
25:DA:2126:A:N6	25:DA:2162:G:O2'	2.13	0.81
8:AH:41:ARG:NH2	8:AH:123:GLU:OE2	2.15	0.80
25:DA:912:C:OP1	36:DQ:8:LYS:NZ	2.14	0.80
1:CA:742:G:OP2	15:CO:35:ARG:NH2	2.14	0.80
3:CC:58:GLU:HB3	10:CJ:92:THR:HG21	1.61	0.80
36:BQ:21:THR:HG21	36:BQ:101:ARG:HD3	1.62	0.80
45:DZ:72:ARG:NH2	45:DZ:97:GLU:O	2.13	0.80
17:CQ:26:GLN:HG2	17:CQ:37:LYS:HG2	1.62	0.80
25:BA:2723:A:OP1	61:BA:4496:HOH:O	2.00	0.80
1:CA:1151:A:HO2'	1:CA:1152:A:H8	1.29	0.80
38:BS:25:ARG:NH1	38:BS:42:ASP:OD1	2.15	0.80
25:DA:2541:A:N7	61:DA:4301:HOH:O	2.14	0.80
1:AA:1182:G:H4'	1:AA:1183:A:H5'	1.61	0.80
1:CA:1352:C:OP1	21:CU:3:LYS:NZ	2.13	0.80
25:DA:994:C:OP1	40:DU:53:ARG:NH2	2.14	0.80
25:DA:2121:G:H1	25:DA:2177:C:H42	1.29	0.80
32:BI:92:VAL:HG13	32:BI:120:ILE:HB	1.65	0.79
47:D1:51:VAL:HG11	47:D1:74:VAL:HG21	1.64	0.79
23:AY:2:C:N3	23:AY:71:G:N2	2.30	0.79
1:CA:953:G:H5'	1:CA:965:A:H61	1.47	0.79
41:DV:40:LEU:HB2	41:DV:46:VAL:HG13	1.65	0.79
1:AA:1008:C:N3	1:AA:1021:G:O6	2.16	0.79
25:BA:2802:C:O2	25:BA:2903:G:N1	2.14	0.79
27:BD:71:ASP:HB3	27:BD:103:ARG:HH22	1.48	0.79
1:CA:838:G:H1	1:CA:848:C:H42	1.30	0.79
25:DA:793:A:O2'	61:DA:4544:HOH:O	1.99	0.79
1:AA:1422:G:H5"	34:BO:48:PRO:HB3	1.65	0.79
3:CC:120:VAL:HA	3:CC:123:GLN:HE21	1.45	0.79
10:CJ:52:GLY:O	14:CN:41:ARG:NH2	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2150:U:H2'	25:DA:2151:G:C8	2.18	0.79
46:D0:10:THR:HG22	46:D0:12:ASN:H	1.47	0.79
1:AA:1503:A:O2'	22:AV:13:A:N1	2.16	0.79
25:BA:615:G:O6	61:BA:5039:HOH:O	1.99	0.79
1:CA:349:A:H2'	1:CA:350:G:H5"	1.64	0.79
29:DF:140:LEU:HD21	29:DF:170:LEU:HD11	1.65	0.79
45:DZ:126:VAL:HG11	45:DZ:161:VAL:HG23	1.64	0.79
25:BA:237:G:OP1	61:BA:5347:HOH:O	2.00	0.78
25:BA:894:U:OP2	61:BA:4544:HOH:O	2.01	0.78
41:BV:72:VAL:HG13	41:BV:85:LYS:HB3	1.66	0.78
1:CA:38:G:H22	1:CA:397:A:H5"	1.48	0.78
15:CO:87:ILE:HG22	15:CO:88:ARG:H	1.48	0.78
25:DA:981:A:OP1	61:DA:4416:HOH:O	2.02	0.78
25:BA:1189:A:OP1	33:BN:25:ARG:NH2	2.16	0.78
1:CA:671:G:H5'	6:CF:77:ARG:HH22	1.48	0.78
23:CY:7:A:N6	23:CY:66:U:H3	1.81	0.78
32:BI:92:VAL:HG11	32:BI:144:VAL:HG11	1.66	0.78
1:AA:160:A:N6	1:AA:345:C:OP2	2.15	0.78
1:CA:504:C:OP1	61:CA:4009:HOH:O	2.02	0.78
51:D5:16:ARG:NH1	51:D5:17:ASP:OD1	2.17	0.78
1:CA:79:G:H1	1:CA:90:U:H3	1.32	0.78
25:DA:956:G:OP2	36:DQ:14:ARG:NH2	2.17	0.78
25:DA:857:C:OP2	46:D0:77:ARG:NH2	2.17	0.77
36:DQ:26:TYR:O	36:DQ:67:ARG:NH1	2.17	0.77
25:BA:1361:C:OP2	61:BA:4775:HOH:O	2.03	0.77
25:DA:1031:G:H5"	55:D9:8:LYS:HE3	1.65	0.77
25:DA:2206:G:H3'	25:DA:2207:G:C8	2.20	0.77
2:AB:155:LEU:HD21	2:AB:159:PRO:HG3	1.65	0.77
23:CW:18:G:O2'	23:CW:57:G:N2	2.15	0.77
25:DA:1970:A:OP1	61:DA:4260:HOH:O	2.02	0.77
9:AI:50:LEU:HD13	9:AI:56:LEU:HA	1.67	0.77
1:AA:1189:C:OP1	10:AJ:51:ARG:NH2	2.15	0.77
25:BA:479:C:OP1	61:BA:4437:HOH:O	2.01	0.77
23:CW:4:C:N3	23:CW:69:G:N2	2.32	0.77
1:CA:656:C:O2'	15:CO:28:GLN:NE2	2.17	0.77
25:DA:1010:A:OP2	61:DA:4483:HOH:O	2.01	0.77
25:BA:2562:G:OP1	61:BA:5207:HOH:O	2.02	0.77
1:AA:1108:G:O6	61:AA:4156:HOH:O	2.03	0.77
25:DA:2123:G:H1	25:DA:2175:C:H42	1.32	0.77
45:DZ:144:LEU:HD22	45:DZ:174:VAL:HG23	1.66	0.77
8:AH:34:GLU:OE1	8:AH:37:ARG:NH1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1083:U:OP2	61:CA:4106:HOH:O	2.02	0.77
1:CA:64:G:H4'	1:CA:65:U:H3'	1.67	0.77
1:CA:1065:U:OP2	1:CA:1190:G:N2	2.17	0.76
25:DA:563:G:OP2	61:DA:4472:HOH:O	2.03	0.76
1:AA:975:A:H4'	1:AA:976:G:H5"	1.66	0.76
25:DA:81:G:N7	61:DA:4462:HOH:O	2.18	0.76
25:DA:1171:G:H1	25:DA:1178:C:H42	1.31	0.76
23:AY:50:U:H3	23:AY:64:A:H2	1.31	0.76
50:B4:53:GLU:C	50:B4:55:ARG:H	1.94	0.76
24:CX:50:U:H3	24:CX:64:G:H1	1.34	0.76
25:DA:250:G:OP2	54:D8:13:ARG:NH2	2.19	0.76
2:CB:179:LYS:HA	8:CH:72:PRO:HG3	1.66	0.76
25:BA:1296:G:OP2	35:BP:21:ARG:NH1	2.18	0.76
43:DX:35:THR:HG22	43:DX:38:GLU:H	1.51	0.76
25:BA:1067:A:H62	25:BA:1186:U:H3	1.34	0.76
25:DA:2285:C:OP2	52:D6:6:ARG:NH1	2.19	0.76
25:DA:2357:U:OP1	46:D0:20:ARG:NH1	2.19	0.76
34:DO:35:VAL:HG11	34:DO:103:ALA:HB3	1.67	0.76
20:AT:10:LEU:HB3	20:AT:12:ALA:H	1.49	0.76
1:CA:1503:A:O2'	22:CV:13:A:N1	2.19	0.76
25:BA:2459:G:OP2	61:BA:4688:HOH:O	2.03	0.75
25:DA:2151:G:H2'	25:DA:2152:G:H8	1.51	0.75
1:CA:1029:C:C4	1:CA:1032:G:C2	2.75	0.75
25:DA:2139:C:H42	25:DA:2152:G:H1	1.32	0.75
23:CY:26:A:N1	23:CY:44:G:O6	2.20	0.75
2:AB:69:LEU:HB3	2:AB:162:ILE:HG22	1.68	0.75
27:DD:238:GLY:O	61:DD:409:HOH:O	2.03	0.75
25:BA:2720:G:H1'	37:BR:71:GLN:HE22	1.51	0.75
25:DA:2171:A:N3	25:DA:2172:U:N3	2.35	0.75
10:CJ:32:ALA:HB1	10:CJ:33:GLN:HA	1.69	0.75
1:CA:975:A:H4'	1:CA:976:G:H5"	1.69	0.75
25:DA:154(A):C:N4	25:DA:171:G:O6	2.20	0.75
20:CT:60:GLU:HG3	20:CT:81:LYS:HD2	1.69	0.75
25:DA:2317:C:N4	25:DA:2318:G:O6	2.20	0.75
1:AA:201:C:H42	1:AA:216:G:H1	1.35	0.74
2:AB:33:TYR:HB2	2:AB:43:ASP:HB2	1.66	0.74
53:B7:34:ARG:NH2	61:B7:201:HOH:O	2.19	0.74
45:DZ:117:LEU:HA	45:DZ:174:VAL:HA	1.67	0.74
1:AA:406:G:H5'	4:AD:5:ILE:HD11	1.69	0.74
25:BA:878:G:O2'	35:BP:38:GLN:NE2	2.21	0.74
9:CI:97:LYS:HA	9:CI:102:LEU:HG	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:CP:51:VAL:HG12	16:CP:53:VAL:H	1.52	0.74
35:DP:126:VAL:HG12	35:DP:148:LEU:HD22	1.69	0.74
15:CO:5:LYS:HZ2	15:CO:5:LYS:H	1.31	0.74
25:DA:847:U:OP2	61:DA:4326:HOH:O	2.04	0.74
10:CJ:8:LEU:HB2	10:CJ:70:ARG:HB2	1.67	0.74
2:CB:98:LEU:HD23	2:CB:101:MET:HE3	1.70	0.74
26:DB:20:C:N4	26:DB:63:G:O6	2.20	0.74
2:AB:16:HIS:CD2	2:AB:17:PHE:H	2.05	0.74
1:CA:152:A:N6	1:CA:169:C:N3	2.35	0.74
23:CW:76:A:OP1	61:DA:4820:HOH:O	2.04	0.74
25:BA:715:G:N7	61:BA:4010:HOH:O	2.20	0.74
25:BA:2479:C:OP2	61:BA:5182:HOH:O	2.05	0.74
42:BW:19:LEU:HB3	51:B5:25:LEU:HD11	1.70	0.74
25:DA:1170:G:H1	25:DA:1179:C:H42	1.36	0.74
1:AA:1069:C:OP2	61:AA:4012:HOH:O	2.05	0.73
23:CY:51:U:O2	23:CY:63:G:N2	2.20	0.73
43:DX:11:PRO:HB3	43:DX:92:LEU:HD11	1.69	0.73
36:DQ:21:THR:HG21	36:DQ:101:ARG:HD3	1.69	0.73
23:AY:26:A:N1	23:AY:44:G:N2	2.35	0.73
43:BX:11:PRO:HB3	43:BX:92:LEU:HD11	1.68	0.73
1:CA:353:A:H5'	1:CA:353:A:H8	1.53	0.73
1:CA:693:G:N7	57:CA:3178:PCY:N16	2.37	0.73
1:AA:742:G:OP2	15:AO:35:ARG:NH2	2.22	0.73
25:BA:1648:U:O4	61:BA:4366:HOH:O	2.05	0.73
25:BA:2849:G:H5'	37:BR:46:GLY:HA2	1.70	0.73
1:CA:838:G:H1	1:CA:848:C:N4	1.87	0.73
25:DA:2287:A:H62	25:DA:2344:U:H3	1.34	0.73
1:AA:677:U:H3	1:AA:713:G:H22	1.36	0.73
45:BZ:139:VAL:HG22	45:BZ:155:LEU:HD11	1.71	0.73
11:CK:93:GLN:HA	11:CK:93:GLN:HE21	1.54	0.73
1:CA:999:C:N3	1:CA:1042:G:N2	2.34	0.73
1:CA:922:G:H4'	5:CE:20:GLN:HA	1.70	0.73
1:CA:1255:G:OP1	10:CJ:45:ARG:NH2	2.22	0.73
45:DZ:45:ASP:OD1	45:DZ:49:ARG:NH1	2.22	0.73
30:BG:108:ASN:HB3	50:B4:22:ILE:HD13	1.71	0.72
1:CA:1000:U:H3	1:CA:1041:A:H61	1.36	0.72
19:CS:50:ALA:HB1	19:CS:57:HIS:HB3	1.71	0.72
23:CW:4:C:N4	23:CW:69:G:N1	2.37	0.72
25:DA:2839:G:H5'	37:DR:46:GLY:HA2	1.70	0.72
1:CA:539:A:OP2	12:CL:115:LYS:NZ	2.22	0.72
1:CA:1028:C:N3	1:CA:1033:G:C6	2.56	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CC:109:PRO:HB3	3:CC:115:LEU:HD23	1.71	0.72
25:DA:2130:U:H4'	25:DA:2133:G:H4'	1.71	0.72
25:DA:2138:C:H42	25:DA:2153:G:H1	1.38	0.72
12:AL:71:PRO:O	12:AL:102:ARG:NH1	2.21	0.72
16:CP:52:ASP:O	16:CP:54:GLU:N	2.20	0.72
25:DA:2100:G:H1	25:DA:2189:U:H3	1.34	0.72
25:BA:1018:A:OP2	61:BA:4279:HOH:O	2.08	0.72
9:CI:5:TYR:H	9:CI:87:GLN:HE22	1.38	0.72
25:DA:1602:U:O4	61:DA:4192:HOH:O	2.07	0.72
1:AA:664:G:H22	1:AA:741:G:H1	1.38	0.72
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.38	0.72
1:AA:1183:A:O2'	1:AA:1184:G:OP1	2.08	0.72
25:BA:542:C:OP1	51:B5:16:ARG:NH2	2.23	0.72
25:BA:839:G:O6	61:BA:4760:HOH:O	2.06	0.72
53:B7:34:ARG:NH1	53:B7:41:ARG:O	2.23	0.72
25:DA:1313:U:OP1	61:DA:4343:HOH:O	2.08	0.72
25:DA:2880:C:O3'	37:DR:90:ARG:NH1	2.23	0.72
2:AB:88:ALA:HB2	2:AB:219:VAL:HG13	1.71	0.72
23:AY:8:4SU:H4'	23:AY:48:C:H4'	1.72	0.72
54:B8:6:THR:HG22	54:B8:63:PRO:HD2	1.72	0.72
24:CX:75:C:OP1	61:CX:4003:HOH:O	2.06	0.72
25:BA:2776:G:OP2	61:BA:4827:HOH:O	2.06	0.72
57:CA:3178:PCY:O19	57:CA:3178:PCY:N2	2.21	0.72
2:CB:88:ALA:HB2	2:CB:219:VAL:HG13	1.70	0.72
25:BA:2145:G:N2	25:BA:2197:C:N3	2.32	0.72
1:CA:1029:C:N4	1:CA:1032:G:N1	2.37	0.72
25:DA:1352:U:OP2	61:DA:4084:HOH:O	2.08	0.72
17:AQ:26:GLN:HG2	17:AQ:37:LYS:HG2	1.70	0.71
4:CD:25:ARG:NH1	4:CD:30:LYS:O	2.23	0.71
25:BA:1001:G:OP2	36:BQ:14:ARG:NH2	2.22	0.71
1:CA:78:G:H2'	1:CA:79:G:H5"	1.71	0.71
28:DE:27:LEU:HD22	39:DT:1:MET:HE1	1.72	0.71
1:AA:1030(C):G:N7	1:AA:1031:G:N2	2.38	0.71
25:BA:2877:G:OP2	39:BT:119:LYS:NZ	2.23	0.71
32:BI:93:THR:HG22	32:BI:119:PRO:HB3	1.72	0.71
25:BA:2162:C:C2	25:BA:2173:G:N2	2.59	0.71
25:BA:2396:G:OP2	46:B0:55:ARG:NH1	2.21	0.71
3:AC:6:HIS:HD2	3:AC:8:ILE:H	1.36	0.71
36:BQ:14:ARG:HG2	36:BQ:41:TRP:HH2	1.55	0.71
9:CI:127:LYS:O	9:CI:128:ARG:HB3	1.91	0.71
24:CX:49:G:H1	24:CX:65:C:H42	1.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DZ:28:MET:HE1	45:DZ:61:LEU:HD21	1.71	0.71
27:BD:148:GLU:HB2	27:BD:151:LYS:HD2	1.73	0.71
1:CA:427:U:OP1	4:CD:13:ARG:NH2	2.24	0.71
15:CO:54:ARG:NH1	15:CO:58:MET:SD	2.63	0.71
25:DA:2110:G:O2'	25:DA:2120:G:OP2	2.08	0.71
42:DW:33:ARG:NH2	42:DW:52:GLU:OE1	2.23	0.71
45:DZ:144:LEU:HD21	45:DZ:173:ALA:HA	1.72	0.71
11:AK:79:SER:HA	11:AK:104:GLN:HB2	1.71	0.70
1:CA:6:G:H4'	1:CA:298:A:H4'	1.73	0.70
25:DA:320:A:OP2	29:DF:137:LYS:NZ	2.20	0.70
57:AA:3231:PCY:N2	57:AA:3231:PCY:O19	2.24	0.70
25:BA:465:G:N7	61:BA:4522:HOH:O	2.24	0.70
25:BA:1378:G:OP1	61:BA:4775:HOH:O	2.08	0.70
25:BA:2157:A:H61	25:BA:2178:G:H1'	1.56	0.70
25:BA:2251:G:OP2	61:BA:4470:HOH:O	2.08	0.70
36:BQ:109:VAL:HG13	36:BQ:113:GLN:HB3	1.71	0.70
25:DA:323:G:O2'	25:DA:1205:U:N3	2.23	0.70
3:AC:78:GLY:HA3	3:AC:83:ARG:H	1.56	0.70
25:BA:2146:G:H1	25:BA:2196:C:H42	1.39	0.70
29:BF:101:LEU:O	29:BF:106:ARG:NH1	2.25	0.70
50:B4:61:ARG:HG3	50:B4:62:ARG:H	1.56	0.70
1:CA:201:C:H42	1:CA:216:G:H1	1.37	0.70
1:CA:346:G:OP1	39:DT:41:ARG:NH2	2.23	0.70
25:DA:1671:U:OP2	61:DA:4069:HOH:O	2.08	0.70
25:BA:1249:A:H2	25:BA:1287:A:H62	1.39	0.70
27:BD:69:ARG:NH2	27:BD:128:GLY:O	2.25	0.70
1:CA:97:G:O2'	1:CA:98:G:O5'	2.09	0.70
23:CY:51:U:N3	23:CY:63:G:N1	2.39	0.70
25:DA:2503:A:O2'	25:DA:2505:G:OP2	2.09	0.70
29:DF:101:LEU:O	29:DF:106:ARG:NH1	2.25	0.70
30:DG:80:PHE:O	30:DG:82:LEU:N	2.24	0.70
25:BA:30:G:OP2	40:BU:5:LYS:NZ	2.23	0.70
25:BA:1700:G:H3'	37:BR:2:ARG:HD3	1.74	0.70
1:CA:1116:C:H2'	1:CA:1117:G:H5"	1.73	0.70
47:D1:76:ARG:HH11	47:D1:97:LEU:HD22	1.56	0.70
5:AE:85:GLY:O	5:AE:87:SER:N	2.24	0.70
1:CA:1118:C:H2'	1:CA:1119:C:H6	1.55	0.70
25:DA:1670:C:OP1	61:DA:4069:HOH:O	2.10	0.70
25:BA:1395:A:OP1	61:BA:5097:HOH:O	2.10	0.70
35:BP:42:SER:O	61:BP:303:HOH:O	2.10	0.70
25:DA:2447:G:OP2	61:DA:4707:HOH:O	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:DD:71:ASP:HB3	27:DD:103:ARG:HH22	1.57	0.70
3:AC:150:LYS:HE2	3:AC:152:ILE:HD11	1.71	0.69
1:CA:559:A:OP1	5:CE:126:ARG:NH2	2.24	0.69
25:BA:2143:G:H1	25:BA:2199:C:H42	1.40	0.69
35:DP:36:LYS:O	61:DP:201:HOH:O	2.09	0.69
9:AI:16:ARG:HB2	9:AI:64:THR:HB	1.74	0.69
44:BY:92:ASN:HB3	44:BY:94:LYS:H	1.56	0.69
25:DA:2355:C:H4'	46:D0:24:LYS:HD3	1.74	0.69
25:BA:2130:C:H2'	25:BA:2131:U:H6	1.57	0.69
25:DA:2682:U:OP2	61:DA:4147:HOH:O	2.10	0.69
1:AA:538:G:H5"	12:AL:114:LYS:HB2	1.73	0.69
1:AA:1353:G:OP1	21:AU:10:ARG:NH1	2.25	0.69
19:AS:63:THR:OG1	19:AS:65:ASN:ND2	2.25	0.69
25:BA:1922:A:OP2	61:BA:4461:HOH:O	2.09	0.69
25:DA:601:C:O2'	29:DF:104:LYS:NZ	2.24	0.69
25:DA:2807:G:N2	25:DA:2893:G:O6	2.25	0.69
1:AA:1129:C:H5"	9:AI:16:ARG:HH12	1.57	0.69
25:BA:1039:G:OP1	40:BU:50:ARG:NH2	2.25	0.69
11:CK:48:ILE:O	11:CK:50:TYR:N	2.22	0.69
1:AA:836:G:OP1	18:AR:61:LYS:NZ	2.23	0.69
25:BA:2081:A:OP2	61:BA:4472:HOH:O	2.11	0.69
1:CA:1125:U:O2'	1:CA:1126:U:H2'	1.93	0.69
11:CK:54:ARG:NH2	23:CY:39:PSU:O2'	2.26	0.69
15:CO:22:THR:OG1	15:CO:23:GLY:N	2.21	0.69
1:AA:812:C:N3	61:AA:4050:HOH:O	2.25	0.69
1:AA:922:G:H4'	5:AE:20:GLN:HA	1.75	0.69
25:DA:1783:A:OP1	61:DA:4516:HOH:O	2.11	0.69
25:DA:2327:A:H2'	25:DA:2328:A:C8	2.28	0.69
23:AY:19:G:N1	23:AY:56:C:N4	2.38	0.69
23:AY:67:C:H2'	23:AY:68:C:C6	2.28	0.69
28:BE:47:VAL:HG21	28:BE:86:PRO:HD2	1.73	0.69
23:CW:2:C:N3	23:CW:71:G:O6	2.26	0.69
25:DA:2125:G:H22	25:DA:2172:U:H5'	1.57	0.69
25:DA:2135:A:H61	25:DA:2157:G:H21	1.37	0.69
37:DR:67:LEU:HD13	37:DR:76:VAL:HG21	1.75	0.69
25:BA:139:A:H8	25:BA:1454:C:HO2'	1.40	0.69
1:CA:1314:C:OP2	19:CS:4:SER:OG	2.08	0.69
25:DA:9:U:H3	25:DA:2629:A:H2	1.39	0.69
25:DA:2122:U:O4	25:DA:2176:A:N1	2.24	0.69
25:DA:2162:G:H4'	25:DA:2172:U:H2'	1.75	0.69
1:AA:200:G:H1	1:AA:217:C:H42	1.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:539:A:OP2	12:AL:115:LYS:NZ	2.26	0.68
1:AA:1423:G:OP1	34:BO:49:ARG:NH2	2.26	0.68
23:AY:44:G:O2'	23:AY:45:U:OP1	2.10	0.68
23:CY:13:C:N3	23:CY:22:G:O6	2.26	0.68
25:DA:1012:U:H5	33:DN:28:THR:HG21	1.59	0.68
25:DA:2167:U:O2'	25:DA:2168:G:N3	2.25	0.68
40:DU:76:TYR:HH	40:DU:92:ARG:NH1	1.91	0.68
25:DA:601:C:OP1	29:DF:108:LYS:NZ	2.27	0.68
25:DA:943:U:OP2	61:DA:4576:HOH:O	2.11	0.68
25:DA:1021:A:H62	25:DA:1141:U:H3	1.39	0.68
1:AA:1034:G:H2'	1:AA:1035:A:C8	2.27	0.68
1:AA:44:G:O6	61:AA:4055:HOH:O	2.09	0.68
25:BA:1717:C:OP2	61:BA:5207:HOH:O	2.12	0.68
42:BW:14:PRO:HG2	42:BW:78:GLU:HG2	1.74	0.68
1:CA:1129:C:OP1	9:CI:16:ARG:NH1	2.25	0.68
25:BA:667:G:N2	25:BA:670:C:OP2	2.27	0.68
23:CW:29:G:H1	23:CW:41:C:H42	1.42	0.68
10:AJ:30:SER:O	10:AJ:81:THR:OG1	2.11	0.68
12:AL:49:ASN:ND2	12:AL:92:ASP:OD2	2.22	0.68
25:DA:1817:G:OP1	27:DD:88:ARG:NH2	2.26	0.68
1:AA:972:C:O2'	10:AJ:55:LYS:O	2.10	0.68
23:AY:50:U:O4	23:AY:64:A:N1	2.27	0.68
25:BA:1044:C:OP1	61:BA:4784:HOH:O	2.11	0.68
25:DA:370:G:OP2	61:DA:4103:HOH:O	2.12	0.68
25:DA:2552:U:H2'	25:DA:2554:U:OP2	1.93	0.68
26:DB:13:A:N1	26:DB:69:G:O2'	2.24	0.68
25:BA:427:G:N7	61:BA:5099:HOH:O	2.26	0.68
25:BA:932:C:H3'	25:BA:933:C:H5"	1.75	0.68
25:BA:2138:G:N7	25:BA:2187:G:N2	2.42	0.68
25:BA:2695:C:O2	34:BO:70:LYS:NZ	2.25	0.68
9:CI:17:VAL:HG11	9:CI:81:ILE:HA	1.76	0.68
25:DA:20:C:OP1	40:DU:22:LYS:NZ	2.23	0.68
25:DA:1031:G:H21	55:D9:36:GLN:HE22	1.40	0.68
48:D2:22:GLU:OE2	48:D2:68:ARG:NH2	2.27	0.68
55:D9:25:VAL:HB	55:D9:34:GLN:HB2	1.76	0.68
1:AA:1297:C:O2'	7:AG:114:ARG:NH2	2.27	0.68
23:CY:52:G:O6	23:CY:62:C:N3	2.27	0.68
25:DA:400:G:N7	61:DA:4682:HOH:O	2.27	0.68
25:DA:805:G:OP1	61:DA:4971:HOH:O	2.12	0.68
25:DA:1271:G:OP2	61:DA:4508:HOH:O	2.11	0.67
4:AD:173:TRP:CE3	4:AD:174:LEU:HG	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2134:A:O2'	25:DA:2159:G:N3	2.26	0.67
39:DT:65:LYS:HE2	39:DT:67:SER:HB2	1.76	0.67
25:BA:2122:G:H1	25:BA:2211:U:H3	1.41	0.67
32:BI:133:HIS:ND1	32:BI:134:PRO:O	2.26	0.67
1:CA:1075:C:OP1	2:CB:179:LYS:NZ	2.26	0.67
8:CH:10:LEU:HD22	8:CH:83:ILE:HD11	1.76	0.67
10:CJ:44:VAL:HG13	10:CJ:66:ARG:HG2	1.76	0.67
26:DB:75:G:N2	45:DZ:87:ASP:OD1	2.25	0.67
1:CA:766:A:OP2	61:CA:4022:HOH:O	2.11	0.67
3:CC:54:ARG:HH11	3:CC:54:ARG:HB3	1.58	0.67
25:DA:2507:C:H5"	25:DA:2573:C:N4	2.09	0.67
1:CA:1301:U:O2'	1:CA:1302:U:H5'	1.94	0.67
28:DE:47:VAL:HG11	28:DE:86:PRO:HD2	1.76	0.67
51:B5:40:LYS:NZ	51:B5:44:THR:O	2.22	0.67
1:CA:7:G:O2'	5:CE:120:THR:O	2.13	0.67
36:DQ:110:THR:HG23	36:DQ:113:GLN:HB2	1.76	0.67
1:AA:1352:C:OP1	21:AU:3:LYS:NZ	2.23	0.67
25:BA:70:A:H3'	25:BA:70:A:OP2	1.94	0.67
10:CJ:5:ARG:N	61:CJ:5101:HOH:O	2.28	0.67
29:DF:21:ALA:HB3	29:DF:22:ALA:HA	1.76	0.67
19:AS:41:VAL:HG12	19:AS:43:GLU:H	1.60	0.67
3:CC:6:HIS:HD2	3:CC:8:ILE:H	1.42	0.67
5:CE:143:ARG:NH1	8:CH:77:GLU:OE1	2.28	0.67
25:DA:796:C:H2'	25:DA:797:C:C6	2.30	0.67
9:AI:20:ARG:O	9:AI:60:ASP:N	2.23	0.67
1:CA:986:A:N3	19:CS:52:TYR:OH	2.25	0.67
1:CA:1312:G:H1	1:CA:1325:C:H42	1.41	0.67
2:CB:69:LEU:HB3	2:CB:162:ILE:HG22	1.76	0.67
3:CC:129:ALA:HB3	3:CC:132:ARG:HB2	1.76	0.67
25:DA:517:C:OP1	51:D5:16:ARG:NH2	2.28	0.67
29:DF:103:LYS:HA	29:DF:106:ARG:HG3	1.76	0.67
29:DF:184:TYR:CE2	29:DF:188:ARG:HD2	2.29	0.67
1:AA:1416:G:N7	61:AA:4106:HOH:O	2.28	0.67
25:BA:701:A:N7	61:BA:4847:HOH:O	2.28	0.67
25:BA:2153:G:H5"	25:BA:2154:U:H3'	1.75	0.67
25:BA:2788:A:N7	61:BA:4672:HOH:O	2.27	0.67
25:BA:2793:G:OP1	61:BA:4974:HOH:O	2.13	0.67
37:BR:67:LEU:HD13	37:BR:76:VAL:HG21	1.77	0.67
18:CR:22:VAL:HB	18:CR:56:THR:HA	1.77	0.67
25:DA:81:G:HO2'	25:DA:295:G:HO2'	1.40	0.67
25:DA:2060:A:N3	61:DA:4409:HOH:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:DD:206:LEU:HD22	27:DD:211:ARG:HG2	1.76	0.67
19:AS:68:GLY:H	50:B4:58:ARG:HH12	1.41	0.66
25:BA:325:G:OP2	44:BY:84:ARG:NH2	2.28	0.66
25:BA:2387:G:N7	61:BA:4876:HOH:O	2.29	0.66
4:CD:140:VAL:HG11	4:CD:146:ILE:HD11	1.77	0.66
32:DI:92:VAL:HG22	32:DI:120:ILE:HB	1.77	0.66
1:AA:572:A:OP1	61:AA:4102:HOH:O	2.12	0.66
1:AA:1392:G:N2	1:AA:1502:A:H8	1.94	0.66
27:BD:237:GLU:OE2	61:BD:412:HOH:O	2.14	0.66
1:CA:947:G:H1	1:CA:1234:C:H42	1.41	0.66
1:CA:1002:G:H1	1:CA:1038:C:H42	1.43	0.66
1:CA:1086:U:H3	1:CA:1099:G:H22	1.43	0.66
25:DA:1218:C:H42	25:DA:1231:G:H1	1.43	0.66
25:DA:2006:C:OP2	61:DA:4803:HOH:O	2.13	0.66
25:DA:2046:G:H5'	51:D5:19:ARG:HA	1.76	0.66
1:AA:1152:A:OP1	10:AJ:68:HIS:ND1	2.27	0.66
1:AA:1238:A:OP2	61:AA:4145:HOH:O	2.12	0.66
26:BB:33:G:H5'	30:BG:2:PRO:HD3	1.77	0.66
25:DA:271(I):G:N2	25:DA:271(O):C:O2	2.27	0.66
25:DA:1188:U:H5"	41:DV:79:VAL:HG13	1.76	0.66
1:AA:953:G:H5'	1:AA:965:A:H61	1.60	0.66
1:AA:1255:G:OP1	10:AJ:45:ARG:NH2	2.29	0.66
1:CA:1360:A:OP2	14:CN:35:ARG:NH2	2.29	0.66
25:DA:1243:G:O2'	35:DP:4:SER:O	2.13	0.66
25:DA:1658:C:OP1	61:DA:4502:HOH:O	2.12	0.66
26:DB:12:C:H2'	46:D0:73:GLY:HA3	1.78	0.66
1:CA:972:C:O2'	10:CJ:55:LYS:O	2.14	0.66
25:DA:1332:G:OP1	61:DA:4468:HOH:O	2.13	0.66
1:CA:67:C:H2'	1:CA:68:G:C8	2.31	0.66
1:CA:1029:C:N3	1:CA:1032:G:N2	2.44	0.66
1:AA:1025:U:O2'	1:AA:1026:G:O4'	2.14	0.66
9:AI:17:VAL:HG23	9:AI:63:ILE:HG12	1.78	0.66
19:AS:68:GLY:HA3	50:B4:58:ARG:HH22	1.61	0.66
31:BH:149:ARG:NH1	31:BH:167:GLU:OE2	2.29	0.66
1:CA:539:A:H2'	1:CA:540:G:C8	2.31	0.66
19:CS:42:PRO:HG3	50:D4:61:ARG:HG3	1.78	0.66
25:DA:304:G:O6	61:DA:4486:HOH:O	2.11	0.66
43:DX:65:ARG:HG3	43:DX:70:LEU:HG	1.77	0.66
23:AW:51:U:H2'	23:AW:52:G:C8	2.30	0.66
27:BD:206:LEU:HD22	27:BD:211:ARG:HG2	1.78	0.66
3:CC:181:ASN:HD21	3:CC:204:LEU:HD12	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:310:G:OP2	16:AP:27:LYS:NZ	2.27	0.66
25:BA:2158:C:N3	25:BA:2177:G:N2	2.43	0.66
28:BE:29:GLY:HA3	61:BE:406:HOH:O	1.96	0.66
45:BZ:72:ARG:NH2	45:BZ:97:GLU:O	2.28	0.66
2:AB:47:THR:HA	2:AB:202:PRO:HG2	1.77	0.66
25:BA:2362:C:OP2	61:BA:4189:HOH:O	2.13	0.66
23:CW:61:C:O2'	23:CW:62:C:O5'	2.09	0.66
25:DA:307:G:N2	25:DA:310:A:O5'	2.26	0.66
25:DA:526:A:OP1	61:DA:4488:HOH:O	2.14	0.66
1:AA:1392:G:H21	1:AA:1502:A:H8	1.45	0.65
4:AD:15:GLU:HG2	4:AD:63:LYS:HB3	1.78	0.65
25:BA:2419:G:OP1	61:BA:4387:HOH:O	2.13	0.65
25:BA:2772:G:N7	61:BA:4262:HOH:O	2.28	0.65
45:BZ:117:LEU:HD11	45:BZ:144:LEU:HB3	1.78	0.65
13:CM:40:ASN:HB3	13:CM:43:THR:HG23	1.78	0.65
1:AA:427:U:OP1	4:AD:13:ARG:NH2	2.29	0.65
1:AA:656:C:O2'	15:AO:28:GLN:NE2	2.30	0.65
1:AA:1530:G:H2'	1:AA:1531:A:O4'	1.96	0.65
25:BA:2184:G:H5"	25:BA:2194:U:H2'	1.78	0.65
39:BT:65:LYS:HE2	39:BT:67:SER:HB2	1.76	0.65
1:CA:79:G:N2	1:CA:90:U:O2	2.27	0.65
10:CJ:77:PRO:O	10:CJ:81:THR:OG1	2.14	0.65
24:CX:64:G:H4'	36:DQ:10:ARG:HH12	1.60	0.65
25:DA:1996:C:H4'	25:DA:1997:G:OP1	1.96	0.65
45:DZ:108:PRO:HB2	45:DZ:111:VAL:HG23	1.77	0.65
1:AA:76:C:N3	1:AA:93:G:O6	2.29	0.65
23:AW:19:G:N2	23:AW:56:C:N3	2.44	0.65
43:BX:31:HIS:HD2	43:BX:33:LYS:H	1.44	0.65
1:CA:1002:G:C4	1:CA:1003:G:H8	2.14	0.65
1:CA:1028:C:C4	1:CA:1033:G:O6	2.49	0.65
25:DA:42:G:OP2	61:DA:4954:HOH:O	2.14	0.65
36:DQ:111:GLU:OE1	36:DQ:133:ARG:NH2	2.26	0.65
1:CA:1218:C:OP2	14:CN:9:LYS:NZ	2.29	0.65
25:DA:30:G:OP2	40:DU:5:LYS:NZ	2.25	0.65
30:DG:114:ILE:HA	30:DG:140:ILE:HD11	1.79	0.65
5:AE:33:VAL:HG21	5:AE:109:ILE:HA	1.77	0.65
13:CM:37:THR:O	13:CM:55:ARG:NH1	2.29	0.65
1:AA:1002:G:H3'	1:AA:1003:G:O4'	1.97	0.65
25:DA:1019:U:H3	25:DA:1142(A):A:H62	1.45	0.65
31:DH:3:ARG:NH2	31:DH:5:GLY:H	1.95	0.65
1:AA:837:G:H1	1:AA:849:C:H42	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AL:24:VAL:HG11	12:AL:27:LEU:HD22	1.78	0.65
55:B9:25:VAL:HB	55:B9:34:GLN:HB2	1.78	0.65
1:CA:1245:A:H61	1:CA:1292:U:H3	1.45	0.65
1:CA:1417:G:O6	61:CA:4051:HOH:O	2.12	0.65
19:CS:28:LYS:HB2	19:CS:29:ARG:HA	1.78	0.65
50:D4:44:THR:O	50:D4:46:GLN:N	2.30	0.65
23:CW:51:U:H3	23:CW:63:G:H1	1.45	0.65
34:DO:68:GLU:HB3	34:DO:78:ARG:HB2	1.79	0.65
2:AB:201:ILE:HG21	2:AB:214:ILE:HG21	1.80	0.64
25:BA:11:G:H2'	25:BA:12:U:H5"	1.79	0.64
2:CB:178:ARG:HH22	8:CH:68:ARG:HH12	1.44	0.64
5:CE:122:GLU:O	5:CE:126:ARG:NH1	2.30	0.64
25:DA:1204:A:H2	25:DA:1241:A:H62	1.46	0.64
30:DG:15:VAL:HG22	30:DG:175:LEU:HB3	1.79	0.64
33:DN:30:ILE:HG22	33:DN:34:LEU:HD22	1.78	0.64
1:AA:78:G:N2	1:AA:91:C:N3	2.46	0.64
25:BA:2340:A:H2'	25:BA:2341:G:C8	2.32	0.64
19:CS:63:THR:OG1	19:CS:65:ASN:ND2	2.30	0.64
25:DA:613:G:O2'	25:DA:614(C):A:N1	2.30	0.64
25:DA:631:A:OP1	35:DP:65:ARG:NH1	2.30	0.64
1:AA:1136:U:H5"	1:AA:1137:C:C4	2.31	0.64
1:CA:1149:C:O2'	1:CA:1280:A:N1	2.31	0.64
48:D2:1:MET:N	48:D2:52:ASP:OD1	2.23	0.64
1:AA:346:G:OP1	39:BT:41:ARG:NH1	2.26	0.64
1:AA:1456:G:O3'	20:AT:39:LYS:NZ	2.30	0.64
3:AC:58:GLU:HB3	10:AJ:92:THR:HG21	1.79	0.64
9:AI:53:VAL:O	9:AI:55:ALA:N	2.31	0.64
4:CD:157:LEU:O	4:CD:161:ASN:ND2	2.30	0.64
1:AA:1008:C:O2	1:AA:1021:G:N1	2.27	0.64
7:AG:111:ARG:NH1	7:AG:113:GLU:OE2	2.27	0.64
25:BA:2164:C:N3	25:BA:2171:G:O6	2.31	0.64
25:DA:1013:C:H2'	25:DA:1014:U:H6	1.62	0.64
1:AA:97:G:O2'	1:AA:98:G:O4'	2.14	0.64
15:AO:25:THR:HG21	15:AO:70:LEU:HB2	1.79	0.64
25:BA:1451:U:H2'	25:BA:1452:U:C6	2.32	0.64
33:BN:67:LEU:HB3	33:BN:88:GLU:HG3	1.79	0.64
37:BR:97:VAL:HG22	37:BR:114:VAL:HG13	1.80	0.64
1:CA:1255:G:HO2'	1:CA:1258:G:HO2'	1.46	0.64
1:CA:1456:G:O6	20:CT:54:LYS:NZ	2.25	0.64
25:DA:1283:G:N2	25:DA:1286:A:OP2	2.31	0.64
25:BA:1222:A:H3'	25:BA:1223:C:C6	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AL:34:ARG:NH2	61:AL:201:HOH:O	2.30	0.64
2:CB:16:HIS:HB2	2:CB:204:ASN:HB3	1.80	0.64
9:CI:16:ARG:HB2	9:CI:64:THR:HG22	1.79	0.64
23:CY:5:G:H1	23:CY:68:C:H42	1.46	0.64
25:DA:2431:U:OP1	61:DA:4215:HOH:O	2.15	0.64
29:DF:24:LEU:HD23	29:DF:115:ALA:HA	1.79	0.64
1:AA:352:C:OP2	61:AA:4109:HOH:O	2.15	0.64
4:AD:177:ASP:HB3	4:AD:182:LYS:HG2	1.78	0.64
23:CY:50:U:O2	23:CY:64:A:N1	2.31	0.64
25:DA:143(A):C:O2'	43:DX:2:LYS:NZ	2.30	0.64
25:DA:2023:G:H5'	25:DA:2617:C:H4'	1.79	0.64
28:DE:111:ARG:HD3	37:DR:1:MET:HE1	1.79	0.64
46:D0:11:ARG:O	46:D0:14:ARG:NH2	2.31	0.64
1:CA:1029:C:C2	1:CA:1032:G:N2	2.66	0.64
3:CC:164:ARG:NH1	3:CC:166:GLU:OE1	2.31	0.64
15:CO:54:ARG:HD3	15:CO:58:MET:HE2	1.80	0.64
25:DA:1958:C:OP2	61:DA:4696:HOH:O	2.15	0.64
1:AA:1183:A:H3'	1:AA:1184:G:H5"	1.80	0.63
23:AW:19:G:H1	23:AW:56:C:H42	1.43	0.63
45:BZ:126:VAL:HG11	45:BZ:161:VAL:HG23	1.81	0.63
45:BZ:138:GLU:H	45:BZ:156:LYS:HD3	1.62	0.63
1:CA:165:C:H2'	1:CA:166:G:H8	1.62	0.63
25:DA:330:A:H2	25:DA:1210:A:HO2'	1.43	0.63
25:DA:1266:G:O5'	42:DW:15:ARG:NH2	2.31	0.63
1:AA:812:C:O2	61:AA:4048:HOH:O	2.14	0.63
16:AP:22:THR:HA	16:AP:33:ILE:HG13	1.80	0.63
25:DA:2123:G:H1	25:DA:2175:C:N4	1.97	0.63
25:DA:2299:G:H2'	25:DA:2300:G:H8	1.64	0.63
25:DA:2360:A:OP2	61:DA:4626:HOH:O	2.15	0.63
25:BA:1219:A:H4'	25:BA:1220:U:OP1	1.97	0.63
25:BA:1431:G:O2'	25:BA:1442:U:O2	2.11	0.63
2:CB:47:THR:HA	2:CB:202:PRO:HG2	1.79	0.63
1:AA:159:G:N2	1:AA:162:A:OP2	2.32	0.63
1:AA:353:A:H8	1:AA:353:A:H5'	1.63	0.63
50:B4:68:ARG:HD2	50:B4:69:LYS:H	1.63	0.63
19:CS:27:GLU:HG2	19:CS:47:HIS:NE2	2.14	0.63
24:CX:76:A:H5'	25:DA:2585:U:H5	1.63	0.63
1:AA:545:C:OP1	4:AD:61:LYS:NZ	2.31	0.63
15:AO:39:LEU:HD13	15:AO:56:LEU:HB2	1.81	0.63
25:BA:1480:A:H61	25:BA:1605:A:H62	1.45	0.63
28:BE:143:ASN:HD22	28:BE:147:PRO:HD3	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1003:G:N2	1:CA:1025:U:O4	2.31	0.63
25:DA:307:G:N1	25:DA:310:A:OP2	2.32	0.63
25:DA:468:G:N7	53:D7:39:ARG:NH2	2.44	0.63
25:DA:2867:G:OP2	39:DT:119:LYS:NZ	2.32	0.63
26:DB:4:C:H42	26:DB:117:G:H1	1.44	0.63
2:AB:118:LEU:HB3	2:AB:142:LEU:HD12	1.79	0.63
1:CA:920:U:H2'	1:CA:921:U:C6	2.33	0.63
26:DB:22:U:H3	26:DB:61:G:H1	1.46	0.63
28:DE:36:ARG:HG2	28:DE:47:VAL:HG12	1.80	0.63
1:AA:78:G:N1	1:AA:91:C:N4	2.47	0.63
25:DA:900:A:H2'	25:DA:901:A:H8	1.64	0.63
25:DA:1220:A:OP2	40:DU:19:LYS:NZ	2.31	0.63
25:BA:302:A:O2'	25:BA:303:C:OP1	2.17	0.63
13:CM:58:GLU:O	13:CM:62:ASN:ND2	2.27	0.63
25:DA:2646:C:OP2	25:DA:2732:G:O2'	2.17	0.63
27:DD:26:LYS:NZ	27:DD:30:GLU:OE1	2.31	0.63
1:AA:134:A:H61	16:AP:25:ARG:NH1	1.97	0.63
23:AY:19:G:H3'	23:AY:20:U:H6	1.64	0.63
25:BA:2164:C:O2	25:BA:2171:G:N1	2.27	0.63
34:BO:35:VAL:HG11	34:BO:103:ALA:HB3	1.80	0.63
37:BR:44:LEU:HD22	37:BR:48:VAL:HG23	1.81	0.63
25:DA:1283:G:O2'	25:DA:1285:G:N7	2.26	0.63
38:BS:59:LYS:HD2	38:BS:60:GLY:H	1.64	0.62
1:CA:1028:C:C2	1:CA:1033:G:N1	2.67	0.62
1:CA:1132:C:H42	1:CA:1142:G:H1	1.46	0.62
25:DA:7:G:H2'	25:DA:8:A:C8	2.34	0.62
25:DA:2502:G:N7	61:DA:4706:HOH:O	2.31	0.62
27:DD:12:SER:HB3	27:DD:208:LYS:HB3	1.80	0.62
10:AJ:37:PRO:HA	10:AJ:72:VAL:HG12	1.80	0.62
23:AW:7:A:H61	23:AW:66:U:H3	1.45	0.62
25:BA:1312:G:O5'	42:BW:15:ARG:NH2	2.32	0.62
25:DA:1815:A:P	27:DD:54:ARG:HH22	2.22	0.62
28:DE:34:VAL:HG11	28:DE:78:LEU:HD11	1.81	0.62
1:AA:1002:G:C4	1:AA:1003:G:H1'	2.34	0.62
1:AA:1103:C:OP1	2:AB:96:ARG:NH2	2.32	0.62
1:CA:345:C:OP2	39:DT:39:ARG:NH2	2.32	0.62
1:CA:1120:G:C6	1:CA:1154:G:N2	2.67	0.62
29:DF:157:VAL:HB	29:DF:194:MET:HG2	1.81	0.62
25:BA:265:U:H2'	25:BA:266:C:C6	2.34	0.62
26:BB:84:C:OP1	49:B3:15:TYR:OH	2.18	0.62
2:CB:178:ARG:NH2	8:CH:68:ARG:HH12	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:D4:24:THR:OG1	50:D4:25:TYR:N	2.32	0.62
1:AA:316:G:OP2	1:AA:351:G:O2'	2.17	0.62
25:BA:2163:G:H1	25:BA:2171:G:H22	1.46	0.62
3:CC:152:ILE:HG23	3:CC:199:LYS:HB2	1.82	0.62
4:CD:191:ARG:NH1	4:CD:191:ARG:O	2.32	0.62
13:CM:33:ALA:HA	13:CM:59:TYR:HE2	1.64	0.62
25:DA:221:A:N1	25:DA:265:A:O2'	2.32	0.62
25:DA:2141:G:O6	25:DA:2150:U:O2	2.17	0.62
1:AA:45:U:H2'	1:AA:46:G:C8	2.35	0.62
1:AA:519:C:OP2	12:AL:50:SER:OG	2.17	0.62
7:AG:27:ILE:HD12	7:AG:40:ALA:HA	1.82	0.62
8:AH:10:LEU:HD22	8:AH:83:ILE:HD11	1.80	0.62
25:BA:278:G:OP1	47:B1:76:ARG:NH1	2.31	0.62
25:BA:2164:C:H2'	25:BA:2165:C:C6	2.35	0.62
2:CB:185:ILE:HG22	2:CB:199:TYR:HB2	1.82	0.62
3:CC:138:VAL:HG23	3:CC:151:VAL:HG23	1.82	0.62
4:CD:15:GLU:OE2	4:CD:66:ARG:NH1	2.31	0.62
24:CX:21:A:H61	24:CX:46:G:H2'	1.65	0.62
25:DA:952:G:OP1	36:DQ:16:ARG:NH2	2.33	0.62
25:DA:2591:C:OP1	27:DD:239:ARG:HD2	2.00	0.62
2:AB:16:HIS:O	2:AB:18:GLY:N	2.32	0.62
9:AI:46:ALA:HB2	9:AI:74:ILE:HG23	1.82	0.62
20:AT:57:ARG:HH12	20:AT:100:ILE:HD12	1.64	0.62
25:BA:1848:G:OP1	27:BD:88:ARG:NH2	2.33	0.62
25:BA:2163:G:C4	25:BA:2164:C:H1'	2.33	0.62
25:DA:1842:G:O2'	27:DD:253:GLN:NE2	2.33	0.62
27:DD:182:LEU:HB2	27:DD:272:ALA:HB3	1.80	0.62
37:DR:97:VAL:HG22	37:DR:114:VAL:HG13	1.80	0.62
25:BA:2801:C:OP1	28:BE:61:ARG:NH2	2.28	0.62
1:CA:266:G:H5"	1:CA:268:C:H41	1.64	0.62
1:CA:352:C:O2'	1:CA:354:G:OP1	2.14	0.62
23:CW:74:C:N4	25:DA:2507:C:O2'	2.31	0.62
25:DA:2141:G:H2'	25:DA:2142:C:O4'	2.00	0.62
36:DQ:109:VAL:HG13	36:DQ:113:GLN:HB3	1.81	0.62
37:DR:104:ARG:HG3	37:DR:111:LEU:HD11	1.82	0.62
54:D8:6:THR:HG22	54:D8:63:PRO:HD2	1.81	0.62
3:AC:3:ASN:OD1	3:AC:3:ASN:N	2.33	0.62
6:AF:42:GLU:OE1	6:AF:59:TYR:OH	2.13	0.62
7:AG:111:ARG:NH2	7:AG:126:ASP:OD2	2.32	0.62
25:BA:493:G:OP1	53:B7:33:ARG:NH1	2.33	0.62
46:B0:18:ALA:HB3	46:B0:20:ARG:HH21	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CR:56:THR:HB	18:CR:58:LEU:HD23	1.81	0.62
45:DZ:92:SER:OG	45:DZ:93:ASP:N	2.27	0.62
25:BA:1223:C:H2'	25:BA:1224:C:H6	1.65	0.62
1:CA:406:G:H5'	4:CD:5:ILE:HD11	1.81	0.62
4:CD:104:VAL:HG11	4:CD:146:ILE:HD13	1.82	0.62
25:DA:910:A:H62	36:DQ:12:GLN:HA	1.65	0.62
38:DS:14:VAL:O	38:DS:18:ILE:HG12	2.00	0.62
1:CA:377:G:OP1	16:CP:3:LYS:HD2	1.99	0.61
1:CA:1129:C:H2'	1:CA:1139:G:N7	2.15	0.61
3:CC:47:LEU:HD12	3:CC:68:VAL:HG11	1.81	0.61
20:CT:57:ARG:HH12	20:CT:100:ILE:HD12	1.65	0.61
25:DA:886:C:O2'	25:DA:889:C:N4	2.32	0.61
25:DA:2141:G:C6	25:DA:2150:U:O2	2.52	0.61
53:D7:34:ARG:NH1	53:D7:41:ARG:O	2.32	0.61
1:AA:1435:G:H2'	1:AA:1436:U:C6	2.35	0.61
8:AH:51:VAL:HG21	8:AH:60:ARG:HH11	1.65	0.61
14:AN:23:ARG:HH11	14:AN:30:ALA:HB2	1.64	0.61
25:BA:1425:A:H4'	25:BA:1426:G:OP2	2.00	0.61
43:BX:31:HIS:CD2	43:BX:33:LYS:H	2.18	0.61
49:B3:3:ARG:NH1	49:B3:60:GLU:OE2	2.29	0.61
1:CA:657:G:H21	15:CO:22:THR:HG1	1.47	0.61
17:CQ:66:SER:O	17:CQ:70:ARG:NH1	2.33	0.61
27:DD:148:GLU:HB2	27:DD:151:LYS:HD2	1.82	0.61
1:AA:189(B):C:H42	1:AA:189(I):G:H1	1.48	0.61
1:AA:452:A:H4'	16:AP:72:ARG:NH1	2.15	0.61
25:BA:1284:G:OP2	61:BA:5106:HOH:O	2.16	0.61
1:CA:148:G:H2'	1:CA:149:A:H8	1.65	0.61
1:CA:942:G:H21	9:CI:124:GLN:NE2	1.98	0.61
4:CD:165:MET:SD	4:CD:168:ARG:NH1	2.72	0.61
23:CW:9:A:H5'	23:CW:46:7MG:HN22	1.64	0.61
25:DA:2121:G:H1	25:DA:2177:C:N4	1.97	0.61
1:CA:1422:G:O3'	34:DO:49:ARG:NH1	2.31	0.61
1:CA:1441:G:H5"	1:CA:1442:G:H5'	1.81	0.61
16:CP:71:ARG:HG3	16:CP:80:PHE:HE2	1.66	0.61
2:AB:53:ARG:NH2	2:AB:198:ASP:O	2.32	0.61
2:AB:93:VAL:HG21	2:AB:97:TRP:CD1	2.36	0.61
20:AT:60:GLU:HG3	20:AT:81:LYS:HD2	1.80	0.61
25:BA:288:U:O2'	25:BA:289:G:OP1	2.17	0.61
25:BA:1993:A:OP1	61:BA:4467:HOH:O	2.15	0.61
25:BA:2121:U:H3	25:BA:2212:G:H1	1.47	0.61
48:B2:65:ASN:OD1	48:B2:69:ARG:NH1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2758:A:C2	25:DA:2759:G:H1'	2.36	0.61
25:DA:2843:G:N7	61:DA:4550:HOH:O	2.31	0.61
1:AA:100:C:H2'	1:AA:101:A:C8	2.36	0.61
1:AA:1305:G:N2	1:AA:1331:G:H1'	2.16	0.61
19:AS:32:LYS:HA	19:AS:50:ALA:HB3	1.83	0.61
7:CG:15:ASP:OD2	7:CG:44:TYR:OH	2.18	0.61
25:DA:2611:U:C4	51:D5:3:LYS:HG2	2.35	0.61
19:AS:68:GLY:H	50:B4:58:ARG:NH1	1.99	0.61
25:BA:2303:U:H2'	25:BA:2304:C:C6	2.36	0.61
4:CD:72:GLU:OE1	4:CD:207:TYR:OH	2.18	0.61
7:CG:32:ARG:HH12	7:CG:109:ASN:HD21	1.47	0.61
15:CO:22:THR:HG1	15:CO:23:GLY:H	1.49	0.61
24:CX:21:A:N6	24:CX:46:G:H2'	2.16	0.61
25:DA:831:G:O2'	35:DP:38:GLN:NE2	2.34	0.61
1:AA:276:G:O3'	17:AQ:68:ARG:NH1	2.33	0.61
2:AB:185:ILE:HG22	2:AB:199:TYR:HB2	1.83	0.61
3:AC:13:GLY:HA3	14:AN:57:ARG:NH2	2.16	0.61
23:AW:18:G:O2'	23:AW:57:G:N2	2.24	0.61
31:BH:3:ARG:HG2	31:BH:6:ARG:HG2	1.82	0.61
36:BQ:108:GLY:HA3	45:BZ:116:VAL:HG13	1.82	0.61
38:BS:27:SER:HA	38:BS:88:ASP:HB3	1.82	0.61
1:CA:992:U:H3	1:CA:1044:A:H62	1.49	0.61
1:CA:1004:A:N6	1:CA:1037:C:C2	2.69	0.61
1:CA:1030(A):G:H2'	1:CA:1030(C):G:OP2	2.00	0.61
13:CM:88:ARG:HG3	13:CM:98:VAL:HG11	1.83	0.61
25:DA:307:G:N7	61:DA:4267:HOH:O	2.31	0.61
25:DA:2110:G:H4'	25:DA:2111:C:OP2	2.00	0.61
2:AB:93:VAL:HG21	2:AB:97:TRP:HD1	1.66	0.61
3:AC:8:ILE:HD13	3:AC:184:TYR:HB3	1.83	0.61
3:AC:162:GLN:NE2	22:AV:24:A:O2'	2.33	0.61
17:AQ:66:SER:O	17:AQ:70:ARG:NH1	2.34	0.61
25:BA:1343:C:OP1	61:BA:4495:HOH:O	2.16	0.61
31:BH:56:SER:HB3	31:BH:61:HIS:ND1	2.16	0.61
1:CA:36:C:N4	61:CA:4168:HOH:O	2.33	0.61
19:CS:4:SER:HB3	19:CS:7:LYS:HG3	1.82	0.61
23:CY:9:A:H5"	23:CY:46:7MG:H1'	1.81	0.61
25:DA:644:A:H4'	25:DA:645:C:C5	2.36	0.61
47:D1:7:ILE:HG23	47:D1:98:LEU:HD11	1.82	0.61
1:AA:559:A:OP1	5:AE:126:ARG:NH2	2.25	0.61
1:AA:1381:U:H1'	7:AG:79:ARG:HG3	1.83	0.61
4:AD:128:VAL:N	4:AD:131:ARG:O	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AW:1:G:O6	23:AW:72:C:N3	2.34	0.61
43:BX:35:THR:HG22	43:BX:38:GLU:H	1.65	0.61
19:CS:32:LYS:HA	19:CS:50:ALA:HB3	1.83	0.61
25:DA:1023:U:OP2	61:DA:4898:HOH:O	2.16	0.61
25:BA:1211:U:H2'	25:BA:1212:C:C6	2.36	0.60
1:CA:148:G:H2'	1:CA:149:A:C8	2.36	0.60
2:CB:15:VAL:O	2:CB:17:PHE:N	2.34	0.60
29:DF:78:ILE:HA	29:DF:83:PHE:CD1	2.36	0.60
31:DH:99:VAL:N	31:DH:102:ALA:O	2.34	0.60
45:DZ:145:GLU:HG3	45:DZ:146:ILE:H	1.66	0.60
1:AA:1441:G:H5"	1:AA:1442:G:H5'	1.82	0.60
1:AA:1442:G:O2'	1:AA:1442(A):G:OP1	2.19	0.60
13:AM:84:ILE:HG13	13:AM:85:GLY:HA2	1.81	0.60
17:AQ:76:LEU:HD21	17:AQ:79:SER:HB2	1.83	0.60
25:BA:354:A:H2	25:BA:1255:A:H2'	1.66	0.60
25:BA:1071:G:C4	25:BA:1180:C:H1'	2.36	0.60
43:BX:60:ARG:HH22	53:B7:47:ARG:HH22	1.49	0.60
25:DA:2118:U:C4	25:DA:2149:G:H1'	2.37	0.60
29:DF:158:THR:O	29:DF:164:ARG:NH1	2.32	0.60
25:BA:956:A:H62	36:BQ:12:GLN:HA	1.66	0.60
3:CC:142:MET:HG3	3:CC:170:GLN:HB3	1.84	0.60
50:D4:50:VAL:O	50:D4:52:THR:N	2.33	0.60
3:AC:12:LEU:HD23	3:AC:16:ARG:HB3	1.83	0.60
10:AJ:26:ALA:O	10:AJ:84:GLN:NE2	2.34	0.60
25:BA:1218:G:O2'	25:BA:1219:A:O4'	2.19	0.60
25:BA:1846:A:P	27:BD:54:ARG:HH22	2.23	0.60
1:CA:1305:G:N2	1:CA:1331:G:H1'	2.17	0.60
19:CS:38:SER:HB2	19:CS:71:LEU:HD22	1.83	0.60
25:DA:509:C:OP1	61:DA:4614:HOH:O	2.15	0.60
32:DI:27:ARG:HD2	47:D1:71:TYR:CE1	2.37	0.60
31:BH:86:GLU:OE2	31:BH:132:ARG:NH2	2.34	0.60
1:CA:1028:C:N3	1:CA:1033:G:O6	2.34	0.60
25:DA:1012:U:C5	33:DN:28:THR:HG21	2.37	0.60
1:AA:800:G:O6	61:AA:4021:HOH:O	2.12	0.60
25:BA:1159:U:H2'	25:BA:1160:G:C8	2.36	0.60
1:CA:1007:C:N3	1:CA:1022:G:O6	2.35	0.60
1:CA:1132:C:H2'	1:CA:1133:G:H8	1.65	0.60
16:CP:22:THR:HA	16:CP:33:ILE:HG13	1.82	0.60
25:DA:993:G:H21	41:DV:89:GLN:HE22	1.50	0.60
25:DA:1355:G:O6	61:DA:4421:HOH:O	2.15	0.60
25:BA:2166:U:O2'	25:BA:2167:C:H2'	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2173:G:H2'	25:BA:2174:G:C8	2.37	0.60
25:DA:299:A:N1	25:DA:322:A:O2'	2.28	0.60
45:DZ:55:HIS:CE1	45:DZ:135:GLU:HG3	2.36	0.60
46:D0:12:ASN:HA	46:D0:14:ARG:HH21	1.66	0.60
1:AA:976:G:H5'	1:AA:1358:U:O2'	2.00	0.60
5:AE:151:LEU:HD22	8:AH:79:VAL:HG22	1.84	0.60
25:BA:1834:A:O2'	27:BD:259:THR:HG21	2.00	0.60
47:B1:7:ILE:HG23	47:B1:98:LEU:HD11	1.83	0.60
1:CA:17:U:H2'	1:CA:18:C:C6	2.37	0.60
25:DA:1297:C:OP2	61:DA:4287:HOH:O	2.15	0.60
27:DD:69:ARG:NH2	27:DD:128:GLY:O	2.35	0.60
27:DD:85:ASP:OD2	27:DD:88:ARG:NH1	2.34	0.60
31:DH:3:ARG:HH22	31:DH:5:GLY:H	1.49	0.60
45:DZ:163:LEU:HG	45:DZ:165:VAL:HG22	1.83	0.60
47:D1:59:THR:O	47:D1:91:LYS:NZ	2.34	0.60
26:BB:6:C:H2'	26:BB:7:G:H5"	1.83	0.60
27:BD:179:SER:O	27:BD:275:LYS:HB2	2.02	0.60
1:CA:1138:G:C6	1:CA:1140:C:H1'	2.37	0.60
2:CB:67:THR:HA	2:CB:90:MET:HE1	1.84	0.60
2:CB:84:GLU:HB3	2:CB:219:VAL:HG21	1.84	0.60
25:DA:322:A:OP2	29:DF:169:ASN:HB2	2.02	0.60
25:DA:392:C:OP1	61:DA:4693:HOH:O	2.16	0.60
25:DA:1721:G:H8	25:DA:1741:A:H62	1.48	0.60
30:DG:150:ASP:OD2	30:DG:153:ARG:NH1	2.35	0.60
20:AT:43:LEU:O	20:AT:47:GLY:N	2.35	0.60
45:BZ:4:ARG:NE	45:BZ:60:GLU:OE1	2.32	0.60
25:DA:987:G:O2'	25:DA:1000:A:N3	2.32	0.60
31:DH:7:LEU:HD12	31:DH:8:PRO:HD2	1.84	0.60
1:AA:625:G:H4'	16:AP:16:HIS:CD2	2.36	0.59
2:AB:84:GLU:HB3	2:AB:219:VAL:HG21	1.84	0.59
7:AG:144:MET:HE1	23:AY:31:A:H1'	1.83	0.59
14:AN:3:ARG:HB3	14:AN:3:ARG:HH21	1.66	0.59
1:CA:1001:A:H2'	1:CA:1001(A):G:H8	1.66	0.59
1:CA:1376:U:H2'	1:CA:1377:A:C8	2.37	0.59
3:CC:30:ARG:HH21	14:CN:38:GLY:HA2	1.67	0.59
25:DA:2495:G:H5"	36:DQ:82:ARG:HG2	1.84	0.59
25:DA:2875:C:O2'	39:DT:2:ASN:OD1	2.19	0.59
29:DF:21:ALA:CB	29:DF:22:ALA:HA	2.32	0.59
4:AD:129:ASN:OD1	4:AD:145:GLU:N	2.33	0.59
5:AE:110:LEU:HD13	5:AE:118:ILE:HG21	1.84	0.59
12:AL:88:GLY:O	12:AL:99:HIS:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AS:20:LEU:HD13	50:B4:69:LYS:HE2	1.84	0.59
25:BA:83:A:H5'	44:BY:8:LYS:HG2	1.83	0.59
1:CA:646:U:H2'	1:CA:647:C:C6	2.36	0.59
1:CA:811:C:N4	61:CA:4024:HOH:O	2.35	0.59
1:CA:909:A:N3	1:CA:1413:A:O2'	2.32	0.59
1:CA:1112:C:H1'	3:CC:179:ARG:HG2	1.83	0.59
9:CI:53:VAL:O	9:CI:55:ALA:N	2.35	0.59
23:CW:29:G:H1	23:CW:41:C:N4	1.99	0.59
25:DA:1639:U:H2'	25:DA:1640:C:H5"	1.84	0.59
25:BA:1201:A:OP1	40:BU:55:ARG:HD3	2.02	0.59
41:BV:76:LYS:HB2	41:BV:81:TYR:HB3	1.84	0.59
51:B5:11:THR:HG23	51:B5:15:ARG:HB3	1.83	0.59
4:CD:98:GLU:HG2	4:CD:189:PRO:HG2	1.83	0.59
35:DP:121:LYS:HB3	35:DP:123:LEU:HG	1.84	0.59
38:DS:25:ARG:NH1	38:DS:42:ASP:OD1	2.35	0.59
25:BA:553:A:N1	25:BA:2064:A:H2'	2.16	0.59
1:CA:934:C:OP1	61:CA:4152:HOH:O	2.17	0.59
2:CB:91:PRO:HD3	2:CB:154:LEU:HD12	1.84	0.59
23:CY:33:U:H2'	23:CY:35:A:OP2	2.01	0.59
25:DA:784:A:C6	27:DD:229:VAL:HG11	2.37	0.59
25:DA:2169:A:H2'	25:DA:2170:A:C8	2.37	0.59
44:BY:102:CYS:SG	44:BY:103:GLY:N	2.75	0.59
54:B8:42:ARG:HD2	61:B8:207:HOH:O	2.02	0.59
1:CA:1412:C:H2'	1:CA:1413:A:C8	2.37	0.59
25:DA:303:U:H2'	25:DA:304:G:H8	1.67	0.59
25:DA:2139:C:N4	25:DA:2152:G:H1	2.00	0.59
25:BA:302:A:H2'	25:BA:303:C:C6	2.38	0.59
45:BZ:152:ALA:HB2	45:BZ:171:ILE:HG21	1.84	0.59
1:CA:450:G:OP1	16:CP:43:LYS:NZ	2.34	0.59
23:CY:62:C:H2'	23:CY:63:G:C8	2.38	0.59
25:DA:1796:U:H2'	25:DA:1797:C:C6	2.38	0.59
25:DA:2135:A:H61	25:DA:2157:G:N2	2.00	0.59
25:DA:2137:C:H42	25:DA:2154:G:H1	1.51	0.59
25:BA:611:U:H2'	25:BA:612:C:C6	2.37	0.59
1:CA:976:G:OP1	14:CN:32:SER:N	2.33	0.59
30:DG:136:ARG:HD2	30:DG:137:GLU:HG3	1.85	0.59
44:DY:102:CYS:SG	44:DY:103:GLY:N	2.76	0.59
1:AA:97:G:O2'	1:AA:98:G:H8	1.86	0.59
25:BA:2584:A:N7	28:BE:144:ARG:HD2	2.18	0.59
6:CF:45:LEU:HD12	6:CF:59:TYR:HD2	1.68	0.59
10:CJ:7:LYS:HE3	10:CJ:71:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:DD:132:PRO:HG2	27:DD:135:PHE:CD2	2.37	0.59
50:D4:59:PHE:HA	50:D4:60:GLN:C	2.27	0.59
3:AC:57:ILE:HG12	3:AC:66:VAL:HG22	1.84	0.59
4:AD:155:LEU:HD13	4:AD:158:ILE:HD11	1.84	0.59
1:CA:1128:C:O2'	1:CA:1129:C:OP1	2.17	0.59
1:CA:1218:C:H2'	1:CA:1219:U:C6	2.38	0.59
4:CD:153:ARG:HB2	4:CD:181:MET:SD	2.43	0.59
25:DA:1800:C:OP2	27:DD:183:ARG:NH2	2.35	0.59
25:DA:2140:C:H1'	25:DA:2152:G:N2	2.18	0.59
28:DE:72:VAL:HG13	28:DE:73:GLU:O	2.03	0.59
1:AA:1492:A:O2'	1:AA:1493:A:O5'	2.10	0.59
45:BZ:24:LEU:HB2	45:BZ:41:LEU:HD23	1.84	0.59
1:CA:448:A:P	1:CA:485:G:H22	2.26	0.59
8:CH:51:VAL:HG21	8:CH:60:ARG:HB2	1.84	0.59
25:DA:957:A:H5'	36:DQ:76:LYS:HG3	1.84	0.59
25:DA:2651:C:H42	25:DA:2669:G:H1	1.51	0.59
30:DG:41:GLN:HE22	30:DG:153:ARG:HB3	1.66	0.59
38:DS:71:ARG:NH1	38:DS:107:GLU:OE1	2.36	0.59
1:AA:97:G:HO2'	1:AA:98:G:H8	1.51	0.58
1:AA:1008:C:N3	1:AA:1021:G:C6	2.71	0.58
1:AA:1125:U:H4'	10:AJ:5:ARG:NH2	2.18	0.58
25:BA:2045:G:H5'	25:BA:2629:C:H4'	1.84	0.58
27:BD:17:THR:O	27:BD:211:ARG:NH2	2.36	0.58
31:BH:7:LEU:HD12	31:BH:8:PRO:HD2	1.85	0.58
1:CA:1059:C:OP2	3:CC:199:LYS:NZ	2.33	0.58
9:CI:50:LEU:HB2	9:CI:56:LEU:HD23	1.84	0.58
25:DA:927:G:H2'	25:DA:928:G:O4'	2.02	0.58
28:BE:3:GLY:HA3	28:BE:81:ILE:HD12	1.83	0.58
10:CJ:30:SER:O	10:CJ:81:THR:HG23	2.04	0.58
24:CX:76:A:OP1	61:CX:4003:HOH:O	2.17	0.58
25:DA:1266:G:O2'	25:DA:2012:G:O6	2.20	0.58
29:DF:116:ASP:OD1	29:DF:119:ARG:NH2	2.35	0.58
5:AE:143:ARG:NH1	8:AH:77:GLU:OE1	2.36	0.58
24:AX:59:A:H2'	24:AX:60:U:H5'	1.83	0.58
25:BA:1232:G:H5"	41:BV:81:TYR:CE1	2.37	0.58
23:CY:36:A:H2'	23:CY:37:MIA:O4'	2.03	0.58
25:BA:1452:U:H2'	25:BA:1453:C:C6	2.38	0.58
28:BE:47:VAL:HG23	28:BE:84:PHE:O	2.03	0.58
32:BI:72:LEU:C	32:BI:74:ASN:H	2.08	0.58
1:CA:405:U:O4	4:CD:2:GLY:N	2.36	0.58
7:CG:27:ILE:HD12	7:CG:40:ALA:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1359:A:H61	25:DA:1372:U:H3	1.50	0.58
25:DA:1803:A:O2'	27:DD:259:THR:HG21	2.03	0.58
32:DI:31:LEU:HD21	32:DI:38:LEU:HG	1.84	0.58
8:AH:73:ASP:OD1	8:AH:75:ARG:HD3	2.03	0.58
25:BA:1218:G:O2'	25:BA:1219:A:O5'	2.21	0.58
17:AQ:45:HIS:CD2	17:AQ:47:PRO:HG3	2.39	0.58
25:BA:2130:C:H2'	25:BA:2131:U:C6	2.37	0.58
32:BI:27:ARG:HD2	47:B1:71:TYR:CE1	2.39	0.58
50:B4:61:ARG:HG3	50:B4:62:ARG:N	2.19	0.58
25:BA:238:C:O2	54:B8:12:LYS:NZ	2.33	0.58
28:BE:111:ARG:HG3	28:BE:160:TYR:CD2	2.39	0.58
1:CA:545:C:OP2	4:CD:65:ARG:NH2	2.37	0.58
25:DA:613:G:N2	25:DA:614(C):A:O2'	2.37	0.58
25:DA:871:U:O2	25:DA:906:G:N2	2.30	0.58
30:DG:144:ILE:HA	30:DG:148:MET:HE1	1.85	0.58
33:DN:15:LEU:HB2	33:DN:135:PRO:HB2	1.85	0.58
1:AA:997:U:H3	1:AA:1044:A:H61	1.51	0.58
1:CA:316:G:OP2	1:CA:351:G:O2'	2.20	0.58
13:CM:33:ALA:HA	13:CM:59:TYR:CE2	2.39	0.58
25:DA:1204:A:H5'	25:DA:1206:G:H1'	1.86	0.58
25:DA:1250:G:OP2	35:DP:21:ARG:NH1	2.37	0.58
25:DA:1711:C:H2'	25:DA:1712:C:C6	2.38	0.58
34:DO:107:ARG:CZ	39:DT:36:GLU:HG2	2.34	0.58
1:AA:200:G:H1	1:AA:217:C:N4	2.02	0.58
25:BA:1272:A:OP1	41:BV:84:LYS:HE2	2.04	0.58
25:BA:1827:U:H2'	25:BA:1828:C:C6	2.39	0.58
50:B4:57:GLU:HB3	50:B4:58:ARG:HG2	1.86	0.58
25:DA:972:G:OP2	25:DA:973:A:O2'	2.17	0.58
25:BA:303:C:H42	25:BA:385:G:H1	1.51	0.58
6:CF:9:VAL:HB	6:CF:87:ARG:HB2	1.85	0.58
12:CL:88:GLY:O	12:CL:99:HIS:HD2	1.85	0.58
25:DA:900:A:H2'	25:DA:901:A:C8	2.38	0.58
25:DA:2291:U:H2'	25:DA:2292:C:C6	2.39	0.58
26:DB:81:G:H1	26:DB:96:U:H3	1.51	0.58
52:D6:14:THR:OG1	52:D6:48:VAL:O	2.22	0.58
9:AI:9:ARG:HG2	9:AI:14:VAL:HG12	1.86	0.57
25:BA:83:A:H5"	44:BY:8:LYS:HE3	1.86	0.57
25:BA:2152:U:H2'	25:BA:2153:G:N2	2.19	0.57
25:BA:2820:A:N6	25:BA:2900:G:O2'	2.36	0.57
32:BI:126:TYR:HB2	32:BI:142:VAL:HG23	1.86	0.57
1:CA:517:G:N1	1:CA:533:A:OP2	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:775:G:N2	1:CA:804:U:O4	2.36	0.57
2:CB:95:GLN:HG3	2:CB:147:LYS:HD3	1.86	0.57
25:DA:131:G:OP1	61:DA:4107:HOH:O	2.17	0.57
3:CC:18:TRP:HE3	3:CC:18:TRP:H	1.52	0.57
8:CH:64:LYS:HG2	8:CH:79:VAL:HG21	1.86	0.57
20:CT:13:LEU:H	20:CT:13:LEU:HD12	1.68	0.57
24:CX:49:G:H1	24:CX:65:C:N4	2.02	0.57
25:DA:324:A:N6	25:DA:338:G:O2'	2.37	0.57
25:DA:2379:G:O2'	38:DS:17:ARG:NH2	2.22	0.57
1:AA:410:G:OP1	4:AD:30:LYS:NZ	2.29	0.57
1:AA:619:U:C2	4:AD:135:LEU:HD22	2.40	0.57
25:BA:129:G:OP1	61:BA:4198:HOH:O	2.17	0.57
50:B4:53:GLU:O	50:B4:55:ARG:N	2.35	0.57
11:CK:31:THR:HG23	11:CK:42:TRP:HB3	1.85	0.57
20:CT:9:ASN:O	20:CT:10:LEU:HB2	2.04	0.57
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.40	0.57
14:AN:27:CYS:SG	14:AN:29:ARG:HB2	2.44	0.57
25:BA:2162:C:C4	25:BA:2173:G:N1	2.71	0.57
25:BA:2299:A:N6	25:BA:2356:U:H3	1.98	0.57
39:BT:24:PRO:HA	39:BT:49:VAL:HG22	1.86	0.57
45:BZ:28:MET:HE1	45:BZ:61:LEU:HD21	1.85	0.57
1:CA:1001:A:H2'	1:CA:1001(A):G:C8	2.38	0.57
25:DA:570:G:H2'	25:DA:2030:A:C5	2.39	0.57
25:DA:833:U:O2	35:DP:55:ARG:NH2	2.36	0.57
24:AX:21:A:N6	24:AX:46:G:H2'	2.19	0.57
25:BA:2227:G:H5'	25:BA:2228:G:N7	2.19	0.57
1:CA:1029:C:N4	1:CA:1032:G:C5	2.72	0.57
1:CA:1348:U:H2'	1:CA:1349:A:H8	1.70	0.57
38:DS:27:SER:HA	38:DS:88:ASP:HB3	1.87	0.57
23:AY:63:G:H2'	23:AY:64:A:O4'	2.05	0.57
35:BP:63:PRO:HG2	54:B8:25:MET:HB2	1.85	0.57
25:DA:1400:G:H2'	25:DA:1401:G:C8	2.38	0.57
25:DA:1539:G:H2'	25:DA:1540:U:O4'	2.04	0.57
35:DP:97:PRO:HD3	35:DP:126:VAL:O	2.04	0.57
1:AA:1191:A:H5"	3:AC:4:LYS:NZ	2.20	0.57
15:AO:11:VAL:HG21	15:AO:34:LEU:HD22	1.86	0.57
25:BA:667:G:H21	25:BA:671:A:H2	1.52	0.57
25:BA:2126:G:H2'	25:BA:2127:C:C6	2.40	0.57
1:CA:1151:A:O4'	10:CJ:39:PRO:HB2	2.03	0.57
11:CK:110:ASP:HB3	18:CR:85:LEU:HB3	1.86	0.57
13:CM:13:LYS:HA	13:CM:44:ARG:HH11	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1400:G:H2'	25:DA:1401:G:H8	1.70	0.57
25:DA:2142:C:H2'	25:DA:2143:C:C6	2.40	0.57
30:DG:39:ILE:HG12	30:DG:157:ILE:HG12	1.87	0.57
50:D4:61:ARG:O	50:D4:63:TYR:N	2.38	0.57
1:AA:222:U:H2'	1:AA:223:U:C6	2.39	0.57
2:AB:178:ARG:HG2	8:AH:72:PRO:HA	1.85	0.57
10:AJ:38:ILE:HD11	10:AJ:71:LEU:HD23	1.87	0.57
23:AY:20:U:H4'	23:AY:21:A:OP1	2.04	0.57
37:BR:28:LEU:HD12	37:BR:48:VAL:HG21	1.87	0.57
38:BS:20:ARG:NH2	46:B0:48:GLY:O	2.37	0.57
7:CG:69:VAL:HG21	7:CG:104:LEU:HD11	1.87	0.57
9:CI:128:ARG:NH2	24:CX:33:U:OP2	2.38	0.57
25:DA:784:A:C5	27:DD:229:VAL:HG11	2.40	0.57
38:DS:87:PHE:CE1	38:DS:102:ALA:HB2	2.40	0.57
48:D2:35:LEU:HD12	48:D2:53:LEU:HD12	1.87	0.57
1:AA:7:G:O2'	5:AE:120:THR:O	2.23	0.57
1:AA:78:G:C6	1:AA:91:C:N4	2.73	0.57
1:AA:1510:U:H2'	1:AA:1511:G:C8	2.40	0.57
6:AF:97:PHE:N	18:AR:30:ASP:OD1	2.37	0.57
25:BA:572:A:H61	41:BV:19:LYS:H	1.53	0.57
29:BF:172:TRP:H	29:BF:172:TRP:CD1	2.23	0.57
1:CA:673:G:H2'	1:CA:674:G:C8	2.40	0.57
1:CA:1030(A):G:N2	1:CA:1030(D):A:OP2	2.37	0.57
1:CA:1317:C:OP1	14:CN:17:LYS:HG2	2.05	0.57
13:CM:81:LEU:HD13	13:CM:88:ARG:HG2	1.87	0.57
25:DA:250:G:P	54:D8:13:ARG:HH22	2.28	0.57
25:DA:639:U:H2'	25:DA:640:C:C6	2.40	0.57
25:DA:1359:A:N6	25:DA:1372:U:H3	2.03	0.57
25:DA:1530:C:N4	25:DA:1539:G:H1	2.03	0.57
29:DF:11:VAL:HG22	29:DF:125:LEU:HB2	1.86	0.57
34:DO:2:ILE:HB	34:DO:33:ALA:HB3	1.87	0.57
1:AA:972:C:OP1	61:AA:4158:HOH:O	2.18	0.57
25:BA:613:A:OP1	29:BF:95:ARG:NH1	2.38	0.57
25:BA:1027:A:OP1	61:BA:4709:HOH:O	2.18	0.57
25:BA:2736:C:OP1	37:BR:3:HIS:ND1	2.22	0.57
27:BD:108:PRO:HB3	27:BD:143:HIS:CE1	2.40	0.57
29:BF:53:THR:HG22	29:BF:55:GLY:H	1.70	0.57
35:BP:81:GLN:NE2	35:BP:105:LEU:O	2.36	0.57
1:CA:1392:G:H21	1:CA:1502:A:H8	1.50	0.57
2:CB:74:LYS:HG3	2:CB:77:ALA:HB3	1.86	0.57
7:CG:78:ARG:NH1	7:CG:79:ARG:HH12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:CJ:78:ASN:O	10:CJ:80:LYS:N	2.38	0.57
26:DB:15:A:OP2	26:DB:69:G:N2	2.37	0.57
25:BA:1346:U:H4'	25:BA:1347:A:C5'	2.35	0.56
25:BA:1475:G:H2'	25:BA:1476:C:C6	2.39	0.56
25:DA:528:A:C2	25:DA:2042:A:H2'	2.40	0.56
34:DO:87:ILE:HD12	34:DO:91:LEU:HA	1.87	0.56
45:DZ:110:GLY:O	45:DZ:146:ILE:HG13	2.04	0.56
1:AA:405:U:OP2	4:AD:3:ARG:NH2	2.38	0.56
1:AA:838:G:H2'	1:AA:839:U:H2'	1.86	0.56
1:AA:977:A:H1'	1:AA:982:U:O4	2.06	0.56
1:AA:1064:G:H4'	1:AA:1065:U:OP1	2.06	0.56
25:BA:346:A:OP1	29:BF:168:ARG:HD2	2.05	0.56
25:BA:1065:U:O2'	25:BA:1067:A:H2	1.88	0.56
25:BA:2331:G:H22	38:BS:3:ARG:NE	2.03	0.56
25:BA:2840:G:OP1	28:BE:76:ARG:NH2	2.38	0.56
31:BH:113:VAL:HG11	31:BH:151:ILE:HD13	1.87	0.56
50:B4:33:VAL:HG12	50:B4:34:GLU:H	1.71	0.56
2:CB:118:LEU:HB3	2:CB:142:LEU:HD12	1.87	0.56
24:CX:76:A:H5'	25:DA:2585:U:C5	2.41	0.56
25:DA:1204:A:N6	25:DA:1240:U:H2'	2.20	0.56
25:DA:1430:C:H2'	25:DA:1431:U:C6	2.39	0.56
25:DA:2138:C:N4	25:DA:2153:G:H1	2.03	0.56
34:DO:115:VAL:HG13	34:DO:121:VAL:HG21	1.87	0.56
3:AC:33:LEU:HD21	14:AN:53:LEU:HD22	1.85	0.56
5:AE:79:GLU:HG3	5:AE:93:PRO:HD2	1.87	0.56
23:AY:33:U:H2'	23:AY:35:A:OP2	2.04	0.56
25:BA:1513:G:H2'	25:BA:1594:C:N4	2.20	0.56
25:BA:1613:A:OP1	27:BD:211:ARG:NH1	2.39	0.56
25:BA:1817:A:H1'	25:BA:1960:A:N6	2.20	0.56
25:BA:2310:A:H2'	25:BA:2311:G:O4'	2.05	0.56
1:CA:1151:A:O2'	1:CA:1152:A:H8	1.88	0.56
3:CC:15:THR:HG21	3:CC:181:ASN:HA	1.87	0.56
8:CH:41:ARG:NH2	8:CH:123:GLU:OE2	2.38	0.56
8:CH:51:VAL:HG11	8:CH:60:ARG:NH1	2.20	0.56
19:CS:30:LEU:HA	19:CS:48:THR:O	2.06	0.56
20:CT:92:LEU:HA	20:CT:95:ALA:HB3	1.87	0.56
23:CY:62:C:H2'	23:CY:63:G:H8	1.69	0.56
25:DA:994:C:OP2	40:DU:54:LYS:NZ	2.33	0.56
25:DA:1300:U:H4'	25:DA:1301:A:H5'	1.88	0.56
25:DA:2506:U:OP1	28:DE:144:ARG:NH2	2.38	0.56
31:DH:96:ALA:HB1	31:DH:103:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DS:68:GLN:HE21	38:DS:71:ARG:HD3	1.69	0.56
52:D6:6:ARG:NH1	52:D6:26:ASN:HB2	2.20	0.56
2:AB:100:GLY:N	2:AB:176:GLU:OE2	2.27	0.56
25:BA:273:G:H4'	25:BA:274:U:OP1	2.04	0.56
29:BF:140:LEU:HD21	29:BF:170:LEU:HD11	1.86	0.56
1:CA:1492:A:O2'	1:CA:1493:A:O5'	2.16	0.56
15:CO:25:THR:HG21	15:CO:70:LEU:HB2	1.86	0.56
25:DA:1434:A:H61	25:DA:1558:A:H62	1.53	0.56
25:DA:1594:G:H2'	25:DA:1595:G:O4'	2.05	0.56
25:DA:2193:G:H2'	25:DA:2194:G:H8	1.71	0.56
1:AA:1007:C:N3	1:AA:1022:G:O6	2.37	0.56
2:AB:15:VAL:HG21	2:AB:209:ARG:HG2	1.87	0.56
3:AC:54:ARG:NH1	3:AC:56:ASP:OD2	2.38	0.56
25:BA:173:C:H2'	25:BA:174:U:C6	2.40	0.56
25:DA:1231:G:H2'	25:DA:1232:G:C8	2.41	0.56
25:DA:1518:U:H2'	25:DA:1519:G:O4'	2.05	0.56
41:DV:43:GLU:N	41:DV:43:GLU:OE2	2.37	0.56
1:AA:17:U:H2'	1:AA:18:C:C6	2.40	0.56
57:AA:3231:PCY:O26	57:AA:3231:PCY:O36	2.22	0.56
4:AD:108:LEU:HD22	4:AD:174:LEU:HD13	1.88	0.56
15:AO:64:ARG:HB3	15:AO:64:ARG:HH11	1.70	0.56
18:AR:56:THR:HB	18:AR:58:LEU:HD23	1.87	0.56
25:BA:1428:G:N7	61:BA:5233:HOH:O	2.33	0.56
25:BA:2825:C:H5'	51:B5:29:THR:HG21	1.87	0.56
29:BF:157:VAL:HB	29:BF:194:MET:HG2	1.88	0.56
36:BQ:111:GLU:OE1	36:BQ:133:ARG:NH2	2.38	0.56
1:CA:201:C:N4	1:CA:216:G:H1	2.04	0.56
1:CA:685:G:N1	1:CA:686:U:O4	2.39	0.56
9:CI:18:PHE:HD2	9:CI:62:TYR:HD2	1.52	0.56
14:CN:12:ARG:HE	14:CN:14:PRO:HB3	1.71	0.56
23:CW:23:A:H2'	23:CW:24:G:C8	2.40	0.56
25:DA:1029:A:N1	25:DA:2465:C:O2'	2.36	0.56
25:DA:2611:U:H5'	25:DA:2611:U:H6	1.71	0.56
30:DG:43:LEU:HD11	30:DG:153:ARG:HG2	1.86	0.56
23:AW:4:C:H2'	23:AW:5:G:H8	1.71	0.56
1:CA:1014:A:OP1	19:CS:18:LYS:NZ	2.30	0.56
18:CR:32:ARG:HA	18:CR:69:THR:HG21	1.86	0.56
36:DQ:111:GLU:O	36:DQ:115:MET:HG2	2.05	0.56
1:AA:924:C:O2'	1:AA:1502:A:N6	2.37	0.56
23:AY:19:G:H3'	23:AY:20:U:C6	2.39	0.56
25:BA:1084:C:H42	25:BA:1163:G:H1	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:CS:22:LEU:HD22	19:CS:31:ILE:HD11	1.86	0.56
25:DA:131:G:OP1	61:DA:4106:HOH:O	2.18	0.56
25:DA:1203:G:OP2	25:DA:1204:A:O2'	2.20	0.56
25:DA:1226:A:OP1	41:DV:84:LYS:HE2	2.05	0.56
29:DF:167:ALA:HB1	29:DF:173:VAL:HG11	1.87	0.56
25:BA:2289:G:OP2	46:B0:10:THR:HG21	2.05	0.56
28:BE:24:THR:HG22	28:BE:186:GLY:O	2.06	0.56
52:B6:35:GLU:OE2	52:B6:50:ARG:NH1	2.39	0.56
2:CB:87:ARG:HH12	2:CB:230:VAL:HG11	1.70	0.56
11:CK:81:ASP:OD1	11:CK:107:SER:OG	2.21	0.56
23:CW:39:PSU:H2'	23:CW:40:C:H6	1.71	0.56
25:DA:649:G:H4'	54:D8:46:ARG:HH22	1.70	0.56
25:DA:1414:G:N2	25:DA:1588:C:O2	2.37	0.56
28:DE:72:VAL:HA	28:DE:73:GLU:HB3	1.88	0.56
37:DR:56:LYS:NZ	37:DR:90:ARG:O	2.39	0.56
13:AM:3:ARG:HD2	13:AM:9:ILE:HG12	1.88	0.56
23:AW:8:4SU:O5'	23:AW:8:4SU:H6	2.06	0.56
25:BA:796:C:OP2	61:BA:5333:HOH:O	2.18	0.56
25:BA:2157:A:N1	25:BA:2178:G:O2'	2.32	0.56
29:BF:125:LEU:HD12	29:BF:194:MET:HB2	1.88	0.56
29:BF:192:LEU:HD13	29:BF:194:MET:HE2	1.88	0.56
38:BS:14:VAL:O	38:BS:18:ILE:HG12	2.06	0.56
1:CA:1029:C:C4	1:CA:1033:G:C6	2.94	0.56
1:CA:1513:A:H2'	1:CA:1514:C:C6	2.41	0.56
9:CI:9:ARG:HG2	9:CI:14:VAL:HG12	1.88	0.56
13:CM:92:HIS:CE1	13:CM:98:VAL:HG21	2.41	0.56
25:DA:1721:G:N1	25:DA:1739:U:OP2	2.39	0.56
25:DA:1798:U:OP2	27:DD:274:ARG:NH2	2.39	0.56
25:DA:2303:G:O2'	30:DG:132:ASN:HB2	2.06	0.56
45:DZ:120:ILE:HG13	45:DZ:173:ALA:HB3	1.88	0.56
2:AB:16:HIS:CG	2:AB:17:PHE:N	2.74	0.55
3:AC:17:ASP:O	3:AC:54:ARG:NH2	2.40	0.55
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.87	0.55
25:BA:795:G:H2'	25:BA:797:A:OP2	2.06	0.55
1:CA:45:U:H2'	1:CA:46:G:C8	2.42	0.55
1:CA:1051:C:H2'	1:CA:1052:U:C6	2.41	0.55
1:CA:1073:U:O2	2:CB:104:ASN:ND2	2.38	0.55
1:CA:1442(A):G:C8	39:DT:118:ARG:HG2	2.41	0.55
2:CB:189:ASP:OD1	2:CB:189:ASP:N	2.34	0.55
45:DZ:33:LEU:HD11	45:DZ:90:VAL:HG21	1.87	0.55
1:AA:60:A:H4'	1:AA:61:G:H5'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BI:72:LEU:O	32:BI:74:ASN:N	2.39	0.55
1:CA:1122:U:N3	1:CA:1123:A:N7	2.55	0.55
11:CK:92:GLU:HB3	11:CK:96:ARG:HH21	1.72	0.55
25:DA:27:G:N2	25:DA:512:G:H1'	2.20	0.55
25:DA:1300:U:H4'	25:DA:1301:A:C5'	2.37	0.55
27:DD:242:ARG:N	27:DD:242:ARG:HD3	2.20	0.55
25:BA:559:U:H2'	25:BA:560:C:C6	2.42	0.55
37:BR:96:ARG:NH1	37:BR:118:GLU:OE2	2.37	0.55
1:CA:352:C:OP2	61:CA:4054:HOH:O	2.17	0.55
1:CA:838:G:N2	1:CA:848:C:N3	2.52	0.55
10:CJ:8:LEU:HB3	10:CJ:16:LEU:HD22	1.88	0.55
19:CS:41:VAL:HG12	19:CS:43:GLU:H	1.71	0.55
20:CT:43:LEU:O	20:CT:47:GLY:N	2.39	0.55
25:DA:330:A:HO2'	25:DA:331:A:H8	1.53	0.55
25:DA:878:A:N6	25:DA:899:A:O2'	2.39	0.55
25:DA:1406:U:H2'	25:DA:1407:C:C6	2.41	0.55
25:DA:2177:C:H2'	25:DA:2178:C:O4'	2.06	0.55
27:DD:218:ARG:HB3	27:DD:219:PRO:HD2	1.88	0.55
36:DQ:37:LEU:HD21	36:DQ:130:LYS:HE2	1.89	0.55
1:AA:1392:G:N2	1:AA:1502:A:C8	2.74	0.55
25:BA:431:C:H4'	25:BA:432:U:H5'	1.87	0.55
25:BA:641:G:OP1	29:BF:40:GLN:HG2	2.07	0.55
1:CA:1469:G:H2'	1:CA:1470:G:C8	2.42	0.55
2:CB:98:LEU:HD22	2:CB:98:LEU:H	1.71	0.55
8:CH:69:ARG:NH2	8:CH:75:ARG:O	2.39	0.55
15:CO:4:THR:OG1	15:CO:7:GLU:OE1	2.20	0.55
25:DA:2273:A:H2'	25:DA:2274:A:C8	2.41	0.55
1:AA:356:A:N3	1:AA:368:U:O2'	2.33	0.55
1:AA:715:A:H2'	1:AA:716:A:C8	2.41	0.55
1:AA:975:A:H5'	1:AA:975:A:H8	1.70	0.55
9:AI:22:GLY:N	9:AI:58:HIS:O	2.31	0.55
25:BA:354:A:H2	25:BA:1255:A:HO2'	1.54	0.55
25:BA:661:G:OP1	35:BP:132:LYS:HE2	2.07	0.55
25:BA:1735:U:O2	25:BA:1747:A:H5'	2.06	0.55
25:DA:2296:U:OP2	38:DS:9:ARG:NH2	2.39	0.55
35:DP:38:GLN:O	35:DP:39:LYS:HB3	2.05	0.55
1:AA:165:C:H2'	1:AA:166:G:C8	2.42	0.55
1:AA:509:A:O2'	1:AA:510:A:OP1	2.18	0.55
6:AF:91:VAL:HG11	18:AR:72:ARG:NH1	2.20	0.55
25:BA:333:G:N3	25:BA:353:G:O2'	2.36	0.55
61:BA:5082:HOH:O	35:BP:39:LYS:HE3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BI:93:THR:OG1	32:BI:96:ASP:OD1	2.16	0.55
47:B1:89:GLU:O	47:B1:93:GLU:HG2	2.07	0.55
1:CA:677:U:H3	1:CA:713:G:H22	1.53	0.55
1:CA:1006:C:H2'	1:CA:1007:C:C6	2.41	0.55
3:CC:54:ARG:HH12	3:CC:56:ASP:CG	2.14	0.55
25:DA:143:G:H4'	43:DX:35:THR:HG21	1.87	0.55
31:DH:30:LYS:HG3	31:DH:80:SER:O	2.06	0.55
25:BA:906:G:O2'	25:BA:962:G:O6	2.21	0.55
25:BA:1222:A:N3	25:BA:1222:A:H2'	2.21	0.55
1:CA:814:A:H2'	1:CA:816:A:H5"	1.87	0.55
1:CA:1469:G:H2'	1:CA:1470:G:H8	1.71	0.55
23:CW:29:G:H2'	23:CW:30:G:H8	1.72	0.55
1:AA:407:G:OP1	4:AD:115:ARG:NH2	2.39	0.55
1:AA:1025:U:C2	1:AA:1036:G:O6	2.59	0.55
4:AD:190:ASP:HB2	4:AD:193:ASP:OD2	2.07	0.55
25:BA:206:G:OP2	61:BA:5143:HOH:O	2.18	0.55
26:BB:66:A:H61	26:BB:109:C:H5'	1.71	0.55
1:CA:1010:G:H2'	1:CA:1011:G:H8	1.71	0.55
3:CC:37:GLN:HE22	3:CC:40:ARG:HD2	1.72	0.55
14:CN:23:ARG:NH1	14:CN:30:ALA:HB2	2.21	0.55
16:CP:58:TYR:O	16:CP:61:SER:OG	2.19	0.55
24:CX:19:G:H4'	24:CX:20:U:OP2	2.07	0.55
25:DA:1579:A:H2'	25:DA:1580:A:C8	2.42	0.55
25:DA:2022:U:O2'	25:DA:2617:C:H5'	2.07	0.55
25:DA:2683:C:P	39:DT:53:ARG:HH22	2.30	0.55
1:AA:1414:U:H3	1:AA:1486:G:H1	1.54	0.55
25:BA:139:A:H8	25:BA:1454:C:O2'	1.90	0.55
25:BA:272:U:OP1	32:BI:50:ARG:NH1	2.40	0.55
25:BA:479:C:O2	25:BA:483:A:O2'	2.23	0.55
25:BA:704:U:H2'	25:BA:705:C:C6	2.42	0.55
50:B4:63:TYR:N	50:B4:64:GLY:HA2	2.20	0.55
1:CA:1370:G:O6	61:CA:4006:HOH:O	2.16	0.55
3:CC:7:PRO:O	3:CC:11:ARG:NH1	2.38	0.55
25:DA:191:A:H2'	25:DA:192:C:C6	2.41	0.55
25:DA:674:G:H1'	29:DF:74:ARG:HD3	1.89	0.55
42:DW:4:LYS:HB2	42:DW:106:ILE:HG12	1.89	0.55
43:DX:31:HIS:CD2	43:DX:33:LYS:H	2.24	0.55
2:AB:189:ASP:OD1	2:AB:189:ASP:N	2.30	0.55
5:AE:91:LEU:HG	5:AE:118:ILE:HD11	1.89	0.55
5:AE:151:LEU:HD11	8:AH:77:GLU:HG2	1.88	0.55
10:AJ:17:ASP:OD1	10:AJ:70:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AT:36:LEU:HD13	20:AT:58:LYS:HG3	1.88	0.55
25:BA:1873:G:O2'	27:BD:253:GLN:NE2	2.39	0.55
33:BN:15:LEU:HD12	33:BN:137:LYS:HG3	1.89	0.55
1:CA:1121:U:C4	1:CA:1122:U:C4	2.96	0.55
3:CC:134:ILE:HG23	3:CC:151:VAL:HB	1.88	0.55
9:CI:23:ASN:HD22	9:CI:25:LYS:HG2	1.72	0.55
10:CJ:38:ILE:HD11	10:CJ:71:LEU:HB3	1.89	0.55
25:DA:829:A:N7	25:DA:2247:A:O2'	2.37	0.55
25:DA:2641:G:H5"	33:DN:76:SER:HB3	1.88	0.55
40:DU:49:HIS:HA	40:DU:52:ARG:HB3	1.88	0.55
43:DX:8:ILE:O	48:D2:36:ARG:NH2	2.40	0.55
1:AA:1007:C:H2'	1:AA:1008:C:H5"	1.88	0.54
9:AI:21:PRO:HA	9:AI:59:PHE:HA	1.90	0.54
1:CA:76:C:H42	1:CA:93:G:H1	1.55	0.54
25:DA:2666:C:N4	31:DH:108:GLY:O	2.39	0.54
31:DH:80:SER:OG	31:DH:81:GLU:N	2.40	0.54
1:AA:69:G:H2'	1:AA:70:G:C8	2.42	0.54
3:AC:134:ILE:HG23	3:AC:151:VAL:HB	1.89	0.54
3:AC:164:ARG:NH1	3:AC:166:GLU:OE1	2.40	0.54
24:AX:19:G:H4'	24:AX:20:U:OP2	2.07	0.54
23:AY:40:C:H2'	23:AY:41:C:H6	1.72	0.54
29:BF:14:PRO:HD2	29:BF:127:GLU:OE2	2.07	0.54
34:BO:64:ARG:NH1	34:BO:81:ASP:OD1	2.40	0.54
34:BO:104:ARG:CZ	39:BT:34:VAL:HG21	2.37	0.54
23:CW:51:U:H2'	23:CW:52:G:H8	1.72	0.54
23:CY:9:A:O3'	23:CY:45:U:O2'	2.25	0.54
23:CY:67:C:H2'	23:CY:68:C:C6	2.42	0.54
25:DA:829:A:N7	25:DA:2248:C:H5'	2.22	0.54
25:DA:896:A:H62	45:DZ:146:ILE:HD13	1.72	0.54
26:DB:19:G:H2'	26:DB:20:C:O4'	2.06	0.54
1:AA:153:C:H2'	1:AA:154:C:C6	2.42	0.54
1:AA:165:C:H2'	1:AA:166:G:H8	1.72	0.54
3:AC:11:ARG:NH2	3:AC:177:THR:O	2.41	0.54
25:BA:714:U:O2	54:B8:2:PRO:HD2	2.06	0.54
39:BT:112:ARG:HG3	39:BT:115:ARG:NH2	2.23	0.54
1:CA:664:G:H22	1:CA:741:G:H1	1.53	0.54
25:DA:807:U:O2'	25:DA:2060:A:N1	2.40	0.54
26:DB:66:A:N6	26:DB:109:C:H5'	2.14	0.54
1:AA:637:G:H2'	1:AA:638:G:H8	1.71	0.54
1:AA:731:G:H5'	1:AA:766:A:H4'	1.89	0.54
1:AA:749:C:H2'	1:AA:750:G:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1112:C:H1'	3:AC:179:ARG:HG2	1.88	0.54
4:AD:98:GLU:HG2	4:AD:189:PRO:HG2	1.88	0.54
25:BA:2146:G:H1	25:BA:2196:C:N4	2.05	0.54
34:BO:80:ASP:OD1	39:BT:64:ARG:NH2	2.40	0.54
1:CA:976:G:H5'	1:CA:1358:U:O2'	2.07	0.54
1:CA:1063:C:OP2	1:CA:1064:G:O2'	2.23	0.54
1:CA:1183:A:O2'	1:CA:1184:G:OP1	2.22	0.54
23:CW:51:U:H2'	23:CW:52:G:C8	2.42	0.54
25:DA:864:G:H21	25:DA:866:A:H61	1.54	0.54
25:DA:1889:A:H2'	25:DA:1890:A:C8	2.43	0.54
25:DA:2167:U:H2'	25:DA:2168:G:H21	1.73	0.54
25:DA:2183:C:H2'	25:DA:2184:G:H8	1.72	0.54
25:DA:2430:A:N3	25:DA:2430:A:H2'	2.22	0.54
29:DF:172:TRP:CD1	29:DF:172:TRP:H	2.26	0.54
2:AB:83:MET:HB3	2:AB:234:PRO:HG2	1.88	0.54
25:BA:602:G:H2'	25:BA:603:C:C6	2.43	0.54
25:BA:2298:A:H4'	25:BA:2299:A:O4'	2.07	0.54
40:BU:108:GLU:O	40:BU:112:ARG:HG2	2.07	0.54
50:B4:53:GLU:HG3	50:B4:55:ARG:H	1.72	0.54
1:CA:448:A:O5'	1:CA:485:G:N2	2.40	0.54
1:CA:1456:G:O3'	20:CT:39:LYS:NZ	2.40	0.54
7:CG:32:ARG:HH12	7:CG:109:ASN:ND2	2.05	0.54
25:DA:2721:A:OP1	61:DA:4147:HOH:O	2.18	0.54
28:DE:116:VAL:HG13	28:DE:122:PHE:HB2	1.90	0.54
45:DZ:70:LEU:O	45:DZ:89:PHE:N	2.38	0.54
23:AY:76:A:N6	25:BA:2434:A:O4'	2.40	0.54
25:BA:552:C:H5	61:BA:4972:HOH:O	1.90	0.54
33:BN:4:TYR:CD2	40:BU:100:VAL:HG11	2.42	0.54
4:CD:162:LEU:HD13	4:CD:181:MET:HG2	1.90	0.54
25:DA:2447:G:N2	25:DA:2450:A:OP2	2.40	0.54
28:DE:73:GLU:O	28:DE:73:GLU:HG3	2.06	0.54
45:DZ:117:LEU:HD12	45:DZ:174:VAL:HG22	1.89	0.54
1:AA:376:G:O3'	16:AP:5:ARG:HD2	2.07	0.54
6:AF:8:ILE:HD11	6:AF:79:LEU:HD13	1.89	0.54
25:BA:2227:G:O2'	25:BA:2228:G:OP1	2.24	0.54
25:BA:2373:A:OP1	54:B8:27:THR:OG1	2.18	0.54
2:CB:201:ILE:HG21	2:CB:214:ILE:HG21	1.89	0.54
19:CS:52:TYR:HB2	19:CS:57:HIS:CE1	2.42	0.54
25:DA:303:U:H2'	25:DA:304:G:C8	2.42	0.54
1:AA:532:A:O2'	1:AA:533:A:OP1	2.22	0.54
2:AB:162:ILE:O	2:AB:185:ILE:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:181:ASN:HD21	3:AC:204:LEU:HD12	1.73	0.54
4:AD:168:ARG:CD	4:AD:168:ARG:H	2.21	0.54
5:AE:85:GLY:C	5:AE:87:SER:H	2.13	0.54
10:AJ:49:VAL:HG23	14:AN:41:ARG:HB2	1.89	0.54
23:AY:55:PSU:C2	23:AY:57:G:H5'	2.43	0.54
25:BA:310:C:H2'	25:BA:311:C:H6	1.72	0.54
25:BA:2255:U:H2'	25:BA:2256:U:C6	2.43	0.54
29:BF:184:TYR:CE2	29:BF:188:ARG:HD2	2.43	0.54
44:BY:20:TYR:CE1	44:BY:43:ASN:HA	2.41	0.54
1:CA:1118:C:H1'	1:CA:1179:A:C5	2.43	0.54
11:CK:22:HIS:HB3	11:CK:29:ILE:HB	1.90	0.54
23:CW:27:G:H2'	23:CW:28:G:C8	2.43	0.54
25:DA:2659:G:H4'	31:DH:175:LYS:HD3	1.88	0.54
28:DE:38:THR:HG23	28:DE:41:LYS:HB3	1.90	0.54
1:CA:1003:G:H1	1:CA:1035:A:N6	2.06	0.54
23:CW:21:A:N6	23:CW:46:7MG:N3	2.56	0.54
39:DT:64:ARG:HB2	39:DT:73:GLU:HG2	1.89	0.54
1:AA:676:A:H1'	11:AK:115:PRO:HB3	1.88	0.54
1:AA:1218:C:H2'	1:AA:1219:U:C6	2.43	0.54
25:BA:2178:G:H2'	25:BA:2179:G:C4	2.42	0.54
25:BA:2227:G:H3'	25:BA:2228:G:C8	2.42	0.54
30:BG:72:ARG:NH1	30:BG:87:PRO:HG3	2.23	0.54
31:BH:56:SER:OG	31:BH:57:ASP:N	2.41	0.54
47:B1:85:LEU:HD22	47:B1:89:GLU:HG3	1.90	0.54
1:CA:35:G:O2'	12:CL:118:SER:O	2.19	0.54
1:CA:41:G:H2'	1:CA:42:G:C8	2.43	0.54
1:CA:41:G:H2'	1:CA:42:G:H8	1.73	0.54
1:CA:160:A:H1'	1:CA:344:A:N7	2.23	0.54
1:CA:1028:C:O2	1:CA:1033:G:N1	2.41	0.54
15:CO:70:LEU:HD11	15:CO:77:ARG:HB2	1.89	0.54
25:DA:319:C:H2'	25:DA:320:A:O4'	2.08	0.54
32:DI:57:ARG:HA	32:DI:61:ARG:HH21	1.72	0.54
36:DQ:16:ARG:HG2	36:DQ:18:LYS:HE2	1.89	0.54
37:DR:21:TYR:CZ	37:DR:43:GLU:HG2	2.43	0.54
1:AA:134:A:H61	16:AP:25:ARG:HH12	1.56	0.53
11:AK:99:GLN:HG2	11:AK:105:VAL:HG21	1.90	0.53
13:AM:93:ARG:HD2	25:BA:935:C:OP1	2.08	0.53
25:BA:1653:C:H4'	25:BA:1654:A:O5'	2.07	0.53
25:BA:2549:U:H2'	25:BA:2550:C:C6	2.43	0.53
31:BH:41:MET:HE2	31:BH:65:HIS:HA	1.90	0.53
34:BO:16:ALA:HB2	34:BO:52:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BZ:92:SER:OG	45:BZ:93:ASP:N	2.31	0.53
1:CA:158:G:N2	1:CA:163:C:O2	2.41	0.53
25:DA:770:G:OP2	61:DA:4559:HOH:O	2.19	0.53
25:DA:2141:G:O4'	25:DA:2151:G:N2	2.41	0.53
27:DD:132:PRO:HD3	27:DD:190:TYR:CZ	2.42	0.53
2:AB:178:ARG:HH21	8:AH:74:PRO:HB3	1.74	0.53
25:BA:354:A:H2	25:BA:1255:A:C2'	2.21	0.53
25:BA:718:C:N4	61:BA:5006:HOH:O	2.40	0.53
25:BA:1740:U:O2'	27:BD:14:ARG:NH2	2.41	0.53
27:BD:145:VAL:HG12	27:BD:146:GLU:O	2.07	0.53
48:B2:24:LEU:HD23	48:B2:60:LEU:HD21	1.89	0.53
1:CA:21:G:H2'	1:CA:22:G:C8	2.43	0.53
30:DG:113:ARG:NH1	30:DG:139:LEU:O	2.37	0.53
31:DH:9:ILE:HG12	31:DH:69:ARG:HD2	1.90	0.53
1:AA:110:C:H2'	1:AA:111:G:O4'	2.07	0.53
1:AA:933:G:O6	7:AG:3:ARG:NH2	2.39	0.53
13:AM:37:THR:O	13:AM:55:ARG:NH1	2.42	0.53
25:BA:236:G:H4'	25:BA:413:G:C5	2.42	0.53
25:BA:794:U:O2	25:BA:2036:A:H1'	2.07	0.53
25:BA:968:U:H2'	25:BA:969:C:C6	2.44	0.53
45:BZ:117:LEU:HD21	45:BZ:144:LEU:HD13	1.89	0.53
1:CA:187:C:O2'	20:CT:89:ARG:NH2	2.39	0.53
1:CA:788:U:O2'	57:CA:3178:PCY:O14	2.20	0.53
7:CG:111:ARG:NH1	7:CG:113:GLU:OE2	2.40	0.53
15:CO:26:GLU:OE2	15:CO:77:ARG:NH2	2.35	0.53
19:CS:27:GLU:HG2	19:CS:47:HIS:CE1	2.43	0.53
23:CW:52:G:H2'	23:CW:53:G:O4'	2.08	0.53
23:CY:8:4SU:H6	23:CY:8:4SU:H5"	1.91	0.53
25:DA:709:U:H2'	25:DA:710:G:C8	2.44	0.53
31:DH:90:LYS:HD3	31:DH:159:GLU:HG2	1.91	0.53
35:DP:84:ASN:OD1	35:DP:117:GLU:HB2	2.08	0.53
41:DV:6:LYS:HB2	41:DV:38:LEU:HD21	1.90	0.53
1:AA:1001:A:H2'	1:AA:1001(A):G:C8	2.43	0.53
1:AA:1305:G:H22	1:AA:1331:G:H1'	1.72	0.53
4:AD:101:LEU:HB2	4:AD:138:TYR:HB3	1.90	0.53
25:BA:927:G:H2'	25:BA:928:G:H8	1.74	0.53
25:BA:1000:C:OP1	36:BQ:87:LYS:HE3	2.08	0.53
25:BA:1067:A:H3'	25:BA:1067:A:C8	2.43	0.53
39:BT:23:ARG:HG3	39:BT:120:ARG:NH1	2.23	0.53
25:DA:660:G:H5'	29:DF:99:TYR:CE2	2.43	0.53
25:DA:811:U:OP2	35:DP:29:LYS:N	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2206:G:H3'	25:DA:2207:G:N7	2.22	0.53
31:DH:103:LEU:HB3	31:DH:115:VAL:HB	1.89	0.53
31:DH:113:VAL:HG11	31:DH:151:ILE:HD13	1.89	0.53
1:AA:1027:C:N4	1:AA:1033:G:O6	2.42	0.53
1:AA:1124:G:N7	1:AA:1145:C:O2'	2.40	0.53
10:AJ:5:ARG:NH2	10:AJ:73:ASP:OD2	2.32	0.53
23:AW:4:C:N3	23:AW:69:G:O6	2.42	0.53
25:BA:1058:U:C5	33:BN:28:THR:HG21	2.44	0.53
1:CA:142:G:H2'	1:CA:143:A:C8	2.44	0.53
1:CA:254:G:OP1	17:CQ:66:SER:OG	2.21	0.53
15:CO:16:ALA:HB1	15:CO:21:ASP:HB3	1.89	0.53
25:DA:247:G:H4'	25:DA:386:G:C5	2.44	0.53
25:DA:1292:U:H2'	25:DA:1293:C:C6	2.44	0.53
25:DA:2483:C:H2'	25:DA:2484:G:O4'	2.07	0.53
26:DB:6:C:H2'	26:DB:7:G:H5"	1.89	0.53
26:DB:17:C:H2'	26:DB:18:G:O4'	2.09	0.53
29:DF:129:PHE:CD2	29:DF:163:VAL:HG21	2.44	0.53
36:DQ:14:ARG:HG2	36:DQ:41:TRP:HH2	1.73	0.53
1:AA:954:G:H21	1:AA:1227:A:H62	1.56	0.53
1:AA:1004:A:H5"	1:AA:1025:U:C5	2.43	0.53
9:AI:86:VAL:HG13	9:AI:96:LEU:HD12	1.91	0.53
23:AW:26:A:H61	23:AW:44:G:H1	1.55	0.53
23:AY:67:C:H2'	23:AY:68:C:H6	1.71	0.53
25:BA:2798:C:OP1	28:BE:41:LYS:NZ	2.39	0.53
27:BD:77:ALA:HB2	27:BD:97:TYR:CD2	2.44	0.53
28:BE:28:ALA:HB3	28:BE:93:VAL:HG12	1.91	0.53
51:B5:16:ARG:NH1	51:B5:17:ASP:OD1	2.41	0.53
1:CA:91:C:H2'	1:CA:92:C:C6	2.43	0.53
1:CA:1192:C:OP2	3:CC:4:LYS:NZ	2.36	0.53
10:CJ:17:ASP:OD1	10:CJ:70:ARG:NH1	2.42	0.53
24:CX:8:4SU:O5'	24:CX:8:4SU:H6	2.08	0.53
27:DD:26:LYS:HE2	27:DD:28:GLU:O	2.08	0.53
36:DQ:85:LYS:HG2	46:D0:7:LEU:HB3	1.90	0.53
1:AA:1176:A:H2'	1:AA:1177:G:C8	2.43	0.53
15:AO:82:ILE:O	15:AO:86:GLY:N	2.41	0.53
25:BA:239:G:OP2	54:B8:13:ARG:NH2	2.42	0.53
25:BA:2589:A:H5"	25:BA:2590:G:H5'	1.90	0.53
44:BY:54:LYS:H	44:BY:56:PRO:HD3	1.73	0.53
1:CA:49:U:O4	1:CA:365:U:H5	1.89	0.53
1:CA:1077:G:N2	1:CA:1080:A:OP2	2.42	0.53
3:CC:37:GLN:NE2	3:CC:40:ARG:HD2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:403:U:H4'	25:DA:404:C:H5'	1.89	0.53
25:DA:774:A:N3	25:DA:774:A:H2'	2.24	0.53
25:DA:1247:A:OP1	29:DF:95:ARG:NH2	2.40	0.53
40:DU:79:PHE:CZ	40:DU:83:LEU:HD21	2.43	0.53
8:AH:4:ASP:OD2	8:AH:85:ARG:NH1	2.41	0.53
9:AI:23:ASN:ND2	9:AI:25:LYS:HG2	2.24	0.53
1:CA:396:G:O2'	1:CA:398:C:OP1	2.09	0.53
16:CP:9:PHE:CE1	16:CP:18:ARG:HD2	2.44	0.53
25:DA:956:G:N2	25:DA:959:A:H3'	2.24	0.53
25:DA:993:G:H21	41:DV:89:GLN:NE2	2.06	0.53
25:DA:1496:A:N3	25:DA:1577:C:O2'	2.40	0.53
25:DA:2567:G:H2'	25:DA:2568:C:C6	2.43	0.53
36:DQ:32:TYR:OH	36:DQ:111:GLU:OE1	2.13	0.53
42:DW:86:LEU:HD22	42:DW:96:ILE:HD11	1.91	0.53
6:AF:68:PRO:HB2	6:AF:71:ARG:HG3	1.90	0.53
23:AY:40:C:H2'	23:AY:41:C:C6	2.44	0.53
25:BA:1154:U:O2'	25:BA:1155:C:O4'	2.27	0.53
25:BA:1338:U:H2'	25:BA:1339:C:C6	2.44	0.53
38:BS:34:HIS:O	38:BS:97:ARG:NH2	2.41	0.53
44:BY:6:HIS:H	44:BY:6:HIS:CD2	2.26	0.53
1:CA:428:G:OP2	4:CD:10:ARG:NH1	2.42	0.53
1:CA:1435:G:H2'	1:CA:1436:U:C6	2.44	0.53
25:DA:39:C:H2'	25:DA:40:C:C6	2.44	0.53
25:DA:323:G:C8	29:DF:171:PRO:HG3	2.44	0.53
25:DA:455:C:N3	25:DA:472:A:H2'	2.24	0.53
26:DB:105:A:OP1	45:DZ:72:ARG:NH1	2.42	0.53
30:DG:16:ARG:O	30:DG:20:ILE:HG13	2.07	0.53
30:DG:115:ARG:HD2	30:DG:136:ARG:HH21	1.73	0.53
40:DU:92:ARG:HA	40:DU:95:LEU:HB2	1.90	0.53
1:AA:78:G:C2	1:AA:91:C:N3	2.77	0.53
1:AA:562:C:H1'	12:AL:15:ARG:HB3	1.91	0.53
1:AA:1149:C:P	9:AI:9:ARG:HH21	2.32	0.53
8:AH:112:LEU:HA	8:AH:134:ILE:HG12	1.91	0.53
25:BA:1634:C:H2'	25:BA:1635:C:H6	1.74	0.53
25:BA:2346:G:H5'	38:BS:9:ARG:HG2	1.90	0.53
25:BA:2604:G:OP1	61:BA:4863:HOH:O	2.18	0.53
39:BT:64:ARG:HB2	39:BT:73:GLU:HG2	1.90	0.53
5:CE:60:TYR:OH	5:CE:64:ARG:NH2	2.41	0.53
25:DA:1405:U:H2'	25:DA:1406:U:C6	2.43	0.53
25:DA:2881:C:H2'	25:DA:2882:A:O4'	2.09	0.53
1:AA:67:C:H2'	1:AA:68:G:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:253:U:OP1	17:AQ:67:LYS:NZ	2.42	0.52
23:AW:20:U:H4'	23:AW:20:U:OP1	2.07	0.52
25:BA:1159:U:H2'	25:BA:1160:G:H8	1.74	0.52
25:BA:1634:C:H2'	25:BA:1635:C:C6	2.44	0.52
25:BA:2364:A:N6	25:BA:2377:G:O2'	2.42	0.52
25:BA:2490:A:H5'	55:B9:31:LYS:HE2	1.92	0.52
39:BT:51:ARG:HG3	39:BT:98:LYS:HD2	1.91	0.52
45:BZ:111:VAL:C	45:BZ:113:ALA:H	2.17	0.52
49:B3:8:LEU:HD13	49:B3:31:LEU:HD23	1.91	0.52
50:B4:15:ILE:O	50:B4:33:VAL:N	2.40	0.52
1:CA:179:A:H2'	1:CA:180:U:C6	2.44	0.52
25:DA:918:A:H5"	26:DB:98:G:O2'	2.09	0.52
25:DA:1278:A:OP1	37:DR:36:THR:HG23	2.08	0.52
25:DA:2727:G:O2'	34:DO:70:LYS:NZ	2.42	0.52
1:AA:1073:U:O2'	2:AB:104:ASN:OD1	2.28	0.52
4:AD:173:TRP:HE1	4:AD:193:ASP:HB3	1.74	0.52
20:AT:90:GLN:O	20:AT:93:GLU:HB3	2.09	0.52
25:BA:599:U:H2'	25:BA:600:G:C8	2.44	0.52
25:BA:1346:U:H4'	25:BA:1347:A:H5'	1.91	0.52
25:BA:2169:G:H2'	25:BA:2170:G:O4'	2.09	0.52
26:BB:83:G:OP1	49:B3:19:GLN:NE2	2.41	0.52
32:BI:65:ALA:HB1	32:BI:136:VAL:HG11	1.91	0.52
35:BP:82:GLY:HA2	35:BP:113:LYS:O	2.09	0.52
43:BX:53:LYS:HB3	43:BX:82:GLN:HB3	1.90	0.52
1:CA:165:C:H2'	1:CA:166:G:C8	2.44	0.52
1:CA:1256:A:N6	1:CA:1278:U:H1'	2.09	0.52
3:CC:54:ARG:NH1	3:CC:56:ASP:OD1	2.42	0.52
6:CF:91:VAL:HG11	18:CR:72:ARG:NH1	2.24	0.52
8:CH:73:ASP:OD1	8:CH:75:ARG:HD3	2.10	0.52
17:CQ:66:SER:OG	17:CQ:69:LYS:HB2	2.08	0.52
25:DA:937:U:H2'	25:DA:938:G:O4'	2.08	0.52
25:DA:2836:U:H2'	25:DA:2837:G:C8	2.44	0.52
28:DE:170:LEU:HB3	28:DE:184:VAL:HG22	1.91	0.52
31:DH:89:ILE:O	31:DH:129:THR:HG23	2.09	0.52
36:DQ:85:LYS:HD3	46:D0:7:LEU:HG	1.92	0.52
40:DU:104:GLN:OE1	40:DU:105:VAL:N	2.39	0.52
1:AA:741:G:H2'	1:AA:742:G:O4'	2.09	0.52
1:AA:1179:A:H4'	9:AI:103:THR:HA	1.90	0.52
2:AB:54:THR:HG21	2:AB:201:ILE:HD11	1.89	0.52
6:AF:45:LEU:HD12	6:AF:59:TYR:HD2	1.74	0.52
11:AK:32:ILE:HG13	11:AK:72:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:934:A:H2	25:BA:936:C:H2'	1.74	0.52
25:BA:2228:G:O2'	25:BA:2229:A:OP1	2.25	0.52
25:BA:2603:C:H2'	25:BA:2604:G:C8	2.44	0.52
29:BF:143:ALA:HB1	29:BF:148:LEU:HB2	1.91	0.52
43:BX:43:VAL:HG21	43:BX:81:VAL:HG11	1.91	0.52
1:CA:833:U:H2'	1:CA:834:C:H6	1.73	0.52
1:CA:1325:C:OP1	21:CU:15:ARG:NE	2.40	0.52
25:DA:220:G:O2'	25:DA:233:A:N3	2.39	0.52
25:DA:1149:G:H2'	25:DA:1150:C:C6	2.45	0.52
42:DW:14:PRO:HG2	42:DW:78:GLU:HG2	1.92	0.52
43:DX:84:ALA:HB3	43:DX:87:GLN:NE2	2.24	0.52
1:AA:1442(B):A:N3	39:BT:118:ARG:NH2	2.57	0.52
10:AJ:35:SER:HB3	10:AJ:73:ASP:HB2	1.91	0.52
13:AM:11:ARG:C	13:AM:13:LYS:H	2.17	0.52
23:AY:18:G:H1	23:AY:55:PSU:H1'	1.74	0.52
25:BA:469:A:H1'	25:BA:1246:C:O4'	2.08	0.52
25:BA:957:A:H2'	36:BQ:9:TYR:OH	2.10	0.52
25:BA:1405:A:H2'	25:BA:1406:A:H5'	1.90	0.52
36:BQ:32:TYR:OH	36:BQ:111:GLU:OE1	2.22	0.52
51:B5:16:ARG:HH11	51:B5:16:ARG:HG2	1.74	0.52
52:B6:34:LEU:HB2	52:B6:51:GLU:HB2	1.91	0.52
1:CA:185:A:N3	20:CT:81:LYS:NZ	2.58	0.52
1:CA:642:A:N3	8:CH:113:SER:OG	2.43	0.52
1:CA:735:C:H2'	1:CA:736:C:H6	1.73	0.52
1:CA:1111:A:N1	3:CC:177:THR:OG1	2.33	0.52
2:CB:163:PHE:HA	2:CB:185:ILE:HG12	1.92	0.52
25:DA:1913:A:H4'	25:DA:1914:C:O5'	2.09	0.52
25:DA:2136:C:O2'	25:DA:2137:C:O5'	2.23	0.52
25:DA:2712:U:H2'	25:DA:2714:G:H5"	1.91	0.52
41:DV:35:LEU:HB2	41:DV:57:VAL:HG22	1.91	0.52
1:AA:438:G:H4'	4:AD:123:HIS:ND1	2.24	0.52
3:AC:16:ARG:NH2	3:AC:183:ASP:OD1	2.36	0.52
5:AE:74:GLY:HA3	5:AE:116:THR:HG22	1.92	0.52
25:BA:153:C:OP2	47:B1:92:LYS:NZ	2.43	0.52
25:BA:847:A:H8	25:BA:847:A:OP1	1.92	0.52
25:BA:924:U:H3	25:BA:945:A:H2	1.56	0.52
25:BA:1094:A:N1	25:BA:1158:G:O2'	2.36	0.52
33:BN:14:VAL:HG11	33:BN:138:LEU:HD12	1.91	0.52
50:B4:53:GLU:C	50:B4:55:ARG:N	2.67	0.52
1:CA:692:U:O2'	1:CA:694:A:N7	2.30	0.52
1:CA:992:U:H3'	1:CA:992:U:OP1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:CA:3178:PCY:H381	7:CG:82:GLY:O	2.10	0.52
5:CE:31:LEU:HD22	5:CE:43:LEU:HD11	1.90	0.52
6:CF:76:ALA:O	6:CF:80:ARG:HG3	2.09	0.52
10:CJ:30:SER:HB2	10:CJ:80:LYS:CB	2.39	0.52
25:DA:192:C:O2'	25:DA:802:A:N3	2.42	0.52
25:DA:361:G:O2'	25:DA:362:U:H5'	2.09	0.52
25:DA:590:A:OP1	29:DF:95:ARG:NH1	2.43	0.52
25:DA:1971:A:OP2	27:DD:242:ARG:NH2	2.42	0.52
33:DN:34:LEU:O	33:DN:49:GLY:HA3	2.09	0.52
36:DQ:34:LEU:HB2	36:DQ:118:LEU:HD22	1.91	0.52
37:DR:44:LEU:HD22	37:DR:48:VAL:HG23	1.91	0.52
1:AA:76:C:H2'	1:AA:77:G:C8	2.44	0.52
1:AA:346:G:C2	1:AA:347:G:H1'	2.44	0.52
1:AA:347:G:H2'	1:AA:348:G:C8	2.44	0.52
1:AA:1320:C:O2	19:AS:36:ARG:NH2	2.38	0.52
1:CA:97:G:O2'	1:CA:98:G:H8	1.93	0.52
1:CA:1002:G:H1	1:CA:1038:C:N4	2.07	0.52
25:DA:1324:G:C2	25:DA:1331:A:C2	2.97	0.52
25:DA:1607:C:H4'	25:DA:1608:A:O5'	2.10	0.52
28:DE:7:VAL:HG12	28:DE:27:LEU:HB3	1.90	0.52
38:DS:77:ALA:HB1	38:DS:82:ILE:HB	1.91	0.52
45:DZ:100:VAL:HG21	45:DZ:134:PRO:HG2	1.91	0.52
1:AA:946:A:H2'	1:AA:947:G:C8	2.44	0.52
1:AA:1158:C:H5	1:AA:1181:G:N1	2.02	0.52
13:AM:3:ARG:HG3	13:AM:8:GLU:HA	1.92	0.52
18:AR:26:LEU:HD23	18:AR:29:PHE:CE2	2.45	0.52
25:BA:1699:A:OP1	37:BR:8:ARG:NH1	2.36	0.52
25:BA:2331:G:H22	38:BS:3:ARG:CZ	2.23	0.52
33:BN:73:THR:HG23	33:BN:82:LEU:HD11	1.91	0.52
47:B1:3:LYS:HB2	47:B1:61:ARG:HH12	1.75	0.52
1:CA:1117:G:N2	1:CA:1180:A:O2'	2.42	0.52
5:CE:12:LEU:HB3	5:CE:31:LEU:HB2	1.91	0.52
8:CH:39:LEU:HD12	8:CH:44:PHE:HB2	1.91	0.52
47:D1:89:GLU:O	47:D1:93:GLU:HG2	2.10	0.52
1:AA:1251:A:H2'	1:AA:1252:A:C8	2.45	0.52
1:AA:1499:A:H1'	1:AA:1520:G:H5'	1.90	0.52
25:BA:482:C:H4'	61:BA:4038:HOH:O	2.09	0.52
25:BA:2148:A:N6	25:BA:2184:G:O2'	2.43	0.52
25:BA:2797:C:H1'	28:BE:37:ARG:NH1	2.25	0.52
38:BS:10:ARG:O	38:BS:14:VAL:HG13	2.09	0.52
1:CA:353:A:H5'	1:CA:353:A:C8	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1222:G:OP1	19:CS:77:THR:HG21	2.10	0.52
6:CF:8:ILE:HD11	6:CF:79:LEU:HD13	1.91	0.52
23:CY:52:G:N1	23:CY:62:C:O2	2.33	0.52
25:DA:190:A:OP2	47:D1:39:LYS:HE3	2.09	0.52
25:DA:492:A:H2'	25:DA:493:G:O4'	2.09	0.52
25:DA:1786:A:H1'	25:DA:1938:A:N6	2.24	0.52
25:DA:2143:C:H2'	25:DA:2144:U:O4'	2.10	0.52
31:DH:90:LYS:HD2	31:DH:163:TYR:CE1	2.45	0.52
8:AH:51:VAL:HG12	8:AH:52:ASP:H	1.75	0.52
26:BB:105:A:OP1	45:BZ:72:ARG:NH1	2.43	0.52
34:BO:2:ILE:HD12	34:BO:6:THR:HG21	1.92	0.52
43:BX:2:LYS:NZ	43:BX:38:GLU:OE2	2.38	0.52
43:BX:54:VAL:HG22	43:BX:81:VAL:HG12	1.92	0.52
2:CB:87:ARG:NH2	2:CB:220:ASP:OD1	2.43	0.52
2:CB:122:PHE:HD1	2:CB:123:ALA:H	1.56	0.52
23:CY:13:C:O2	23:CY:22:G:N1	2.33	0.52
1:AA:189(I):G:H2'	1:AA:189(J):G:H5"	1.92	0.52
15:AO:26:GLU:OE2	15:AO:77:ARG:NE	2.31	0.52
25:BA:310:C:H2'	25:BA:311:C:C6	2.45	0.52
25:BA:427:G:O6	61:BA:5098:HOH:O	2.16	0.52
25:BA:1804:A:OP2	61:BA:4855:HOH:O	2.19	0.52
45:BZ:55:HIS:CE1	45:BZ:135:GLU:HG3	2.45	0.52
1:CA:110:C:H2'	1:CA:111:G:O4'	2.10	0.52
4:CD:173:TRP:CD1	4:CD:189:PRO:HG3	2.45	0.52
6:CF:42:GLU:OE1	6:CF:59:TYR:OH	2.24	0.52
25:DA:242:G:C8	54:D8:5:LYS:HG2	2.45	0.52
25:DA:1296:G:OP1	25:DA:2709:G:O2'	2.25	0.52
25:DA:1859:A:N6	25:DA:1883:G:O2'	2.42	0.52
25:DA:1939:U:OP1	25:DA:2604:U:O2'	2.27	0.52
25:DA:2820:A:O2'	25:DA:2821:A:OP1	2.27	0.52
44:DY:23:ARG:HG2	44:DY:42:VAL:HG22	1.91	0.52
45:DZ:117:LEU:HD23	45:DZ:119:GLU:HG2	1.92	0.52
1:AA:309:G:O2'	1:AA:607:A:N1	2.42	0.51
19:AS:27:GLU:H	19:AS:27:GLU:CD	2.18	0.51
25:BA:2339:A:H2'	25:BA:2340:A:C8	2.45	0.51
43:BX:31:HIS:CD2	43:BX:33:LYS:HB2	2.45	0.51
1:CA:1120:G:C6	1:CA:1121:U:C4	2.98	0.51
1:CA:1512:U:H2'	1:CA:1513:A:C8	2.46	0.51
2:CB:71:VAL:HB	2:CB:164:VAL:HA	1.91	0.51
13:CM:3:ARG:N	50:D4:34:GLU:OE1	2.43	0.51
17:CQ:78:GLU:OE2	17:CQ:81:ARG:NH1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:812:C:H2'	25:DA:813:U:H6	1.74	0.51
25:DA:911:A:H2'	36:DQ:9:TYR:OH	2.10	0.51
25:DA:1028:A:N6	25:DA:1125:G:H2'	2.24	0.51
25:DA:1386:C:H2'	25:DA:1387:C:C6	2.45	0.51
29:DF:20:LEU:HD12	29:DF:125:LEU:HD13	1.92	0.51
34:DO:80:ASP:OD1	39:DT:64:ARG:NH2	2.43	0.51
37:DR:36:THR:HG22	37:DR:37:THR:H	1.75	0.51
1:AA:250:A:H4'	1:AA:251:G:O5'	2.10	0.51
1:AA:583:A:OP2	61:AA:4025:HOH:O	2.19	0.51
6:AF:67:MET:HE1	6:AF:75:LEU:HD12	1.92	0.51
13:AM:19:LEU:HD21	13:AM:56:LEU:HD11	1.91	0.51
24:AX:59:A:C2'	24:AX:60:U:H5'	2.40	0.51
25:BA:572:A:N6	41:BV:19:LYS:H	2.07	0.51
25:BA:595:A:OP2	41:BV:78:LYS:NZ	2.43	0.51
27:BD:242:ARG:HD3	27:BD:242:ARG:N	2.25	0.51
1:CA:1312:G:H1	1:CA:1325:C:N4	2.07	0.51
2:CB:185:ILE:HG22	2:CB:199:TYR:CD2	2.45	0.51
16:CP:43:LYS:HA	16:CP:48:TRP:HB3	1.91	0.51
25:DA:668:G:H5'	25:DA:669:G:OP2	2.11	0.51
25:DA:938:G:OP1	54:D8:52:LYS:HD2	2.10	0.51
25:DA:1429:G:H2'	25:DA:1430:C:C6	2.45	0.51
51:D5:16:ARG:HG2	51:D5:16:ARG:HH11	1.74	0.51
1:AA:28:G:O2'	1:AA:296:U:OP1	2.26	0.51
2:AB:77:ALA:HB2	2:AB:165:VAL:HG11	1.92	0.51
7:AG:48:LYS:O	7:AG:52:GLU:HG2	2.11	0.51
20:AT:54:LYS:HB2	20:AT:100:ILE:HD11	1.93	0.51
25:BA:1604:C:OP2	25:BA:1605:A:O2'	2.22	0.51
25:BA:2623:U:C4	51:B5:3:LYS:HG2	2.44	0.51
28:BE:105:THR:OG1	28:BE:199:ARG:NH2	2.43	0.51
6:CF:41:GLU:OE1	18:CR:35:ARG:NH2	2.42	0.51
7:CG:50:ILE:HD11	7:CG:58:PRO:HA	1.93	0.51
7:CG:138:LYS:NZ	7:CG:142:GLU:OE1	2.42	0.51
23:CW:4:C:N4	23:CW:69:G:C6	2.77	0.51
25:DA:330:A:H2	25:DA:1210:A:O2'	1.93	0.51
1:AA:1036:G:H3'	1:AA:1037:C:C6	2.45	0.51
9:AI:77:ILE:O	9:AI:81:ILE:HG22	2.10	0.51
23:AY:34:G:H2'	23:AY:35:A:C8	2.45	0.51
25:BA:489:G:O6	61:BA:4635:HOH:O	2.18	0.51
25:BA:1212:C:O2'	61:BA:4755:HOH:O	2.19	0.51
37:BR:21:TYR:OH	37:BR:43:GLU:HG2	2.10	0.51
1:CA:1014:A:C2	1:CA:1219:U:H1'	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1005:C:H2'	25:DA:1006:C:C6	2.44	0.51
42:DW:12:ILE:HD13	42:DW:17:VAL:HG13	1.93	0.51
45:DZ:97:GLU:HB2	45:DZ:125:LEU:HD11	1.92	0.51
54:D8:63:PRO:HG2	54:D8:64:TYR:CD2	2.44	0.51
1:AA:49:U:O4	1:AA:365:U:H5	1.94	0.51
9:AI:93:ARG:HH11	9:AI:93:ARG:HB2	1.75	0.51
16:AP:19:ILE:HG22	16:AP:37:GLY:C	2.36	0.51
25:BA:1091:A:OP1	25:BA:1091:A:H4'	2.10	0.51
25:BA:2143:G:H1	25:BA:2199:C:N4	2.08	0.51
25:BA:2797:C:H1'	28:BE:37:ARG:HH12	1.74	0.51
26:BB:2:C:H2'	26:BB:3:C:C6	2.45	0.51
38:BS:15:ARG:O	38:BS:19:LYS:HG2	2.09	0.51
1:CA:142:G:H2'	1:CA:143:A:H8	1.75	0.51
1:CA:920:U:H2'	1:CA:921:U:H6	1.72	0.51
1:CA:1053:G:N7	1:CA:1200:C:H5"	2.26	0.51
3:CC:121:ALA:O	3:CC:125:GLU:HG3	2.11	0.51
8:CH:121:ASP:N	8:CH:121:ASP:OD1	2.41	0.51
18:CR:24:ALA:O	18:CR:26:LEU:N	2.39	0.51
25:DA:580:C:H2'	25:DA:581:C:H6	1.74	0.51
25:DA:637:A:H5"	35:DP:117:GLU:HG2	1.92	0.51
25:DA:1771:C:OP1	61:DA:4530:HOH:O	2.19	0.51
26:DB:14:U:OP2	26:DB:70:C:O2'	2.25	0.51
28:DE:72:VAL:HA	28:DE:73:GLU:CB	2.41	0.51
38:BS:15:ARG:NE	38:BS:88:ASP:OD2	2.37	0.51
40:BU:104:GLN:H	40:BU:104:GLN:CD	2.18	0.51
44:BY:92:ASN:N	44:BY:93:GLY:HA2	2.26	0.51
1:CA:56:U:H2'	1:CA:57:G:C8	2.45	0.51
1:CA:461:A:O2'	1:CA:471:G:N7	2.42	0.51
1:CA:1132:C:H2'	1:CA:1133:G:C8	2.45	0.51
1:CA:1512:U:H2'	1:CA:1513:A:H8	1.76	0.51
25:DA:852:G:H2'	25:DA:853:G:C8	2.45	0.51
25:DA:2640:G:N7	61:DA:4154:HOH:O	2.34	0.51
29:DF:24:LEU:HD21	29:DF:114:VAL:HG12	1.92	0.51
29:DF:156:LEU:HD21	29:DF:163:VAL:HG12	1.92	0.51
31:DH:80:SER:OG	31:DH:81:GLU:OE1	2.26	0.51
40:DU:66:ASN:O	40:DU:70:ARG:HG3	2.10	0.51
1:AA:581:G:OP1	15:AO:65:ARG:NH2	2.43	0.51
1:AA:757:U:H2'	1:AA:758:G:O4'	2.11	0.51
6:AF:70:ASP:OD1	6:AF:70:ASP:N	2.36	0.51
14:AN:23:ARG:NH1	14:AN:30:ALA:HB2	2.25	0.51
15:AO:21:ASP:OD2	15:AO:24:SER:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AP:71:ARG:HG3	16:AP:80:PHE:HE2	1.75	0.51
25:BA:1223:C:H2'	25:BA:1224:C:C6	2.45	0.51
28:BE:9:VAL:HB	39:BT:3:ARG:HG2	1.93	0.51
30:BG:145:THR:OG1	30:BG:148:MET:SD	2.63	0.51
3:CC:3:ASN:OD1	3:CC:3:ASN:N	2.41	0.51
9:CI:3:GLN:OE1	9:CI:20:ARG:NH2	2.43	0.51
25:DA:625:G:O6	35:DP:107:LYS:NZ	2.35	0.51
25:DA:2299:G:N1	25:DA:2318:G:N7	2.59	0.51
33:DN:19:GLU:HA	33:DN:59:LYS:HB2	1.93	0.51
35:DP:44:GLY:CA	35:DP:45:LEU:HB2	2.40	0.51
1:AA:381:C:H2'	1:AA:382:A:O4'	2.10	0.51
1:AA:1202:G:O4'	14:AN:29:ARG:NH1	2.43	0.51
2:AB:21:ARG:H	2:AB:21:ARG:HH21	1.59	0.51
23:AW:18:G:N2	23:AW:57:G:H2'	2.25	0.51
23:AW:18:G:H4'	23:AW:60:U:C5	2.46	0.51
25:BA:720:C:OP1	29:BF:54:ARG:NH1	2.42	0.51
54:B8:23:VAL:HG11	54:B8:47:LYS:HD3	1.93	0.51
1:CA:833:U:H2'	1:CA:834:C:C6	2.46	0.51
25:DA:362:U:O2'	25:DA:363:G:H5"	2.11	0.51
25:DA:1507:A:O2'	25:DA:1508:A:O5'	2.28	0.51
25:DA:1530:C:H42	25:DA:1539:G:H1	1.58	0.51
25:DA:2630:G:H2'	25:DA:2631:G:C8	2.45	0.51
1:AA:437:U:H5'	4:AD:155:LEU:HD21	1.93	0.51
1:AA:1277:C:O2'	1:AA:1279:A:H1'	2.10	0.51
1:AA:1318:A:H5"	19:AS:3:ARG:NH1	2.26	0.51
19:AS:65:ASN:HD22	19:AS:65:ASN:N	2.07	0.51
25:BA:704:U:H2'	25:BA:705:C:H6	1.76	0.51
28:BE:11:MET:HG2	28:BE:24:THR:HB	1.93	0.51
28:BE:12:THR:HG22	28:BE:13:ARG:H	1.76	0.51
37:BR:57:ARG:NE	37:BR:59:ASP:OD1	2.44	0.51
47:B1:85:LEU:HB3	47:B1:89:GLU:HG3	1.93	0.51
2:CB:95:GLN:HB2	2:CB:148:TYR:HD1	1.76	0.51
12:CL:28:LYS:N	12:CL:29:GLY:HA2	2.26	0.51
25:DA:608:A:H2'	25:DA:609:A:C8	2.45	0.51
25:DA:2193:G:H2'	25:DA:2194:G:C8	2.46	0.51
39:DT:16:ARG:NH2	39:DT:83:ILE:O	2.43	0.51
6:AF:37:VAL:HA	6:AF:65:VAL:HG12	1.92	0.51
25:BA:771:U:H2'	25:BA:772:G:O4'	2.11	0.51
25:BA:865:G:O6	61:BA:4412:HOH:O	2.19	0.51
25:BA:2044:U:O2'	25:BA:2629:C:H5'	2.11	0.51
32:BI:81:VAL:O	32:BI:146:ALA:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:748:C:H4'	1:CA:749:C:O5'	2.11	0.51
1:CA:1010:G:N2	1:CA:1020:U:H1'	2.25	0.51
2:CB:134:GLU:O	2:CB:138:LEU:HG	2.10	0.51
30:DG:5:VAL:HG22	30:DG:8:LYS:H	1.76	0.51
31:DH:20:ALA:HB1	31:DH:21:PRO:HD2	1.92	0.51
1:AA:92:C:H2'	1:AA:93:G:C8	2.46	0.50
1:AA:174:C:H2'	1:AA:175:C:H6	1.77	0.50
1:AA:1001:A:H2'	1:AA:1001(A):G:H8	1.76	0.50
6:AF:33:TYR:CD2	6:AF:75:LEU:HD23	2.46	0.50
11:AK:84:VAL:HG11	11:AK:91:ARG:HD2	1.93	0.50
12:AL:117:ARG:HB3	12:AL:122:THR:HB	1.93	0.50
13:AM:11:ARG:HA	13:AM:45:VAL:HB	1.92	0.50
20:AT:56:MET:HE2	20:AT:85:MET:HA	1.93	0.50
25:BA:407:U:OP1	61:BA:4339:HOH:O	2.19	0.50
27:BD:85:ASP:OD2	27:BD:88:ARG:NH1	2.39	0.50
1:CA:953:G:H5'	1:CA:965:A:N6	2.23	0.50
1:CA:986:A:H2'	1:CA:987:G:C8	2.47	0.50
2:CB:15:VAL:HG13	2:CB:209:ARG:HB3	1.93	0.50
25:DA:1025:G:C4	25:DA:1135:C:H1'	2.46	0.50
25:DA:2183:C:H2'	25:DA:2184:G:C8	2.46	0.50
25:DA:2819:G:N7	61:DA:4376:HOH:O	2.34	0.50
27:DD:17:THR:O	27:DD:211:ARG:NH2	2.41	0.50
57:AA:3231:PCY:H40	23:AY:35:A:C2	2.45	0.50
3:AC:164:ARG:HG2	3:AC:165:THR:H	1.76	0.50
17:AQ:67:LYS:HA	17:AQ:70:ARG:HH12	1.76	0.50
25:BA:801:C:H2'	25:BA:802:C:C6	2.46	0.50
25:BA:1040:C:OP1	40:BU:53:ARG:NH2	2.44	0.50
26:BB:82:G:N7	61:BB:3110:HOH:O	2.34	0.50
30:BG:16:ARG:HH21	30:BG:31:VAL:HG11	1.75	0.50
30:BG:75:LYS:HA	30:BG:84:LYS:HE2	1.92	0.50
40:BU:76:TYR:CZ	40:BU:80:ILE:HG13	2.46	0.50
2:CB:47:THR:O	2:CB:51:LEU:N	2.44	0.50
15:CO:87:ILE:HG22	15:CO:88:ARG:N	2.23	0.50
23:CW:4:C:N4	23:CW:69:G:H1	2.10	0.50
25:DA:981:A:N1	25:DA:2027:G:O2'	2.39	0.50
25:DA:992:C:OP1	41:DV:74:LYS:NZ	2.36	0.50
25:DA:2031:A:N3	25:DA:2455:G:O2'	2.38	0.50
25:DA:2846:G:H2'	25:DA:2847:U:O4'	2.11	0.50
31:DH:56:SER:OG	31:DH:57:ASP:N	2.43	0.50
37:DR:29:LEU:HB3	37:DR:75:LEU:HD11	1.93	0.50
2:AB:231:GLU:HB3	2:AB:232:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AY:6:G:O6	23:AY:7:A:N6	2.45	0.50
25:BA:510:C:H2'	25:BA:511:C:C6	2.47	0.50
25:BA:1002:A:H5'	36:BQ:76:LYS:HG3	1.92	0.50
25:BA:1269:G:N2	25:BA:1272:A:OP2	2.36	0.50
37:BR:118:GLU:CD	37:BR:118:GLU:H	2.18	0.50
45:BZ:52:SER:OG	45:BZ:53:ILE:N	2.45	0.50
1:CA:78:G:C2'	1:CA:79:G:H5"	2.37	0.50
1:CA:1035:A:H2'	1:CA:1036:G:H8	1.77	0.50
23:CW:8:4SU:O2'	23:CW:21:A:N6	2.41	0.50
25:DA:531:C:H4'	25:DA:532:A:H5"	1.94	0.50
25:DA:1448:G:H4'	25:DA:1542:A:OP1	2.10	0.50
52:D6:34:LEU:HB2	52:D6:51:GLU:HB2	1.92	0.50
9:AI:50:LEU:HD23	9:AI:81:ILE:HD11	1.94	0.50
2:CB:80:ILE:HD11	2:CB:212:GLN:HA	1.93	0.50
23:CY:2:C:H2'	23:CY:3:C:C6	2.46	0.50
25:DA:76:C:O3'	48:D2:59:ARG:HG3	2.11	0.50
25:DA:443:A:H1'	25:DA:1201:C:O4'	2.10	0.50
1:AA:1254:C:H41	10:AJ:43:ARG:HH12	1.58	0.50
4:AD:127:THR:HA	4:AD:132:ARG:HA	1.93	0.50
8:AH:121:ASP:OD2	8:AH:121:ASP:N	2.43	0.50
13:AM:88:ARG:HG3	13:AM:98:VAL:CG1	2.42	0.50
25:BA:385:G:N1	25:BA:386:U:O4	2.44	0.50
25:BA:721:G:O2'	29:BF:74:ARG:HD3	2.10	0.50
25:BA:2148:A:N6	25:BA:2184:G:HO2'	2.09	0.50
1:CA:1179:A:H4'	9:CI:103:THR:HA	1.93	0.50
6:CF:70:ASP:OD1	6:CF:70:ASP:N	2.27	0.50
9:CI:9:ARG:O	9:CI:104:ARG:HG3	2.12	0.50
9:CI:9:ARG:H	9:CI:79:LEU:HD23	1.77	0.50
17:CQ:95:TYR:HA	17:CQ:98:LEU:HD22	1.94	0.50
25:DA:263:C:O2'	25:DA:429:A:N3	2.42	0.50
25:DA:1946:U:H2'	25:DA:1947:C:C6	2.45	0.50
25:DA:2334:G:H5'	38:DS:9:ARG:HG2	1.93	0.50
25:DA:2830:G:OP1	28:DE:76:ARG:NH2	2.45	0.50
30:DG:23:PHE:HB2	30:DG:25:TYR:CZ	2.47	0.50
31:DH:144:VAL:O	31:DH:148:ILE:HG12	2.12	0.50
1:AA:93:G:H2'	1:AA:96:U:O4'	2.12	0.50
5:AE:50:GLU:HB2	5:AE:53:LEU:HD13	1.94	0.50
20:AT:34:LYS:HZ2	20:AT:80:ARG:HH12	1.59	0.50
23:AY:5:G:H1'	23:AY:69:G:N2	2.25	0.50
25:BA:470:C:H5"	61:BA:4091:HOH:O	2.10	0.50
25:BA:1744:G:OP2	25:BA:1745:A:O2'	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2132:G:C2	25:BA:2142:G:H1'	2.47	0.50
41:BV:40:LEU:HB2	41:BV:46:VAL:HG13	1.93	0.50
1:CA:9:G:H2'	1:CA:10:A:H8	1.77	0.50
1:CA:297:G:N2	1:CA:300:A:OP2	2.45	0.50
1:CA:1186:G:H21	14:CN:61:TRP:C	2.20	0.50
2:CB:224:GLN:HG2	2:CB:225:ALA:N	2.27	0.50
8:CH:82:HIS:N	8:CH:138:TRP:O	2.42	0.50
25:DA:2655:G:O2'	25:DA:2664:G:O6	2.28	0.50
28:DE:111:ARG:HG3	28:DE:160:TYR:CD2	2.46	0.50
30:DG:48:GLU:O	30:DG:51:ARG:HG3	2.12	0.50
35:DP:81:GLN:NE2	35:DP:105:LEU:O	2.44	0.50
1:AA:8:A:H5'	5:AE:101:ILE:HG22	1.93	0.50
1:AA:69:G:H2'	1:AA:70:G:H8	1.76	0.50
1:AA:96:U:O2'	1:AA:97:G:H5'	2.11	0.50
1:AA:833:U:H2'	1:AA:834:C:C6	2.47	0.50
1:AA:1027:C:N3	1:AA:1034:G:C6	2.80	0.50
1:AA:1027:C:O2	1:AA:1034:G:C2	2.65	0.50
1:AA:1318:A:H5"	19:AS:3:ARG:HH12	1.77	0.50
11:AK:45:GLY:O	11:AK:50:TYR:HB2	2.11	0.50
23:AW:56:C:P	25:BA:943:C:H5'	2.52	0.50
25:BA:2235:G:OP1	27:BD:172:TYR:OH	2.24	0.50
25:BA:2389:A:H2'	25:BA:2390:A:C8	2.47	0.50
25:BA:2885:C:O2'	39:BT:2:ASN:OD1	2.26	0.50
38:BS:15:ARG:HE	38:BS:88:ASP:CG	2.19	0.50
1:CA:1310:G:H5'	13:CM:77:ASN:ND2	2.26	0.50
1:CA:1399:C:H4'	1:CA:1400:C:O5'	2.12	0.50
23:CY:26:A:N1	23:CY:44:G:C6	2.79	0.50
26:DB:9:G:H1	26:DB:112:U:H3	1.58	0.50
39:DT:85:LYS:NZ	39:DT:87:ASP:OD2	2.43	0.50
1:AA:21:G:OP1	61:AA:4120:HOH:O	2.19	0.50
2:AB:109:SER:HA	2:AB:112:VAL:HG13	1.94	0.50
8:AH:21:LYS:O	8:AH:65:TYR:OH	2.27	0.50
25:BA:555:G:O4'	25:BA:555:G:N3	2.43	0.50
25:BA:1298:G:OP1	40:BU:36:ARG:NH2	2.45	0.50
25:BA:2155:G:H21	25:BA:2180:A:H62	1.58	0.50
33:BN:62:VAL:HG22	33:BN:66:LYS:HD2	1.92	0.50
44:BY:55:TYR:N	44:BY:55:TYR:CD2	2.80	0.50
1:CA:222:U:H2'	1:CA:223:U:C6	2.46	0.50
1:CA:1346:A:N1	1:CA:1374:A:H5"	2.27	0.50
2:CB:13:ALA:C	2:CB:15:VAL:H	2.20	0.50
25:DA:1009:A:H5'	40:DU:59:ARG:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:D4:46:GLN:C	50:D4:48:ARG:H	2.20	0.50
10:AJ:11:PHE:HE1	10:AJ:67:THR:HG22	1.76	0.50
25:BA:489:G:OP2	61:BA:5265:HOH:O	2.20	0.50
25:BA:2116:G:P	32:BI:22:LYS:HD2	2.52	0.50
35:BP:59:LEU:HD22	54:B8:13:ARG:HD2	1.94	0.50
40:BU:86:ALA:O	41:BV:49:THR:HG23	2.12	0.50
1:CA:349:A:C2'	1:CA:350:G:H5"	2.38	0.50
1:CA:1004:A:H5"	1:CA:1025:U:C5	2.47	0.50
1:CA:1347:G:N2	1:CA:1373:G:H2'	2.27	0.50
3:CC:78:GLY:HA3	3:CC:83:ARG:H	1.77	0.50
4:CD:149:ALA:HB3	4:CD:152:SER:HB2	1.94	0.50
5:CE:140:ARG:O	5:CE:143:ARG:NH2	2.45	0.50
6:CF:45:LEU:HD12	6:CF:59:TYR:CD2	2.46	0.50
9:CI:121:ARG:NH1	9:CI:122:ALA:O	2.44	0.50
23:CY:8:4SU:S4	23:CY:14:A:N7	2.85	0.50
25:DA:274:G:H2'	25:DA:275:G:C8	2.46	0.50
45:DZ:111:VAL:HG13	45:DZ:117:LEU:H	1.77	0.50
1:AA:1068:G:OP2	1:AA:1068:G:H8	1.95	0.49
1:AA:1122:U:H2'	1:AA:1123:A:O4'	2.12	0.49
4:AD:164:ALA:C	4:AD:168:ARG:HH11	2.19	0.49
25:BA:2495:C:N3	36:BQ:124:LYS:NZ	2.58	0.49
32:BI:66:GLU:HA	32:BI:69:LYS:HB3	1.94	0.49
38:BS:34:HIS:ND1	38:BS:53:SER:OG	2.35	0.49
50:B4:56:VAL:O	50:B4:60:GLN:HG3	2.12	0.49
1:CA:811:C:O2'	1:CA:901:A:N1	2.41	0.49
1:CA:947:G:H1	1:CA:1234:C:N4	2.09	0.49
1:CA:1123:A:O3'	10:CJ:36:GLY:HA3	2.12	0.49
15:CO:15:PHE:CE2	15:CO:84:LYS:HD3	2.47	0.49
20:CT:77:ALA:O	20:CT:81:LYS:HG3	2.11	0.49
25:DA:587:C:OP2	35:DP:21:ARG:NH2	2.45	0.49
25:DA:1155:A:H3'	61:DA:4617:HOH:O	2.11	0.49
25:DA:2124:G:N2	25:DA:2174:C:N3	2.58	0.49
25:DA:2313:C:H4'	30:DG:91:ARG:HG3	1.94	0.49
25:DA:2331:G:O2'	25:DA:2336:A:N1	2.37	0.49
25:DA:2502:G:H5"	25:DA:2503:A:H5"	1.94	0.49
25:DA:2741:A:H2'	25:DA:2742:C:O4'	2.12	0.49
28:DE:174:ASP:OD1	28:DE:175:VAL:N	2.45	0.49
42:DW:71:VAL:HA	42:DW:107:LEU:HD12	1.94	0.49
1:AA:174:C:H2'	1:AA:175:C:C6	2.47	0.49
1:AA:524:G:H2'	1:AA:525:C:C6	2.47	0.49
1:AA:590:C:O2	1:AA:649:G:N2	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:922:G:C6	1:AA:923:A:C6	3.00	0.49
2:AB:231:GLU:HB3	2:AB:232:PRO:CD	2.42	0.49
25:BA:1517:G:H5"	25:BA:1518:A:OP1	2.12	0.49
30:BG:131:TYR:HB3	30:BG:159:VAL:HG13	1.93	0.49
31:BH:154:PRO:HB3	31:BH:163:TYR:CZ	2.47	0.49
1:CA:973:G:H3'	1:CA:974:A:H5"	1.94	0.49
1:CA:1035:A:H2'	1:CA:1036:G:C8	2.47	0.49
7:CG:111:ARG:NH2	7:CG:126:ASP:OD2	2.45	0.49
24:CX:76:A:H3'	25:DA:2585:U:C5	2.47	0.49
25:DA:1639:U:H4'	25:DA:2699:C:H4'	1.93	0.49
25:DA:2148:G:H2'	25:DA:2149:G:C8	2.47	0.49
36:DQ:108:GLY:HA3	45:DZ:116:VAL:HG13	1.93	0.49
38:DS:93:LYS:CD	38:DS:95:HIS:HB2	2.42	0.49
1:AA:1060:C:C5	3:AC:2:GLY:HA3	2.48	0.49
3:AC:87:LEU:O	3:AC:91:LEU:N	2.36	0.49
25:BA:1155:C:H5'	25:BA:1156:G:OP2	2.11	0.49
32:BI:106:GLY:HA2	32:BI:107:VAL:O	2.12	0.49
1:CA:532:A:H2	1:CA:1206:G:H21	1.60	0.49
1:CA:1104:G:H4'	2:CB:111:ARG:NH1	2.26	0.49
23:CW:25:C:H2'	23:CW:26:A:H8	1.76	0.49
25:DA:921:G:H4'	25:DA:2269:A:C5	2.47	0.49
30:DG:108:ASN:HB3	50:D4:22:ILE:HD13	1.95	0.49
38:DS:78:LEU:HD11	38:DS:108:GLY:O	2.12	0.49
11:AK:81:ASP:OD1	11:AK:107:SER:OG	2.25	0.49
23:AW:4:C:H2'	23:AW:5:G:C8	2.46	0.49
25:BA:1067:A:H3'	25:BA:1067:A:H8	1.77	0.49
25:BA:2357:G:H4'	25:BA:2358:A:H5"	1.94	0.49
25:BA:2710:U:H2'	25:BA:2711:C:C6	2.47	0.49
28:BE:170:LEU:HB3	28:BE:184:VAL:HG22	1.93	0.49
31:BH:164:TYR:N	31:BH:167:GLU:OE1	2.42	0.49
32:BI:77:LEU:HB3	32:BI:142:VAL:HG12	1.94	0.49
1:CA:185:A:H5'	20:CT:74:LYS:HE2	1.94	0.49
1:CA:1178:G:N2	1:CA:1180:A:H3'	2.28	0.49
2:CB:185:ILE:HG22	2:CB:199:TYR:HD2	1.77	0.49
5:CE:38:GLN:N	5:CE:38:GLN:HE21	2.10	0.49
25:DA:276:A:H5"	25:DA:277:C:H5'	1.94	0.49
25:DA:657:U:H2'	25:DA:658:C:C6	2.46	0.49
25:DA:1589:C:H2'	25:DA:1590:U:H6	1.77	0.49
25:DA:2529:G:H5"	25:DA:2530:A:H5"	1.94	0.49
25:DA:2537:U:H2'	25:DA:2538:C:C6	2.47	0.49
31:DH:4:ILE:HG22	31:DH:69:ARG:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:DI:130:TYR:HD2	32:DI:138:ILE:HD12	1.78	0.49
1:AA:1399:C:C2	1:AA:1502:A:N6	2.81	0.49
2:AB:17:PHE:HB2	2:AB:44:LEU:HD21	1.94	0.49
2:AB:59:GLU:HB2	2:AB:221:LEU:HG	1.94	0.49
6:AF:89:MET:HE1	18:AR:72:ARG:HB3	1.94	0.49
19:AS:3:ARG:HE	19:AS:7:LYS:HB2	1.78	0.49
25:BA:125:A:H5"	25:BA:126:C:C6	2.48	0.49
25:BA:739:C:O2'	27:BD:38:LYS:NZ	2.46	0.49
25:BA:2626:A:OP1	61:BA:4516:HOH:O	2.19	0.49
32:BI:129:THR:HG22	32:BI:139:GLN:HE22	1.76	0.49
48:B2:16:LEU:O	48:B2:67:LYS:NZ	2.46	0.49
53:B7:12:ARG:NH2	53:B7:44:PRO:HB3	2.27	0.49
1:CA:184:G:H2'	1:CA:185:A:H8	1.77	0.49
1:CA:193:C:H2'	1:CA:194:C:C6	2.47	0.49
1:CA:787:A:C2	57:CA:3178:PCY:H111	2.48	0.49
12:CL:70:ILE:HD13	12:CL:77:LEU:HD12	1.94	0.49
18:CR:53:ARG:HH21	18:CR:59:SER:HA	1.77	0.49
25:DA:839:U:H2'	25:DA:840:C:C6	2.46	0.49
25:DA:2125:G:H1	25:DA:2172:U:P	2.35	0.49
29:DF:165:ARG:HG2	29:DF:168:ARG:NH2	2.28	0.49
39:DT:19:LEU:HD22	39:DT:86:ILE:HG13	1.93	0.49
47:D1:24:ALA:HA	47:D1:32:LYS:HD2	1.95	0.49
1:AA:1025:U:O2	1:AA:1036:G:C6	2.62	0.49
1:AA:1034:G:H2'	1:AA:1035:A:H8	1.72	0.49
2:AB:98:LEU:HD12	2:AB:101:MET:HE3	1.94	0.49
4:AD:175:SER:HB3	4:AD:186:LEU:HD11	1.93	0.49
25:BA:630:U:OP1	29:BF:102:PRO:HA	2.12	0.49
25:BA:779:C:OP1	61:BA:4829:HOH:O	2.19	0.49
25:BA:801:C:H2'	25:BA:802:C:H6	1.78	0.49
25:BA:1553:A:O2'	25:BA:1554:A:O4'	2.30	0.49
25:BA:1589:A:O2'	61:BA:5331:HOH:O	2.20	0.49
27:BD:107:ALA:O	61:BD:416:HOH:O	2.20	0.49
29:BF:89:VAL:HG12	29:BF:90:PHE:CD2	2.48	0.49
44:BY:35:TYR:CE2	44:BY:69:ALA:HB3	2.47	0.49
1:CA:153:C:H2'	1:CA:154:C:C6	2.47	0.49
1:CA:1016:A:H2'	1:CA:1017:G:O4'	2.12	0.49
1:CA:1030:C:N4	1:CA:1032:G:O6	2.45	0.49
1:CA:1305:G:H5'	21:CU:4:GLY:HA3	1.94	0.49
57:CA:3178:PCY:O21	57:CA:3178:PCY:O36	2.29	0.49
4:CD:111:ALA:HB1	4:CD:116:GLN:HB3	1.94	0.49
8:CH:64:LYS:HD2	8:CH:79:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:CU:13:ILE:HG12	21:CU:22:ARG:NH2	2.28	0.49
24:CX:47:U:N3	24:CX:50:U:OP1	2.45	0.49
25:DA:184:C:H2'	25:DA:185:U:C6	2.47	0.49
25:DA:271(O):C:H2'	25:DA:271(P):C:C6	2.48	0.49
25:DA:1006:C:C2	25:DA:1138:G:N2	2.81	0.49
45:DZ:52:SER:OG	45:DZ:54:HIS:ND1	2.42	0.49
45:DZ:53:ILE:HD13	45:DZ:99:TYR:HB2	1.94	0.49
1:AA:131:C:H2'	1:AA:132:C:C6	2.48	0.49
1:AA:1066:C:O2'	1:AA:1067:A:H5'	2.13	0.49
4:AD:163:GLU:C	4:AD:165:MET:H	2.21	0.49
25:BA:2348:A:H61	46:B0:43:THR:HG22	1.78	0.49
27:BD:2:ALA:HA	27:BD:200:ASP:OD2	2.12	0.49
27:BD:12:SER:HB3	27:BD:208:LYS:HB3	1.94	0.49
39:BT:11:GLU:OE1	39:BT:57:PHE:HB3	2.13	0.49
52:B6:6:ARG:NH1	52:B6:26:ASN:HB2	2.27	0.49
1:CA:519:C:OP2	12:CL:50:SER:OG	2.31	0.49
1:CA:1149:C:H2'	1:CA:1150:U:C6	2.48	0.49
1:CA:1305:G:O2'	1:CA:1331:G:N2	2.45	0.49
25:DA:298:G:H5"	25:DA:299:A:OP1	2.13	0.49
25:DA:576:U:OP1	61:DA:4464:HOH:O	2.19	0.49
25:DA:643:A:N1	25:DA:2369:A:O2'	2.43	0.49
29:DF:192:LEU:HD13	29:DF:194:MET:HE2	1.95	0.49
31:DH:3:ARG:HD3	31:DH:54:ARG:HH12	1.76	0.49
3:AC:11:ARG:HB3	3:AC:15:THR:HB	1.94	0.49
13:AM:79:LYS:HA	13:AM:82:MET:HE2	1.93	0.49
17:AQ:62:SER:HB3	17:AQ:72:ARG:HD2	1.94	0.49
24:AX:8:4SU:O5'	24:AX:8:4SU:H6	2.13	0.49
25:BA:709:G:H5"	35:BP:16:ARG:HG2	1.93	0.49
25:BA:860:U:H2'	25:BA:861:C:C6	2.48	0.49
25:BA:1424:A:OP1	53:B7:10:ARG:NH2	2.46	0.49
25:BA:2856:G:H2'	25:BA:2857:U:O4'	2.13	0.49
28:BE:59:VAL:HG21	28:BE:74:PRO:HB3	1.93	0.49
29:BF:53:THR:CG2	29:BF:55:GLY:H	2.25	0.49
1:CA:1028:C:C2	1:CA:1033:G:C6	3.00	0.49
2:CB:48:MET:HA	2:CB:51:LEU:HB2	1.95	0.49
17:CQ:13:ASP:C	17:CQ:15:MET:H	2.20	0.49
25:DA:2137:C:H2'	25:DA:2138:C:C6	2.47	0.49
25:DA:2650:U:H2'	25:DA:2651:C:C6	2.47	0.49
25:DA:2784:C:H1'	28:DE:37:ARG:HH12	1.77	0.49
26:DB:75:G:HO2'	45:DZ:85:HIS:CE1	2.27	0.49
35:DP:95:VAL:HG13	35:DP:125:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DQ:37:LEU:HD11	36:DQ:130:LYS:HB2	1.94	0.49
37:DR:2:ARG:NH1	37:DR:5:LYS:O	2.46	0.49
25:BA:2245:U:H2'	25:BA:2246:G:C8	2.47	0.49
25:BA:2784:C:H2'	25:BA:2785:C:C6	2.48	0.49
25:BA:2880:C:H2'	25:BA:2881:C:O4'	2.13	0.49
50:B4:63:TYR:N	50:B4:63:TYR:CD1	2.78	0.49
1:CA:946:A:H2'	1:CA:947:G:C8	2.48	0.49
1:CA:1009:G:H22	1:CA:1021:G:H1'	1.75	0.49
1:CA:1106:G:H5"	3:CC:172:ARG:HG2	1.94	0.49
2:CB:17:PHE:HB2	2:CB:44:LEU:HD11	1.95	0.49
6:CF:67:MET:HE1	6:CF:75:LEU:HD12	1.95	0.49
10:CJ:42:THR:HG23	10:CJ:68:HIS:HA	1.94	0.49
19:CS:49:ILE:HD13	19:CS:62:ILE:HD13	1.95	0.49
25:DA:71:A:N7	43:DX:31:HIS:HE1	2.11	0.49
25:DA:146:G:O6	61:DA:4857:HOH:O	2.17	0.49
25:DA:1782:C:O2	25:DA:2608:G:O2'	2.31	0.49
25:DA:2078:C:C4	25:DA:2079:U:C4	3.01	0.49
25:DA:2647:U:H2'	25:DA:2648:C:C6	2.48	0.49
26:DB:13:A:O2'	26:DB:14:U:H3'	2.12	0.49
29:DF:116:ASP:OD2	35:DP:1:MET:N	2.40	0.49
38:DS:15:ARG:O	38:DS:19:LYS:HG2	2.12	0.49
1:AA:1244:C:OP1	21:AU:9:ARG:HB2	2.13	0.49
2:AB:128:GLU:HB2	2:AB:135:GLN:NE2	2.28	0.49
5:AE:140:ARG:O	5:AE:143:ARG:NH2	2.46	0.49
17:AQ:45:HIS:NE2	17:AQ:47:PRO:HG3	2.28	0.49
25:BA:956:A:N1	25:BA:2289:G:H1'	2.28	0.49
29:BF:51:THR:O	29:BF:93:LYS:HE2	2.13	0.49
44:BY:86:ARG:HH11	44:BY:100:ALA:HB1	1.78	0.49
1:CA:202:U:O2'	1:CA:203:U:O5'	2.26	0.49
1:CA:662:G:H2'	1:CA:663:A:C8	2.48	0.49
1:CA:1000:U:H3	1:CA:1041:A:N6	2.05	0.49
2:CB:52:GLU:HG2	2:CB:56:ARG:HH22	1.78	0.49
11:CK:45:GLY:O	11:CK:50:TYR:HB2	2.12	0.49
25:DA:861:A:N3	26:DB:79:C:O2'	2.41	0.49
25:DA:1168:G:H2'	25:DA:1169:G:C8	2.48	0.49
25:DA:2116:G:H5'	25:DA:2117:A:OP2	2.13	0.49
25:DA:2156:G:H2'	25:DA:2157:G:C2	2.48	0.49
26:DB:24:G:H4'	26:DB:25:A:C8	2.47	0.49
30:DG:68:PRO:HB3	30:DG:92:VAL:HB	1.95	0.49
45:DZ:126:VAL:CG1	45:DZ:161:VAL:HG23	2.40	0.49
1:AA:972:C:OP2	10:AJ:57:LYS:NZ	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:32:ILE:HD13	2:AB:40:HIS:CD2	2.48	0.48
23:AY:48:C:C2	23:AY:59:U:H1'	2.48	0.48
25:BA:625:G:O2'	25:BA:702:A:N6	2.46	0.48
25:BA:1815:A:OP2	61:BA:4831:HOH:O	2.20	0.48
28:BE:31:CYS:HB3	28:BE:49:LEU:HG	1.95	0.48
29:BF:185:ASP:HA	29:BF:188:ARG:HD3	1.95	0.48
34:BO:87:ILE:HD12	34:BO:91:LEU:HA	1.94	0.48
1:CA:189(F):U:O2	17:CQ:63:ARG:NH2	2.46	0.48
1:CA:434:U:H2'	1:CA:435:C:C6	2.47	0.48
25:DA:897:C:H3'	25:DA:898:C:C6	2.46	0.48
25:DA:947:G:H2'	25:DA:948:G:C8	2.48	0.48
25:DA:1430:C:H2'	25:DA:1431:U:H6	1.76	0.48
25:DA:1507:A:O2'	25:DA:1508:A:O4'	2.31	0.48
25:DA:2756:U:H1'	25:DA:2757:A:H5"	1.95	0.48
25:DA:2820:A:O5'	37:DR:4:LEU:HD23	2.13	0.48
30:DG:72:ARG:NH1	30:DG:87:PRO:HG3	2.28	0.48
1:AA:346:G:H3'	1:AA:347:G:H4'	1.94	0.48
1:AA:1236:A:H4'	1:AA:1304:G:H4'	1.94	0.48
25:BA:1733:C:H2'	25:BA:1734:G:O4'	2.13	0.48
25:BA:2073:A:H5'	25:BA:2590:G:O4'	2.13	0.48
25:BA:2203:G:O2'	25:BA:2204:G:OP1	2.26	0.48
36:BQ:1:MET:HE2	36:BQ:45:GLN:HA	1.95	0.48
1:CA:26:A:N6	1:CA:558:G:O2'	2.43	0.48
1:CA:194:C:O3'	20:CT:68:LYS:HD2	2.13	0.48
1:CA:1316:G:N1	1:CA:1319:A:OP2	2.46	0.48
5:CE:78:HIS:HA	8:CH:105:ARG:HG3	1.96	0.48
9:CI:77:ILE:O	9:CI:81:ILE:HG22	2.13	0.48
19:CS:20:LEU:HD23	19:CS:23:ASN:HD22	1.77	0.48
23:CW:34:G:H2'	23:CW:35:A:C8	2.47	0.48
25:DA:307:G:H21	25:DA:330:A:H62	1.61	0.48
25:DA:819:A:OP2	25:DA:1187:G:N2	2.31	0.48
25:DA:1231:G:H2'	25:DA:1232:G:H8	1.78	0.48
25:DA:1335:U:OP1	43:DX:65:ARG:NH2	2.46	0.48
25:DA:1641:A:H2'	25:DA:1642:G:O4'	2.13	0.48
25:DA:2365:G:O6	54:D8:39:LYS:HE3	2.12	0.48
45:DZ:110:GLY:O	45:DZ:174:VAL:HG11	2.13	0.48
54:D8:31:HIS:ND1	54:D8:32:LEU:HD13	2.28	0.48
1:AA:347:G:H3'	1:AA:348:G:H5"	1.96	0.48
1:AA:473:G:H2'	1:AA:474:G:H8	1.78	0.48
1:AA:1298:C:H4'	1:AA:1299:A:O4'	2.13	0.48
10:AJ:11:PHE:HB3	14:AN:55:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AN:6:LEU:HB3	14:AN:23:ARG:NH2	2.28	0.48
25:BA:933:C:OP1	25:BA:933:C:H4'	2.13	0.48
27:BD:39:LYS:NZ	27:BD:57:GLY:O	2.44	0.48
35:BP:121:LYS:HB3	35:BP:123:LEU:HG	1.95	0.48
42:BW:71:VAL:HA	42:BW:107:LEU:HD12	1.96	0.48
42:BW:79:GLY:HA3	42:BW:100:THR:HG22	1.94	0.48
1:CA:337:C:H2'	1:CA:338:A:C8	2.48	0.48
1:CA:1004:A:H2'	1:CA:1038:C:H1'	1.95	0.48
1:CA:1228:C:H2'	1:CA:1229:A:H8	1.78	0.48
1:CA:1457:G:H5"	20:CT:35:THR:HG21	1.95	0.48
23:CW:76:A:H4'	25:DA:2506:U:O2'	2.12	0.48
25:DA:443:A:N7	29:DF:45:ARG:HG2	2.28	0.48
25:DA:1778:U:H2'	25:DA:1784:A:N6	2.27	0.48
25:DA:2128:C:H1'	25:DA:2173:A:O2'	2.12	0.48
28:DE:9:VAL:HG22	28:DE:25:VAL:HB	1.95	0.48
28:DE:11:MET:HG2	28:DE:24:THR:HB	1.96	0.48
28:DE:119:ARG:HB3	28:DE:120:TRP:CD1	2.48	0.48
35:DP:2:LYS:HG2	35:DP:5:ASP:CG	2.38	0.48
1:AA:447:G:H2'	1:AA:485:G:N2	2.28	0.48
1:AA:620:C:H2'	1:AA:621:A:O4'	2.14	0.48
8:AH:82:HIS:N	8:AH:138:TRP:O	2.47	0.48
23:AW:62:C:H2'	23:AW:63:G:H8	1.79	0.48
25:BA:63:A:H1'	43:BX:66:LEU:HB2	1.94	0.48
25:BA:1038:C:OP1	41:BV:74:LYS:NZ	2.39	0.48
25:BA:2033:U:OP1	42:BW:42:ARG:NH1	2.43	0.48
25:BA:2486:C:H5"	25:BA:2487:C:OP2	2.13	0.48
30:BG:7:LEU:HD11	30:BG:107:LEU:HD12	1.96	0.48
32:BI:116:LEU:HD21	32:BI:119:PRO:HA	1.96	0.48
1:CA:1002:G:C5	1:CA:1003:G:C8	3.02	0.48
1:CA:1126:U:H3	10:CJ:40:LEU:HD11	1.78	0.48
1:CA:1317:C:OP2	14:CN:17:LYS:HE3	2.13	0.48
5:CE:24:ARG:NH1	22:CV:24:A:OP2	2.46	0.48
6:CF:2:ARG:NE	6:CF:69:GLU:HG2	2.28	0.48
19:CS:28:LYS:HB2	19:CS:29:ARG:CA	2.42	0.48
25:DA:2245:U:O2'	25:DA:2436:G:OP2	2.30	0.48
3:AC:35:GLU:CD	3:AC:59:ARG:HH22	2.22	0.48
15:AO:5:LYS:H	15:AO:5:LYS:HD2	1.78	0.48
23:AY:33:U:H3'	23:AY:34:G:H5"	1.95	0.48
25:BA:390:G:H2'	25:BA:391:G:C8	2.49	0.48
25:BA:2482:G:OP1	36:BQ:56:ARG:NH2	2.47	0.48
42:BW:25:ARG:NH2	42:BW:74:ALA:O	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:601:C:H2'	1:CA:602:A:C8	2.49	0.48
1:CA:986:A:H1'	19:CS:55:LYS:HA	1.95	0.48
1:CA:1002:G:C4	1:CA:1003:G:C8	2.99	0.48
1:CA:1316:G:H22	1:CA:1319:A:H5"	1.79	0.48
1:CA:1442:G:O2'	1:CA:1442(A):G:OP1	2.30	0.48
9:CI:23:ASN:HB2	9:CI:25:LYS:HE3	1.94	0.48
25:DA:143:G:C2	25:DA:143(A):C:C2	3.02	0.48
30:DG:179:PRO:HB2	50:D4:42:PHE:HE1	1.78	0.48
33:DN:123:TYR:HH	33:DN:130:HIS:CD2	2.27	0.48
1:AA:486:U:H2'	1:AA:487:A:H8	1.77	0.48
1:AA:628:G:H2'	1:AA:629:G:C8	2.49	0.48
1:AA:1029:C:N3	1:AA:1032:G:O6	2.46	0.48
25:BA:1093:G:H2'	25:BA:1156:G:H22	1.77	0.48
42:BW:48:ALA:O	42:BW:52:GLU:HB2	2.13	0.48
1:CA:73:G:C6	1:CA:97:G:C6	3.02	0.48
1:CA:174:C:H2'	1:CA:175:C:H6	1.79	0.48
1:CA:522:C:OP2	12:CL:69:TYR:OH	2.25	0.48
1:CA:1008:C:H2'	1:CA:1009:G:O4'	2.13	0.48
1:CA:1103:C:OP1	2:CB:96:ARG:NH2	2.47	0.48
7:CG:113:GLU:CG	7:CG:119:ARG:HG2	2.44	0.48
11:CK:15:ALA:HA	11:CK:76:GLY:O	2.13	0.48
25:DA:1354:A:H2'	25:DA:1355:G:O4'	2.13	0.48
25:DA:1358:G:O2'	25:DA:1359:A:H5"	2.14	0.48
25:DA:1991:U:H2'	25:DA:1992:G:H5"	1.95	0.48
25:DA:2042:A:OP1	61:DA:4181:HOH:O	2.20	0.48
1:AA:738:C:H2'	1:AA:739:C:H6	1.78	0.48
1:AA:750:G:O2'	15:AO:22:THR:O	2.25	0.48
1:AA:1292:U:OP2	7:AG:41:ARG:NH2	2.47	0.48
3:AC:18:TRP:HE3	3:AC:18:TRP:H	1.60	0.48
7:AG:153:HIS:HA	7:AG:155:ARG:NH2	2.29	0.48
25:BA:185:A:N3	25:BA:185:A:H2'	2.29	0.48
25:BA:671:A:H2'	25:BA:672:G:O4'	2.13	0.48
25:BA:821:A:N3	25:BA:821:A:H2'	2.29	0.48
25:BA:1845:G:H4'	27:BD:51:VAL:HG21	1.96	0.48
25:BA:2760:G:O6	25:BA:2768:C:H5"	2.13	0.48
25:BA:2802:C:O2'	25:BA:2803:A:H4'	2.14	0.48
26:BB:7:G:H5"	26:BB:7:G:H8	1.78	0.48
43:BX:60:ARG:HA	43:BX:75:ASP:OD2	2.14	0.48
1:CA:171:A:H2'	1:CA:172:A:C8	2.49	0.48
1:CA:1051:C:H2'	1:CA:1052:U:H6	1.79	0.48
1:CA:1064:G:O6	1:CA:1191:A:N6	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1129:C:H1'	1:CA:1130:A:N7	2.28	0.48
24:CX:59:A:H2'	24:CX:60:U:H5'	1.95	0.48
25:DA:322:A:H5'	25:DA:340:A:H1'	1.95	0.48
25:DA:997:G:OP1	40:DU:92:ARG:HG2	2.12	0.48
25:DA:1204:A:H61	25:DA:1240:U:H2'	1.79	0.48
25:DA:2059:A:O2'	29:DF:69:HIS:HD2	1.97	0.48
33:DN:82:LEU:HD23	33:DN:84:LYS:HE2	1.96	0.48
39:DT:11:GLU:O	39:DT:15:VAL:HG23	2.14	0.48
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.49	0.48
3:AC:181:ASN:HD22	3:AC:204:LEU:HB2	1.77	0.48
25:BA:2627:U:H2'	25:BA:2628:C:H6	1.79	0.48
29:BF:164:ARG:O	29:BF:168:ARG:HB2	2.14	0.48
35:BP:59:LEU:HD21	54:B8:10:ALA:HA	1.95	0.48
36:BQ:135:ASP:N	36:BQ:138:ASP:OD2	2.34	0.48
45:BZ:65:GLN:HB3	45:BZ:67:LEU:HD21	1.95	0.48
50:B4:53:GLU:HG3	50:B4:55:ARG:N	2.29	0.48
4:CD:150:GLU:HA	4:CD:153:ARG:HE	1.79	0.48
7:CG:132:GLY:O	7:CG:136:LYS:HG2	2.14	0.48
9:CI:24:GLY:HA2	9:CI:59:PHE:O	2.14	0.48
25:DA:249:C:O2	54:D8:12:LYS:NZ	2.43	0.48
1:AA:486:U:H2'	1:AA:487:A:C8	2.49	0.48
1:AA:1053:G:H4'	1:AA:1054:C:H5'	1.94	0.48
7:AG:111:ARG:HB3	7:AG:113:GLU:OE2	2.14	0.48
10:AJ:6:ILE:HA	10:AJ:97:GLU:O	2.14	0.48
19:AS:51:VAL:O	19:AS:58:VAL:N	2.43	0.48
25:BA:2327:G:H2'	25:BA:2328:C:C6	2.49	0.48
42:BW:14:PRO:HG2	42:BW:78:GLU:CG	2.43	0.48
44:BY:99:CYS:HB2	44:BY:106:LEU:HD21	1.95	0.48
1:CA:757:U:H2'	1:CA:758:G:O4'	2.13	0.48
1:CA:973:G:OP1	10:CJ:57:LYS:NZ	2.42	0.48
1:CA:976:G:C8	1:CA:1358:U:C2	3.02	0.48
1:CA:1060:C:H5'	10:CJ:51:ARG:HB3	1.96	0.48
2:CB:16:HIS:HB2	2:CB:204:ASN:CB	2.43	0.48
18:CR:33:ASP:OD2	18:CR:36:ASN:HB2	2.14	0.48
23:CY:38:A:H2'	23:CY:39:PSU:O4'	2.13	0.48
25:DA:322:A:OP1	29:DF:168:ARG:HD2	2.13	0.48
25:DA:2029:G:H2'	25:DA:2031:A:OP1	2.14	0.48
25:DA:2334:G:O6	46:D0:74:ARG:NH2	2.46	0.48
28:DE:24:THR:HG23	28:DE:184:VAL:HG12	1.96	0.48
29:DF:164:ARG:O	29:DF:168:ARG:HB2	2.14	0.48
31:DH:90:LYS:HD2	31:DH:163:TYR:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:60:ASP:O	2:AB:64:ARG:HB2	2.14	0.48
2:AB:95:GLN:HG3	2:AB:147:LYS:HD3	1.96	0.48
5:AE:144:THR:OG1	5:AE:147:ASP:OD2	2.26	0.48
7:AG:72:ARG:H	7:AG:72:ARG:HG2	1.42	0.48
13:AM:23:TYR:HB3	13:AM:67:GLU:HA	1.95	0.48
31:BH:4:ILE:O	31:BH:69:ARG:HG2	2.14	0.48
1:CA:12:U:H4'	1:CA:526:C:O2'	2.13	0.48
1:CA:275:G:H5'	17:CQ:14:LYS:HB3	1.96	0.48
1:CA:299:G:H2'	1:CA:300:A:C8	2.49	0.48
1:CA:779:C:H2'	1:CA:780:A:O4'	2.13	0.48
1:CA:1388:C:H2'	1:CA:1389:C:C6	2.49	0.48
3:CC:39:ILE:HG23	3:CC:91:LEU:HD11	1.96	0.48
3:CC:109:PRO:C	3:CC:111:LEU:H	2.22	0.48
3:CC:164:ARG:HG2	3:CC:165:THR:H	1.79	0.48
4:CD:173:TRP:CZ3	4:CD:193:ASP:HB3	2.49	0.48
25:DA:534:U:H2'	25:DA:535:C:C6	2.49	0.48
25:DA:910:A:C5	36:DQ:13:GLN:HG3	2.48	0.48
32:DI:57:ARG:HA	32:DI:61:ARG:NH2	2.28	0.48
41:DV:29:PRO:HG3	41:DV:63:GLY:HA2	1.95	0.48
1:AA:56:U:H2'	1:AA:57:G:C8	2.49	0.47
1:AA:1118:C:H1'	1:AA:1179:A:C4	2.49	0.47
1:AA:1399:C:H4'	1:AA:1400:C:O5'	2.14	0.47
2:AB:115:LEU:O	2:AB:119:GLU:HG2	2.14	0.47
3:AC:36:ASP:O	3:AC:40:ARG:HG3	2.14	0.47
5:AE:38:GLN:HE21	5:AE:38:GLN:HB2	1.55	0.47
10:AJ:8:LEU:HD22	10:AJ:96:ILE:HG12	1.95	0.47
25:BA:1938:A:H2'	25:BA:1939:U:O4'	2.13	0.47
31:BH:3:ARG:CG	31:BH:6:ARG:HG2	2.44	0.47
1:CA:96:U:O2'	1:CA:97:G:H5'	2.14	0.47
1:CA:376:G:H4'	16:CP:5:ARG:HD3	1.96	0.47
1:CA:921:U:O2	5:CE:19:MET:HB2	2.13	0.47
1:CA:1176:A:H2'	1:CA:1177:G:O4'	2.14	0.47
1:CA:1286:A:C8	1:CA:1287:A:H4'	2.49	0.47
19:CS:80:TYR:CZ	19:CS:82:GLY:HA2	2.49	0.47
25:DA:623:G:H2'	25:DA:624:C:C6	2.49	0.47
25:DA:1257:C:H4'	29:DF:83:PHE:CD2	2.49	0.47
26:DB:41:U:H5	30:DG:70:VAL:H	1.60	0.47
29:DF:117:ARG:HH12	35:DP:1:MET:H2	1.62	0.47
38:DS:105:ALA:O	38:DS:110:LEU:HB2	2.14	0.47
45:DZ:52:SER:OG	45:DZ:53:ILE:N	2.43	0.47
1:AA:1057:G:OP2	61:AA:4034:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:659:C:H2'	25:BA:660:C:C6	2.48	0.47
28:BE:40:GLU:H	28:BE:40:GLU:CD	2.22	0.47
31:BH:90:LYS:HD3	31:BH:159:GLU:HG2	1.96	0.47
1:CA:646:U:H2'	1:CA:647:C:H6	1.78	0.47
1:CA:865:A:H5'	1:CA:1078:U:C5	2.49	0.47
1:CA:1239:A:H62	1:CA:1299:A:H62	1.62	0.47
3:CC:180:ALA:O	3:CC:181:ASN:C	2.56	0.47
13:CM:50:GLU:HA	13:CM:53:VAL:HB	1.96	0.47
25:DA:315:G:H2'	25:DA:316:C:C6	2.49	0.47
25:DA:851:U:O2'	49:D3:42:ALA:O	2.32	0.47
25:DA:1263:U:C4	25:DA:1264:G:C6	3.02	0.47
25:DA:2331:G:O2'	46:D0:43:THR:HG22	2.14	0.47
28:DE:1:MET:HE1	28:DE:199:ARG:HD2	1.96	0.47
25:BA:185:A:H62	35:BP:38:GLN:HE22	1.62	0.47
25:BA:346:A:OP2	29:BF:169:ASN:HB2	2.14	0.47
25:BA:1513:G:H2'	25:BA:1594:C:H41	1.80	0.47
25:BA:1882:U:H2'	25:BA:1883:C:O4'	2.14	0.47
28:BE:101:ARG:CZ	28:BE:171:GLU:HB2	2.44	0.47
29:BF:18:ARG:NH2	29:BF:127:GLU:OE1	2.46	0.47
30:BG:126:ASP:OD2	30:BG:130:ASN:ND2	2.38	0.47
1:CA:9:G:H2'	1:CA:10:A:C8	2.49	0.47
3:CC:32:LEU:HD22	3:CC:32:LEU:H	1.79	0.47
12:CL:33:ARG:HD3	12:CL:62:SER:HB3	1.96	0.47
13:CM:122:LYS:CD	13:CM:123:ALA:H	2.27	0.47
23:CW:46:7MG:O2'	23:CW:47:U:O5'	2.29	0.47
25:DA:1685:C:H2'	25:DA:1686:C:C6	2.49	0.47
25:DA:2127:G:N2	25:DA:2161:C:N3	2.63	0.47
25:DA:2651:C:C2'	25:DA:2652:C:H5'	2.45	0.47
25:DA:2651:C:H2'	25:DA:2652:C:H5'	1.97	0.47
44:DY:5:MET:HE2	44:DY:5:MET:HB2	1.71	0.47
45:DZ:53:ILE:HG22	45:DZ:71:VAL:O	2.14	0.47
45:DZ:156:LYS:HG2	45:DZ:158:PRO:HD3	1.97	0.47
1:AA:342:C:C2	1:AA:348:G:N2	2.82	0.47
1:AA:642:A:N3	8:AH:113:SER:OG	2.46	0.47
1:AA:833:U:H2'	1:AA:834:C:H6	1.79	0.47
4:AD:166:LYS:HB2	4:AD:168:ARG:NH2	2.30	0.47
6:AF:69:GLU:O	6:AF:72:VAL:HG12	2.14	0.47
13:AM:96:LEU:O	13:AM:110:ARG:NH1	2.32	0.47
15:AO:16:ALA:HB1	15:AO:21:ASP:HB3	1.97	0.47
25:BA:211:A:H3'	25:BA:448:U:H5'	1.96	0.47
25:BA:2138:G:N1	25:BA:2184:G:OP1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2139:A:O2'	25:BA:2140:U:H5"	2.14	0.47
25:BA:2163:G:H1	25:BA:2171:G:N2	2.12	0.47
25:BA:2658:C:H2'	25:BA:2659:U:O4'	2.14	0.47
44:BY:86:ARG:NH1	44:BY:100:ALA:HB1	2.29	0.47
49:B3:23:LEU:HD13	49:B3:50:VAL:HG11	1.96	0.47
1:CA:1084:G:H5'	1:CA:1102:A:OP2	2.13	0.47
4:CD:150:GLU:CD	4:CD:151:LYS:H	2.22	0.47
9:CI:85:LEU:HB3	9:CI:92:TYR:HD2	1.78	0.47
23:CW:23:A:H2'	23:CW:24:G:H8	1.80	0.47
25:DA:852:G:H2'	25:DA:853:G:H8	1.77	0.47
25:DA:1011:G:OP2	40:DU:70:ARG:NH2	2.48	0.47
25:DA:1503:U:H2'	25:DA:1504:C:C6	2.50	0.47
25:DA:2532:G:H1'	25:DA:2663:G:N2	2.29	0.47
25:DA:2684:U:O2'	34:DO:68:GLU:OE1	2.32	0.47
25:DA:2849:U:H4'	25:DA:2868:A:C2	2.49	0.47
25:DA:2886:G:N7	61:DA:4437:HOH:O	2.35	0.47
31:DH:18:GLU:HG2	31:DH:19:VAL:N	2.29	0.47
31:DH:126:PRO:HG2	31:DH:130:ARG:HD2	1.96	0.47
32:DI:40:THR:O	32:DI:44:LEU:HB2	2.14	0.47
1:AA:184:G:H2'	1:AA:185:A:C8	2.50	0.47
1:AA:625:G:H2'	1:AA:626:U:C6	2.50	0.47
1:AA:1370:G:O6	61:AA:4100:HOH:O	2.20	0.47
12:AL:7:ILE:O	12:AL:11:VAL:HG23	2.14	0.47
25:BA:211:A:H5"	25:BA:448:U:OP1	2.14	0.47
25:BA:1153:G:N3	25:BA:1153:G:H2'	2.29	0.47
29:BF:33:LEU:HD22	29:BF:112:MET:HE3	1.96	0.47
30:BG:43:LEU:HD11	30:BG:153:ARG:HG2	1.95	0.47
31:BH:90:LYS:HD2	31:BH:163:TYR:CD1	2.49	0.47
38:BS:11:LYS:O	38:BS:15:ARG:HG3	2.14	0.47
1:CA:232:G:H1'	1:CA:262:A:N1	2.29	0.47
1:CA:250:A:H4'	1:CA:251:G:O5'	2.13	0.47
1:CA:1399:C:C2	1:CA:1502:A:N6	2.83	0.47
5:CE:84:PHE:N	5:CE:87:SER:O	2.48	0.47
9:CI:23:ASN:ND2	9:CI:23:ASN:H	2.12	0.47
19:CS:51:VAL:O	19:CS:58:VAL:N	2.40	0.47
25:DA:194:G:H2'	25:DA:195:A:O4'	2.14	0.47
25:DA:2320:A:H2'	25:DA:2320:A:N3	2.28	0.47
25:DA:2336:A:H61	46:D0:43:THR:HG22	1.79	0.47
25:DA:2461:C:H2'	25:DA:2462:U:C6	2.50	0.47
25:DA:2704:C:H2'	25:DA:2705:A:O4'	2.15	0.47
1:AA:6:G:H4'	1:AA:298:A:H4'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:438:G:H4'	4:AD:123:HIS:HD1	1.79	0.47
1:AA:501:C:H2'	1:AA:502:G:C8	2.50	0.47
1:AA:695:A:H2'	1:AA:696:A:C8	2.49	0.47
1:AA:1004:A:H5"	1:AA:1025:U:H5	1.79	0.47
1:AA:1029:C:N4	1:AA:1030:C:H41	2.13	0.47
4:AD:79:PHE:HE1	4:AD:204:ILE:HD13	1.80	0.47
4:AD:162:LEU:CD1	4:AD:181:MET:HG2	2.45	0.47
13:AM:96:LEU:C	13:AM:110:ARG:HG2	2.39	0.47
25:BA:274:U:H3'	25:BA:275:C:C5'	2.44	0.47
25:BA:898:U:O2'	49:B3:42:ALA:O	2.30	0.47
25:BA:2096:U:H2'	25:BA:2097:U:C6	2.49	0.47
25:BA:2175:G:N3	25:BA:2175:G:H2'	2.29	0.47
27:BD:26:LYS:HE2	27:BD:28:GLU:O	2.14	0.47
39:BT:112:ARG:HG3	39:BT:115:ARG:HH21	1.78	0.47
40:BU:66:ASN:O	40:BU:70:ARG:HG3	2.15	0.47
45:BZ:105:VAL:O	45:BZ:140:ASP:HA	2.14	0.47
45:BZ:126:VAL:CG1	45:BZ:161:VAL:HG23	2.43	0.47
50:B4:44:THR:O	50:B4:46:GLN:N	2.47	0.47
1:CA:109:A:C6	1:CA:326:G:C6	3.03	0.47
1:CA:1378:C:H5	1:CA:1379:G:H1'	1.79	0.47
1:CA:1391:U:H2'	1:CA:1392:G:C8	2.50	0.47
1:CA:1392:G:N2	1:CA:1502:A:H8	2.12	0.47
19:CS:27:GLU:HB2	19:CS:28:LYS:NZ	2.28	0.47
25:DA:1386:C:H2'	25:DA:1387:C:H6	1.79	0.47
25:DA:1667:G:O2'	25:DA:1991:U:O4	2.26	0.47
25:DA:2299:G:H2'	25:DA:2300:G:C8	2.47	0.47
25:DA:2748:A:H5'	31:DH:4:ILE:HD12	1.96	0.47
29:DF:12:LEU:HB2	29:DF:124:LEU:HD11	1.96	0.47
33:DN:67:LEU:HB3	33:DN:88:GLU:HG3	1.97	0.47
36:DQ:111:GLU:CD	36:DQ:133:ARG:HH21	2.18	0.47
43:DX:54:VAL:HG22	43:DX:81:VAL:HG12	1.95	0.47
47:D1:54:ALA:HB1	47:D1:83:GLU:HG3	1.96	0.47
1:AA:164:U:H2'	1:AA:165:C:C6	2.50	0.47
1:AA:193:C:H2'	1:AA:194:C:C6	2.49	0.47
1:AA:841:U:C5	1:AA:848:C:H1'	2.49	0.47
1:AA:1494:G:O2'	25:BA:1934:A:O2'	2.27	0.47
2:AB:76:GLN:CD	2:AB:76:GLN:H	2.21	0.47
9:AI:26:VAL:HG13	9:AI:61:ALA:HB3	1.96	0.47
10:AJ:76:ASN:HA	10:AJ:77:PRO:HD2	1.68	0.47
23:AW:7:A:N6	23:AW:66:U:H3	2.10	0.47
25:BA:670:C:H5'	25:BA:671:A:OP2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1640:G:H2'	25:BA:1641:G:O4'	2.14	0.47
25:BA:1756:U:H2'	25:BA:1757:C:C6	2.50	0.47
25:BA:1814:A:N7	61:BA:5150:HOH:O	2.35	0.47
25:BA:1993:A:OP2	27:BD:242:ARG:NH2	2.48	0.47
25:BA:2021:C:H5"	25:BA:2736:C:O2'	2.15	0.47
25:BA:2641:A:H1'	25:BA:2642:G:H5"	1.95	0.47
31:BH:20:ALA:HB1	31:BH:21:PRO:HD2	1.96	0.47
39:BT:33:LYS:O	39:BT:82:LEU:HD23	2.15	0.47
45:BZ:145:GLU:H	45:BZ:148:ASP:HB2	1.79	0.47
52:B6:10:LEU:HG	52:B6:54:ILE:HG13	1.97	0.47
1:CA:235:C:H5'	17:CQ:70:ARG:HG2	1.95	0.47
1:CA:408:A:H4'	4:CD:112:VAL:HG21	1.97	0.47
1:CA:538:G:H5"	12:CL:114:LYS:HB2	1.96	0.47
1:CA:886:G:O6	61:CA:4005:HOH:O	2.18	0.47
1:CA:1132:C:N4	1:CA:1142:G:H1	2.12	0.47
1:CA:1187:G:P	9:CI:113:LYS:HZ1	2.38	0.47
2:CB:17:PHE:HB2	2:CB:44:LEU:HD21	1.96	0.47
2:CB:19:HIS:ND1	2:CB:20:GLU:HG2	2.29	0.47
2:CB:48:MET:O	2:CB:52:GLU:N	2.48	0.47
2:CB:87:ARG:HD3	2:CB:234:PRO:HD2	1.97	0.47
2:CB:207:ALA:HB3	2:CB:210:SER:HB3	1.95	0.47
3:CC:19:GLU:HB3	3:CC:40:ARG:NH2	2.29	0.47
7:CG:103:TRP:CH2	7:CG:141:VAL:HG21	2.50	0.47
12:CL:34:ARG:HG3	12:CL:105:TYR:CE2	2.50	0.47
24:CX:47:U:H5'	24:CX:48:C:H5'	1.97	0.47
25:DA:116:C:H2'	25:DA:117:G:O4'	2.15	0.47
25:DA:1297:C:OP1	25:DA:2710:C:H4'	2.14	0.47
25:DA:1926:U:O2'	25:DA:1928:A:N7	2.37	0.47
25:DA:1952:A:OP1	34:DO:42:SER:OG	2.32	0.47
25:DA:2316:C:H1'	30:DG:128:ARG:HH21	1.79	0.47
25:DA:2635:C:H5"	28:DE:78:LEU:O	2.15	0.47
28:DE:5:LEU:HD11	28:DE:79:ARG:HB2	1.96	0.47
31:DH:11:VAL:HG13	31:DH:15:VAL:HG13	1.96	0.47
31:DH:46:GLU:HB2	31:DH:49:VAL:HG13	1.97	0.47
36:DQ:77:LYS:NZ	36:DQ:86:GLY:O	2.46	0.47
38:DS:80:LEU:HD12	38:DS:80:LEU:HA	1.76	0.47
39:DT:117:ASP:OD2	39:DT:120:ARG:NE	2.39	0.47
41:DV:16:PRO:HD3	41:DV:99:ILE:HD11	1.95	0.47
41:DV:60:GLU:HB3	41:DV:95:LEU:HB3	1.97	0.47
45:DZ:52:SER:HG	45:DZ:54:HIS:HD1	1.57	0.47
1:AA:920:U:H2'	1:AA:921:U:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:152:ALA:O	7:AG:155:ARG:HB3	2.15	0.47
20:AT:77:ALA:O	20:AT:81:LYS:HG3	2.14	0.47
23:AY:54:5MU:O2	23:AY:58:A:N7	2.48	0.47
25:BA:2141:A:C2	25:BA:2192:A:H2'	2.50	0.47
26:BB:75:G:H5"	26:BB:75:G:H8	1.79	0.47
1:CA:741:G:H2'	1:CA:742:G:O4'	2.15	0.47
1:CA:955:U:O2'	19:CS:83:HIS:HD2	1.98	0.47
1:CA:997:U:H3	1:CA:1044:A:H61	1.62	0.47
1:CA:1054:C:C5	23:CW:34:G:H1'	2.49	0.47
1:CA:1245:A:N6	1:CA:1292:U:H3	2.13	0.47
8:CH:51:VAL:HG11	8:CH:60:ARG:HH12	1.79	0.47
8:CH:51:VAL:HG12	8:CH:52:ASP:H	1.80	0.47
25:DA:271(D):G:H2'	25:DA:271(E):U:C6	2.50	0.47
25:DA:889:C:O2'	25:DA:890:A:O5'	2.29	0.47
25:DA:1019:U:H2'	25:DA:1020:A:H8	1.79	0.47
25:DA:2080:G:H2'	25:DA:2081:C:C6	2.49	0.47
32:DI:4:ILE:HG12	32:DI:18:VAL:HG22	1.97	0.47
45:DZ:45:ASP:OD2	45:DZ:49:ARG:HD2	2.15	0.47
2:AB:61:LEU:HD23	2:AB:68:ILE:HD11	1.97	0.47
18:AR:38:GLU:HA	18:AR:41:LYS:HD2	1.97	0.47
23:AW:51:U:H2'	23:AW:52:G:H8	1.75	0.47
23:AY:2:C:N4	23:AY:71:G:N1	2.39	0.47
25:BA:1537:G:O2'	27:BD:101:GLU:HB2	2.15	0.47
25:BA:1694:G:OP1	61:BA:5334:HOH:O	2.20	0.47
25:BA:2230:U:O2	47:B1:52:ARG:NH2	2.48	0.47
25:BA:2274:U:OP1	25:BA:2399:U:O2'	2.29	0.47
25:BA:2398:C:O2'	61:BA:5405:HOH:O	2.20	0.47
34:BO:68:GLU:HB3	34:BO:78:ARG:HB2	1.96	0.47
34:BO:107:ARG:CZ	39:BT:36:GLU:HG2	2.45	0.47
39:BT:118:ARG:HA	39:BT:118:ARG:HD2	1.66	0.47
1:CA:685:G:C2	1:CA:686:U:C4	3.03	0.47
1:CA:1262:C:H2'	1:CA:1263:C:C6	2.49	0.47
7:CG:114:ARG:HB2	7:CG:115:ARG:HH21	1.80	0.47
15:CO:48:LYS:HA	15:CO:48:LYS:HD3	1.69	0.47
23:CW:39:PSU:H2'	23:CW:40:C:C6	2.50	0.47
25:DA:271(E):U:H2'	25:DA:271(F):C:C6	2.50	0.47
25:DA:493:G:H2'	25:DA:494:G:O4'	2.14	0.47
25:DA:1471:A:H3'	25:DA:1472:A:H8	1.79	0.47
25:DA:1786:A:OP1	25:DA:1980:G:N2	2.39	0.47
25:DA:2124:G:H1	25:DA:2174:C:H42	1.59	0.47
25:DA:2356:C:P	46:D0:24:LYS:HZ1	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2390:U:OP2	54:D8:35:GLN:NE2	2.32	0.47
1:AA:748:C:H4'	1:AA:749:C:O5'	2.15	0.47
1:AA:1028:C:H2'	1:AA:1029:C:H4'	1.97	0.47
2:AB:145:LEU:O	2:AB:149:LEU:HB2	2.14	0.47
6:AF:75:LEU:O	6:AF:79:LEU:HG	2.15	0.47
13:AM:11:ARG:O	13:AM:13:LYS:N	2.46	0.47
25:BA:905:U:O2	25:BA:2280:A:H2'	2.15	0.47
25:BA:2527:C:O2'	25:BA:2528:G:H5'	2.15	0.47
39:BT:127:ALA:O	39:BT:128:GLU:HB2	2.15	0.47
1:CA:576:G:O6	1:CA:880:C:O2'	2.31	0.47
1:CA:750:G:H1'	15:CO:22:THR:OG1	2.15	0.47
1:CA:784:C:H4'	25:DA:1837:C:OP1	2.15	0.47
1:CA:1226:C:O2'	13:CM:111:LYS:NZ	2.49	0.47
2:CB:187:LEU:HA	2:CB:201:ILE:HB	1.97	0.47
3:CC:70:VAL:O	3:CC:106:VAL:N	2.48	0.47
7:CG:26:PHE:CE1	7:CG:30:ILE:HD11	2.50	0.47
13:CM:65:LYS:HA	50:D4:50:VAL:HG11	1.97	0.47
25:DA:286:C:H2'	25:DA:287:C:C6	2.50	0.47
25:DA:2572:A:C8	28:DE:144:ARG:HD2	2.50	0.47
25:DA:2584:U:H2'	25:DA:2585:U:H2'	1.97	0.47
25:DA:2631:G:N2	25:DA:2787:C:O2	2.38	0.47
26:DB:78:A:C2	26:DB:100:A:C4	3.03	0.47
1:AA:473:G:H2'	1:AA:474:G:C8	2.50	0.46
1:AA:1456:G:O6	20:AT:54:LYS:NZ	2.35	0.46
24:AX:13:C:O2'	25:BA:1946:C:H4'	2.15	0.46
29:BF:129:PHE:CD2	29:BF:163:VAL:HG21	2.50	0.46
31:BH:33:LEU:HD21	31:BH:136:ILE:HG13	1.97	0.46
32:BI:60:GLU:HG3	32:BI:61:ARG:HD2	1.97	0.46
2:CB:105:PHE:O	2:CB:109:SER:OG	2.26	0.46
11:CK:99:GLN:HG2	11:CK:105:VAL:HG21	1.96	0.46
14:CN:47:LEU:O	14:CN:51:GLY:N	2.48	0.46
25:DA:221:A:C8	25:DA:266:G:C6	3.03	0.46
25:DA:478:A:N1	25:DA:500:G:H4'	2.30	0.46
25:DA:817:C:O2'	25:DA:839:U:OP1	2.32	0.46
25:DA:963:U:OP1	61:DA:4058:HOH:O	2.21	0.46
25:DA:2271:G:C5	25:DA:2272:U:C5	3.03	0.46
26:DB:80:U:H2'	26:DB:81:G:C8	2.49	0.46
35:DP:68:GLN:HG3	54:D8:12:LYS:HG2	1.97	0.46
1:AA:662:G:H2'	1:AA:663:A:C8	2.49	0.46
1:AA:1237:C:HO2'	1:AA:1300:G:H1	1.62	0.46
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:32:ILE:HG21	2:AB:40:HIS:HD2	1.79	0.46
4:AD:133:VAL:HG12	4:AD:135:LEU:H	1.79	0.46
25:BA:1475:G:H2'	25:BA:1476:C:H6	1.79	0.46
25:BA:1891:G:H2'	25:BA:1892:G:O4'	2.15	0.46
25:BA:2561:G:O6	61:BA:4141:HOH:O	2.20	0.46
25:BA:2720:G:H1'	37:BR:71:GLN:NE2	2.26	0.46
25:BA:2834:C:H5	61:BA:4097:HOH:O	1.98	0.46
1:CA:1039:C:C4	1:CA:1040:U:C4	3.03	0.46
1:CA:1118:C:H2'	1:CA:1119:C:C6	2.42	0.46
1:CA:1133:G:C4	1:CA:1134:G:C8	3.04	0.46
3:CC:113:ALA:HB2	3:CC:202:ILE:HG13	1.97	0.46
7:CG:144:MET:HE1	23:CY:31:A:H1'	1.97	0.46
9:CI:23:ASN:ND2	9:CI:25:LYS:HG2	2.30	0.46
25:DA:223:A:O2'	25:DA:420:C:O2	2.29	0.46
25:DA:300:A:P	44:DY:86:ARG:HH22	2.38	0.46
25:DA:392:C:H5"	25:DA:409:C:H5"	1.97	0.46
25:DA:900:A:O2'	25:DA:901:A:OP1	2.33	0.46
25:DA:955:C:OP1	36:DQ:87:LYS:HE3	2.16	0.46
25:DA:1015:G:H2'	25:DA:1016:G:H8	1.80	0.46
43:DX:9:LEU:HA	48:D2:36:ARG:HH21	1.80	0.46
1:AA:76:C:O2	1:AA:93:G:N1	2.32	0.46
1:AA:236:G:H5"	17:AQ:42:TYR:OH	2.15	0.46
1:AA:376:G:P	16:AP:67:THR:HG21	2.56	0.46
2:AB:62:ALA:HB3	2:AB:225:ALA:HB3	1.97	0.46
8:AH:39:LEU:HB3	8:AH:45:ILE:HG12	1.96	0.46
13:AM:57:ARG:CZ	50:B4:34:GLU:HB3	2.45	0.46
24:AX:8:4SU:O2	24:AX:21:A:H2	1.98	0.46
23:AY:19:G:H1	23:AY:56:C:N4	2.09	0.46
25:BA:733:G:C4	53:B7:11:LYS:HG2	2.50	0.46
32:BI:96:ASP:OD1	32:BI:96:ASP:N	2.47	0.46
47:B1:86:SER:OG	47:B1:89:GLU:OE1	2.24	0.46
53:B7:30:VAL:O	53:B7:34:ARG:HG3	2.15	0.46
1:CA:735:C:H2'	1:CA:736:C:C6	2.50	0.46
1:CA:1057:G:H2'	1:CA:1058:G:O4'	2.16	0.46
7:CG:48:LYS:O	7:CG:52:GLU:HG2	2.16	0.46
7:CG:79:ARG:HB3	7:CG:79:ARG:CZ	2.45	0.46
15:CO:5:LYS:H	15:CO:5:LYS:NZ	2.06	0.46
25:DA:144:C:H2'	25:DA:145:G:H8	1.80	0.46
25:DA:1151:G:H4'	40:DU:81:HIS:CG	2.51	0.46
25:DA:1857:G:C6	25:DA:1858:G:C6	3.03	0.46
25:DA:2379:G:HO2'	38:DS:17:ARG:HH21	1.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DB:12:C:O2'	46:D0:74:ARG:HG2	2.15	0.46
44:DY:20:TYR:CE1	44:DY:43:ASN:HA	2.50	0.46
45:DZ:3:TYR:O	45:DZ:57:ILE:HA	2.16	0.46
19:AS:3:ARG:HH21	19:AS:7:LYS:HB3	1.79	0.46
23:AY:3:C:H42	23:AY:70:G:H1	1.64	0.46
25:BA:305:G:O2'	25:BA:383:A:N6	2.45	0.46
25:BA:876:A:N7	25:BA:2260:C:H5'	2.31	0.46
25:BA:2331:G:N2	38:BS:3:ARG:HA	2.31	0.46
25:BA:2541:G:H5"	25:BA:2542:A:H5"	1.98	0.46
41:BV:52:VAL:HG22	41:BV:55:ALA:HB3	1.98	0.46
1:CA:918:A:H2'	1:CA:919:A:O4'	2.16	0.46
1:CA:1226:C:H4'	19:CS:80:TYR:OH	2.14	0.46
2:CB:54:THR:HG21	2:CB:201:ILE:HD11	1.97	0.46
8:CH:91:ARG:NH1	17:CQ:33:GLY:HA3	2.30	0.46
9:CI:46:ALA:HB2	9:CI:74:ILE:HG23	1.97	0.46
19:CS:51:VAL:HB	19:CS:75:ALA:HB2	1.97	0.46
23:CW:75:C:H2'	23:CW:76:A:C4	2.50	0.46
25:DA:477:A:H2'	25:DA:478:A:C8	2.51	0.46
25:DA:1803:A:H4'	27:DD:259:THR:HG23	1.98	0.46
43:DX:92:LEU:C	43:DX:94:GLY:H	2.23	0.46
48:D2:16:LEU:O	48:D2:67:LYS:NZ	2.49	0.46
1:AA:870:U:H4'	1:AA:871:U:H5"	1.97	0.46
5:AE:121:LYS:HG3	5:AE:123:LEU:HG	1.98	0.46
12:AL:84:LEU:HB2	12:AL:105:TYR:CE2	2.50	0.46
25:BA:864:C:H4'	25:BA:977:G:C5	2.51	0.46
25:BA:1221:G:H21	25:BA:1222:A:H4'	1.80	0.46
25:BA:1496:A:H5'	25:BA:1497:G:OP2	2.15	0.46
25:BA:2285:A:H2'	25:BA:2286:A:C8	2.49	0.46
25:BA:2504:U:H2'	25:BA:2505:U:C6	2.51	0.46
25:BA:2660:C:H2'	25:BA:2661:U:C6	2.50	0.46
1:CA:407:G:OP1	4:CD:115:ARG:HD2	2.16	0.46
1:CA:1187:G:OP1	9:CI:113:LYS:NZ	2.49	0.46
1:CA:1202:G:O4'	14:CN:29:ARG:NH1	2.49	0.46
1:CA:1243:C:H42	1:CA:1294:G:H1	1.63	0.46
2:CB:35:GLU:OE2	2:CB:38:GLY:HA2	2.16	0.46
2:CB:201:ILE:O	2:CB:203:GLY:N	2.48	0.46
17:CQ:9:VAL:HG13	17:CQ:56:VAL:HG22	1.97	0.46
23:CW:29:G:H2'	23:CW:30:G:C8	2.51	0.46
23:CY:71:G:H4'	25:DA:1851:U:H4'	1.97	0.46
25:DA:521:G:H2'	25:DA:522:G:H8	1.80	0.46
25:DA:1434:A:H61	25:DA:1558:A:N6	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DB:33:G:C2	26:DB:50:G:C2	3.04	0.46
27:DD:108:PRO:HB3	27:DD:143:HIS:CE1	2.50	0.46
29:DF:187:VAL:HG11	35:DP:6:LEU:HD11	1.97	0.46
35:DP:47:ASP:OD2	35:DP:50:ARG:HD3	2.16	0.46
47:D1:83:GLU:HA	47:D1:84:GLY:HA2	1.64	0.46
1:AA:202:U:O2'	1:AA:203:U:O5'	2.29	0.46
1:AA:614:A:H2'	1:AA:615:C:O4'	2.15	0.46
1:AA:1278:U:H3'	1:AA:1278:U:H6	1.81	0.46
2:AB:16:HIS:CG	2:AB:17:PHE:H	2.30	0.46
4:AD:53:ASP:O	4:AD:57:ARG:HG3	2.16	0.46
9:AI:4:TYR:CE1	9:AI:88:TYR:HD1	2.34	0.46
25:BA:1289:G:O2'	35:BP:7:ARG:NH2	2.49	0.46
25:BA:2160:C:O2	25:BA:2160:C:H2'	2.15	0.46
25:BA:2209:G:H2'	25:BA:2210:C:O4'	2.15	0.46
42:BW:18:ARG:NH1	42:BW:76:VAL:O	2.49	0.46
1:CA:573:A:N3	1:CA:883:C:O2'	2.45	0.46
1:CA:1006:C:OP1	1:CA:1037:C:O2'	2.33	0.46
3:CC:8:ILE:HD13	3:CC:184:TYR:HB3	1.98	0.46
3:CC:11:ARG:HB3	3:CC:15:THR:HB	1.97	0.46
24:CX:23:C:H2'	24:CX:24:U:C6	2.50	0.46
24:CX:59:A:C2'	24:CX:60:U:H5'	2.46	0.46
24:CX:64:G:H4'	36:DQ:10:ARG:NH1	2.27	0.46
23:CY:51:U:O4	23:CY:63:G:O6	2.33	0.46
23:CY:71:G:H2'	23:CY:72:C:C6	2.51	0.46
25:DA:740:U:H2'	25:DA:741:G:C8	2.51	0.46
25:DA:989:G:H4'	25:DA:990:A:OP1	2.15	0.46
25:DA:1378:A:OP1	53:D7:10:ARG:NH2	2.49	0.46
33:DN:67:LEU:C	33:DN:88:GLU:HG3	2.41	0.46
34:DO:15:GLY:O	34:DO:47:ILE:HG12	2.14	0.46
49:D3:6:VAL:HG13	49:D3:56:VAL:HG22	1.97	0.46
50:D4:26:SER:OG	50:D4:27:THR:N	2.49	0.46
1:AA:189(D):C:H2'	1:AA:189(E):U:O4'	2.16	0.46
1:AA:345:C:H6	1:AA:345:C:O5'	1.98	0.46
1:AA:600:C:H5'	8:AH:129:VAL:HA	1.98	0.46
2:AB:17:PHE:CB	2:AB:44:LEU:HD21	2.46	0.46
9:AI:5:TYR:O	9:AI:87:GLN:NE2	2.49	0.46
13:AM:65:LYS:NZ	13:AM:73:GLU:HG3	2.31	0.46
19:AS:80:TYR:CZ	19:AS:82:GLY:HA2	2.51	0.46
25:BA:139:A:C8	25:BA:1454:C:O2'	2.67	0.46
25:BA:932:C:H3'	25:BA:933:C:C5'	2.44	0.46
25:BA:2297:C:OP2	52:B6:6:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2325:C:H4'	30:BG:91:ARG:HG3	1.96	0.46
27:BD:142:VAL:HG13	27:BD:191:ALA:HB1	1.98	0.46
29:BF:126:VAL:HG21	29:BF:129:PHE:CZ	2.50	0.46
29:BF:195:ASP:HB3	29:BF:198:ALA:H	1.81	0.46
42:BW:4:LYS:HB2	42:BW:106:ILE:HG12	1.96	0.46
1:CA:1128:C:C2'	1:CA:1129:C:H5"	2.46	0.46
1:CA:1161:C:H2'	1:CA:1162:C:C6	2.51	0.46
1:CA:1327:C:H2'	1:CA:1328:C:C6	2.51	0.46
57:CA:3178:PCY:N16	57:CA:3178:PCY:O5	2.45	0.46
12:CL:34:ARG:HE	12:CL:34:ARG:HB3	1.44	0.46
15:CO:17:ARG:HH11	15:CO:17:ARG:HG3	1.81	0.46
25:DA:1292:U:H2'	25:DA:1293:C:H6	1.79	0.46
25:DA:1336:A:H2'	25:DA:1337:G:C8	2.51	0.46
25:DA:2112:G:H2'	25:DA:2113:U:O4'	2.15	0.46
29:DF:120:GLU:HB2	29:DF:122:LYS:HG2	1.97	0.46
30:DG:49:ASP:OD1	30:DG:49:ASP:N	2.45	0.46
30:DG:114:ILE:HG23	30:DG:136:ARG:NH2	2.30	0.46
31:DH:124:GLU:OE1	31:DH:132:ARG:HD2	2.15	0.46
35:DP:101:VAL:HA	35:DP:106:LEU:O	2.16	0.46
53:D7:1:MET:HE2	53:D7:1:MET:HB2	1.64	0.46
1:AA:184:G:H2'	1:AA:185:A:H8	1.81	0.46
12:AL:33:ARG:HH11	12:AL:62:SER:HB3	1.81	0.46
23:AW:2:C:H2'	23:AW:3:C:C6	2.51	0.46
23:AY:26:A:N6	23:AY:44:G:N1	2.42	0.46
25:BA:231:G:C8	54:B8:5:LYS:HG2	2.50	0.46
25:BA:2018:C:H4'	25:BA:2019:G:OP1	2.15	0.46
25:BA:2486:C:OP2	25:BA:2487:C:N4	2.41	0.46
38:BS:39:ILE:HB	38:BS:49:VAL:HG13	1.98	0.46
45:BZ:145:GLU:O	45:BZ:147:GLY:HA2	2.16	0.46
50:B4:15:ILE:HD12	50:B4:21:VAL:HG22	1.98	0.46
1:CA:23:C:H5	1:CA:561:U:O4	1.98	0.46
1:CA:447:G:O6	1:CA:485:G:O2'	2.29	0.46
1:CA:1307:U:H2'	1:CA:1308:U:C6	2.51	0.46
1:CA:1410:G:H2'	1:CA:1411:C:C6	2.51	0.46
2:CB:125:PRO:O	2:CB:127:ILE:N	2.49	0.46
5:CE:57:LYS:HG2	5:CE:61:TYR:CE2	2.51	0.46
6:CF:69:GLU:O	6:CF:72:VAL:HG12	2.16	0.46
23:CW:33:U:N3	23:CW:36:A:OP2	2.46	0.46
25:DA:1325:G:OP1	25:DA:1647:G:O2'	2.21	0.46
25:DA:2170:A:H2'	25:DA:2171:A:H5'	1.98	0.46
25:DA:2203:U:H4'	27:DD:151:LYS:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DH:117:PRO:HG3	31:DH:123:PHE:CD2	2.51	0.46
32:DI:101:LEU:HD12	32:DI:105:HIS:HD2	1.81	0.46
39:DT:27:THR:HB	39:DT:89:VAL:HG22	1.97	0.46
45:DZ:97:GLU:HA	45:DZ:126:VAL:O	2.16	0.46
1:AA:573:A:OP2	61:AA:4006:HOH:O	2.20	0.46
1:AA:1030(D):A:H2'	1:AA:1031:G:O4'	2.16	0.46
4:AD:98:GLU:O	4:AD:103:ASN:ND2	2.48	0.46
8:AH:101:PRO:HG3	8:AH:133:LEU:HD11	1.98	0.46
15:AO:7:GLU:O	15:AO:11:VAL:HG23	2.16	0.46
20:AT:87:LYS:O	20:AT:91:LEU:HG	2.16	0.46
23:AW:9:A:O2'	23:AW:10:G:N7	2.49	0.46
25:BA:397:G:H8	25:BA:397:G:OP2	1.99	0.46
25:BA:1513:G:O2'	25:BA:1593:C:O2'	2.23	0.46
25:BA:1535:U:HO2'	25:BA:1536:A:H8	1.63	0.46
25:BA:2021:C:H4'	25:BA:2736:C:O2	2.15	0.46
25:BA:2135:U:O4	25:BA:2136:A:N6	2.46	0.46
25:BA:2697:G:H5'	34:BO:68:GLU:OE1	2.16	0.46
31:BH:126:PRO:HB2	31:BH:130:ARG:HH21	1.81	0.46
35:BP:138:LEU:HD23	35:BP:145:PRO:HG3	1.98	0.46
47:B1:72:GLU:O	47:B1:76:ARG:HG3	2.16	0.46
50:B4:46:GLN:HE21	50:B4:46:GLN:HB3	1.60	0.46
1:CA:943:U:H2'	1:CA:944:G:H5'	1.97	0.46
1:CA:1004:A:H8	1:CA:1005:A:H4'	1.79	0.46
1:CA:1069:C:O2'	1:CA:1192:C:H1'	2.16	0.46
1:CA:1118:C:OP1	9:CI:9:ARG:HD2	2.16	0.46
1:CA:1194:U:H2'	1:CA:1195:C:C6	2.51	0.46
1:CA:1251:A:H2'	1:CA:1252:A:C8	2.50	0.46
3:CC:83:ARG:O	3:CC:87:LEU:HG	2.16	0.46
12:CL:83:VAL:HG23	12:CL:107:ALA:HB2	1.98	0.46
17:CQ:5:VAL:HG22	17:CQ:60:ILE:HG13	1.97	0.46
25:DA:479:A:H4'	25:DA:480:A:OP1	2.15	0.46
25:DA:639:U:H2'	25:DA:640:C:H6	1.80	0.46
25:DA:747:U:O2	25:DA:2014:A:H1'	2.14	0.46
25:DA:1449:A:OP2	25:DA:1449:A:H8	1.98	0.46
25:DA:2179:C:C2'	25:DA:2180:U:H5'	2.46	0.46
25:DA:2815:C:H5'	51:D5:29:THR:HG21	1.98	0.46
30:DG:70:VAL:HA	30:DG:90:LEU:HD23	1.97	0.46
40:DU:16:LYS:HB3	40:DU:16:LYS:HE2	1.69	0.46
55:D9:10:ILE:HD12	55:D9:32:HIS:HA	1.97	0.46
1:AA:38:G:H22	1:AA:397:A:H5"	1.81	0.46
1:AA:197:A:C6	1:AA:221:C:H4'	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:922:G:H2'	1:AA:923:A:C8	2.51	0.46
1:AA:1183:A:HO2'	1:AA:1184:G:P	2.39	0.46
2:AB:59:GLU:HG2	2:AB:63:MET:HE2	1.98	0.46
2:AB:166:ASP:OD2	2:AB:169:LYS:HB2	2.16	0.46
7:AG:15:ASP:OD1	7:AG:20:ASP:N	2.40	0.46
7:AG:113:GLU:HG3	7:AG:118:VAL:HG12	1.98	0.46
20:AT:10:LEU:HD13	20:AT:12:ALA:HB2	1.98	0.46
25:BA:63:A:O3'	43:BX:71:GLY:HA3	2.16	0.46
27:BD:95:LEU:HD11	27:BD:105:ILE:HD13	1.97	0.46
35:BP:62:LEU:O	54:B8:13:ARG:HD3	2.15	0.46
36:BQ:85:LYS:HG2	46:B0:7:LEU:HB3	1.98	0.46
1:CA:544:G:P	4:CD:62:GLN:HE21	2.37	0.46
1:CA:1004:A:C2	1:CA:1038:C:C4	3.04	0.46
1:CA:1030(A):G:O2'	1:CA:1030(C):G:N7	2.45	0.46
1:CA:1269:A:N1	1:CA:1312:G:O2'	2.44	0.46
1:CA:1314:C:OP1	19:CS:6:LYS:NZ	2.39	0.46
1:CA:1318:A:OP1	19:CS:3:ARG:NH2	2.43	0.46
4:CD:22:LYS:HB2	4:CD:26:CYS:SG	2.56	0.46
10:CJ:27:ALA:HA	10:CJ:81:THR:HG22	1.97	0.46
12:CL:7:ILE:O	12:CL:11:VAL:HG23	2.16	0.46
25:DA:887:A:H5'	25:DA:888:C:OP1	2.16	0.46
25:DA:896:A:H61	45:DZ:114:GLY:HA3	1.81	0.46
25:DA:2336:A:H61	46:D0:43:THR:CG2	2.29	0.46
25:DA:2552:U:C2	25:DA:2554:U:H5"	2.51	0.46
31:DH:2:SER:O	31:DH:3:ARG:HG2	2.15	0.46
41:DV:62:LEU:HD21	41:DV:95:LEU:HB2	1.97	0.46
50:D4:16:CYS:SG	50:D4:17:GLY:N	2.89	0.46
1:AA:707:C:OP1	11:AK:85:ARG:NH1	2.48	0.45
57:AA:3231:PCY:N20	57:AA:3231:PCY:O21	2.49	0.45
7:AG:15:ASP:O	7:AG:19:GLY:HA2	2.16	0.45
9:AI:49:PRO:HG3	9:AI:101:PHE:CD2	2.51	0.45
25:BA:265:U:H2'	25:BA:266:C:H6	1.80	0.45
25:BA:439:A:H8	25:BA:439:A:O5'	1.99	0.45
25:BA:505:A:N3	25:BA:507:G:H5"	2.31	0.45
31:BH:13:LYS:HA	31:BH:14:GLY:HA2	1.54	0.45
39:BT:127:ALA:C	39:BT:129:ARG:H	2.24	0.45
1:CA:583:A:H2'	1:CA:584:G:O4'	2.16	0.45
1:CA:713:G:H2'	1:CA:714:G:C8	2.51	0.45
1:CA:718:G:H5'	11:CK:117:ASN:CG	2.41	0.45
1:CA:865:A:H2	1:CA:918:A:H4'	1.81	0.45
4:CD:112:VAL:HG13	4:CD:161:ASN:OD1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CE:100:VAL:O	5:CE:107:ARG:NH2	2.28	0.45
25:DA:265:A:H1'	25:DA:266:G:O4'	2.16	0.45
25:DA:305:U:H2'	25:DA:306:U:C6	2.51	0.45
25:DA:588:U:H2'	25:DA:589:C:C6	2.51	0.45
25:DA:695:G:OP1	25:DA:1380:G:O2'	2.32	0.45
25:DA:1669:A:H5"	25:DA:2550:G:OP1	2.16	0.45
25:DA:2666:C:N4	31:DH:109:PHE:HA	2.31	0.45
25:DA:2712:U:OP1	25:DA:2714:G:H4'	2.17	0.45
28:DE:1:MET:HE1	28:DE:199:ARG:HB3	1.97	0.45
28:DE:112:GLY:O	28:DE:159:HIS:HA	2.16	0.45
41:DV:15:GLU:O	41:DV:18:LEU:HB2	2.16	0.45
50:D4:15:ILE:HG23	50:D4:21:VAL:HG22	1.96	0.45
1:AA:204:U:H4'	1:AA:216:G:O5'	2.15	0.45
19:AS:3:ARG:NH2	19:AS:7:LYS:HE2	2.31	0.45
23:AY:28:G:H1	23:AY:42:C:H42	1.64	0.45
25:BA:484:G:O2'	25:BA:495:G:O6	2.29	0.45
25:BA:549:U:H2'	25:BA:550:U:C6	2.51	0.45
25:BA:2430:A:H2'	25:BA:2431:U:C6	2.51	0.45
28:BE:73:GLU:H	28:BE:73:GLU:HG3	1.55	0.45
33:BN:75:TYR:CE2	33:BN:77:GLY:HA2	2.51	0.45
36:BQ:18:LYS:O	36:BQ:98:LYS:NZ	2.31	0.45
46:B0:10:THR:HG22	46:B0:12:ASN:N	2.20	0.45
47:B1:3:LYS:HB3	47:B1:4:VAL:H	1.41	0.45
1:CA:62:U:H2'	1:CA:63:C:C6	2.51	0.45
1:CA:1066:C:O2'	1:CA:1067:A:H5'	2.15	0.45
2:CB:230:VAL:HG22	2:CB:231:GLU:H	1.80	0.45
10:CJ:32:ALA:CB	10:CJ:33:GLN:HA	2.43	0.45
23:CW:2:C:H2'	23:CW:3:C:H6	1.81	0.45
25:DA:1782:C:H1'	25:DA:2609:U:H5"	1.98	0.45
25:DA:2191:G:H2'	25:DA:2192:G:O4'	2.16	0.45
31:DH:4:ILE:O	31:DH:69:ARG:HG2	2.17	0.45
44:DY:9:LYS:HA	44:DY:10:GLY:HA2	1.57	0.45
50:D4:49:PHE:HB3	50:D4:50:VAL:H	1.52	0.45
1:AA:434:U:H2'	1:AA:435:C:C6	2.51	0.45
1:AA:455:C:O5'	1:AA:455:C:H6	2.00	0.45
1:AA:738:C:H2'	1:AA:739:C:C6	2.50	0.45
2:AB:80:ILE:HD13	2:AB:211:ILE:HG22	1.98	0.45
3:AC:15:THR:HG21	3:AC:181:ASN:HA	1.99	0.45
7:AG:76:ARG:HB3	7:AG:156:TRP:HH2	1.82	0.45
23:AY:48:C:OP1	23:AY:48:C:H2'	2.17	0.45
23:AY:58:A:O2'	23:AY:60:U:OP2	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:80:G:HO2'	25:BA:319:G:HO2'	1.63	0.45
25:BA:555:G:C5	25:BA:2044:U:H5"	2.51	0.45
25:BA:581:G:OP1	33:BN:111:PRO:HD2	2.17	0.45
25:BA:942:A:N7	45:BZ:146:ILE:HD12	2.31	0.45
25:BA:2168:C:H4'	25:BA:2169:G:N3	2.31	0.45
25:BA:2357:G:N3	25:BA:2393:C:H2'	2.31	0.45
49:B3:5:LYS:HE3	49:B3:55:ARG:HH12	1.82	0.45
50:B4:26:SER:OG	50:B4:27:THR:N	2.49	0.45
1:CA:50:A:H1'	1:CA:52:G:C8	2.52	0.45
1:CA:529:G:O6	12:CL:49:ASN:HA	2.16	0.45
1:CA:630:G:O2'	1:CA:631:G:H5'	2.16	0.45
1:CA:1022:G:H4'	1:CA:1022:G:OP1	2.16	0.45
1:CA:1273:G:H3'	1:CA:1274:G:H8	1.81	0.45
1:CA:1388:C:H2'	1:CA:1389:C:H6	1.81	0.45
5:CE:57:LYS:HG2	5:CE:61:TYR:HE2	1.82	0.45
25:DA:892:G:H2'	25:DA:893:C:C4'	2.46	0.45
25:DA:1187:G:H5'	41:DV:81:TYR:CE1	2.51	0.45
25:DA:2080:G:H2'	25:DA:2081:C:H6	1.81	0.45
25:DA:2127:G:N1	25:DA:2161:C:N4	2.64	0.45
25:DA:2519:U:C6	25:DA:2542:A:N6	2.84	0.45
25:DA:2728:U:H2'	25:DA:2729:G:C8	2.51	0.45
29:DF:37:VAL:O	29:DF:41:LEU:HG	2.17	0.45
34:DO:16:ALA:HB2	34:DO:52:VAL:HG21	1.98	0.45
43:DX:44:GLU:O	43:DX:48:LYS:N	2.49	0.45
47:D1:53:VAL:HG22	47:D1:74:VAL:HG13	1.97	0.45
1:AA:872:A:C8	1:AA:874:G:C8	3.05	0.45
4:AD:164:ALA:O	4:AD:168:ARG:HD3	2.16	0.45
19:AS:22:LEU:C	19:AS:27:GLU:HG3	2.41	0.45
23:AW:19:G:H1	23:AW:56:C:N4	2.10	0.45
25:BA:266:C:H2'	25:BA:267:C:O4'	2.16	0.45
25:BA:1170:C:H1'	55:B9:36:GLN:NE2	2.31	0.45
25:BA:1834:A:H4'	27:BD:259:THR:HG23	1.97	0.45
25:BA:2745:G:H3'	25:BA:2746:A:O4'	2.16	0.45
26:BB:12:C:H2'	46:B0:73:GLY:HA3	1.97	0.45
35:BP:50:ARG:HD3	54:B8:7:HIS:CD2	2.51	0.45
45:BZ:138:GLU:N	45:BZ:156:LYS:HD3	2.30	0.45
1:CA:200:G:H2'	1:CA:201:C:O4'	2.15	0.45
1:CA:1128:C:H2'	1:CA:1129:C:H5"	1.99	0.45
3:CC:148:GLY:HA3	3:CC:172:ARG:O	2.16	0.45
5:CE:68:GLU:OE1	5:CE:70:PRO:HG3	2.16	0.45
25:DA:182:A:N3	25:DA:433:C:O2'	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:196:A:H62	35:DP:38:GLN:HE22	1.63	0.45
25:DA:2683:C:O2	34:DO:70:LYS:NZ	2.39	0.45
28:DE:24:THR:HG22	28:DE:186:GLY:O	2.16	0.45
29:DF:126:VAL:HG21	29:DF:129:PHE:CZ	2.52	0.45
31:DH:6:ARG:HH22	31:DH:54:ARG:NH2	2.14	0.45
33:DN:73:THR:HA	33:DN:83:LYS:O	2.16	0.45
37:DR:44:LEU:HD23	37:DR:44:LEU:HA	1.74	0.45
1:AA:390:C:H2'	1:AA:391:G:C8	2.51	0.45
1:AA:1131:G:C2'	1:AA:1132:C:H5'	2.47	0.45
4:AD:23:GLY:HA3	4:AD:112:VAL:CG1	2.46	0.45
9:AI:121:ARG:NH1	9:AI:122:ALA:O	2.50	0.45
17:AQ:67:LYS:O	17:AQ:68:ARG:HB3	2.16	0.45
25:BA:843:C:H2'	25:BA:844:C:C6	2.50	0.45
25:BA:904:C:N4	25:BA:905:U:O4	2.49	0.45
25:BA:1199:C:H2'	25:BA:1200:G:O4'	2.16	0.45
25:BA:2119:C:H2'	25:BA:2120:U:O4'	2.16	0.45
25:BA:2162:C:O2'	25:BA:2174:G:N2	2.49	0.45
36:BQ:16:ARG:HG3	36:BQ:17:LEU:H	1.81	0.45
51:B5:17:ASP:OD2	61:B5:205:HOH:O	2.21	0.45
1:CA:67:C:H2'	1:CA:68:G:H8	1.81	0.45
1:CA:426:G:OP1	4:CD:38:TYR:OH	2.21	0.45
1:CA:1073:U:H2'	1:CA:1074:G:H8	1.82	0.45
1:CA:1122:U:C4	1:CA:1123:A:N7	2.84	0.45
12:CL:75:HIS:HA	12:CL:102:ARG:HH22	1.80	0.45
12:CL:117:ARG:NH2	12:CL:124:LYS:HB2	2.31	0.45
23:CW:47:U:O2'	23:CW:48:C:OP1	2.33	0.45
23:CY:57:G:N3	23:CY:57:G:H2'	2.32	0.45
23:CY:69:G:H2'	23:CY:70:G:O4'	2.17	0.45
25:DA:38:A:H2'	25:DA:39:C:C6	2.51	0.45
25:DA:500:G:N1	25:DA:503:A:OP2	2.50	0.45
25:DA:818:G:O2'	25:DA:819:A:O4'	2.30	0.45
25:DA:1703:G:H2'	25:DA:1704:G:C8	2.51	0.45
25:DA:1857:G:C6	25:DA:1858:G:N1	2.84	0.45
25:DA:2792:G:H2'	25:DA:2792:G:N3	2.32	0.45
27:DD:182:LEU:HD23	27:DD:182:LEU:HA	1.81	0.45
30:DG:137:GLU:HG2	30:DG:152:LEU:HD23	1.99	0.45
31:DH:35:VAL:O	31:DH:37:VAL:HG23	2.17	0.45
44:DY:88:LYS:NZ	44:DY:89:PHE:O	2.38	0.45
1:AA:130:A:O2'	1:AA:131:C:O5'	2.30	0.45
1:AA:626:U:C2	1:AA:627:G:C8	3.04	0.45
3:AC:82:GLU:HG2	3:AC:85:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:121:ALA:O	3:AC:125:GLU:HG3	2.17	0.45
25:BA:940:C:H2'	25:BA:941:U:O4'	2.16	0.45
25:BA:2699:U:OP2	61:BA:4975:HOH:O	2.21	0.45
29:BF:30:PRO:HB3	35:BP:1:MET:HE1	1.99	0.45
29:BF:170:LEU:HG	29:BF:172:TRP:NE1	2.32	0.45
35:BP:101:VAL:HA	35:BP:106:LEU:O	2.16	0.45
44:BY:92:ASN:OD1	44:BY:94:LYS:HG3	2.16	0.45
54:B8:23:VAL:CG1	54:B8:47:LYS:HD3	2.46	0.45
1:CA:264:U:H4'	17:CQ:63:ARG:HD2	1.99	0.45
2:CB:16:HIS:CD2	2:CB:204:ASN:HB3	2.51	0.45
2:CB:63:MET:CG	2:CB:225:ALA:HB1	2.47	0.45
23:CW:21:A:N6	23:CW:46:7MG:C4	2.85	0.45
25:DA:117:G:C6	25:DA:119:A:C6	3.05	0.45
25:DA:433:C:H2'	25:DA:434:U:C6	2.51	0.45
25:DA:656:G:H2'	25:DA:657:U:O4'	2.17	0.45
25:DA:1709:U:H1'	25:DA:2860:A:N3	2.32	0.45
25:DA:2514:U:H2'	25:DA:2515:C:C6	2.52	0.45
25:DA:2724:C:OP1	28:DE:118:LYS:NZ	2.44	0.45
27:DD:71:ASP:CB	27:DD:103:ARG:HH22	2.28	0.45
30:DG:41:GLN:NE2	30:DG:153:ARG:HB3	2.32	0.45
33:DN:39:ARG:HA	33:DN:40:PRO:HD3	1.78	0.45
1:AA:171:A:H2'	1:AA:172:A:C8	2.52	0.45
1:AA:277:C:H5"	17:AQ:68:ARG:NH2	2.31	0.45
1:AA:691:G:H2'	1:AA:692:U:C6	2.51	0.45
4:AD:157:LEU:HD22	4:AD:161:ASN:HD21	1.81	0.45
11:AK:20:TYR:CZ	11:AK:83:ILE:HD12	2.52	0.45
11:AK:34:ASP:HB3	11:AK:40:ILE:HD11	1.99	0.45
14:AN:6:LEU:HD12	14:AN:6:LEU:HA	1.88	0.45
25:BA:939:C:H2'	25:BA:940:C:C6	2.51	0.45
25:BA:1213:U:H2'	25:BA:1214:G:C8	2.52	0.45
34:BO:120:GLU:OE1	39:BT:67:SER:OG	2.19	0.45
36:BQ:37:LEU:HD21	36:BQ:130:LYS:HE2	1.98	0.45
38:BS:3:ARG:HA	38:BS:3:ARG:HE	1.82	0.45
1:CA:130:A:O2'	1:CA:131:C:O5'	2.35	0.45
1:CA:256:U:H2'	1:CA:257:G:C8	2.51	0.45
1:CA:1230:C:H2'	1:CA:1231:G:H8	1.82	0.45
2:CB:219:VAL:HA	2:CB:222:ILE:CG1	2.47	0.45
23:CW:61:C:O2'	23:CW:62:C:H6	1.99	0.45
24:CX:72:A:H2'	24:CX:73:A:C8	2.52	0.45
23:CY:59:U:O5'	23:CY:59:U:H6	1.99	0.45
25:DA:724:U:H2'	25:DA:725:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1218:C:N4	25:DA:1231:G:H1	2.13	0.45
25:DA:1227:G:N2	25:DA:1228:G:H1'	2.32	0.45
25:DA:1417:C:H2'	25:DA:1418:G:O4'	2.16	0.45
35:DP:59:LEU:HD23	54:D8:58:ILE:HD13	1.98	0.45
36:DQ:35:VAL:HG12	36:DQ:130:LYS:O	2.16	0.45
42:DW:83:LYS:HE2	42:DW:97:LYS:HD3	1.99	0.45
49:D3:7:LYS:HB2	49:D3:34:GLU:HG2	1.98	0.45
1:AA:119:A:H4'	1:AA:120:A:C8	2.52	0.45
2:AB:24:TRP:CD1	2:AB:24:TRP:H	2.35	0.45
2:AB:103:THR:HA	2:AB:180:LEU:HD11	1.99	0.45
2:AB:215:LEU:O	2:AB:219:VAL:HG23	2.17	0.45
43:BX:66:LEU:HD23	43:BX:66:LEU:HA	1.68	0.45
45:BZ:152:ALA:HA	45:BZ:155:LEU:HD22	1.98	0.45
1:CA:258:G:O6	61:CA:4159:HOH:O	2.21	0.45
1:CA:1154:G:H8	1:CA:1154:G:H3'	1.81	0.45
1:CA:1359:C:H1'	1:CA:1362:C:H41	1.82	0.45
2:CB:63:MET:HG3	2:CB:225:ALA:HB1	1.99	0.45
4:CD:166:LYS:HD3	4:CD:178:VAL:HG11	1.99	0.45
14:CN:21:TYR:HE2	14:CN:23:ARG:NE	2.15	0.45
19:CS:27:GLU:HG2	19:CS:47:HIS:HE2	1.81	0.45
25:DA:30:G:H2'	25:DA:31:C:C6	2.52	0.45
25:DA:572:A:OP2	41:DV:78:LYS:NZ	2.50	0.45
25:DA:1341:U:O2	43:DX:80:ILE:HD12	2.16	0.45
25:DA:2120:G:H2'	25:DA:2121:G:H8	1.82	0.45
25:DA:2275:C:H6	25:DA:2275:C:H5'	1.82	0.45
25:DA:2518:A:OP2	61:DA:4302:HOH:O	2.21	0.45
27:DD:10:THR:OG1	27:DD:13:ARG:HG2	2.17	0.45
30:DG:167:GLU:H	30:DG:167:GLU:CD	2.25	0.45
35:DP:100:LEU:HD12	35:DP:112:LEU:HD11	1.97	0.45
45:DZ:6:LYS:HD2	45:DZ:8:TYR:OH	2.16	0.45
1:AA:149:A:H2'	1:AA:150:C:C6	2.52	0.45
1:AA:1002:G:O6	1:AA:1003:G:N2	2.50	0.45
1:AA:1128:C:H2'	1:AA:1129:C:H5'	1.98	0.45
1:AA:1145:C:H4'	1:AA:1146:A:H5"	1.98	0.45
23:AY:50:U:N3	23:AY:64:A:C2	2.77	0.45
25:BA:274:U:H3'	25:BA:275:C:H5'	1.99	0.45
25:BA:327:U:H2'	25:BA:328:G:H8	1.81	0.45
25:BA:360:C:HO2'	44:BY:35:TYR:HH	1.60	0.45
25:BA:909:G:H2'	25:BA:910:A:O4'	2.17	0.45
25:BA:2149:G:H1	25:BA:2183:C:N4	2.15	0.45
25:BA:2545:A:H2'	25:BA:2546:A:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BQ:7:MET:HB2	36:BQ:7:MET:HE3	1.51	0.45
37:BR:41:ALA:HB1	37:BR:114:VAL:HG22	1.99	0.45
38:BS:3:ARG:HE	38:BS:3:ARG:CA	2.30	0.45
1:CA:542:G:OP1	4:CD:10:ARG:NH2	2.43	0.45
1:CA:715:A:H2'	1:CA:716:A:C8	2.52	0.45
1:CA:1072:G:H2'	1:CA:1073:U:C6	2.52	0.45
3:CC:131:ARG:HH21	3:CC:166:GLU:HB3	1.82	0.45
3:CC:179:ARG:NH1	3:CC:206:GLU:OE1	2.50	0.45
8:CH:86:ILE:HG12	8:CH:135:CYS:HA	1.99	0.45
23:CY:51:U:H2'	23:CY:52:G:O4'	2.17	0.45
25:DA:83:G:N1	25:DA:102:G:O2'	2.31	0.45
25:DA:463:G:N2	25:DA:466:A:OP2	2.46	0.45
25:DA:1152:C:H2'	25:DA:1153:C:C6	2.51	0.45
25:DA:1529:G:C6	25:DA:1530:C:N4	2.85	0.45
25:DA:1826:G:H4'	27:DD:242:ARG:CZ	2.47	0.45
25:DA:2149:G:H3'	25:DA:2150:U:H6	1.82	0.45
25:DA:2317:C:N3	25:DA:2318:G:N7	2.65	0.45
25:DA:2399:G:H2'	25:DA:2400:G:O4'	2.16	0.45
25:DA:2693:A:H2'	25:DA:2694:G:H8	1.81	0.45
46:D0:38:VAL:HG12	46:D0:40:GLN:HG2	1.99	0.45
1:AA:345:C:H4'	1:AA:346:G:N3	2.31	0.45
1:AA:1151:A:O4'	10:AJ:39:PRO:HB2	2.17	0.45
1:AA:1286:A:H2	21:AU:18:TYR:OH	2.00	0.45
23:AW:37:MIA:H162	23:AW:37:MIA:H122	1.87	0.45
25:BA:553:A:H3'	25:BA:553:A:C8	2.52	0.45
25:BA:2054:G:O2'	28:BE:145:LYS:HE3	2.17	0.45
25:BA:2658:C:OP2	25:BA:2745:G:O2'	2.33	0.45
29:BF:197:ASP:OD1	29:BF:197:ASP:N	2.49	0.45
30:BG:41:GLN:HE22	30:BG:153:ARG:HB3	1.82	0.45
44:BY:1:MET:HB2	44:BY:2:ARG:H	1.65	0.45
47:B1:2:SER:HB3	47:B1:46:LEU:HD12	1.99	0.45
1:CA:1251:A:N1	1:CA:1354:C:O2'	2.50	0.45
10:CJ:6:ILE:HG12	10:CJ:98:ILE:HG13	1.99	0.45
13:CM:122:LYS:HD3	13:CM:123:ALA:H	1.82	0.45
23:CW:4:C:N3	23:CW:69:G:C2	2.84	0.45
25:DA:224:G:H2'	25:DA:225:A:O4'	2.17	0.45
25:DA:2526:G:H5'	25:DA:2742:C:O2'	2.17	0.45
27:DD:166:GLN:HB2	27:DD:174:ILE:HG22	1.99	0.45
29:DF:125:LEU:HD22	29:DF:199:TRP:HB2	1.99	0.45
31:DH:13:LYS:HA	31:DH:14:GLY:HA2	1.61	0.45
31:DH:44:VAL:O	31:DH:50:VAL:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DP:63:PRO:HD3	54:D8:27:THR:HG22	1.97	0.45
1:AA:198:G:H2'	1:AA:199:G:H8	1.83	0.44
1:AA:1036:G:H5"	1:AA:1037:C:C5	2.52	0.44
1:AA:1118:C:H2'	1:AA:1119:C:H6	1.82	0.44
1:AA:1182:G:C4'	1:AA:1183:A:H5'	2.39	0.44
25:BA:997:G:OP1	36:BQ:16:ARG:NH2	2.48	0.44
25:BA:1639:G:H2'	25:BA:1640:G:C8	2.53	0.44
25:BA:2023:A:H2'	25:BA:2024:G:C8	2.51	0.44
25:BA:2799:U:O2'	28:BE:62:PRO:O	2.29	0.44
37:BR:83:ILE:O	37:BR:86:ARG:HG2	2.17	0.44
45:BZ:7:ALA:HB3	45:BZ:61:LEU:HD12	1.99	0.44
1:CA:357:G:OP1	1:CA:367:U:H5"	2.17	0.44
1:CA:532:A:H2	1:CA:1206:G:N2	2.14	0.44
1:CA:1010:G:H2'	1:CA:1011:G:C8	2.50	0.44
2:CB:95:GLN:HB2	2:CB:148:TYR:CD1	2.52	0.44
25:DA:93:G:H2'	25:DA:94:C:C6	2.52	0.44
25:DA:383:U:H2'	25:DA:385:C:H5	1.81	0.44
25:DA:646:A:H2'	25:DA:647:G:O4'	2.17	0.44
25:DA:864:G:H2'	25:DA:865:C:C6	2.53	0.44
25:DA:2168:G:H2'	25:DA:2169:A:C8	2.52	0.44
27:DD:169:GLU:O	27:DD:169:GLU:HG3	2.17	0.44
29:DF:7:TYR:O	29:DF:22:ALA:N	2.50	0.44
35:DP:122:PRO:HB3	35:DP:141:ALA:O	2.17	0.44
40:DU:65:ILE:HD11	40:DU:95:LEU:HB3	1.99	0.44
41:DV:72:VAL:CG1	41:DV:85:LYS:HD2	2.47	0.44
43:DX:47:PHE:O	43:DX:49:VAL:HG13	2.18	0.44
46:D0:68:GLU:OE1	46:D0:82:ARG:HD2	2.17	0.44
54:D8:63:PRO:HG2	54:D8:64:TYR:CE2	2.53	0.44
1:AA:262:A:H2'	1:AA:263:A:C8	2.52	0.44
1:AA:371:G:H2'	1:AA:372:C:O4'	2.17	0.44
1:AA:673:G:H2'	1:AA:674:G:C8	2.52	0.44
1:AA:1054:C:C4	23:AW:34:G:H1'	2.52	0.44
1:AA:1241:G:H2'	1:AA:1242:C:C6	2.52	0.44
1:AA:1262:C:H2'	1:AA:1263:C:C6	2.53	0.44
1:AA:1302:U:OP1	13:AM:13:LYS:HE3	2.17	0.44
2:AB:178:ARG:HH22	8:AH:68:ARG:HH22	1.66	0.44
7:AG:26:PHE:CE2	7:AG:30:ILE:HD11	2.53	0.44
25:BA:1320:A:N3	25:BA:1343:C:H1'	2.32	0.44
25:BA:2735:G:H2'	25:BA:2736:C:C6	2.52	0.44
27:BD:223:GLY:HA3	27:BD:231:HIS:CE1	2.52	0.44
28:BE:174:ASP:OD1	28:BE:175:VAL:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BN:67:LEU:HD13	33:BN:87:LEU:HD13	1.98	0.44
39:BT:6:LEU:O	39:BT:10:VAL:HG23	2.18	0.44
44:BY:92:ASN:HB3	44:BY:94:LYS:N	2.30	0.44
1:CA:664:G:N2	1:CA:741:G:H1	2.14	0.44
1:CA:944:G:O2'	1:CA:1339:A:N6	2.49	0.44
1:CA:1136:U:H5"	1:CA:1137:C:C5	2.52	0.44
1:CA:1468:A:H2'	1:CA:1469:G:O4'	2.18	0.44
1:CA:1530:G:H2'	1:CA:1531:A:O4'	2.18	0.44
19:CS:28:LYS:HB3	19:CS:28:LYS:HZ3	1.83	0.44
25:DA:212:G:H5'	25:DA:213:A:OP2	2.17	0.44
25:DA:848:G:N9	25:DA:933:A:H8	2.15	0.44
25:DA:980:A:N3	25:DA:2037:G:O2'	2.48	0.44
25:DA:1019:U:H2'	25:DA:1020:A:C8	2.51	0.44
25:DA:1127:A:C2'	25:DA:1128:A:H5"	2.48	0.44
25:DA:1165:U:H2'	25:DA:1166:C:C6	2.52	0.44
25:DA:2268:A:OP1	61:DA:4433:HOH:O	2.21	0.44
26:DB:24:G:N3	26:DB:26:A:N6	2.65	0.44
33:DN:67:LEU:O	33:DN:88:GLU:HG3	2.17	0.44
42:DW:34:ASN:OD1	42:DW:37:ARG:NH1	2.40	0.44
1:AA:98:G:H5'	1:AA:99:U:OP2	2.17	0.44
1:AA:161:A:H2'	1:AA:162:A:C8	2.52	0.44
1:AA:192:U:H2'	1:AA:193:C:C6	2.52	0.44
1:AA:767:A:H2'	1:AA:768:A:O4'	2.17	0.44
1:AA:973:G:H3'	1:AA:974:A:H5"	1.99	0.44
1:AA:1016:A:H2'	1:AA:1017:G:O4'	2.18	0.44
4:AD:168:ARG:H	4:AD:168:ARG:NE	2.15	0.44
23:AY:19:G:H4'	23:AY:57:G:H22	1.82	0.44
23:AY:69:G:H2'	23:AY:70:G:O4'	2.17	0.44
25:BA:174:U:H2'	25:BA:175:G:C8	2.52	0.44
25:BA:831:A:C8	25:BA:839:G:C5	3.05	0.44
25:BA:1324:A:OP1	37:BR:36:THR:HG23	2.17	0.44
25:BA:2123:G:H1	25:BA:2210:C:H42	1.65	0.44
34:BO:36:GLY:HA3	34:BO:109:LYS:HD2	1.99	0.44
39:BT:37:GLY:HA2	39:BT:38:ASN:HA	1.67	0.44
45:BZ:155:LEU:HD12	45:BZ:156:LYS:H	1.82	0.44
48:B2:1:MET:HG2	48:B2:5:GLU:OE1	2.17	0.44
1:CA:203:U:H2'	1:CA:203:U:OP2	2.17	0.44
1:CA:1315:U:H2'	1:CA:1316:G:O4'	2.17	0.44
2:CB:7:VAL:HB	2:CB:8:LYS:H	1.55	0.44
2:CB:77:ALA:HA	2:CB:80:ILE:HG22	1.98	0.44
9:CI:21:PRO:HA	9:CI:59:PHE:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:CI:55:ALA:HA	9:CI:58:HIS:CD2	2.52	0.44
25:DA:286:C:H2'	25:DA:287:C:H6	1.83	0.44
25:DA:422:A:OP2	61:DA:4103:HOH:O	2.21	0.44
25:DA:910:A:N1	25:DA:2277:G:H1'	2.33	0.44
25:DA:1184:G:OP1	49:D3:30:ARG:HD2	2.17	0.44
25:DA:1900:A:N1	25:DA:1970:A:C6	2.85	0.44
25:DA:2108:C:H2'	25:DA:2109:U:H6	1.82	0.44
25:DA:2141:G:O6	25:DA:2150:U:C2	2.70	0.44
25:DA:2648:C:H2'	25:DA:2649:U:C6	2.52	0.44
28:DE:101:ARG:NH1	28:DE:169:ASN:O	2.43	0.44
29:DF:150:GLY:HA2	29:DF:172:TRP:CD2	2.52	0.44
32:DI:38:LEU:HD12	32:DI:38:LEU:H	1.82	0.44
39:DT:99:LEU:HD22	39:DT:101:PHE:HE1	1.81	0.44
43:DX:31:HIS:HD2	43:DX:33:LYS:H	1.65	0.44
45:DZ:138:GLU:H	45:DZ:156:LYS:HD3	1.82	0.44
51:D5:16:ARG:HD2	51:D5:20:ARG:NH1	2.33	0.44
52:D6:18:ARG:HD2	52:D6:42:TRP:CE2	2.52	0.44
1:AA:664:G:OP1	18:AR:64:ARG:NE	2.46	0.44
1:AA:1014:A:OP1	19:AS:18:LYS:NZ	2.36	0.44
1:AA:1129:C:O2'	1:AA:1139:G:N7	2.50	0.44
1:AA:1270:C:OP2	21:AU:24:ARG:NH2	2.51	0.44
2:AB:170:GLU:O	2:AB:174:VAL:HG23	2.18	0.44
25:BA:1360:C:OP1	61:BA:4775:HOH:O	2.21	0.44
25:BA:2221:A:OP2	25:BA:2222:C:H5	2.00	0.44
25:BA:2453:C:OP2	25:BA:2598:C:O2'	2.34	0.44
25:BA:2574:U:H1'	34:BO:23:ARG:HD3	2.00	0.44
25:BA:2661:U:H2'	25:BA:2662:U:C6	2.52	0.44
25:BA:2731:G:O2'	25:BA:2857:U:OP1	2.25	0.44
37:BR:33:ARG:NH2	51:B5:57:VAL:O	2.46	0.44
43:BX:31:HIS:HD2	43:BX:33:LYS:HB2	1.83	0.44
48:B2:21:LEU:HB2	48:B2:64:LEU:HD23	2.00	0.44
50:B4:57:GLU:HA	50:B4:58:ARG:HA	1.61	0.44
1:CA:779:C:O2'	11:CK:120:ARG:HD3	2.17	0.44
2:CB:19:HIS:NE2	2:CB:206:ASP:HB2	2.32	0.44
4:CD:58:LEU:HD22	4:CD:62:GLN:HG2	1.98	0.44
15:CO:39:LEU:HD13	15:CO:56:LEU:HB2	1.99	0.44
25:DA:307:G:H22	25:DA:310:A:P	2.39	0.44
25:DA:908:C:OP1	36:DQ:22:LYS:HB3	2.18	0.44
25:DA:1015:G:H2'	25:DA:1016:G:C8	2.53	0.44
25:DA:2532:G:H1'	25:DA:2663:G:H22	1.83	0.44
25:DA:2871:C:N4	61:DA:4551:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:DH:25:LYS:HE2	31:DH:34:GLU:OE2	2.17	0.44
52:D6:11:LEU:HB2	52:D6:21:TYR:HB2	1.99	0.44
1:AA:154:C:C2'	1:AA:155:C:H5'	2.48	0.44
1:AA:257:G:C6	1:AA:258:G:C5	3.05	0.44
1:AA:1131:G:O2'	1:AA:1132:C:H5'	2.18	0.44
1:AA:1169:A:C6	1:AA:1170:A:C6	3.06	0.44
4:AD:155:LEU:HB3	4:AD:158:ILE:HD11	1.99	0.44
13:AM:84:ILE:HD12	19:AS:74:PHE:CE2	2.53	0.44
16:AP:14:ASN:OD1	16:AP:42:ARG:NH2	2.50	0.44
18:AR:33:ASP:OD2	18:AR:36:ASN:HB2	2.17	0.44
23:AW:31:A:H2'	23:AW:32:PSU:O4'	2.17	0.44
23:AY:19:G:C2	23:AY:56:C:N3	2.86	0.44
23:AY:25:C:H2'	23:AY:26:A:H8	1.82	0.44
25:BA:270:C:H4'	25:BA:271:U:OP1	2.18	0.44
25:BA:1552:C:O2'	25:BA:1553:A:H5'	2.17	0.44
25:BA:2707:C:H2'	25:BA:2708:U:C6	2.52	0.44
25:BA:2707:C:H2'	25:BA:2708:U:H6	1.82	0.44
35:BP:135:LEU:HA	35:BP:135:LEU:HD23	1.70	0.44
36:BQ:4:PRO:HB2	36:BQ:7:MET:HE2	2.00	0.44
38:BS:26:LEU:HB2	38:BS:85:VAL:HG21	1.99	0.44
44:BY:56:PRO:C	44:BY:58:GLY:H	2.25	0.44
54:B8:6:THR:HG23	54:B8:64:TYR:HD2	1.83	0.44
1:CA:564:C:C4	1:CA:565:U:C4	3.06	0.44
1:CA:1244:C:H42	1:CA:1293:G:H1	1.65	0.44
2:CB:112:VAL:O	2:CB:116:GLU:HB2	2.18	0.44
7:CG:79:ARG:NE	7:CG:80:VAL:H	2.16	0.44
23:CW:9:A:O2'	23:CW:10:G:N7	2.47	0.44
23:CW:24:G:C2'	23:CW:25:C:H5'	2.46	0.44
25:DA:57:C:H2'	25:DA:58:G:O4'	2.18	0.44
25:DA:510:C:H2'	25:DA:511:U:O4'	2.18	0.44
25:DA:887:A:H4'	25:DA:888:C:C5	2.51	0.44
25:DA:1453:U:O2'	25:DA:1455:G:N7	2.43	0.44
25:DA:2872:G:O2'	25:DA:2873:A:H5'	2.18	0.44
35:DP:63:PRO:HG2	54:D8:25:MET:HB2	2.00	0.44
36:DQ:18:LYS:HE3	36:DQ:18:LYS:HB2	1.74	0.44
55:D9:29:ASN:HD22	55:D9:32:HIS:CE1	2.35	0.44
1:AA:376:G:OP2	16:AP:67:THR:HG21	2.17	0.44
1:AA:1124:G:O2'	1:AA:1145:C:C4	2.71	0.44
1:AA:1226:C:H4'	19:AS:80:TYR:OH	2.17	0.44
2:AB:51:LEU:HD23	2:AB:201:ILE:HD12	1.99	0.44
5:AE:8:GLU:OE2	5:AE:63:ARG:NH2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AS:68:GLY:N	50:B4:58:ARG:HH12	2.13	0.44
20:AT:92:LEU:O	20:AT:96:GLY:HA2	2.18	0.44
20:AT:100:ILE:HB	20:AT:101:GLY:H	1.63	0.44
25:BA:934:A:O2'	25:BA:935:C:OP2	2.31	0.44
25:BA:1809:U:H2'	25:BA:1815:A:N6	2.33	0.44
25:BA:2062:C:H2'	25:BA:2063:U:O4'	2.18	0.44
25:BA:2376:C:H2'	25:BA:2377:G:O4'	2.18	0.44
35:BP:76:LYS:HE3	35:BP:76:LYS:HB3	1.78	0.44
1:CA:532:A:O2'	1:CA:533:A:P	2.75	0.44
2:CB:62:ALA:HB1	2:CB:225:ALA:HB3	2.00	0.44
3:CC:32:LEU:O	3:CC:36:ASP:HB2	2.17	0.44
3:CC:113:ALA:N	3:CC:183:ASP:OD2	2.45	0.44
9:CI:53:VAL:HG21	9:CI:92:TYR:CE1	2.53	0.44
23:CY:33:U:OP2	23:CY:33:U:H6	2.00	0.44
25:DA:416:C:H2'	25:DA:417:C:O4'	2.17	0.44
25:DA:528:A:N1	25:DA:2042:A:H2'	2.33	0.44
25:DA:583:G:OP2	40:DU:10:ARG:HD2	2.17	0.44
25:DA:973:A:H5'	25:DA:1188:U:H1'	1.99	0.44
25:DA:1557:C:H5"	25:DA:1558:A:OP2	2.17	0.44
25:DA:2094:G:OP1	32:DI:22:LYS:HD2	2.18	0.44
25:DA:2557:G:H2'	25:DA:2558:C:C6	2.52	0.44
42:DW:68:ARG:HH11	42:DW:111:HIS:HA	1.81	0.44
49:D3:26:LEU:O	49:D3:35:ARG:HD3	2.18	0.44
1:AA:555:C:H2'	1:AA:556:C:C6	2.53	0.44
1:AA:1004:A:H5'	1:AA:1024:G:O6	2.17	0.44
1:AA:1006:C:H2'	1:AA:1007:C:C6	2.53	0.44
1:AA:1047:G:H5"	14:AN:4:LYS:HD2	2.00	0.44
6:AF:19:LEU:HD21	6:AF:59:TYR:CE1	2.53	0.44
19:AS:66:MET:HB2	19:AS:74:PHE:CZ	2.53	0.44
24:AX:20:U:H5"	24:AX:21:A:OP2	2.18	0.44
23:AY:9:A:O3'	23:AY:45:U:O2'	2.26	0.44
25:BA:895:G:H2'	25:BA:896:A:C8	2.53	0.44
25:BA:1343:C:OP1	25:BA:2722:C:H4'	2.18	0.44
25:BA:2295:C:H2'	25:BA:2296:C:O4'	2.17	0.44
31:BH:167:GLU:HA	31:BH:168:PRO:HD3	1.83	0.44
32:BI:110:ASP:HA	32:BI:111:PRO:HD2	1.67	0.44
1:CA:91:C:H2'	1:CA:92:C:H6	1.83	0.44
1:CA:390:C:H2'	1:CA:391:G:C8	2.53	0.44
25:DA:309:G:N3	25:DA:329:G:O2'	2.47	0.44
25:DA:903:C:H2'	25:DA:904:C:C6	2.52	0.44
25:DA:1239:G:H2'	25:DA:1240:U:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1632:A:O5'	25:DA:1632:A:H8	1.99	0.44
25:DA:2207:G:H3'	25:DA:2208:A:H5"	1.99	0.44
25:DA:2340:G:H2'	25:DA:2341:G:H8	1.82	0.44
25:DA:2818:G:OP2	37:DR:42:LYS:NZ	2.46	0.44
25:DA:2849:U:OP2	39:DT:95:ARG:NH1	2.51	0.44
29:DF:51:THR:HG23	29:DF:92:PRO:HG2	1.99	0.44
30:DG:86:MET:HA	30:DG:87:PRO:HD3	1.89	0.44
45:DZ:110:GLY:HA3	45:DZ:144:LEU:O	2.18	0.44
47:D1:94:LEU:HD23	47:D1:94:LEU:HA	1.76	0.44
1:AA:376:G:H5"	16:AP:5:ARG:CG	2.38	0.44
1:AA:1286:A:C8	1:AA:1287:A:H4'	2.53	0.44
57:AA:3231:PCY:H37	23:AY:34:G:O6	2.17	0.44
8:AH:86:ILE:HG13	8:AH:133:LEU:HD22	2.00	0.44
13:AM:115:LYS:HE2	13:AM:115:LYS:HB2	1.84	0.44
25:BA:1210:G:H2'	25:BA:1211:U:C6	2.53	0.44
25:BA:2343:G:O2'	46:B0:43:THR:HG22	2.18	0.44
29:BF:33:LEU:HB3	35:BP:6:LEU:HD21	2.00	0.44
31:BH:11:VAL:HG21	31:BH:50:VAL:HG23	1.99	0.44
50:B4:58:ARG:C	50:B4:60:GLN:H	2.25	0.44
1:CA:160:A:H1'	1:CA:344:A:C8	2.53	0.44
1:CA:603:U:H2'	1:CA:604:G:H8	1.83	0.44
1:CA:936:C:H2'	1:CA:937:A:O4'	2.18	0.44
1:CA:1068:G:H8	1:CA:1068:G:OP2	2.01	0.44
1:CA:1105:A:H2'	1:CA:1106:G:H8	1.83	0.44
1:CA:1327:C:H2'	1:CA:1328:C:H6	1.83	0.44
4:CD:184:LYS:HE3	4:CD:186:LEU:HD23	2.00	0.44
25:DA:885:C:H2'	25:DA:886:C:H4'	1.98	0.44
25:DA:1449:A:O2'	25:DA:1529:G:N2	2.23	0.44
25:DA:1450(A):C:N4	25:DA:1451:C:H41	2.15	0.44
25:DA:2023:G:H4'	25:DA:2617:C:O3'	2.18	0.44
25:DA:2591:C:H2'	25:DA:2592:G:C8	2.53	0.44
26:DB:24:G:N2	26:DB:27:C:N3	2.47	0.44
37:DR:63:ARG:O	37:DR:67:LEU:HB2	2.18	0.44
49:D3:7:LYS:NZ	49:D3:32:GLN:O	2.50	0.44
1:AA:840:C:H4'	1:AA:841:U:OP1	2.18	0.44
1:AA:1003:G:C2	1:AA:1004:A:N3	2.86	0.44
1:AA:1032:G:H2'	1:AA:1033:G:C8	2.53	0.44
1:AA:1353:G:H2'	1:AA:1354:C:H6	1.83	0.44
4:AD:178:VAL:C	4:AD:180:GLY:H	2.26	0.44
5:AE:92:LYS:HB3	5:AE:119:LEU:HB2	1.99	0.44
25:BA:280:C:H2'	25:BA:281:G:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:537:G:OP1	25:BA:1280:U:O2'	2.23	0.44
25:BA:664:U:H2'	25:BA:665:C:C6	2.53	0.44
25:BA:1822:A:H8	25:BA:1822:A:OP2	2.00	0.44
25:BA:2148:A:H4'	25:BA:2149:G:H5'	2.00	0.44
25:BA:2371:C:H2'	25:BA:2372:A:O4'	2.18	0.44
25:BA:2695:C:OP1	39:BT:53:ARG:NH2	2.51	0.44
25:BA:2762:A:P	31:BH:3:ARG:HH21	2.39	0.44
38:BS:110:LEU:HD12	38:BS:110:LEU:HA	1.73	0.44
43:BX:50:LYS:N	43:BX:87:GLN:OE1	2.47	0.44
1:CA:1005:A:H3'	1:CA:1006:C:O4'	2.17	0.44
1:CA:1256:A:OP2	3:CC:26:LYS:NZ	2.51	0.44
2:CB:19:HIS:HD1	2:CB:20:GLU:HG2	1.83	0.44
6:CF:3:ARG:HD3	6:CF:64:GLN:NE2	2.32	0.44
7:CG:27:ILE:HD11	7:CG:43:PHE:HB3	2.00	0.44
12:CL:71:PRO:O	12:CL:102:ARG:HD2	2.18	0.44
23:CY:8:4SU:H5'	23:CY:49:C:H5"	2.00	0.44
25:DA:528:A:C2'	25:DA:529:A:H5"	2.48	0.44
25:DA:721:C:H2'	25:DA:722:A:C8	2.53	0.44
45:DZ:29:TYR:HB3	45:DZ:34:ASN:HD22	1.83	0.44
50:D4:64:GLY:C	50:D4:66:SER:H	2.26	0.44
1:AA:167:G:H2'	1:AA:168:G:H8	1.82	0.43
1:AA:736:C:H2'	1:AA:737:A:C8	2.53	0.43
1:AA:1008:C:H2'	1:AA:1009:G:O4'	2.17	0.43
3:AC:82:GLU:HA	3:AC:85:ARG:CZ	2.48	0.43
4:AD:170:VAL:CG1	4:AD:174:LEU:HB2	2.48	0.43
4:AD:174:LEU:HD23	4:AD:185:PHE:HA	2.00	0.43
23:AY:34:G:C6	23:AY:35:A:C6	3.06	0.43
23:AY:46:7MG:H81	23:AY:46:7MG:H2'	1.75	0.43
25:BA:831:A:C6	27:BD:229:VAL:HG11	2.52	0.43
25:BA:1836:U:O2	27:BD:50:THR:HB	2.17	0.43
45:BZ:152:ALA:O	45:BZ:155:LEU:HB2	2.18	0.43
4:CD:64:LEU:HD22	4:CD:198:VAL:HG11	1.99	0.43
6:CF:35:ALA:HA	6:CF:67:MET:HB3	2.00	0.43
25:DA:1013:C:O2'	25:DA:1014:U:H5'	2.18	0.43
25:DA:2572:A:N7	28:DE:145:LYS:HB2	2.33	0.43
30:DG:43:LEU:HD12	30:DG:43:LEU:HA	1.85	0.43
36:DQ:56:ARG:O	36:DQ:56:ARG:HD3	2.18	0.43
42:DW:84:ARG:O	42:DW:96:ILE:N	2.50	0.43
45:DZ:150:LEU:HD12	45:DZ:150:LEU:HA	1.80	0.43
1:AA:72:C:H2'	1:AA:73:G:O4'	2.17	0.43
1:AA:109:A:H2'	1:AA:326:G:N2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:429:U:H4'	1:AA:430:A:O5'	2.18	0.43
1:AA:1129:C:H5"	9:AI:16:ARG:NH1	2.29	0.43
7:AG:65:ALA:O	7:AG:69:VAL:HG23	2.17	0.43
10:AJ:11:PHE:CE1	10:AJ:67:THR:HG22	2.53	0.43
25:BA:1086:C:H2'	25:BA:1087:C:O4'	2.17	0.43
25:BA:1218:G:H2'	25:BA:1218:G:OP2	2.18	0.43
25:BA:2173:G:C2	25:BA:2174:G:C6	3.06	0.43
30:BG:179:PRO:HG3	50:B4:43:TYR:OH	2.18	0.43
41:BV:49:THR:O	41:BV:49:THR:HG22	2.19	0.43
45:BZ:100:VAL:HG21	45:BZ:134:PRO:HG2	2.00	0.43
45:BZ:125:LEU:HG	45:BZ:164:ALA:HB3	2.00	0.43
46:B0:38:VAL:HG12	46:B0:40:GLN:HG2	1.99	0.43
50:B4:58:ARG:C	50:B4:60:GLN:N	2.76	0.43
1:CA:184:G:H2'	1:CA:185:A:C8	2.53	0.43
1:CA:1121:U:H2'	1:CA:1122:U:O4'	2.18	0.43
1:CA:1123:A:H4'	10:CJ:37:PRO:HD2	2.00	0.43
1:CA:1210:C:H2'	1:CA:1211:U:H5"	1.99	0.43
1:CA:1353:G:OP1	21:CU:10:ARG:NH1	2.51	0.43
3:CC:155:GLY:O	3:CC:157:ILE:N	2.48	0.43
4:CD:81:GLU:O	4:CD:85:LYS:HB2	2.18	0.43
6:CF:100:ASN:HB2	18:CR:28:GLU:HA	2.00	0.43
7:CG:99:LEU:HD22	7:CG:103:TRP:CZ2	2.54	0.43
8:CH:82:HIS:CE1	8:CH:84:ARG:HG2	2.53	0.43
14:CN:3:ARG:O	14:CN:7:ILE:HG23	2.17	0.43
16:CP:49:LEU:HD22	16:CP:73:LEU:HD22	1.99	0.43
17:CQ:27:PHE:CE2	17:CQ:36:ILE:HD11	2.52	0.43
25:DA:528:A:H2'	25:DA:529:A:H5"	1.99	0.43
25:DA:848:G:C4	25:DA:933:A:H8	2.36	0.43
25:DA:2474:C:H5"	25:DA:2475:C:OP2	2.17	0.43
38:DS:25:ARG:HD3	38:DS:42:ASP:OD2	2.17	0.43
38:DS:30:ARG:HG3	38:DS:35:ILE:HD12	2.00	0.43
39:DT:78:LEU:HD12	39:DT:79:HIS:NE2	2.33	0.43
44:DY:83:THR:HG21	44:DY:99:CYS:HB2	2.01	0.43
45:DZ:146:ILE:H	45:DZ:146:ILE:HD12	1.83	0.43
45:DZ:158:PRO:HA	45:DZ:159:PRO:HD3	1.90	0.43
45:DZ:166:SER:O	45:DZ:169:GLU:HB2	2.18	0.43
1:AA:532:A:N6	1:AA:1206:G:O2'	2.52	0.43
1:AA:1458:G:OP1	20:AT:35:THR:OG1	2.33	0.43
2:AB:155:LEU:HD11	2:AB:159:PRO:HD3	2.00	0.43
10:AJ:13:HIS:HB3	10:AJ:68:HIS:CE1	2.54	0.43
25:BA:692:C:H2'	25:BA:693:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:956:A:C5	36:BQ:13:GLN:HG3	2.53	0.43
25:BA:1476:C:H2'	25:BA:1477:U:C6	2.52	0.43
25:BA:1547:C:O4'	27:BD:100:GLY:HA2	2.17	0.43
25:BA:2651:A:OP2	61:BA:4267:HOH:O	2.21	0.43
30:BG:16:ARG:HB2	30:BG:17:PRO:HD3	1.99	0.43
45:BZ:19:ARG:NH1	45:BZ:84:GLU:O	2.51	0.43
49:B3:5:LYS:NZ	49:B3:34:GLU:OE2	2.51	0.43
1:CA:393:A:OP2	16:CP:12:LYS:HD2	2.17	0.43
1:CA:875:C:H1'	8:CH:15:ASN:HD21	1.82	0.43
1:CA:1040:U:H2'	1:CA:1041:A:H5"	2.00	0.43
1:CA:1352:C:H2'	1:CA:1353:G:C8	2.52	0.43
3:CC:130:VAL:O	3:CC:134:ILE:HG12	2.18	0.43
7:CG:22:LEU:HG	7:CG:62:PHE:CE2	2.54	0.43
16:CP:8:ARG:HB3	16:CP:28:ARG:NH1	2.32	0.43
23:CY:5:G:H1	23:CY:68:C:N4	2.12	0.43
25:DA:11:G:N7	61:DA:4572:HOH:O	2.36	0.43
25:DA:141:A:C8	25:DA:1408:C:O2'	2.70	0.43
25:DA:468:G:H5"	29:DF:60:SER:HB2	2.00	0.43
25:DA:662:G:H5"	35:DP:16:ARG:HG2	2.00	0.43
25:DA:1038:C:C4	25:DA:1039:G:N7	2.86	0.43
25:DA:1157:G:C2	25:DA:1158:C:C2	3.06	0.43
25:DA:2135:A:C6	25:DA:2136:C:N4	2.86	0.43
25:DA:2533:A:OP1	25:DA:2665:A:O2'	2.34	0.43
25:DA:2538:C:H2'	25:DA:2539:C:H6	1.83	0.43
25:DA:2590:A:OP2	27:DD:238:GLY:HA2	2.18	0.43
30:DG:150:ASP:CG	30:DG:153:ARG:HH12	2.26	0.43
41:DV:55:ALA:HA	41:DV:100:ARG:O	2.18	0.43
1:AA:7:G:H5'	1:AA:298:A:O4'	2.18	0.43
1:AA:44:G:C2	1:AA:45:U:H1'	2.53	0.43
1:AA:159:G:N2	1:AA:161:A:H3'	2.33	0.43
1:AA:1317:C:N3	19:AS:37:ARG:NH2	2.65	0.43
8:AH:72:PRO:O	8:AH:74:PRO:HD3	2.19	0.43
12:AL:39:VAL:HG11	12:AL:41:ARG:NH1	2.33	0.43
14:AN:24:CYS:HB2	14:AN:40:CYS:HB3	1.99	0.43
16:AP:48:TRP:HH2	16:AP:76:GLN:HE22	1.65	0.43
25:BA:201:G:H2'	25:BA:202:A:O4'	2.19	0.43
25:BA:645:G:N3	25:BA:645:G:H5'	2.33	0.43
25:BA:1501:U:O2'	25:BA:1502:G:N7	2.51	0.43
25:BA:2879:G:H2'	25:BA:2880:C:O4'	2.19	0.43
49:B3:19:GLN:OE1	49:B3:52:HIS:NE2	2.48	0.43
50:B4:40:HIS:HA	50:B4:41:PRO:HD2	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:B8:62:LEU:HB3	54:B8:65:GLU:HG2	2.00	0.43
1:CA:60:A:N6	1:CA:110:C:N3	2.64	0.43
1:CA:719:C:N4	18:CR:71:LYS:HE2	2.33	0.43
4:CD:88:VAL:HA	5:CE:97:GLY:HA3	1.99	0.43
12:CL:11:VAL:HG11	17:CQ:36:ILE:HG21	2.00	0.43
15:CO:82:ILE:HB	15:CO:87:ILE:HB	2.00	0.43
17:CQ:81:ARG:NH2	17:CQ:84:LEU:HD21	2.32	0.43
19:CS:64:GLU:HB2	50:D4:59:PHE:CE1	2.53	0.43
20:CT:63:ILE:HD13	20:CT:80:ARG:HB3	1.99	0.43
23:CW:32:PSU:H2'	23:CW:32:PSU:O4	2.18	0.43
25:DA:94(A):G:C6	25:DA:95:G:C5	3.06	0.43
25:DA:196:A:H2'	25:DA:196:A:N3	2.33	0.43
25:DA:207:A:H2'	25:DA:208:C:O4'	2.18	0.43
25:DA:614(B):G:H2'	29:DF:44:ARG:HH11	1.82	0.43
25:DA:2018:G:H2'	25:DA:2019:A:O4'	2.18	0.43
36:DQ:16:ARG:HG3	36:DQ:17:LEU:H	1.82	0.43
38:DS:5:THR:OG1	38:DS:8:GLU:OE2	2.23	0.43
44:DY:35:TYR:CE2	44:DY:69:ALA:HB3	2.54	0.43
1:AA:481:G:O2'	1:AA:483:C:N4	2.48	0.43
1:AA:814:A:H2'	1:AA:816:A:H5"	2.00	0.43
1:AA:1346:A:N6	1:AA:1375:A:OP2	2.51	0.43
1:AA:1493:A:H5"	1:AA:1494:G:OP2	2.19	0.43
6:AF:2:ARG:NE	6:AF:69:GLU:HG2	2.33	0.43
10:AJ:40:LEU:HB2	10:AJ:69:ASN:HB2	2.00	0.43
11:AK:34:ASP:OD2	11:AK:38:ASN:HB2	2.18	0.43
11:AK:48:ILE:O	11:AK:50:TYR:N	2.46	0.43
19:AS:30:LEU:HG	19:AS:31:ILE:N	2.33	0.43
25:BA:1490:G:N2	25:BA:1595:C:C2	2.87	0.43
25:BA:1921:G:H2'	25:BA:1921:G:N3	2.33	0.43
26:BB:13:A:N1	26:BB:69:G:O2'	2.40	0.43
26:BB:114:C:H4'	38:BS:46:VAL:HG22	2.00	0.43
29:BF:32:LEU:HB3	29:BF:112:MET:HE1	1.99	0.43
1:CA:552:U:O3'	12:CL:87:GLY:HA3	2.19	0.43
1:CA:1134:G:H2'	1:CA:1134:G:N3	2.33	0.43
25:DA:140:G:N2	25:DA:1596:A:H4'	2.34	0.43
25:DA:616:G:OP2	29:DF:106:ARG:NE	2.40	0.43
25:DA:866:A:C2	25:DA:867:C:C5	3.06	0.43
25:DA:974:G:N2	25:DA:989:G:H1'	2.34	0.43
25:DA:1359:A:N1	25:DA:1372:U:O4	2.52	0.43
25:DA:1886:C:H2'	25:DA:1887:C:H6	1.84	0.43
25:DA:2096:U:H2'	25:DA:2097:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2243:U:H2'	25:DA:2244:U:C6	2.54	0.43
25:DA:2391:G:O6	25:DA:2425:A:H8	2.02	0.43
25:DA:2507:C:H2'	25:DA:2508:G:O4'	2.18	0.43
25:DA:2854:G:H2'	25:DA:2855:C:C6	2.53	0.43
29:DF:178:PRO:HB3	29:DF:198:ALA:HA	2.00	0.43
1:AA:269:C:H2'	1:AA:270:A:C8	2.54	0.43
2:AB:16:HIS:C	2:AB:17:PHE:HD1	2.27	0.43
2:AB:87:ARG:NE	2:AB:233:SER:HB3	2.33	0.43
2:AB:170:GLU:HB3	2:AB:173:ALA:HB3	2.01	0.43
4:AD:107:ARG:HA	4:AD:107:ARG:HD2	1.88	0.43
5:AE:31:LEU:HD23	5:AE:31:LEU:HA	1.91	0.43
8:AH:25:ASP:OD1	8:AH:60:ARG:HG3	2.18	0.43
25:BA:180:A:H2'	25:BA:181:C:C6	2.53	0.43
25:BA:1040:C:OP2	40:BU:54:LYS:NZ	2.49	0.43
25:BA:2334:A:H2'	25:BA:2335:G:O4'	2.19	0.43
25:BA:2346:G:H4'	25:BA:2347:A:OP2	2.19	0.43
26:BB:7:G:H8	26:BB:7:G:C5'	2.32	0.43
28:BE:51:PHE:O	28:BE:77:ILE:HD12	2.18	0.43
30:BG:11:TYR:CZ	30:BG:16:ARG:HD3	2.54	0.43
41:BV:21:ARG:HG2	41:BV:91:TYR:CD1	2.54	0.43
43:BX:92:LEU:HD12	43:BX:92:LEU:HA	1.79	0.43
1:CA:189(D):C:H2'	1:CA:189(E):U:O4'	2.19	0.43
1:CA:694:A:N1	1:CA:787:A:O2'	2.52	0.43
1:CA:979:C:H2'	1:CA:980:C:H5'	2.01	0.43
2:CB:76:GLN:HG3	2:CB:206:ASP:O	2.18	0.43
4:CD:166:LYS:HD3	4:CD:166:LYS:HA	1.73	0.43
7:CG:15:ASP:O	7:CG:19:GLY:HA2	2.18	0.43
7:CG:15:ASP:OD1	7:CG:20:ASP:N	2.43	0.43
10:CJ:16:LEU:HD23	10:CJ:16:LEU:HA	1.85	0.43
13:CM:19:LEU:HD21	13:CM:56:LEU:HD11	2.00	0.43
13:CM:115:LYS:HE2	13:CM:115:LYS:HB2	1.72	0.43
17:CQ:54:GLY:O	17:CQ:81:ARG:N	2.46	0.43
25:DA:456:C:H4'	61:DA:4011:HOH:O	2.18	0.43
25:DA:567:A:H4'	25:DA:808:G:OP1	2.19	0.43
25:DA:637:A:H8	35:DP:117:GLU:HG3	1.84	0.43
25:DA:658:C:H2'	25:DA:659:C:C6	2.53	0.43
25:DA:699:A:H2'	25:DA:700:G:O4'	2.17	0.43
25:DA:763:G:H1'	25:DA:765:G:O4'	2.18	0.43
25:DA:820:A:N3	25:DA:943:U:H4'	2.33	0.43
25:DA:1155:A:H5"	40:DU:55:ARG:HD3	2.00	0.43
25:DA:2572:A:N7	28:DE:144:ARG:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2685:G:P	39:DT:51:ARG:HH12	2.42	0.43
25:DA:2693:A:H2'	25:DA:2694:G:C8	2.54	0.43
32:DI:88:ILE:O	32:DI:121:LYS:NZ	2.34	0.43
33:DN:48:MET:HE3	33:DN:48:MET:HB2	1.94	0.43
51:D5:16:ARG:NH1	51:D5:16:ARG:HG2	2.34	0.43
1:AA:232:G:H1'	1:AA:262:A:N1	2.33	0.43
1:AA:664:G:N2	1:AA:741:G:H1	2.11	0.43
1:AA:936:C:H2'	1:AA:937:A:O4'	2.18	0.43
2:AB:67:THR:HA	2:AB:90:MET:HE1	2.01	0.43
4:AD:173:TRP:CZ3	4:AD:174:LEU:HG	2.53	0.43
8:AH:64:LYS:HG2	8:AH:79:VAL:HG21	1.99	0.43
13:AM:15:VAL:HG22	13:AM:43:THR:O	2.18	0.43
25:BA:9:U:O4	25:BA:2641:A:H2	2.02	0.43
25:BA:313:A:N6	25:BA:375:G:O2'	2.52	0.43
25:BA:609:A:N1	25:BA:856:G:O2'	2.44	0.43
25:BA:1810:U:H2'	61:BA:5150:HOH:O	2.17	0.43
25:BA:1994:A:H2'	25:BA:1995:G:H8	1.83	0.43
25:BA:2168:C:H4'	25:BA:2169:G:C4	2.54	0.43
25:BA:2627:U:H2'	25:BA:2628:C:C6	2.54	0.43
29:BF:164:ARG:HD2	29:BF:175:THR:HG23	2.00	0.43
30:BG:121:ASN:HA	30:BG:122:PRO:HD3	1.90	0.43
1:CA:308:C:H2'	1:CA:309:G:C8	2.54	0.43
1:CA:580:U:H5"	15:CO:58:MET:HG2	2.01	0.43
1:CA:603:U:H2'	1:CA:604:G:C8	2.53	0.43
1:CA:1004:A:N6	1:CA:1037:C:N3	2.66	0.43
1:CA:1150:U:C2'	1:CA:1151:A:H5'	2.48	0.43
1:CA:1297:C:H1'	1:CA:1298:C:H5	1.83	0.43
1:CA:1410:G:H2'	1:CA:1411:C:H6	1.83	0.43
2:CB:219:VAL:HA	2:CB:222:ILE:HG12	2.01	0.43
20:CT:18:GLN:O	20:CT:22:ARG:HG3	2.19	0.43
23:CY:56:C:H2'	23:CY:57:G:C8	2.35	0.43
25:DA:244:A:C2	25:DA:255:A:C4	3.07	0.43
25:DA:812:C:H1'	25:DA:1250:G:C2	2.53	0.43
25:DA:1371:G:H2'	25:DA:1372:U:H5	1.83	0.43
25:DA:1608:A:H1'	25:DA:1610:A:OP2	2.19	0.43
25:DA:1688:U:O2	25:DA:1700:A:H5'	2.19	0.43
25:DA:2802:G:H2'	25:DA:2803:C:O4'	2.19	0.43
29:DF:64:ILE:HG21	29:DF:78:ILE:HG23	1.99	0.43
29:DF:117:ARG:HH12	35:DP:1:MET:N	2.16	0.43
39:DT:60:THR:HG22	39:DT:77:PRO:HA	2.00	0.43
45:DZ:111:VAL:CG2	45:DZ:117:LEU:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:D3:7:LYS:HZ3	49:D3:34:GLU:HG3	1.83	0.43
50:D4:40:HIS:HA	50:D4:41:PRO:HD2	1.79	0.43
52:D6:10:LEU:HG	52:D6:54:ILE:HG13	2.00	0.43
1:AA:456:C:H2'	1:AA:457:C:C6	2.53	0.43
1:AA:974:A:H8	1:AA:974:A:OP1	2.01	0.43
1:AA:1149:C:H2'	1:AA:1150:U:C6	2.53	0.43
1:AA:1164:G:H2'	1:AA:1165:C:C6	2.53	0.43
1:AA:1302:U:C5	13:AM:17:VAL:HG21	2.53	0.43
3:AC:19:GLU:HB3	3:AC:40:ARG:NH2	2.34	0.43
4:AD:99:SER:O	4:AD:140:VAL:HG23	2.19	0.43
4:AD:157:LEU:HD22	4:AD:161:ASN:ND2	2.34	0.43
23:AY:25:C:H2'	23:AY:26:A:C8	2.54	0.43
23:AY:71:G:H2'	23:AY:72:C:C6	2.54	0.43
25:BA:561:A:H2'	25:BA:562:C:C6	2.54	0.43
25:BA:964:A:H5"	26:BB:98:G:O2'	2.19	0.43
25:BA:1587:U:H2'	25:BA:1588:G:O4'	2.18	0.43
25:BA:2102:G:OP1	47:B1:35:THR:HG21	2.18	0.43
25:BA:2284:U:H5"	25:BA:2285:A:OP1	2.18	0.43
27:BD:130:ALA:C	27:BD:131:LEU:HD12	2.43	0.43
27:BD:145:VAL:HB	27:BD:155:LEU:HB2	2.00	0.43
29:BF:150:GLY:HA2	29:BF:172:TRP:CE3	2.53	0.43
30:BG:49:ASP:O	30:BG:51:ARG:N	2.51	0.43
32:BI:93:THR:O	32:BI:97:ILE:HG13	2.19	0.43
33:BN:34:LEU:HD21	33:BN:120:LEU:HB2	2.01	0.43
34:BO:115:VAL:HG13	34:BO:121:VAL:HG21	2.01	0.43
36:BQ:16:ARG:HG2	36:BQ:18:LYS:HE2	2.00	0.43
39:BT:60:THR:HG22	39:BT:77:PRO:HA	1.99	0.43
41:BV:62:LEU:HD21	41:BV:95:LEU:HB2	2.01	0.43
44:BY:14:LEU:HB2	44:BY:75:ILE:HD11	2.01	0.43
45:BZ:151:HIS:O	45:BZ:153:SER:N	2.49	0.43
52:B6:40:CYS:HA	52:B6:41:PRO:HD3	1.84	0.43
1:CA:130:A:H1'	1:CA:263:A:O2'	2.18	0.43
1:CA:707:C:H2'	1:CA:708:C:C6	2.53	0.43
1:CA:788:U:O3'	57:CA:3178:PCY:H25	2.18	0.43
2:CB:42:ILE:HG21	2:CB:202:PRO:O	2.19	0.43
11:CK:80:VAL:HG13	11:CK:103:LEU:HD12	1.99	0.43
19:CS:66:MET:HB2	19:CS:74:PHE:CZ	2.54	0.43
25:DA:379:G:O2'	25:DA:2232:U:OP1	2.34	0.43
25:DA:686:G:N2	25:DA:788:A:H61	2.17	0.43
25:DA:892:G:H2'	25:DA:893:C:O4'	2.19	0.43
25:DA:994:C:O2'	25:DA:996:A:OP1	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1418:G:OP1	25:DA:1588:C:H4'	2.19	0.43
25:DA:1528(A):A:H2'	25:DA:1529:G:O4'	2.19	0.43
25:DA:2238:G:H2'	25:DA:2238:G:N3	2.33	0.43
25:DA:2432:A:C6	25:DA:2433:A:C6	3.07	0.43
25:DA:2487:G:H2'	25:DA:2488:A:C8	2.53	0.43
25:DA:2722:G:H2'	25:DA:2723:C:C6	2.53	0.43
25:DA:2729:G:C6	25:DA:2730:C:C4	3.06	0.43
27:DD:80:ALA:HB3	27:DD:94:LEU:HB3	2.01	0.43
31:DH:8:PRO:HA	31:DH:51:ARG:HG2	2.00	0.43
35:DP:138:LEU:HD23	35:DP:145:PRO:HG3	2.01	0.43
37:DR:97:VAL:CG2	37:DR:114:VAL:HG13	2.49	0.43
38:DS:93:LYS:HD3	38:DS:95:HIS:HB2	1.99	0.43
45:DZ:108:PRO:HG3	45:DZ:141:VAL:HB	2.00	0.43
1:AA:1240:U:O2'	7:AG:32:ARG:NH2	2.51	0.43
1:AA:1316:G:H22	1:AA:1319:A:H5"	1.84	0.43
2:AB:196:LEU:HD12	2:AB:196:LEU:HA	1.80	0.43
3:AC:45:LYS:HG3	3:AC:46:GLU:N	2.34	0.43
5:AE:145:LYS:O	5:AE:149:GLU:HG2	2.19	0.43
13:AM:2:ALA:N	13:AM:8:GLU:OE1	2.52	0.43
18:AR:32:ARG:HA	18:AR:69:THR:HG21	2.01	0.43
23:AW:62:C:H2'	23:AW:63:G:C8	2.54	0.43
25:BA:200:A:H2'	25:BA:201:G:O4'	2.18	0.43
25:BA:212:A:O4'	25:BA:449:A:H5'	2.19	0.43
25:BA:1440:U:H2'	25:BA:1441:A:O4'	2.19	0.43
25:BA:2250:G:H2'	25:BA:2250:G:N3	2.34	0.43
25:BA:2398:C:H2'	25:BA:2399:U:C6	2.54	0.43
25:BA:2897:U:H2'	25:BA:2898:C:C6	2.54	0.43
42:BW:4:LYS:HE2	42:BW:6:ILE:HD11	2.00	0.43
1:CA:228:A:H2'	1:CA:229:U:O4'	2.19	0.43
1:CA:789:U:H2'	1:CA:791:G:OP2	2.19	0.43
1:CA:1054:C:C4	23:CW:34:G:H1'	2.54	0.43
9:CI:5:TYR:OH	9:CI:16:ARG:HG2	2.19	0.43
11:CK:38:ASN:HA	11:CK:39:PRO:HD3	1.77	0.43
12:CL:113:ARG:NE	12:CL:115:LYS:O	2.43	0.43
20:CT:50:GLU:O	20:CT:100:ILE:HD11	2.18	0.43
25:DA:576:U:H2'	25:DA:577:G:C8	2.54	0.43
25:DA:1164:G:H2'	25:DA:1165:U:C6	2.54	0.43
25:DA:1363:C:H2'	25:DA:1364:G:H8	1.82	0.43
25:DA:1533:G:H22	25:DA:1536:C:H1'	1.82	0.43
25:DA:1741:A:H2'	25:DA:1742:G:O4'	2.18	0.43
25:DA:2026:C:H2'	25:DA:2027:G:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2443:C:H2'	25:DA:2444:G:H8	1.84	0.43
25:DA:2683:C:H4'	28:DE:13:ARG:CZ	2.49	0.43
25:DA:2787:C:H1'	28:DE:62:PRO:HG3	2.01	0.43
25:DA:2875:C:OP1	39:DT:3:ARG:NH2	2.51	0.43
28:DE:9:VAL:HG13	28:DE:25:VAL:O	2.19	0.43
29:DF:93:LYS:HD3	29:DF:93:LYS:HA	1.79	0.43
36:DQ:135:ASP:OD2	45:DZ:49:ARG:NH2	2.51	0.43
37:DR:2:ARG:HG2	37:DR:5:LYS:HB2	2.01	0.43
44:DY:43:ASN:OD1	44:DY:65:ALA:HB3	2.19	0.43
50:D4:1:MET:HE2	50:D4:6:HIS:CD2	2.54	0.43
1:AA:411:A:OP2	4:AD:30:LYS:HD2	2.19	0.43
1:AA:955:U:O2'	19:AS:83:HIS:HD2	2.01	0.43
1:AA:1118:C:H2'	1:AA:1119:C:C6	2.53	0.43
1:AA:1315:U:H2'	1:AA:1316:G:O4'	2.19	0.43
6:AF:81:ILE:HD11	27:BD:125:ILE:HB	2.00	0.43
11:AK:99:GLN:HE21	11:AK:108:ILE:HD11	1.83	0.43
15:AO:61:GLY:O	15:AO:65:ARG:HG3	2.19	0.43
23:AY:54:5MU:C4	23:AY:55:PSU:C2	3.07	0.43
25:BA:343:C:H2'	25:BA:344:A:O4'	2.19	0.43
25:BA:596:G:N1	25:BA:2053:A:OP2	2.38	0.43
25:BA:1566:U:H2'	25:BA:1567:G:O4'	2.19	0.43
27:BD:5:LYS:HB3	27:BD:5:LYS:HE3	1.80	0.43
28:BE:119:ARG:HD2	28:BE:120:TRP:CE2	2.54	0.43
44:BY:6:HIS:HE1	44:BY:72:VAL:O	2.02	0.43
1:CA:347:G:H8	1:CA:347:G:OP2	2.01	0.43
1:CA:1236:A:H2'	1:CA:1237:C:C6	2.54	0.43
1:CA:1258:G:O2'	1:CA:1259:C:H5'	2.18	0.43
2:CB:98:LEU:HB2	2:CB:101:MET:HG3	2.01	0.43
7:CG:26:PHE:O	7:CG:30:ILE:HG13	2.18	0.43
8:CH:119:LEU:HB3	8:CH:123:GLU:HB3	2.01	0.43
12:CL:39:VAL:HG11	12:CL:41:ARG:NH1	2.34	0.43
25:DA:845:G:OP2	25:DA:845:G:N2	2.41	0.43
25:DA:2086:U:H2'	25:DA:2087:G:C8	2.54	0.43
25:DA:2141:G:C8	25:DA:2151:G:N2	2.86	0.43
27:DD:5:LYS:HE3	27:DD:5:LYS:HB3	1.81	0.43
31:DH:116:GLU:HA	31:DH:117:PRO:HD3	1.79	0.43
44:DY:86:ARG:NH1	44:DY:100:ALA:HB1	2.34	0.43
49:D3:7:LYS:HE3	49:D3:32:GLN:NE2	2.34	0.43
1:AA:113:G:H2'	1:AA:114:U:C6	2.54	0.42
1:AA:154:C:N3	1:AA:168:G:C2	2.87	0.42
1:AA:448:A:O5'	1:AA:485:G:N2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:553:A:H2'	1:AA:554:C:C6	2.54	0.42
2:AB:73:THR:OG1	2:AB:170:GLU:OE1	2.31	0.42
2:AB:178:ARG:HH22	8:AH:68:ARG:HH12	1.66	0.42
5:AE:152:ARG:NH2	8:AH:107:LEU:O	2.52	0.42
13:AM:84:ILE:HD12	19:AS:74:PHE:CZ	2.54	0.42
24:AX:12:G:H4'	25:BA:1930:C:O2	2.19	0.42
25:BA:1087:C:H42	25:BA:1160:G:H1	1.67	0.42
25:BA:1831:C:OP2	27:BD:183:ARG:NH2	2.51	0.42
25:BA:2724:U:OP1	25:BA:2727:G:H4'	2.19	0.42
31:BH:97:ARG:NE	31:BH:104:GLU:OE1	2.40	0.42
44:BY:19:LYS:HB3	44:BY:19:LYS:HE2	1.90	0.42
44:BY:98:VAL:HG12	44:BY:105:ALA:HA	2.00	0.42
52:B6:37:ARG:O	52:B6:38:LYS:HD2	2.19	0.42
1:CA:170:U:O2'	1:CA:171:A:H5'	2.19	0.42
1:CA:376:G:H5"	16:CP:5:ARG:HB2	2.00	0.42
1:CA:1005:A:H5"	1:CA:1006:C:C5	2.54	0.42
1:CA:1226:C:H4'	19:CS:80:TYR:CZ	2.53	0.42
1:CA:1236:A:O2'	1:CA:1304:G:H4'	2.19	0.42
1:CA:1432:G:O6	61:CA:4070:HOH:O	2.21	0.42
4:CD:112:VAL:HG22	4:CD:116:GLN:OE1	2.18	0.42
10:CJ:8:LEU:CD2	10:CJ:96:ILE:HG12	2.49	0.42
21:CU:9:ARG:O	21:CU:13:ILE:HG13	2.18	0.42
25:DA:152:G:H2'	25:DA:153:C:C6	2.54	0.42
25:DA:265:A:C8	25:DA:266:G:H1'	2.54	0.42
25:DA:271(H):G:O6	25:DA:271(Q):G:C6	2.72	0.42
25:DA:446:G:OP1	40:DU:3:ARG:NH1	2.52	0.42
25:DA:511:U:O4	25:DA:512:G:N1	2.51	0.42
25:DA:775:G:N3	61:DA:4545:HOH:O	2.37	0.42
25:DA:959:A:N3	25:DA:2457:U:O2'	2.43	0.42
25:DA:2161:C:H2'	25:DA:2162:G:C8	2.54	0.42
25:DA:2350:C:H2'	25:DA:2351:G:O4'	2.19	0.42
25:DA:2543:G:H2'	25:DA:2544:G:C8	2.54	0.42
26:DB:80:U:H2'	26:DB:81:G:N7	2.34	0.42
31:DH:56:SER:HB3	31:DH:61:HIS:ND1	2.33	0.42
32:DI:12:LEU:HD22	32:DI:19:VAL:HG21	2.01	0.42
35:DP:82:GLY:HA2	35:DP:113:LYS:O	2.19	0.42
41:DV:28:GLU:H	41:DV:28:GLU:HG2	1.58	0.42
1:AA:149:A:H2'	1:AA:150:C:H6	1.84	0.42
1:AA:993:G:H2'	1:AA:995:C:H41	1.84	0.42
1:AA:1446:U:O2'	1:AA:1447:A:O5'	2.37	0.42
3:AC:6:HIS:CD2	3:AC:8:ILE:HB	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:22:TRP:CZ2	14:AN:54:PRO:HG3	2.55	0.42
25:BA:239:G:C6	25:BA:240:A:C6	3.08	0.42
25:BA:1846:A:H8	25:BA:1846:A:OP1	2.02	0.42
25:BA:2724:U:H2'	25:BA:2727:G:H5"	2.00	0.42
38:BS:59:LYS:CD	38:BS:60:GLY:H	2.30	0.42
1:CA:581:G:O2'	1:CA:582:U:H5'	2.19	0.42
1:CA:619:U:N3	4:CD:134:ASP:OD1	2.45	0.42
1:CA:859:A:H2'	1:CA:860:A:O4'	2.19	0.42
25:DA:117:G:C6	25:DA:119:A:N6	2.87	0.42
25:DA:1010:A:N3	25:DA:1153:C:H1'	2.35	0.42
25:DA:1012:U:O2	33:DN:25:ARG:NH2	2.50	0.42
25:DA:1027:A:C2	25:DA:2488:A:H5'	2.54	0.42
25:DA:1255:U:O5'	25:DA:1256:G:H5"	2.20	0.42
25:DA:1268:A:C2	25:DA:2013:A:C4	3.06	0.42
25:DA:1903:G:OP1	27:DD:241:PRO:HB2	2.19	0.42
25:DA:2184:G:H2'	25:DA:2185:C:C6	2.54	0.42
25:DA:2203:U:O4'	27:DD:151:LYS:HE2	2.19	0.42
25:DA:2648:C:H2'	25:DA:2649:U:H6	1.83	0.42
25:DA:2820:A:OP1	37:DR:2:ARG:NH2	2.51	0.42
27:DD:132:PRO:HG2	27:DD:135:PHE:HD2	1.80	0.42
29:DF:31:HIS:HB2	35:DP:9:ASN:OD1	2.20	0.42
30:DG:33:ARG:O	30:DG:161:THR:HG23	2.19	0.42
36:DQ:7:MET:HE2	36:DQ:7:MET:HB3	1.76	0.42
38:DS:10:ARG:O	38:DS:14:VAL:HG13	2.19	0.42
44:DY:52:SER:HB2	44:DY:53:PRO:HD2	2.02	0.42
1:AA:1343:G:H2'	1:AA:1344:C:C6	2.54	0.42
2:AB:88:ALA:O	2:AB:226:ARG:NH1	2.52	0.42
6:AF:6:VAL:HG13	6:AF:90:VAL:HG22	2.01	0.42
13:AM:80:ARG:HH21	19:AS:69:HIS:HE1	1.66	0.42
15:AO:56:LEU:O	15:AO:60:VAL:HG23	2.19	0.42
19:AS:23:ASN:HA	19:AS:27:GLU:CD	2.44	0.42
23:AY:51:U:O2	23:AY:63:G:N2	2.47	0.42
25:BA:1081:U:H2'	25:BA:1082:G:C8	2.53	0.42
25:BA:1093:G:H2'	25:BA:1156:G:N2	2.34	0.42
25:BA:1857:G:H2'	25:BA:1858:C:O4'	2.18	0.42
27:BD:228:PRO:HD3	27:BD:235:GLY:CA	2.49	0.42
30:BG:67:LYS:HE3	30:BG:68:PRO:O	2.19	0.42
33:BN:108:PRO:O	33:BN:113:GLY:HA3	2.18	0.42
35:BP:98:GLU:OE1	35:BP:102:ARG:NH1	2.53	0.42
45:BZ:150:LEU:HD12	45:BZ:150:LEU:HA	1.86	0.42
1:CA:93:G:O2'	1:CA:96:U:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:97:G:HO2'	1:CA:98:G:P	2.42	0.42
1:CA:300:A:H1'	1:CA:565:U:O2	2.19	0.42
1:CA:828:A:H5"	1:CA:859:A:C2	2.54	0.42
1:CA:978:A:O2'	1:CA:1322:C:N3	2.40	0.42
1:CA:1005:A:H5"	1:CA:1006:C:C6	2.53	0.42
1:CA:1142:G:H2'	1:CA:1143:G:O4'	2.18	0.42
1:CA:1241:G:H2'	1:CA:1242:C:C6	2.54	0.42
1:CA:1510:U:H2'	1:CA:1511:G:C8	2.54	0.42
4:CD:163:GLU:C	4:CD:165:MET:H	2.26	0.42
5:CE:91:LEU:HG	5:CE:118:ILE:HD11	2.02	0.42
7:CG:59:LEU:HD11	7:CG:63:LYS:HE2	2.00	0.42
8:CH:20:TYR:HA	8:CH:65:TYR:CZ	2.54	0.42
9:CI:89:ASN:O	9:CI:92:TYR:HB2	2.19	0.42
25:DA:39:C:H2'	25:DA:40:C:H6	1.82	0.42
25:DA:208:C:H2'	25:DA:209:C:C6	2.54	0.42
25:DA:411:G:C5	35:DP:72:PRO:HB3	2.54	0.42
25:DA:529:A:H62	25:DA:2041:U:H3	1.67	0.42
25:DA:566:U:H5"	35:DP:29:LYS:HE3	2.01	0.42
25:DA:580:C:H2'	25:DA:581:C:C6	2.53	0.42
25:DA:784:A:C8	25:DA:792:G:C5	3.07	0.42
25:DA:816:C:O2'	25:DA:932:G:O6	2.31	0.42
25:DA:1308:A:H2'	25:DA:1309:G:O4'	2.19	0.42
25:DA:1668:A:O2'	25:DA:1674:G:N7	2.43	0.42
29:DF:13:SER:OG	29:DF:16:GLY:O	2.23	0.42
31:DH:3:ARG:CZ	31:DH:5:GLY:H	2.32	0.42
31:DH:38:SER:HA	31:DH:39:PRO:HD3	1.83	0.42
31:DH:44:VAL:HG12	31:DH:46:GLU:HG2	2.00	0.42
35:DP:45:LEU:HD22	35:DP:45:LEU:HA	1.61	0.42
35:DP:88:LEU:HD11	35:DP:114:ILE:HD12	2.01	0.42
44:DY:38:ILE:HD11	44:DY:66:PRO:HG3	2.00	0.42
1:AA:377:G:OP1	16:AP:3:LYS:HD2	2.19	0.42
1:AA:975:A:H5'	1:AA:975:A:C8	2.53	0.42
3:AC:142:MET:HG3	3:AC:170:GLN:HB3	2.00	0.42
4:AD:170:VAL:HG12	4:AD:174:LEU:HB2	2.01	0.42
5:AE:36:ASP:OD2	5:AE:40:ARG:HB2	2.19	0.42
5:AE:148:VAL:HG21	8:AH:107:LEU:HB3	2.00	0.42
15:AO:26:GLU:H	15:AO:26:GLU:HG2	1.38	0.42
19:AS:63:THR:O	19:AS:66:MET:HG2	2.18	0.42
25:BA:605:G:H2'	25:BA:606:G:C8	2.54	0.42
25:BA:1199:C:OP1	40:BU:92:ARG:NH1	2.52	0.42
25:BA:1700:G:O3'	37:BR:2:ARG:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BD:242:ARG:HG2	27:BD:246:PRO:HG3	2.01	0.42
48:B2:32:LEU:HD13	48:B2:36:ARG:HH11	1.84	0.42
53:B7:11:LYS:HE3	53:B7:15:THR:OG1	2.18	0.42
1:CA:1022:G:C6	1:CA:1023:G:C6	3.07	0.42
1:CA:1227:A:OP2	13:CM:111:LYS:HE3	2.19	0.42
1:CA:1262:C:H2'	1:CA:1263:C:H6	1.83	0.42
1:CA:1353:G:C2	1:CA:1370:G:C2	3.07	0.42
1:CA:1366:C:H2'	1:CA:1367:C:C6	2.54	0.42
2:CB:59:GLU:HG2	2:CB:63:MET:HE2	2.00	0.42
2:CB:82:ARG:HB3	2:CB:94:ASN:OD1	2.20	0.42
23:CW:68:C:H2'	23:CW:69:G:H8	1.85	0.42
23:CY:12:U:C2	23:CY:13:C:H1'	2.53	0.42
25:DA:598:G:C6	25:DA:599:G:C5	3.07	0.42
25:DA:995:C:N3	33:DN:2:LYS:HA	2.34	0.42
25:DA:1473:G:C6	25:DA:1474:C:C4	3.07	0.42
25:DA:1618:A:H5'	61:DA:4351:HOH:O	2.19	0.42
25:DA:2328:A:H2'	25:DA:2329:G:C8	2.55	0.42
25:DA:2740:A:C6	25:DA:2764:A:C8	3.07	0.42
25:DA:2847:U:OP1	39:DT:98:LYS:HE3	2.19	0.42
26:DB:89:G:C6	26:DB:90:A:C6	3.07	0.42
31:DH:106:THR:HG23	31:DH:112:PRO:HB3	2.01	0.42
1:AA:922:G:N3	1:AA:1398:A:H2	2.18	0.42
1:AA:1219:U:OP1	14:AN:19:ARG:NH2	2.47	0.42
4:AD:138:TYR:HE1	4:AD:140:VAL:HA	1.83	0.42
10:AJ:70:ARG:HD3	10:AJ:70:ARG:HA	1.71	0.42
12:AL:28:LYS:HE2	12:AL:64:TYR:CE1	2.54	0.42
25:BA:746:A:H2'	25:BA:747:G:O4'	2.20	0.42
25:BA:1549:U:H2'	25:BA:1550:C:C6	2.54	0.42
25:BA:1644:C:H2'	25:BA:1645:C:H6	1.85	0.42
25:BA:1683:C:H2'	25:BA:1684:A:C8	2.54	0.42
25:BA:2699:U:H2'	25:BA:2700:U:O4'	2.20	0.42
28:BE:116:VAL:HG13	28:BE:122:PHE:HB2	2.00	0.42
28:BE:143:ASN:HD22	28:BE:147:PRO:CD	2.31	0.42
45:BZ:111:VAL:HG13	45:BZ:117:LEU:H	1.84	0.42
48:B2:22:GLU:OE2	48:B2:68:ARG:NH2	2.53	0.42
1:CA:8:A:H5'	5:CE:101:ILE:HG22	2.01	0.42
1:CA:189(C):C:H2'	1:CA:189(D):C:O4'	2.20	0.42
1:CA:241:C:C2	1:CA:286:G:C2	3.08	0.42
1:CA:381:C:H2'	1:CA:382:A:O4'	2.19	0.42
1:CA:429:U:H4'	1:CA:430:A:O5'	2.19	0.42
1:CA:519:C:H2'	1:CA:520:A:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:532:A:HO2'	1:CA:533:A:P	2.37	0.42
1:CA:719:C:O2'	18:CR:49:LYS:HB3	2.20	0.42
1:CA:1003:G:H2'	1:CA:1004:A:H1'	2.01	0.42
1:CA:1319:A:H61	1:CA:1361:G:H21	1.67	0.42
2:CB:16:HIS:CG	2:CB:17:PHE:N	2.87	0.42
2:CB:130:ARG:HA	2:CB:131:PRO:HD3	1.92	0.42
4:CD:58:LEU:O	4:CD:62:GLN:HG2	2.19	0.42
10:CJ:7:LYS:HB2	10:CJ:97:GLU:HB2	2.01	0.42
11:CK:93:GLN:HE21	11:CK:93:GLN:CA	2.28	0.42
24:CX:10:G:C2	24:CX:26:G:H1'	2.54	0.42
25:DA:444:C:H4'	29:DF:49:ALA:HB2	2.01	0.42
25:DA:570:G:H2'	25:DA:2030:A:N7	2.35	0.42
25:DA:856:C:O4'	46:D0:27:GLU:HB3	2.19	0.42
25:DA:1171:G:H1	25:DA:1178:C:N4	2.06	0.42
25:DA:1264:G:H2'	25:DA:2014:A:N6	2.33	0.42
25:DA:2134:A:O2'	25:DA:2135:A:OP1	2.37	0.42
25:DA:2136:C:O2'	25:DA:2137:C:H6	2.02	0.42
25:DA:2271:G:OP1	46:D0:18:ALA:HB1	2.20	0.42
25:DA:2659:G:H2'	25:DA:2661:G:OP2	2.19	0.42
25:DA:2723:C:OP2	28:DE:109:LYS:NZ	2.52	0.42
27:DD:68:LYS:O	27:DD:69:ARG:HB2	2.18	0.42
31:DH:11:VAL:HG21	31:DH:50:VAL:HG23	2.02	0.42
31:DH:40:GLU:O	31:DH:55:PRO:HG3	2.20	0.42
33:DN:123:TYR:OH	33:DN:130:HIS:NE2	2.18	0.42
35:DP:21:ARG:HD3	35:DP:21:ARG:HA	1.68	0.42
37:DR:29:LEU:HD12	37:DR:29:LEU:HA	1.81	0.42
41:DV:8:GLY:O	41:DV:10:LYS:NZ	2.50	0.42
1:AA:123:C:OP1	1:AA:311:C:O2'	2.32	0.42
1:AA:598:U:O4	61:AA:4079:HOH:O	2.21	0.42
1:AA:1030(A):G:O2'	1:AA:1030(C):G:N7	2.53	0.42
1:AA:1314:C:H2'	1:AA:1315:U:C6	2.54	0.42
2:AB:211:ILE:HG22	2:AB:215:LEU:HD12	2.00	0.42
10:AJ:45:ARG:HG2	10:AJ:47:PHE:CZ	2.55	0.42
16:AP:20:VAL:HG21	16:AP:32:TYR:CD2	2.55	0.42
19:AS:40:ILE:HD12	19:AS:69:HIS:C	2.45	0.42
25:BA:2418:U:H6	25:BA:2418:U:H2'	1.70	0.42
25:BA:2576:A:C2	25:BA:2659:U:H4'	2.54	0.42
29:BF:132:VAL:HA	29:BF:138:GLU:HB3	2.01	0.42
39:BT:33:LYS:HA	39:BT:42:ILE:HD13	2.00	0.42
47:B1:50:ARG:HG2	47:B1:59:THR:HB	2.02	0.42
1:CA:114:U:H1'	1:CA:353:A:H1'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:273:A:N6	1:CA:274:A:C6	2.87	0.42
1:CA:767:A:H2'	1:CA:768:A:O4'	2.20	0.42
1:CA:1064:G:H4'	1:CA:1065:U:O5'	2.20	0.42
2:CB:76:GLN:CD	2:CB:76:GLN:H	2.28	0.42
2:CB:91:PRO:HA	2:CB:151:GLY:O	2.19	0.42
2:CB:210:SER:OG	2:CB:211:ILE:N	2.52	0.42
2:CB:211:ILE:O	2:CB:215:LEU:HB2	2.20	0.42
4:CD:158:ILE:HG22	4:CD:162:LEU:HD12	2.02	0.42
5:CE:36:ASP:C	5:CE:38:GLN:H	2.27	0.42
8:CH:9:MET:SD	8:CH:32:LYS:HD3	2.59	0.42
9:CI:111:ARG:O	9:CI:113:LYS:HD2	2.19	0.42
14:CN:24:CYS:HB2	14:CN:40:CYS:HB3	2.01	0.42
23:CW:61:C:H2'	23:CW:61:C:OP2	2.20	0.42
25:DA:141:A:H8	25:DA:1408:C:O2'	2.01	0.42
25:DA:800:A:H8	25:DA:800:A:OP1	2.03	0.42
25:DA:1027:A:N6	25:DA:1126:A:C4	2.87	0.42
25:DA:1992:G:C8	25:DA:1992:G:O5'	2.73	0.42
25:DA:2393:A:H2'	25:DA:2394:C:O4'	2.19	0.42
29:DF:64:ILE:HG13	29:DF:65:TRP:N	2.34	0.42
29:DF:150:GLY:HA2	29:DF:172:TRP:CE3	2.54	0.42
31:DH:69:ARG:HG3	31:DH:70:THR:N	2.33	0.42
31:DH:121:ILE:HD11	31:DH:140:LYS:HG2	1.99	0.42
50:D4:33:VAL:HG12	50:D4:34:GLU:H	1.85	0.42
1:AA:262:A:C6	1:AA:263:A:C6	3.08	0.42
1:AA:757:U:O2'	1:AA:879:C:O2	2.34	0.42
1:AA:1169:A:H2'	1:AA:1170:A:C8	2.54	0.42
1:AA:1316:G:N1	1:AA:1319:A:OP2	2.49	0.42
2:AB:69:LEU:HD12	2:AB:91:PRO:O	2.19	0.42
4:AD:188:LEU:HA	4:AD:189:PRO:HD3	1.85	0.42
15:AO:17:ARG:HH11	15:AO:17:ARG:HG3	1.84	0.42
19:AS:36:ARG:HB3	19:AS:72:GLY:HA3	2.02	0.42
25:BA:1405:A:C2	25:BA:1418:U:O4	2.72	0.42
25:BA:1495:G:H1'	25:BA:1574:A:N1	2.34	0.42
25:BA:1527:G:C6	25:BA:1528:U:C4	3.08	0.42
29:BF:93:LYS:HD3	29:BF:93:LYS:HA	1.79	0.42
32:BI:57:ARG:O	32:BI:61:ARG:HD3	2.20	0.42
37:BR:96:ARG:HD2	37:BR:115:GLU:OE1	2.20	0.42
42:BW:9:TYR:HA	42:BW:100:THR:HG23	2.01	0.42
45:BZ:111:VAL:O	45:BZ:113:ALA:N	2.49	0.42
1:CA:189(D):C:H6	1:CA:189(D):C:O5'	2.03	0.42
1:CA:195:A:OP1	20:CT:68:LYS:NZ	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:890:G:O2'	1:CA:906:G:O6	2.27	0.42
1:CA:1227:A:P	13:CM:111:LYS:HZ1	2.42	0.42
1:CA:1348:U:H4'	9:CI:120:ARG:HD2	2.02	0.42
1:CA:1423:G:P	34:DO:49:ARG:HH12	2.42	0.42
57:CA:3178:PCY:H24	57:CA:3178:PCY:H17	1.67	0.42
3:CC:13:GLY:C	3:CC:14:ILE:HD12	2.45	0.42
3:CC:112:SER:O	3:CC:116:VAL:HG23	2.20	0.42
9:CI:16:ARG:HD3	9:CI:64:THR:HG21	2.01	0.42
20:CT:65:LYS:HA	20:CT:68:LYS:HD3	2.00	0.42
25:DA:807:U:OP2	35:DP:41:ARG:NH2	2.52	0.42
25:DA:1356:G:OP1	61:DA:4817:HOH:O	2.21	0.42
25:DA:1794:U:H2'	25:DA:1795:C:C6	2.55	0.42
25:DA:2004:G:H2'	25:DA:2005:A:O4'	2.20	0.42
25:DA:2805:G:H2'	25:DA:2807:G:C8	2.54	0.42
31:DH:3:ARG:HB3	31:DH:6:ARG:HG2	2.01	0.42
31:DH:8:PRO:O	31:DH:69:ARG:NH1	2.53	0.42
32:DI:93:THR:HG22	32:DI:119:PRO:HB3	2.01	0.42
35:DP:2:LYS:HG2	35:DP:5:ASP:OD2	2.20	0.42
40:DU:97:ASP:OD1	40:DU:101:ARG:HD2	2.20	0.42
45:DZ:24:LEU:N	45:DZ:39:VAL:O	2.50	0.42
47:D1:78:LYS:HB2	47:D1:78:LYS:HE3	1.86	0.42
1:AA:918:A:H2'	1:AA:919:A:O4'	2.19	0.42
1:AA:1118:C:H1'	1:AA:1179:A:C5	2.54	0.42
5:AE:145:LYS:HB3	5:AE:145:LYS:HE2	1.82	0.42
18:AR:47:THR:HG23	18:AR:49:LYS:HG3	2.02	0.42
20:AT:13:LEU:HD12	20:AT:14:LYS:N	2.35	0.42
25:BA:495:G:O6	53:B7:37:LYS:HE2	2.20	0.42
25:BA:886:U:H1'	25:BA:1236:G:H1'	2.02	0.42
25:BA:1553:A:O2'	25:BA:1554:A:O5'	2.25	0.42
25:BA:1821:C:H5"	25:BA:1822:A:OP1	2.20	0.42
25:BA:2108:U:H2'	25:BA:2109:G:C8	2.55	0.42
34:BO:6:THR:HG22	34:BO:8:LEU:HD22	2.01	0.42
35:BP:1:MET:HE3	35:BP:5:ASP:HB3	2.01	0.42
1:CA:431:A:OP2	61:CA:4140:HOH:O	2.21	0.42
1:CA:457:C:H2'	1:CA:458:C:C6	2.54	0.42
1:CA:736:C:H2'	1:CA:737:A:C8	2.55	0.42
1:CA:1018:C:H2'	1:CA:1019:C:O4'	2.20	0.42
1:CA:1278:U:H5'	1:CA:1279:A:C5'	2.50	0.42
2:CB:58:ILE:HD13	2:CB:58:ILE:HA	1.83	0.42
5:CE:93:PRO:HG2	8:CH:105:ARG:HE	1.85	0.42
9:CI:105:ASP:HB2	9:CI:107:ARG:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:CM:65:LYS:N	50:D4:50:VAL:HG21	2.35	0.42
18:CR:43:PHE:C	18:CR:51:LEU:HD12	2.45	0.42
23:CW:13:C:O2'	23:CW:14:A:O5'	2.34	0.42
25:DA:141:A:H8	25:DA:1408:C:HO2'	1.57	0.42
25:DA:262:A:H2'	25:DA:263:C:O4'	2.20	0.42
25:DA:471:A:H2'	25:DA:472:A:O4'	2.20	0.42
25:DA:568:U:H5'	25:DA:945:A:N1	2.34	0.42
25:DA:796:C:H2'	25:DA:797:C:H6	1.80	0.42
25:DA:921:G:H2'	25:DA:922:U:H6	1.85	0.42
25:DA:1364:G:C5	47:D1:3:LYS:HE2	2.55	0.42
25:DA:1983:C:H4'	25:DA:2606:C:H4'	2.00	0.42
25:DA:2061:G:H5"	25:DA:2503:A:C2	2.54	0.42
29:DF:9:ILE:HA	29:DF:10:PRO:HD3	1.79	0.42
30:DG:106:LEU:HA	30:DG:110:ALA:HB3	2.01	0.42
35:DP:85:LEU:HD13	35:DP:120:ALA:HB2	2.02	0.42
37:DR:98:LEU:HB2	37:DR:113:LEU:HD11	2.02	0.42
45:DZ:111:VAL:HG22	45:DZ:174:VAL:HG22	2.02	0.42
47:D1:3:LYS:HB3	47:D1:4:VAL:H	1.58	0.42
53:D7:34:ARG:NH2	61:D7:203:HOH:O	2.53	0.42
1:AA:501:C:H2'	1:AA:502:G:H8	1.84	0.42
1:AA:1002:G:C5	1:AA:1003:G:H1'	2.54	0.42
1:AA:1291:G:O2'	9:AI:38:GLN:OE1	2.30	0.42
1:AA:1530:G:OP1	1:AA:1530:G:H4'	2.19	0.42
4:AD:22:LYS:HB2	4:AD:26:CYS:SG	2.60	0.42
25:BA:669:A:H4'	25:BA:670:C:H5	1.85	0.42
25:BA:895:G:O6	25:BA:974:G:H2'	2.20	0.42
25:BA:2086:C:H2'	25:BA:2087:C:C6	2.55	0.42
25:BA:2826:C:O2	25:BA:2893:A:O2'	2.38	0.42
26:BB:2:C:H2'	26:BB:3:C:H6	1.85	0.42
27:BD:143:HIS:ND1	27:BD:194:GLY:O	2.43	0.42
32:BI:131:LYS:H	32:BI:138:ILE:H	1.67	0.42
41:BV:72:VAL:HG11	41:BV:85:LYS:HD2	2.01	0.42
45:BZ:7:ALA:O	45:BZ:62:PRO:HD3	2.20	0.42
48:B2:35:LEU:HD23	48:B2:35:LEU:HA	1.84	0.42
50:B4:53:GLU:HG2	50:B4:55:ARG:HD2	2.02	0.42
50:B4:55:ARG:HA	50:B4:55:ARG:HD2	1.83	0.42
1:CA:324:G:N2	1:CA:326:G:H3'	2.35	0.42
1:CA:769:G:H4'	1:CA:1513:A:H4'	2.02	0.42
1:CA:1273:G:H3'	1:CA:1274:G:C8	2.54	0.42
2:CB:52:GLU:HG2	2:CB:56:ARG:NH2	2.34	0.42
3:CC:181:ASN:ND2	3:CC:204:LEU:HD12	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CF:22:GLU:O	6:CF:26:ILE:HG13	2.20	0.42
11:CK:93:GLN:HA	11:CK:93:GLN:NE2	2.29	0.42
23:CW:25:C:H2'	23:CW:26:A:C8	2.54	0.42
23:CW:29:G:N2	23:CW:41:C:N3	2.67	0.42
25:DA:667:U:O2	54:D8:2:PRO:HD2	2.20	0.42
25:DA:1187:G:H8	25:DA:1187:G:OP2	2.02	0.42
25:DA:1796:U:H2'	25:DA:1797:C:H6	1.84	0.42
25:DA:2335:A:C8	25:DA:2337:G:C5	3.08	0.42
25:DA:2419:U:H2'	25:DA:2420:C:C6	2.55	0.42
25:DA:2646:C:O5'	25:DA:2646:C:H6	2.03	0.42
25:DA:2652:C:O2	25:DA:2668:G:N2	2.32	0.42
30:DG:111:LEU:HB3	30:DG:117:PHE:CE2	2.55	0.42
36:DQ:79:LEU:HD23	36:DQ:79:LEU:HA	1.94	0.42
52:D6:37:ARG:O	52:D6:38:LYS:HD2	2.20	0.42
1:AA:107:G:H2'	1:AA:108:G:O4'	2.20	0.42
1:AA:130:A:H5'	17:AQ:63:ARG:NE	2.35	0.42
1:AA:431:A:H2'	1:AA:432:A:O4'	2.20	0.42
2:AB:220:ASP:O	2:AB:224:GLN:HG3	2.20	0.42
2:AB:230:VAL:HG22	2:AB:231:GLU:H	1.84	0.42
3:AC:6:HIS:CD2	3:AC:8:ILE:H	2.27	0.42
8:AH:29:SER:HB3	8:AH:32:LYS:HG3	2.02	0.42
19:AS:63:THR:OG1	19:AS:66:MET:HE3	2.20	0.42
25:BA:196:A:H2'	25:BA:197:C:O4'	2.18	0.42
25:BA:213:G:H2'	25:BA:214:A:O4'	2.19	0.42
25:BA:316:C:C2	25:BA:373:G:C2	3.08	0.42
25:BA:329:U:H2'	25:BA:330:U:C6	2.55	0.42
25:BA:1405:A:H61	25:BA:1418:U:H3	1.68	0.42
25:BA:1945:U:H2'	25:BA:1946:C:C6	2.54	0.42
30:BG:163:ALA:HB1	30:BG:168:GLU:HB2	2.01	0.42
32:BI:40:THR:O	32:BI:44:LEU:HB2	2.19	0.42
33:BN:96:GLU:H	33:BN:96:GLU:CD	2.27	0.42
35:BP:99:LEU:HD22	35:BP:102:ARG:NH2	2.35	0.42
35:BP:100:LEU:HD23	35:BP:100:LEU:HA	1.85	0.42
41:BV:18:LEU:HD13	41:BV:20:LEU:HB2	2.02	0.42
43:BX:92:LEU:O	43:BX:94:GLY:N	2.44	0.42
1:CA:397:A:H3'	1:CA:397:A:N3	2.34	0.42
1:CA:625:G:H2'	1:CA:626:U:C6	2.55	0.42
1:CA:714:G:H2'	1:CA:715:A:C8	2.55	0.42
1:CA:737:A:H2'	1:CA:738:C:C6	2.55	0.42
1:CA:1111:A:H2'	1:CA:1112:C:C6	2.54	0.42
1:CA:1120:G:O6	1:CA:1154:G:N2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CF:82:ARG:HA	6:CF:82:ARG:HD2	1.90	0.42
8:CH:73:ASP:OD2	8:CH:75:ARG:NH1	2.53	0.42
10:CJ:37:PRO:HA	10:CJ:72:VAL:HG12	2.02	0.42
25:DA:848:G:H2'	25:DA:849:A:C8	2.54	0.42
25:DA:1027:A:C6	25:DA:1126:A:C4	3.07	0.42
25:DA:1171:G:H8	25:DA:1171:G:OP2	2.03	0.42
25:DA:1913:A:H4'	25:DA:1914:C:C5'	2.50	0.42
25:DA:2135:A:N6	25:DA:2157:G:H21	2.12	0.42
25:DA:2149:G:H3'	25:DA:2150:U:C6	2.55	0.42
25:DA:2514:U:H2'	25:DA:2515:C:H6	1.84	0.42
25:DA:2787:C:H2'	25:DA:2788:C:C6	2.55	0.42
26:DB:14:U:H1'	26:DB:108:U:O2'	2.20	0.42
27:DD:118:VAL:HG22	27:DD:119:ALA:H	1.85	0.42
28:DE:31:CYS:HA	28:DE:32:PRO:HD2	1.86	0.42
30:DG:165:THR:OG1	30:DG:168:GLU:HG3	2.20	0.42
37:DR:55:ALA:HB2	37:DR:79:LEU:HD13	2.02	0.42
43:DX:12:VAL:HG22	43:DX:29:TRP:CE2	2.55	0.42
1:AA:31:G:O2'	1:AA:48:C:N4	2.53	0.41
1:AA:50:A:H1'	1:AA:52:G:C8	2.55	0.41
1:AA:1106:G:C6	1:AA:1107:C:C4	3.08	0.41
1:AA:1368:G:OP2	9:AI:112:LYS:HG3	2.19	0.41
2:AB:133:LYS:O	2:AB:137:ARG:HG3	2.19	0.41
5:AE:36:ASP:OD1	5:AE:38:GLN:N	2.41	0.41
5:AE:41:VAL:HG11	5:AE:109:ILE:O	2.20	0.41
8:AH:19:VAL:HG23	8:AH:21:LYS:HD3	2.02	0.41
8:AH:56:LYS:HA	8:AH:56:LYS:HD3	1.87	0.41
10:AJ:90:LEU:HA	10:AJ:91:PRO:HD3	1.95	0.41
12:AL:92:ASP:O	12:AL:94:PRO:HD3	2.19	0.41
20:AT:48:LYS:HA	20:AT:48:LYS:HD3	1.85	0.41
23:AW:26:A:N6	23:AW:44:G:H1	2.18	0.41
25:BA:553:A:C2	25:BA:2065:C:H4'	2.55	0.41
25:BA:766:C:H2'	25:BA:767:C:C6	2.54	0.41
25:BA:1855:G:O3'	27:BD:249:PRO:HD3	2.20	0.41
25:BA:2348:A:H61	46:B0:43:THR:CG2	2.33	0.41
25:BA:2696:U:O2'	34:BO:68:GLU:OE1	2.30	0.41
25:BA:2815:C:H2'	25:BA:2816:G:C8	2.55	0.41
31:BH:144:VAL:O	31:BH:148:ILE:HG13	2.20	0.41
39:BT:118:ARG:HH11	39:BT:118:ARG:HG3	1.85	0.41
45:BZ:146:ILE:HA	45:BZ:147:GLY:HA2	1.77	0.41
1:CA:620:C:H2'	1:CA:621:A:O4'	2.20	0.41
1:CA:718:G:H5'	11:CK:117:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1394:A:N1	1:CA:1500:A:O2'	2.50	0.41
2:CB:229:VAL:HG12	2:CB:230:VAL:N	2.35	0.41
5:CE:13:ILE:HA	5:CE:29:GLY:O	2.19	0.41
7:CG:113:GLU:HG2	7:CG:119:ARG:HG2	2.01	0.41
8:CH:39:LEU:HD13	8:CH:39:LEU:HA	1.85	0.41
9:CI:6:GLY:HA3	9:CI:80:GLY:O	2.19	0.41
13:CM:64:TRP:HB2	13:CM:66:LEU:HD21	2.00	0.41
16:CP:43:LYS:HB3	16:CP:48:TRP:CD1	2.55	0.41
17:CQ:94:ASN:O	17:CQ:98:LEU:HD13	2.20	0.41
25:DA:25:U:H2'	25:DA:26:G:O4'	2.20	0.41
25:DA:1213:A:H1'	25:DA:1238:G:N3	2.35	0.41
25:DA:2114:A:H2'	25:DA:2114:A:N3	2.35	0.41
30:DG:131:TYR:HB3	30:DG:159:VAL:CG2	2.50	0.41
33:DN:4:TYR:HB2	40:DU:101:ARG:NH1	2.35	0.41
1:AA:1292:U:H5'	9:AI:38:GLN:OE1	2.19	0.41
2:AB:134:GLU:O	2:AB:138:LEU:HG	2.20	0.41
9:AI:93:ARG:HB2	9:AI:93:ARG:NH1	2.35	0.41
16:AP:52:ASP:HB3	16:AP:55:ARG:HB2	2.02	0.41
25:BA:239:G:P	54:B8:13:ARG:HH22	2.43	0.41
25:BA:327:U:H2'	25:BA:328:G:C8	2.54	0.41
25:BA:1506:G:C6	25:BA:1508:G:C5	3.08	0.41
25:BA:1506:G:H5"	25:BA:1507:A:OP2	2.20	0.41
25:BA:2126:G:H2'	25:BA:2127:C:H6	1.82	0.41
28:BE:7:VAL:HG12	28:BE:27:LEU:HB3	2.02	0.41
37:BR:21:TYR:CZ	37:BR:43:GLU:HG2	2.55	0.41
45:BZ:54:HIS:HD2	45:BZ:99:TYR:O	2.03	0.41
50:B4:47:GLN:HG2	50:B4:49:PHE:H	1.85	0.41
1:CA:7:G:H5'	1:CA:298:A:O4'	2.20	0.41
1:CA:277:C:P	17:CQ:41:LYS:HZ1	2.43	0.41
1:CA:344:A:H4'	1:CA:345:C:OP2	2.21	0.41
1:CA:399:G:H2'	1:CA:400:C:C6	2.54	0.41
1:CA:407:G:H5"	4:CD:115:ARG:HB3	2.02	0.41
4:CD:65:ARG:HD3	4:CD:70:ILE:O	2.20	0.41
4:CD:98:GLU:OE1	4:CD:103:ASN:ND2	2.37	0.41
5:CE:51:VAL:HG23	5:CE:52:PRO:HD3	2.01	0.41
9:CI:19:LEU:HD23	9:CI:19:LEU:HA	1.89	0.41
10:CJ:49:VAL:HG23	14:CN:41:ARG:HB2	2.01	0.41
15:CO:32:LEU:HD13	15:CO:63:ARG:HB2	2.02	0.41
15:CO:36:ILE:HG23	15:CO:56:LEU:HD11	2.02	0.41
23:CY:2:C:H2'	23:CY:3:C:H6	1.85	0.41
25:DA:1274:A:N3	25:DA:1297:C:H1'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1336:A:H2'	25:DA:1337:G:H8	1.84	0.41
25:DA:1404:C:O2'	25:DA:1405:U:H5'	2.20	0.41
25:DA:1848:A:C4	25:DA:1849:G:C8	3.09	0.41
25:DA:2144:U:O2	25:DA:2148:G:N1	2.54	0.41
25:DA:2526:G:H2'	25:DA:2527:C:H6	1.85	0.41
25:DA:2769:C:H2'	25:DA:2770:G:O4'	2.20	0.41
26:DB:4:C:N4	26:DB:117:G:H1	2.15	0.41
26:DB:61:G:C6	26:DB:62:C:C4	3.08	0.41
27:DD:79:VAL:O	27:DD:113:VAL:HG23	2.19	0.41
27:DD:164:GLN:NE2	27:DD:176:ARG:HH22	2.17	0.41
28:DE:51:PHE:O	28:DE:77:ILE:HD12	2.20	0.41
30:DG:47:LYS:HB3	30:DG:48:GLU:H	1.58	0.41
31:DH:27:LYS:NZ	31:DH:32:GLU:OE2	2.45	0.41
34:DO:66:LYS:HA	34:DO:79:PHE:O	2.21	0.41
35:DP:97:PRO:HG3	35:DP:112:LEU:HD12	2.02	0.41
1:AA:92:C:H2'	1:AA:93:G:H8	1.84	0.41
1:AA:266:G:O2'	1:AA:267:C:OP2	2.33	0.41
1:AA:1022:G:OP1	1:AA:1022:G:H4'	2.21	0.41
1:AA:1278:U:H5'	1:AA:1279:A:C5'	2.50	0.41
3:AC:130:VAL:O	3:AC:134:ILE:HG13	2.20	0.41
4:AD:166:LYS:HB2	4:AD:168:ARG:CZ	2.50	0.41
24:AX:21:A:H61	24:AX:46:G:H2'	1.84	0.41
23:AY:69:G:C2	23:AY:70:G:H1'	2.55	0.41
25:BA:18:C:O2'	25:BA:577:U:OP1	2.33	0.41
25:BA:1249:A:N6	25:BA:1286:U:H2'	2.36	0.41
25:BA:1686:U:O2'	25:BA:1687:C:H5'	2.20	0.41
25:BA:2122:G:H2'	25:BA:2123:G:C8	2.56	0.41
25:BA:2584:A:C8	28:BE:144:ARG:HD2	2.55	0.41
31:BH:104:GLU:HG3	31:BH:114:VAL:HG22	2.03	0.41
38:BS:19:LYS:HE3	38:BS:42:ASP:OD1	2.20	0.41
43:BX:84:ALA:HB3	43:BX:87:GLN:NE2	2.35	0.41
1:CA:552:U:H4'	12:CL:86:ARG:HD2	2.02	0.41
1:CA:984:C:O5'	1:CA:984:C:H6	2.03	0.41
2:CB:158:LEU:HA	2:CB:159:PRO:HD3	1.88	0.41
4:CD:45:GLN:HB2	4:CD:46:LYS:H	1.73	0.41
5:CE:33:VAL:HA	5:CE:42:GLY:O	2.20	0.41
7:CG:108:ALA:HA	7:CG:111:ARG:HD2	2.02	0.41
9:CI:5:TYR:CE2	9:CI:7:THR:HG23	2.55	0.41
9:CI:100:GLY:O	9:CI:103:THR:HG22	2.20	0.41
12:CL:24:VAL:HG12	12:CL:98:TYR:CE1	2.56	0.41
13:CM:11:ARG:C	13:CM:13:LYS:H	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:CO:69:TYR:O	15:CO:73:GLU:HG2	2.21	0.41
15:CO:74:ASP:OD1	15:CO:76:GLU:HB2	2.20	0.41
25:DA:1614:A:C2	42:DW:93:ALA:HB2	2.54	0.41
25:DA:2097:C:H2'	25:DA:2098:U:O4'	2.20	0.41
25:DA:2135:A:H2'	25:DA:2136:C:C6	2.55	0.41
25:DA:2156:G:H2'	25:DA:2157:G:N3	2.35	0.41
30:DG:115:ARG:HH11	30:DG:115:ARG:H	1.68	0.41
30:DG:179:PRO:HG3	50:D4:43:TYR:OH	2.20	0.41
39:DT:88:ILE:HG13	39:DT:91:ARG:NH2	2.35	0.41
44:DY:90:LEU:HD11	44:DY:96:ILE:HG23	2.02	0.41
1:AA:362:G:O3'	12:AL:33:ARG:NH2	2.53	0.41
1:AA:601:C:H2'	1:AA:602:A:H8	1.84	0.41
1:AA:658:G:H2'	1:AA:659:U:C6	2.55	0.41
1:AA:865:A:H2	1:AA:918:A:H4'	1.85	0.41
1:AA:911:U:OP1	12:AL:95:GLY:HA2	2.20	0.41
1:AA:1028:C:N3	1:AA:1029:C:H1'	2.35	0.41
57:AA:3231:PCY:H40	23:AY:35:A:N1	2.36	0.41
5:AE:83:GLU:HG2	5:AE:88:LYS:HB2	2.02	0.41
7:AG:14:PRO:HG3	7:AG:21:VAL:HG13	2.02	0.41
14:AN:13:THR:HA	14:AN:14:PRO:HD3	1.95	0.41
18:AR:59:SER:OG	18:AR:62:GLU:HG2	2.20	0.41
23:AW:1:G:H2'	23:AW:1:G:N3	2.34	0.41
25:BA:288:U:O2'	25:BA:289:G:P	2.79	0.41
25:BA:543:G:H2'	25:BA:544:U:C6	2.55	0.41
25:BA:1074:A:N6	25:BA:1171:G:H2'	2.36	0.41
25:BA:1091:A:C8	25:BA:1093:G:N2	2.88	0.41
25:BA:1221:G:H1'	25:BA:1222:A:O5'	2.21	0.41
25:BA:2186:C:H5	25:BA:2187:G:C4	2.37	0.41
25:BA:2574:U:H1'	34:BO:23:ARG:HH11	1.86	0.41
25:BA:2849:G:C5'	37:BR:46:GLY:HA2	2.46	0.41
27:BD:132:PRO:HG3	27:BD:190:TYR:CE1	2.55	0.41
30:BG:56:ALA:HA	30:BG:153:ARG:HH21	1.85	0.41
34:BO:118:ALA:HA	34:BO:119:PRO:HD2	1.80	0.41
40:BU:83:LEU:HD13	40:BU:113:ALA:HB2	2.01	0.41
1:CA:129(A):G:C6	1:CA:189(E):U:H4'	2.55	0.41
1:CA:1158:C:O3'	2:CB:133:LYS:NZ	2.54	0.41
1:CA:1313:U:P	19:CS:5:LEU:HG	2.60	0.41
1:CA:1441:G:H8	1:CA:1441:G:O5'	2.04	0.41
2:CB:16:HIS:HB3	2:CB:210:SER:HB3	2.03	0.41
4:CD:15:GLU:OE1	4:CD:63:LYS:HG3	2.21	0.41
10:CJ:5:ARG:HA	10:CJ:73:ASP:OD1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:CK:85:ARG:HG2	11:CK:112:THR:HA	2.02	0.41
23:CY:3:C:H6	23:CY:3:C:O5'	2.04	0.41
25:DA:271(H):G:N3	25:DA:271(I):G:C8	2.88	0.41
25:DA:2001:A:H2'	25:DA:2002:G:C8	2.55	0.41
25:DA:2815:C:H2'	25:DA:2816:C:H6	1.85	0.41
26:DB:66:A:N6	26:DB:108:U:H3'	2.34	0.41
27:DD:3:VAL:HG13	27:DD:17:THR:HB	2.02	0.41
28:DE:28:ALA:HB3	28:DE:93:VAL:HG12	2.02	0.41
30:DG:61:ALA:O	50:D4:7:PRO:HG2	2.21	0.41
32:DI:93:THR:O	32:DI:97:ILE:HG13	2.20	0.41
33:DN:15:LEU:HB2	33:DN:135:PRO:CB	2.49	0.41
33:DN:110:GLY:O	33:DN:114:ARG:HG3	2.20	0.41
37:DR:87:TYR:OH	37:DR:116:LEU:HB3	2.20	0.41
39:DT:91:ARG:HD2	39:DT:120:ARG:NH1	2.36	0.41
45:DZ:97:GLU:H	45:DZ:97:GLU:HG2	1.61	0.41
47:D1:25:LYS:C	47:D1:27:GLU:H	2.27	0.41
1:AA:691:G:OP2	11:AK:26:ASN:ND2	2.43	0.41
1:AA:892:A:O2'	1:AA:1415:G:H4'	2.20	0.41
1:AA:1001(A):G:C6	1:AA:1002:G:N7	2.89	0.41
1:AA:1049:U:OP1	14:AN:3:ARG:HB2	2.20	0.41
1:AA:1125:U:H4'	10:AJ:5:ARG:HH22	1.83	0.41
1:AA:1516:G:H2'	1:AA:1518:A:OP2	2.21	0.41
3:AC:131:ARG:NE	3:AC:166:GLU:OE2	2.53	0.41
3:AC:152:ILE:HG23	3:AC:167:TRP:HB3	2.02	0.41
6:AF:89:MET:HE3	6:AF:91:VAL:HG21	2.02	0.41
10:AJ:5:ARG:HE	10:AJ:73:ASP:CG	2.28	0.41
25:BA:1183:G:H2'	25:BA:1184:G:O4'	2.20	0.41
25:BA:2195:A:N3	25:BA:2195:A:H2'	2.35	0.41
25:BA:2827:G:OP1	37:BR:99:LYS:HE2	2.21	0.41
42:BW:68:ARG:NH1	42:BW:112:GLY:H	2.19	0.41
45:BZ:151:HIS:C	45:BZ:153:SER:H	2.28	0.41
50:B4:58:ARG:CZ	50:B4:58:ARG:HB3	2.49	0.41
1:CA:89:C:H2'	1:CA:90:U:O4'	2.21	0.41
1:CA:982:U:O2	1:CA:1222:G:N1	2.39	0.41
1:CA:1023:G:C5	1:CA:1024:G:C8	3.08	0.41
1:CA:1360:A:H2'	1:CA:1361:G:O4'	2.21	0.41
1:CA:1414:U:H3	1:CA:1486:G:H1	1.68	0.41
2:CB:133:LYS:O	2:CB:137:ARG:HG3	2.20	0.41
11:CK:120:ARG:HA	11:CK:121:PRO:HD3	1.95	0.41
19:CS:27:GLU:CD	19:CS:27:GLU:H	2.24	0.41
24:CX:15:G:H2'	24:CX:59:A:N1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:248:G:C2	25:DA:2431:U:H4'	2.55	0.41
25:DA:579:G:H2'	25:DA:580:C:C6	2.56	0.41
25:DA:930:U:O4'	25:DA:931:G:C2	2.74	0.41
25:DA:1005:C:H4'	25:DA:1012:U:C6	2.55	0.41
25:DA:1127:A:H2'	25:DA:1128:A:H5"	2.02	0.41
25:DA:1131:G:N2	25:DA:1132:A:N3	2.68	0.41
25:DA:1159:U:O2'	25:DA:1160:G:H5'	2.20	0.41
25:DA:1270:C:H5"	25:DA:1271:G:O5'	2.20	0.41
25:DA:1706:U:O2	25:DA:1757:U:H5'	2.20	0.41
25:DA:1707:G:C5	25:DA:1756:G:C6	3.08	0.41
25:DA:1817:G:H2'	25:DA:1818:U:H5'	2.03	0.41
25:DA:2319:G:N2	38:DS:3:ARG:HA	2.35	0.41
25:DA:2356:C:O3'	46:D0:20:ARG:HD3	2.21	0.41
25:DA:2758:A:H2'	25:DA:2759:G:O4'	2.21	0.41
31:DH:9:ILE:HD13	31:DH:72:ILE:HG21	2.03	0.41
38:DS:11:LYS:O	38:DS:15:ARG:HG3	2.20	0.41
40:DU:79:PHE:CE2	40:DU:83:LEU:HD21	2.55	0.41
43:DX:43:VAL:HG21	43:DX:81:VAL:HG11	2.03	0.41
45:DZ:8:TYR:HB2	45:DZ:38:TYR:CE2	2.55	0.41
45:DZ:44:PHE:CZ	45:DZ:86:VAL:HG11	2.56	0.41
50:D4:68:ARG:O	50:D4:69:LYS:HB3	2.20	0.41
1:AA:1145:C:H4'	1:AA:1146:A:C5'	2.51	0.41
4:AD:163:GLU:O	4:AD:166:LYS:HG2	2.20	0.41
9:AI:24:GLY:HA2	9:AI:59:PHE:O	2.20	0.41
16:AP:27:LYS:HE3	16:AP:27:LYS:HB2	1.72	0.41
25:BA:308:U:H2'	25:BA:309:C:C6	2.55	0.41
25:BA:982:U:H2'	25:BA:983:G:O4'	2.21	0.41
25:BA:2162:C:H1'	25:BA:2174:G:H22	1.85	0.41
25:BA:2591:C:O5'	25:BA:2591:C:H6	2.04	0.41
39:BT:53:ARG:HB3	39:BT:53:ARG:NH1	2.35	0.41
45:BZ:107:THR:HA	45:BZ:108:PRO:HD3	1.63	0.41
45:BZ:136:PHE:O	45:BZ:137:ILE:HG13	2.20	0.41
1:CA:164:U:H2'	1:CA:165:C:C6	2.56	0.41
1:CA:542:G:P	4:CD:10:ARG:HH22	2.43	0.41
5:CE:84:PHE:CE2	5:CE:133:TYR:HD2	2.39	0.41
9:CI:18:PHE:CD2	9:CI:62:TYR:HD2	2.36	0.41
20:CT:16:HIS:O	20:CT:19:SER:OG	2.27	0.41
25:DA:42:G:H2'	25:DA:43:A:O4'	2.19	0.41
25:DA:263:C:H2'	25:DA:264:C:O4'	2.21	0.41
25:DA:271(H):G:O2'	25:DA:271(I):G:C8	2.69	0.41
25:DA:1593:G:H2'	25:DA:1594:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:1810:A:H2'	25:DA:1811:G:O4'	2.20	0.41
28:DE:48:GLN:HA	28:DE:80:GLU:HA	2.03	0.41
36:DQ:42:ILE:HD13	36:DQ:97:VAL:HB	2.02	0.41
41:DV:24:LYS:HA	41:DV:92:THR:OG1	2.21	0.41
44:DY:94:LYS:HD2	44:DY:94:LYS:HA	1.84	0.41
45:DZ:156:LYS:HE2	45:DZ:158:PRO:HB3	2.02	0.41
46:D0:50:ASN:HA	46:D0:62:LEU:HD12	2.03	0.41
46:D0:56:ASP:O	46:D0:57:PHE:HB2	2.20	0.41
50:D4:14:ILE:HB	50:D4:22:ILE:HB	2.03	0.41
50:D4:28:LYS:HA	50:D4:29:PRO:HD3	1.93	0.41
53:D7:26:GLY:O	53:D7:30:VAL:HG23	2.21	0.41
55:D9:17:ILE:HA	55:D9:17:ILE:HD12	1.82	0.41
3:AC:148:GLY:HA3	3:AC:172:ARG:O	2.20	0.41
4:AD:138:TYR:CD1	4:AD:138:TYR:C	2.99	0.41
5:AE:122:GLU:O	5:AE:126:ARG:NH1	2.53	0.41
14:AN:33:VAL:HA	14:AN:40:CYS:HA	2.03	0.41
25:BA:354:A:H2	25:BA:1255:A:O2'	2.03	0.41
25:BA:715:G:H5'	25:BA:716:G:OP2	2.20	0.41
25:BA:1065:U:H3	25:BA:1188:A:H62	1.66	0.41
26:BB:17:C:H2'	26:BB:18:G:O4'	2.21	0.41
37:BR:1:MET:HB2	37:BR:2:ARG:H	1.74	0.41
1:CA:302:G:N3	1:CA:556:C:H4'	2.35	0.41
1:CA:411:A:OP2	4:CD:25:ARG:NH2	2.54	0.41
1:CA:583:A:N6	1:CA:758:G:O2'	2.54	0.41
1:CA:1028:C:O2	1:CA:1034:G:H1'	2.20	0.41
1:CA:1055:A:C5	1:CA:1206:G:C2	3.09	0.41
2:CB:16:HIS:CB	2:CB:204:ASN:HB3	2.50	0.41
2:CB:80:ILE:HD11	2:CB:212:GLN:CA	2.51	0.41
4:CD:92:VAL:O	4:CD:96:LEU:HD22	2.21	0.41
13:CM:87:TYR:O	13:CM:91:ARG:HG2	2.21	0.41
14:CN:13:THR:HA	14:CN:14:PRO:HD3	1.88	0.41
20:CT:89:ARG:O	20:CT:93:GLU:HB2	2.20	0.41
24:CX:67:C:H2'	24:CX:68:C:H5'	2.03	0.41
23:CY:18:G:O6	23:CY:55:PSU:O2'	2.33	0.41
25:DA:673:C:H5"	29:DF:81:PRO:HD2	2.02	0.41
25:DA:1316:U:H2'	25:DA:1317:A:C8	2.55	0.41
25:DA:1379:A:H4'	25:DA:1380:G:OP2	2.21	0.41
25:DA:1494:A:C6	25:DA:1495:A:C6	3.09	0.41
25:DA:2489:G:C2'	25:DA:2490:G:H5'	2.51	0.41
25:DA:2516:G:C6	25:DA:2517:C:C4	3.08	0.41
25:DA:2643:G:H2'	25:DA:2644:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DF:64:ILE:HD11	29:DF:75:HIS:HB2	2.02	0.41
43:DX:84:ALA:HB3	43:DX:87:GLN:CD	2.45	0.41
44:DY:86:ARG:HH11	44:DY:100:ALA:HB1	1.85	0.41
45:DZ:129:SER:HA	45:DZ:130:PRO:HD3	1.92	0.41
1:AA:674:G:H2'	1:AA:675:A:C8	2.56	0.41
1:AA:1261:A:H3'	1:AA:1262:C:C6	2.56	0.41
6:AF:44:GLY:HA2	6:AF:59:TYR:CE2	2.56	0.41
6:AF:91:VAL:HG11	18:AR:72:ARG:HH12	1.86	0.41
8:AH:4:ASP:CG	8:AH:85:ARG:HH11	2.29	0.41
16:AP:69:THR:O	16:AP:73:LEU:HG	2.21	0.41
17:AQ:45:HIS:O	17:AQ:73:VAL:HG23	2.21	0.41
20:AT:8:ARG:O	20:AT:9:ASN:HB2	2.21	0.41
23:AY:47:U:O2'	23:AY:50:U:OP1	2.32	0.41
23:AY:64:A:H2'	23:AY:65:G:C8	2.56	0.41
25:BA:492:A:N3	25:BA:730:C:H1'	2.35	0.41
25:BA:1076:G:OP2	36:BQ:128:LYS:NZ	2.49	0.41
25:BA:1334:U:C4	25:BA:1373:C:H1'	2.56	0.41
25:BA:2141:A:N1	25:BA:2192:A:H2'	2.36	0.41
25:BA:2159:C:H2'	25:BA:2160:C:C6	2.56	0.41
25:BA:2853:G:N7	61:BA:4892:HOH:O	2.37	0.41
37:BR:61:HIS:O	37:BR:65:LEU:HD22	2.21	0.41
50:B4:40:HIS:HB3	50:B4:43:TYR:CD2	2.55	0.41
1:CA:109:A:H5'	1:CA:110:C:C5	2.56	0.41
1:CA:657:G:H4'	15:CO:28:GLN:HG2	2.02	0.41
1:CA:788:U:O2	1:CA:795:C:N4	2.53	0.41
1:CA:1029:C:N4	1:CA:1032:G:C2	2.87	0.41
1:CA:1116:C:C2'	1:CA:1117:G:H5"	2.46	0.41
1:CA:1424:C:H2'	1:CA:1425:U:O4'	2.21	0.41
2:CB:94:ASN:HD22	2:CB:94:ASN:HA	1.54	0.41
3:CC:120:VAL:HA	3:CC:123:GLN:NE2	2.25	0.41
9:CI:55:ALA:HA	9:CI:58:HIS:HD2	1.86	0.41
9:CI:70:LYS:O	9:CI:74:ILE:HG13	2.21	0.41
15:CO:80:ALA:O	15:CO:83:GLU:HB3	2.21	0.41
25:DA:247:G:H4'	25:DA:386:G:C6	2.55	0.41
25:DA:636:G:OP1	35:DP:132:LYS:HE2	2.21	0.41
25:DA:746:A:H2'	25:DA:2612:C:H5"	2.03	0.41
25:DA:784:A:O4'	27:DD:227:ASN:ND2	2.53	0.41
25:DA:861:A:C2	25:DA:917:A:C4	3.09	0.41
25:DA:1794:U:H2'	25:DA:1795:C:H6	1.86	0.41
25:DA:2120:G:H2'	25:DA:2121:G:C8	2.56	0.41
25:DA:2153:G:H2'	25:DA:2154:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:2431:U:O2'	25:DA:2433:A:N7	2.50	0.41
31:DH:59:ARG:O	31:DH:63:SER:OG	2.29	0.41
31:DH:98:LEU:HD12	31:DH:98:LEU:HA	1.85	0.41
31:DH:154:PRO:HB3	31:DH:163:TYR:CZ	2.54	0.41
40:DU:49:HIS:O	40:DU:53:ARG:N	2.54	0.41
45:DZ:107:THR:HA	45:DZ:108:PRO:HD3	1.81	0.41
49:D3:31:LEU:HD23	49:D3:31:LEU:HA	1.92	0.41
54:D8:10:ALA:HB3	54:D8:62:LEU:HD21	2.02	0.41
1:AA:189:G:H1	1:AA:189(K):U:H3	1.68	0.41
1:AA:216:G:C2	1:AA:217:C:C4	3.08	0.41
1:AA:308:C:H2'	1:AA:309:G:C8	2.56	0.41
1:AA:621:A:H2'	1:AA:622:A:C8	2.56	0.41
1:AA:826:C:H4'	8:AH:12:ARG:HG2	2.02	0.41
1:AA:974:A:OP2	14:AN:29:ARG:NH2	2.53	0.41
1:AA:1077:G:N2	1:AA:1080:A:OP2	2.45	0.41
1:AA:1121:U:H2'	1:AA:1122:U:O4'	2.21	0.41
1:AA:1191:A:OP1	3:AC:4:LYS:NZ	2.45	0.41
1:AA:1213:A:O2'	1:AA:1215:G:N7	2.47	0.41
1:AA:1223:C:P	19:AS:78:ARG:HH21	2.43	0.41
1:AA:1261:A:H5"	1:AA:1262:C:OP2	2.21	0.41
57:AA:3231:PCY:H17	57:AA:3231:PCY:H24	1.77	0.41
2:AB:105:PHE:CZ	2:AB:155:LEU:HD12	2.56	0.41
2:AB:223:ILE:HD12	2:AB:230:VAL:HG12	2.03	0.41
5:AE:110:LEU:HD13	5:AE:118:ILE:HD13	2.02	0.41
6:AF:2:ARG:HG3	6:AF:69:GLU:HG3	2.03	0.41
8:AH:49:GLU:HG2	8:AH:62:TYR:HE1	1.86	0.41
10:AJ:35:SER:N	10:AJ:73:ASP:O	2.38	0.41
13:AM:3:ARG:HD3	13:AM:4:ILE:HG22	2.02	0.41
23:AY:44:G:H3'	23:AY:45:U:C6	2.56	0.41
25:BA:70:A:N7	43:BX:31:HIS:HE1	2.18	0.41
25:BA:119:G:H4'	25:BA:149:A:H5'	2.03	0.41
25:BA:142:G:H4'	43:BX:35:THR:HG21	2.01	0.41
25:BA:722:A:C8	25:BA:851:A:C6	3.09	0.41
25:BA:776:G:C6	27:BD:208:LYS:HB2	2.56	0.41
25:BA:798:A:H5'	42:BW:90:ARG:HA	2.03	0.41
25:BA:904:C:H1'	46:B0:26:TYR:CE2	2.56	0.41
25:BA:1466:U:O2'	25:BA:1467:G:OP1	2.33	0.41
25:BA:1481:G:H2'	25:BA:1482:G:O4'	2.20	0.41
25:BA:2132:G:OP1	25:BA:2140:U:N3	2.51	0.41
25:BA:2205:C:C2	25:BA:2206:G:C8	3.09	0.41
25:BA:2283:G:OP1	46:B0:18:ALA:HB1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2418:U:N3	35:BP:73:GLY:O	2.37	0.41
25:BA:2664:C:H2'	25:BA:2665:U:O4'	2.21	0.41
27:BD:26:LYS:HB3	27:BD:83:GLU:HG2	2.02	0.41
27:BD:182:LEU:HD23	27:BD:182:LEU:HA	1.77	0.41
28:BE:36:ARG:NH2	28:BE:88:GLY:O	2.54	0.41
28:BE:101:ARG:HA	28:BE:170:LEU:O	2.21	0.41
43:BX:31:HIS:HA	43:BX:32:PRO:HD3	1.93	0.41
1:CA:100:C:H2'	1:CA:101:A:O4'	2.20	0.41
1:CA:175:C:H2'	1:CA:176:C:C6	2.56	0.41
1:CA:269:C:H2'	1:CA:270:A:C8	2.56	0.41
1:CA:309:G:H1'	1:CA:608:A:C2	2.56	0.41
1:CA:429:U:H3'	4:CD:9:CYS:SG	2.60	0.41
1:CA:866:C:O2'	1:CA:919:A:OP1	2.26	0.41
1:CA:976:G:H22	1:CA:1363:C:H5"	1.86	0.41
1:CA:993:G:N3	1:CA:993:G:H2'	2.36	0.41
2:CB:118:LEU:HD13	2:CB:142:LEU:HB2	2.03	0.41
3:CC:45:LYS:HG3	3:CC:46:GLU:N	2.36	0.41
4:CD:196:LEU:O	4:CD:198:VAL:N	2.48	0.41
7:CG:52:GLU:HG2	7:CG:52:GLU:H	1.47	0.41
9:CI:85:LEU:HB3	9:CI:92:TYR:CD2	2.56	0.41
10:CJ:16:LEU:HD23	10:CJ:94:VAL:HG13	2.03	0.41
11:CK:16:SER:O	11:CK:35:PRO:HD3	2.21	0.41
25:DA:97:C:O3'	48:D2:2:LYS:HA	2.20	0.41
25:DA:299:A:N3	25:DA:319:C:O2'	2.51	0.41
25:DA:311:A:C6	25:DA:328:U:C4	3.09	0.41
25:DA:464:U:H2'	25:DA:465:G:O4'	2.21	0.41
25:DA:483:A:O2'	44:DY:59:GLY:N	2.53	0.41
25:DA:715:G:H2'	25:DA:716:A:O4'	2.21	0.41
25:DA:1149:G:H2'	25:DA:1150:C:H6	1.85	0.41
25:DA:1151:G:C6	25:DA:1152:C:N3	2.89	0.41
25:DA:1207:C:H2'	25:DA:1208:C:C6	2.56	0.41
25:DA:1379:A:O5'	25:DA:1379:A:H8	2.04	0.41
25:DA:1899:G:H2'	25:DA:1899:G:N3	2.36	0.41
25:DA:2070:G:H2'	25:DA:2071:A:O4'	2.21	0.41
25:DA:2323:G:C6	25:DA:2324:C:C4	3.09	0.41
25:DA:2364:C:H2'	25:DA:2365:G:O4'	2.21	0.41
25:DA:2365:G:H4'	46:D0:60:PHE:CZ	2.56	0.41
25:DA:2418:A:C2	25:DA:2419:U:C2	3.09	0.41
25:DA:2671:A:H2'	25:DA:2672:G:O4'	2.21	0.41
26:DB:5:C:H42	26:DB:116:G:H1	1.69	0.41
26:DB:95:C:H2'	26:DB:96:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DF:53:THR:HG23	29:DF:55:GLY:N	2.23	0.41
30:DG:43:LEU:HB3	30:DG:44:GLY:H	1.53	0.41
30:DG:91:ARG:HE	30:DG:91:ARG:HB3	1.60	0.41
31:DH:17:VAL:HG11	31:DH:50:VAL:HG21	2.03	0.41
31:DH:18:GLU:OE2	31:DH:25:LYS:HD3	2.21	0.41
32:DI:102:SER:O	32:DI:106:GLY:N	2.54	0.41
35:DP:2:LYS:HG3	35:DP:4:SER:OG	2.21	0.41
35:DP:90:ARG:HG2	35:DP:91:PHE:CD1	2.55	0.41
39:DT:6:LEU:O	39:DT:10:VAL:HG23	2.21	0.41
40:DU:92:ARG:HG2	40:DU:92:ARG:H	1.56	0.41
42:DW:18:ARG:NH1	42:DW:76:VAL:O	2.54	0.41
44:DY:6:HIS:H	44:DY:6:HIS:CD2	2.39	0.41
45:DZ:8:TYR:HB2	45:DZ:38:TYR:CZ	2.56	0.41
54:D8:37:SER:OG	54:D8:39:LYS:HB3	2.21	0.41
1:AA:61:G:H2'	1:AA:62:U:O4'	2.21	0.41
1:AA:193:C:H2'	1:AA:194:C:H6	1.85	0.41
1:AA:542:G:H5'	4:AD:41:GLY:HA3	2.03	0.41
1:AA:601:C:H2'	1:AA:602:A:C8	2.56	0.41
2:AB:189:ASP:HB2	2:AB:190:THR:H	1.73	0.41
3:AC:65:ALA:HA	3:AC:100:ALA:HB3	2.03	0.41
3:AC:108:ASN:HB3	3:AC:111:LEU:HD12	2.03	0.41
4:AD:134:ASP:O	4:AD:136:PRO:HD3	2.21	0.41
10:AJ:35:SER:CB	10:AJ:73:ASP:HB2	2.49	0.41
19:AS:20:LEU:HD23	19:AS:23:ASN:ND2	2.23	0.41
20:AT:99:LEU:HA	20:AT:100:ILE:O	2.21	0.41
25:BA:223:C:H2'	25:BA:224:U:H6	1.85	0.41
25:BA:331:G:H21	25:BA:354:A:H62	1.69	0.41
25:BA:616:G:H4'	54:B8:4:MET:HE2	2.02	0.41
25:BA:865:G:H4'	25:BA:885:C:O3'	2.21	0.41
25:BA:1073:A:C6	25:BA:1172:A:C4	3.09	0.41
25:BA:1781:G:O2'	25:BA:2870:A:N1	2.49	0.41
25:BA:2148:A:N6	25:BA:2185:C:O4'	2.54	0.41
25:BA:2304:C:H2'	25:BA:2305:C:C6	2.56	0.41
30:BG:49:ASP:O	30:BG:50:ALA:C	2.63	0.41
34:BO:2:ILE:HG23	34:BO:6:THR:HG21	2.02	0.41
40:BU:50:ARG:HH12	41:BV:72:VAL:HA	1.85	0.41
45:BZ:44:PHE:CZ	45:BZ:86:VAL:HG11	2.56	0.41
1:CA:790:A:C6	1:CA:791:G:C6	3.09	0.41
1:CA:1002:G:C5	1:CA:1003:G:H8	2.39	0.41
1:CA:1129:C:O2'	1:CA:1139:G:O6	2.31	0.41
3:CC:54:ARG:HB3	3:CC:54:ARG:NH1	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CD:173:TRP:CD1	4:CD:174:LEU:HG	2.56	0.41
5:CE:31:LEU:HD23	5:CE:31:LEU:HA	1.93	0.41
11:CK:84:VAL:HG21	11:CK:95:ILE:HD11	2.03	0.41
25:DA:79:G:C6	25:DA:80:G:C5	3.09	0.41
25:DA:108:U:OP1	25:DA:293:U:O2'	2.36	0.41
25:DA:127:A:H5"	25:DA:128:C:C6	2.55	0.41
25:DA:530:G:N3	25:DA:530:G:O4'	2.53	0.41
25:DA:582:G:H2'	25:DA:583:G:C8	2.56	0.41
25:DA:974:G:OP1	25:DA:1187:G:O2'	2.21	0.41
25:DA:1374:G:H2'	25:DA:1375:C:C6	2.56	0.41
26:DB:76:G:N2	26:DB:101:G:O6	2.42	0.41
27:DD:29:PRO:HA	27:DD:83:GLU:OE1	2.20	0.41
27:DD:73:VAL:HG13	27:DD:120:GLY:HA3	2.03	0.41
43:DX:94:GLY:N	43:DX:95:LEU:HA	2.36	0.41
45:DZ:145:GLU:HG3	45:DZ:146:ILE:N	2.36	0.41
1:AA:1003:G:O3'	1:AA:1004:A:H4'	2.22	0.40
1:AA:1263:C:H5"	1:AA:1264:C:OP2	2.21	0.40
2:AB:19:HIS:HE1	2:AB:189:ASP:HB3	1.86	0.40
23:AY:35:A:H2'	23:AY:36:A:C8	2.57	0.40
25:BA:1314:A:C2	25:BA:2035:A:C4	3.09	0.40
25:BA:2163:G:N1	25:BA:2164:C:O2	2.55	0.40
25:BA:2353:G:H2'	25:BA:2354:C:C6	2.57	0.40
27:BD:68:LYS:O	27:BD:69:ARG:HB2	2.21	0.40
31:BH:24:VAL:HG22	31:BH:35:VAL:HB	2.03	0.40
33:BN:39:ARG:HA	33:BN:40:PRO:HD3	1.91	0.40
45:BZ:158:PRO:HA	45:BZ:159:PRO:HD3	1.85	0.40
47:B1:80:LEU:HD22	47:B1:97:LEU:HD11	2.03	0.40
47:B1:86:SER:O	47:B1:89:GLU:HG2	2.20	0.40
50:B4:59:PHE:C	50:B4:61:ARG:H	2.28	0.40
50:B4:69:LYS:HE3	50:B4:69:LYS:HB3	1.83	0.40
1:CA:509:A:N3	1:CA:543:C:O2'	2.51	0.40
1:CA:865:A:C2	1:CA:918:A:H4'	2.56	0.40
1:CA:1005:A:N6	1:CA:1024:G:O2'	2.54	0.40
1:CA:1201:A:H4'	1:CA:1202:G:O5'	2.21	0.40
1:CA:1358:U:H2'	1:CA:1359:C:O4'	2.21	0.40
4:CD:174:LEU:HD23	4:CD:185:PHE:HA	2.03	0.40
5:CE:53:LEU:O	5:CE:57:LYS:HB2	2.21	0.40
23:CW:9:A:H5'	23:CW:46:7MG:N2	2.34	0.40
24:CX:9:G:H21	24:CX:45:G:H3'	1.86	0.40
24:CX:13:C:O2'	25:DA:1924:C:H4'	2.21	0.40
23:CY:8:4SU:S4	23:CY:14:A:C8	3.14	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:DA:19:C:H2'	25:DA:20:C:C6	2.55	0.40
25:DA:84:A:N1	25:DA:98:G:O2'	2.46	0.40
25:DA:144:C:H2'	25:DA:145:G:C8	2.56	0.40
25:DA:314:A:H2'	25:DA:315:G:C8	2.57	0.40
25:DA:566:U:O2'	25:DA:809:G:OP2	2.27	0.40
25:DA:912:C:N4	25:DA:913:U:O4	2.54	0.40
25:DA:1140:C:O3'	33:DN:25:ARG:NH1	2.53	0.40
25:DA:1171:G:N2	25:DA:1178:C:N3	2.50	0.40
25:DA:1495:A:H2'	25:DA:1496:A:C8	2.56	0.40
25:DA:1790:C:H5"	25:DA:1791:A:OP1	2.20	0.40
25:DA:1877:A:H8	25:DA:1877:A:OP2	2.04	0.40
25:DA:2108:C:H2'	25:DA:2109:U:C6	2.55	0.40
25:DA:2320:A:H1'	25:DA:2321:G:C2	2.56	0.40
33:DN:71:ILE:HA	33:DN:86:PRO:HA	2.02	0.40
43:DX:92:LEU:HD12	43:DX:92:LEU:HA	1.91	0.40
1:AA:179:A:C5	1:AA:180:U:C4	3.09	0.40
1:AA:1007:C:N3	1:AA:1022:G:C6	2.89	0.40
1:AA:1128:C:C2'	1:AA:1129:C:H5'	2.51	0.40
5:AE:82:VAL:HG21	5:AE:138:ALA:HA	2.03	0.40
5:AE:105:VAL:HB	5:AE:106:PRO:HD3	2.03	0.40
10:AJ:62:HIS:HB3	14:AN:59:ALA:HB3	2.03	0.40
23:AW:43:C:H2'	23:AW:44:G:C8	2.56	0.40
25:BA:12:U:O2	25:BA:12:U:H2'	2.21	0.40
25:BA:624:C:O2'	25:BA:628:C:H5"	2.21	0.40
25:BA:2331:G:C2	38:BS:3:ARG:HA	2.56	0.40
25:BA:2332:A:H2'	25:BA:2332:A:N3	2.37	0.40
25:BA:2624:C:OP2	51:B5:2:ALA:N	2.54	0.40
25:BA:2672:A:N7	31:BH:175:LYS:NZ	2.68	0.40
25:BA:2812:A:N3	25:BA:2904:U:H1'	2.37	0.40
36:BQ:85:LYS:HD3	46:B0:7:LEU:HG	2.02	0.40
38:BS:59:LYS:H	38:BS:59:LYS:HG3	1.77	0.40
48:B2:65:ASN:OD1	48:B2:69:ARG:HD3	2.22	0.40
50:B4:55:ARG:HB2	50:B4:56:VAL:C	2.45	0.40
55:B9:17:ILE:HD12	55:B9:17:ILE:HA	1.90	0.40
1:CA:69:G:H2'	1:CA:70:G:C8	2.56	0.40
1:CA:174:C:H2'	1:CA:175:C:C6	2.56	0.40
1:CA:560:U:H5'	1:CA:566:G:N2	2.36	0.40
1:CA:683:G:O6	61:CA:4133:HOH:O	2.21	0.40
1:CA:1060:C:N4	3:CC:2:GLY:HA2	2.36	0.40
2:CB:33:TYR:HB2	2:CB:43:ASP:HB2	2.02	0.40
3:CC:16:ARG:HD2	3:CC:16:ARG:HA	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:CJ:40:LEU:HD23	10:CJ:40:LEU:HA	1.93	0.40
15:CO:87:ILE:CG2	15:CO:88:ARG:H	2.26	0.40
25:DA:660:G:C6	25:DA:661:C:C4	3.10	0.40
25:DA:815:C:N3	25:DA:1193:G:C2	2.89	0.40
25:DA:1288:U:C2	25:DA:1327:C:O2	2.74	0.40
25:DA:1668:A:H4'	25:DA:1669:A:O5'	2.21	0.40
25:DA:1711:C:H2'	25:DA:1712:C:H6	1.85	0.40
25:DA:1777:U:O2'	25:DA:1778:U:H5'	2.21	0.40
25:DA:1971:A:OP1	61:DA:4260:HOH:O	2.21	0.40
25:DA:2529:G:O6	55:D9:31:LYS:NZ	2.54	0.40
25:DA:2679:A:C2	25:DA:2729:G:C2	3.09	0.40
25:DA:2684:U:H1'	34:DO:70:LYS:HD2	2.03	0.40
27:DD:264:LYS:HA	27:DD:265:PRO:HD3	1.95	0.40
29:DF:78:ILE:HA	29:DF:83:PHE:CE1	2.56	0.40
29:DF:154:VAL:HG22	29:DF:191:ARG:HB2	2.03	0.40
31:DH:85:LYS:O	31:DH:132:ARG:HA	2.21	0.40
31:DH:137:ASP:O	31:DH:141:VAL:HG23	2.21	0.40
32:DI:47:LEU:O	32:DI:51:ILE:HG13	2.21	0.40
38:DS:105:ALA:HB1	38:DS:110:LEU:HD23	2.02	0.40
39:DT:65:LYS:O	39:DT:72:VAL:N	2.47	0.40
43:DX:31:HIS:HB3	43:DX:34:ALA:HB2	2.03	0.40
45:DZ:67:LEU:HA	45:DZ:68:PRO:HD3	1.77	0.40
50:D4:62:ARG:C	50:D4:64:GLY:H	2.29	0.40
1:AA:374:A:C6	1:AA:375:U:C4	3.09	0.40
1:AA:461:A:O2'	1:AA:470:C:H5'	2.22	0.40
1:AA:769:G:H4'	1:AA:1513:A:H4'	2.04	0.40
1:AA:1068:G:N2	1:AA:1191:A:N3	2.60	0.40
4:AD:63:LYS:HG3	4:AD:64:LEU:H	1.87	0.40
7:AG:8:GLU:H	7:AG:8:GLU:HG3	1.63	0.40
16:AP:4:ILE:HB	16:AP:66:PRO:HA	2.03	0.40
17:AQ:66:SER:OG	17:AQ:69:LYS:HB2	2.22	0.40
20:AT:10:LEU:HD22	20:AT:11:SER:H	1.86	0.40
25:BA:34:C:H5"	25:BA:35:G:OP2	2.22	0.40
25:BA:866:A:C4	25:BA:1234:A:C2	3.09	0.40
25:BA:2236:G:H4'	25:BA:2238:C:C2	2.56	0.40
25:BA:2359:C:H2'	25:BA:2360:U:C6	2.56	0.40
26:BB:16:G:C6	26:BB:69:G:C2	3.09	0.40
27:BD:136:ILE:HA	27:BD:137:PRO:HD3	1.88	0.40
28:BE:162:ALA:HB3	61:BE:409:HOH:O	2.21	0.40
30:BG:106:LEU:HA	30:BG:110:ALA:HB3	2.01	0.40
32:BI:10:GLU:O	32:BI:12:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BX:41:ASN:O	43:BX:45:THR:HG23	2.21	0.40
1:CA:486:U:H2'	1:CA:487:A:C8	2.57	0.40
1:CA:731:G:OP1	1:CA:766:A:H1'	2.22	0.40
1:CA:1125:U:C2	10:CJ:38:ILE:HD13	2.56	0.40
1:CA:1381:U:H1'	7:CG:79:ARG:HD3	2.03	0.40
3:CC:6:HIS:HA	3:CC:7:PRO:HD3	1.84	0.40
5:CE:106:PRO:O	5:CE:110:LEU:HG	2.21	0.40
8:CH:51:VAL:CG2	8:CH:60:ARG:HB2	2.51	0.40
15:CO:5:LYS:HD3	15:CO:5:LYS:N	2.36	0.40
16:CP:57:ARG:HH21	16:CP:79:VAL:HA	1.85	0.40
18:CR:66:LEU:O	18:CR:70:ILE:HG13	2.21	0.40
25:DA:41:C:H2'	25:DA:42:G:H8	1.86	0.40
25:DA:857:C:H2'	25:DA:858:U:C6	2.56	0.40
25:DA:1344:G:C2	25:DA:1385:G:C8	3.09	0.40
25:DA:1434:A:H2'	25:DA:1435:G:C8	2.56	0.40
25:DA:1446:C:H42	25:DA:1465:G:H1	1.69	0.40
25:DA:1692:U:O2'	25:DA:1693:U:H2'	2.21	0.40
25:DA:1789:A:H2'	25:DA:1790:C:O4'	2.21	0.40
25:DA:1866:C:H6	25:DA:1866:C:O5'	2.05	0.40
25:DA:2140:C:O2	25:DA:2140:C:H2'	2.22	0.40
25:DA:2666:C:H42	31:DH:109:PHE:HA	1.86	0.40
27:DD:69:ARG:C	27:DD:71:ASP:N	2.78	0.40
29:DF:27:GLU:OE2	29:DF:27:GLU:HA	2.20	0.40
30:DG:67:LYS:HG2	30:DG:68:PRO:HD2	2.04	0.40
31:DH:105:LEU:N	31:DH:113:VAL:O	2.45	0.40
32:DI:101:LEU:HG	32:DI:107:VAL:HB	2.03	0.40
36:DQ:43:THR:OG1	36:DQ:45:GLN:HG2	2.22	0.40
37:DR:22:ARG:O	37:DR:26:LYS:HG3	2.21	0.40
39:DT:109:GLU:HG2	39:DT:112:ARG:NH2	2.36	0.40
54:D8:50:LEU:HD23	54:D8:50:LEU:HA	1.86	0.40
1:AA:235:C:H5'	17:AQ:70:ARG:HG2	2.03	0.40
1:AA:1035:A:H2	1:AA:1036:G:C5	2.39	0.40
11:AK:38:ASN:HA	11:AK:39:PRO:HD3	1.79	0.40
13:AM:13:LYS:O	13:AM:44:ARG:HA	2.22	0.40
23:AW:63:G:H2'	23:AW:64:A:O4'	2.21	0.40
25:BA:155:C:O5'	25:BA:155:C:H6	2.03	0.40
25:BA:174:U:H2'	25:BA:175:G:H8	1.85	0.40
25:BA:207:A:C2	25:BA:224:U:H4'	2.57	0.40
25:BA:1271:G:OP1	41:BV:69:LYS:NZ	2.45	0.40
25:BA:1857:G:H4'	27:BD:242:ARG:CZ	2.51	0.40
25:BA:2155:G:H21	25:BA:2180:A:N6	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2162:C:O2	25:BA:2162:C:H2'	2.21	0.40
25:BA:2520:G:H2'	25:BA:2521:G:O4'	2.22	0.40
25:BA:2765:C:O5'	25:BA:2765:C:H6	2.05	0.40
30:BG:45:GLU:H	30:BG:45:GLU:HG2	1.53	0.40
30:BG:67:LYS:HG2	30:BG:68:PRO:HD2	2.03	0.40
31:BH:69:ARG:HG3	31:BH:70:THR:N	2.35	0.40
1:CA:617:G:H4'	16:CP:44:THR:O	2.22	0.40
2:CB:16:HIS:O	2:CB:18:GLY:N	2.55	0.40
2:CB:84:GLU:OE1	2:CB:216:SER:HA	2.21	0.40
4:CD:162:LEU:HD23	4:CD:162:LEU:HA	1.89	0.40
7:CG:76:ARG:HG2	7:CG:156:TRP:CH2	2.55	0.40
10:CJ:74:ILE:HG22	61:CJ:5101:HOH:O	2.20	0.40
24:CX:43:A:H2'	24:CX:44:A:C8	2.56	0.40
25:DA:90:U:H1'	25:DA:92:A:C8	2.56	0.40
25:DA:875:G:N2	25:DA:903:C:C2	2.89	0.40
25:DA:921:G:H2'	25:DA:922:U:C6	2.57	0.40
25:DA:1000:A:C6	25:DA:1155:A:C8	3.09	0.40
25:DA:1116:C:H2'	25:DA:1117:G:C8	2.57	0.40
25:DA:1653:G:C4	37:DR:9:LYS:HD2	2.56	0.40
25:DA:1786:A:C4	25:DA:1938:A:C6	3.09	0.40
25:DA:1922:G:H2'	25:DA:1923:U:O4'	2.21	0.40
25:DA:2176:A:H2'	25:DA:2177:C:C5	2.56	0.40
25:DA:2461:C:H2'	25:DA:2462:U:H6	1.85	0.40
25:DA:2550:G:C6	25:DA:2551:C:C4	3.09	0.40
25:DA:2699:C:H2'	25:DA:2700:C:O4'	2.21	0.40
30:DG:97:ASP:HA	30:DG:100:TRP:HD1	1.86	0.40
30:DG:106:LEU:O	30:DG:110:ALA:HB3	2.21	0.40
34:DO:22:ILE:HD11	34:DO:40:VAL:HG12	2.03	0.40
35:DP:65:ARG:HG3	54:D8:25:MET:CG	2.52	0.40
36:DQ:137:TYR:HB3	45:DZ:76:LEU:HD21	2.04	0.40
46:D0:18:ALA:HB3	46:D0:20:ARG:HH21	1.87	0.40
1:AA:355:C:C4	1:AA:356:A:N7	2.89	0.40
1:AA:580:U:H5"	15:AO:58:MET:HG2	2.03	0.40
1:AA:1288:A:H2'	1:AA:1289:A:C8	2.57	0.40
17:AQ:46:ASP:CG	17:AQ:51:TYR:HD2	2.29	0.40
24:AX:4:G:H2'	24:AX:5:G:C8	2.55	0.40
23:AY:57:G:N3	23:AY:57:G:H2'	2.35	0.40
25:BA:831:A:O4'	27:BD:227:ASN:ND2	2.54	0.40
25:BA:1790:A:H1'	25:BA:2723:A:C2	2.57	0.40
61:BA:4080:HOH:O	33:BN:28:THR:HG23	2.21	0.40
28:BE:56:PRO:HG3	28:BE:74:PRO:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BX:61:GLY:HA3	43:BX:73:ARG:O	2.22	0.40
54:B8:54:GLU:O	54:B8:58:ILE:HG13	2.22	0.40
1:CA:634:C:H2'	1:CA:635:G:H8	1.86	0.40
1:CA:1004:A:H5"	1:CA:1024:G:H22	1.87	0.40
1:CA:1133:G:H2'	1:CA:1134:G:O4'	2.22	0.40
1:CA:1327:C:OP1	21:CU:20:LYS:N	2.55	0.40
1:CA:1427:U:H2'	1:CA:1428:A:C8	2.56	0.40
2:CB:20:GLU:HB2	2:CB:190:THR:OG1	2.22	0.40
2:CB:110:GLN:O	2:CB:110:GLN:HG2	2.21	0.40
4:CD:128:VAL:N	4:CD:131:ARG:O	2.51	0.40
5:CE:33:VAL:HG21	5:CE:109:ILE:HA	2.02	0.40
8:CH:56:LYS:HD3	8:CH:56:LYS:HA	1.82	0.40
15:CO:11:VAL:O	15:CO:15:PHE:HD1	2.04	0.40
21:CU:13:ILE:HG12	21:CU:22:ARG:CZ	2.51	0.40
23:CW:53:G:H1	23:CW:61:C:H42	1.69	0.40
24:CX:38:A:H8	24:CX:38:A:O5'	2.04	0.40
23:CY:58:A:H1'	23:CY:60:U:O2	2.22	0.40
25:DA:858:U:O2	25:DA:2268:A:H2'	2.21	0.40
25:DA:947:G:H2'	25:DA:948:G:H8	1.87	0.40
25:DA:2021:C:OP1	51:D5:12:SER:OG	2.38	0.40
25:DA:2055:C:H5'	25:DA:2056:G:O5'	2.22	0.40
25:DA:2126:A:H4'	25:DA:2127:G:OP1	2.20	0.40
25:DA:2133:G:O2'	25:DA:2134:A:P	2.79	0.40
25:DA:2359:C:H2'	25:DA:2360:A:O4'	2.21	0.40
26:DB:75:G:H21	45:DZ:85:HIS:HD1	1.68	0.40
30:DG:31:VAL:HA	30:DG:32:PRO:HD2	1.78	0.40
30:DG:113:ARG:HD2	30:DG:140:ILE:O	2.21	0.40
32:DI:26:ALA:O	32:DI:31:LEU:HB2	2.22	0.40
40:DU:85:LYS:HE2	40:DU:85:LYS:HB3	1.82	0.40
41:DV:58:VAL:HG21	41:DV:100:ARG:HH11	1.87	0.40
44:DY:12:THR:OG1	44:DY:26:LYS:HE2	2.22	0.40
50:D4:15:ILE:HB	50:D4:32:TYR:CD1	2.56	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%)	200 (87%)	19 (8%)	10 (4%)	2 1
2	CB	229/256 (90%)	195 (85%)	24 (10%)	10 (4%)	2 1
3	AC	204/239 (85%)	184 (90%)	17 (8%)	3 (2%)	8 10
3	CC	204/239 (85%)	180 (88%)	22 (11%)	2 (1%)	12 17
4	AD	206/209 (99%)	192 (93%)	12 (6%)	2 (1%)	12 17
4	CD	206/209 (99%)	189 (92%)	16 (8%)	1 (0%)	24 34
5	AE	146/162 (90%)	134 (92%)	9 (6%)	3 (2%)	5 5
5	CE	146/162 (90%)	138 (94%)	7 (5%)	1 (1%)	18 25
6	AF	98/101 (97%)	97 (99%)	1 (1%)	0	100 100
6	CF	98/101 (97%)	96 (98%)	2 (2%)	0	100 100
7	AG	153/156 (98%)	143 (94%)	8 (5%)	2 (1%)	9 12
7	CG	153/156 (98%)	140 (92%)	9 (6%)	4 (3%)	4 3
8	AH	135/138 (98%)	129 (96%)	6 (4%)	0	100 100
8	CH	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	18 25
9	AI	125/128 (98%)	111 (89%)	11 (9%)	3 (2%)	4 4
9	CI	125/128 (98%)	114 (91%)	8 (6%)	3 (2%)	4 4
10	AJ	95/105 (90%)	83 (87%)	9 (10%)	3 (3%)	3 2
10	CJ	94/105 (90%)	81 (86%)	10 (11%)	3 (3%)	3 2
11	AK	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	6 7
11	CK	112/129 (87%)	107 (96%)	3 (3%)	2 (2%)	6 7
12	AL	120/132 (91%)	115 (96%)	5 (4%)	0	100 100
12	CL	120/132 (91%)	116 (97%)	4 (3%)	0	100 100
13	AM	121/126 (96%)	110 (91%)	9 (7%)	2 (2%)	7 8
13	CM	120/126 (95%)	108 (90%)	9 (8%)	3 (2%)	4 4
14	AN	58/61 (95%)	54 (93%)	4 (7%)	0	100 100
14	CN	58/61 (95%)	53 (91%)	5 (9%)	0	100 100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100 100
15	CO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5 4
16	AP	80/88 (91%)	78 (98%)	2 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	CP	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	9 12
17	AQ	97/105 (92%)	90 (93%)	7 (7%)	0	100 100
17	CQ	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	12 17
18	AR	66/88 (75%)	64 (97%)	2 (3%)	0	100 100
18	CR	66/88 (75%)	65 (98%)	0	1 (2%)	8 10
19	AS	81/93 (87%)	72 (89%)	9 (11%)	0	100 100
19	CS	81/93 (87%)	71 (88%)	10 (12%)	0	100 100
20	AT	94/106 (89%)	84 (89%)	3 (3%)	7 (7%)	1 0
20	CT	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	1 0
21	AU	21/27 (78%)	18 (86%)	3 (14%)	0	100 100
21	CU	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2 1
27	BD	273/276 (99%)	257 (94%)	15 (6%)	1 (0%)	30 39
27	DD	273/276 (99%)	258 (94%)	13 (5%)	2 (1%)	18 25
28	BE	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24 34
28	DE	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	12 17
29	BF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	24 34
29	DF	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	12 17
30	BG	179/182 (98%)	167 (93%)	7 (4%)	5 (3%)	4 3
30	DG	179/182 (98%)	165 (92%)	7 (4%)	7 (4%)	2 1
31	BH	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	21 29
31	DH	172/180 (96%)	157 (91%)	13 (8%)	2 (1%)	10 13
32	BI	144/148 (97%)	123 (85%)	16 (11%)	5 (4%)	3 1
32	DI	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	18 25
33	BN	138/140 (99%)	134 (97%)	4 (3%)	0	100 100
33	DN	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	18 25
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%)	138 (94%)	8 (5%)	1 (1%)	18 25
35	DP	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	9 11
36	BQ	139/141 (99%)	133 (96%)	6 (4%)	0	100 100
36	DQ	139/141 (99%)	129 (93%)	8 (6%)	2 (1%)	9 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BR	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
37	DR	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
38	BS	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
38	DS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	14	20
39	BT	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16	22
39	DT	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	16	22
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%)	94 (95%)	4 (4%)	1 (1%)	12	17
41	DV	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	17
42	BW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
42	DW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
43	BX	93/96 (97%)	90 (97%)	1 (1%)	2 (2%)	5	5
43	DX	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	11	15
44	BY	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
44	DY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
45	BZ	169/206 (82%)	143 (85%)	24 (14%)	2 (1%)	10	13
45	DZ	172/206 (84%)	149 (87%)	22 (13%)	1 (1%)	21	29
46	B0	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	10	13
46	D0	81/85 (95%)	75 (93%)	6 (7%)	0	100	100
47	B1	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
47	D1	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
48	B2	68/72 (94%)	68 (100%)	0	0	100	100
48	D2	68/72 (94%)	68 (100%)	0	0	100	100
49	B3	57/60 (95%)	57 (100%)	0	0	100	100
49	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
50	B4	67/71 (94%)	50 (75%)	11 (16%)	6 (9%)	0	0
50	D4	67/71 (94%)	51 (76%)	12 (18%)	4 (6%)	1	0
51	B5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
51	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
52	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	45 (98%)	0	1 (2%)	5 5
54	B8	62/65 (95%)	62 (100%)	0	0	100 100
54	D8	62/65 (95%)	61 (98%)	1 (2%)	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	11409/12128 (94%)	10643 (93%)	629 (6%)	137 (1%)	10 13

All (137) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL
2	AB	16	HIS
2	AB	17	PHE
2	AB	126	GLU
2	AB	231	GLU
3	AC	65	ALA
9	AI	44	VAL
9	AI	54	ASP
10	AJ	77	PRO
20	AT	47	GLY
27	BD	275	LYS
29	BF	130	ALA
30	BG	50	ALA
50	B4	55	ARG
50	B4	57	GLU
2	CB	16	HIS
2	CB	17	PHE
2	CB	126	GLU
7	CG	7	ALA
9	CI	44	VAL
9	CI	54	ASP
10	CJ	79	ARG
13	CM	107	ALA
20	CT	10	LEU
29	DF	21	ALA
29	DF	130	ALA
30	DG	47	LYS

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Mol	Chain	Res	Type
30	DG	81	LYS
31	DH	29	PRO
31	DH	126	PRO
32	DI	10	GLU
35	DP	45	LEU
50	D4	45	GLY
50	D4	51	ASP
50	D4	62	ARG
53	D7	46	VAL
3	AC	66	VAL
5	AE	85	GLY
5	AE	86	ALA
9	AI	43	ALA
10	AJ	31	GLY
10	AJ	91	PRO
11	AK	49	GLY
30	BG	43	LEU
30	BG	126	ASP
31	BH	126	PRO
32	BI	11	ASN
32	BI	106	GLY
41	BV	79	VAL
45	BZ	152	ALA
45	BZ	159	PRO
50	B4	45	GLY
50	B4	54	GLY
50	B4	68	ARG
2	CB	10	LEU
3	CC	181	ASN
7	CG	81	GLY
10	CJ	77	PRO
11	CK	49	GLY
13	CM	106	ASN
15	CO	23	GLY
16	CP	53	VAL
20	CT	47	GLY
28	DE	73	GLU
30	DG	43	LEU
30	DG	51	ARG
30	DG	126	ASP
41	DV	79	VAL
45	DZ	117	LEU

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Mol	Chain	Res	Type
2	AB	150	SER
4	AD	166	LYS
4	AD	173	TRP
13	AM	12	ASN
20	AT	9	ASN
20	AT	10	LEU
20	AT	94	ALA
20	AT	100	ILE
20	AT	102	GLY
28	BE	52	LEU
46	B0	13	GLY
2	CB	8	LYS
2	CB	150	SER
4	CD	45	GLN
5	CE	69	VAL
8	CH	73	ASP
9	CI	11	LYS
20	CT	99	LEU
27	DD	3	VAL
28	DE	52	LEU
33	DN	2	LYS
36	DQ	28	ALA
38	DS	84	GLN
2	AB	10	LEU
3	AC	107	GLN
5	AE	69	VAL
7	AG	80	VAL
13	AM	11	ARG
30	BG	32	PRO
30	BG	51	ARG
32	BI	73	GLU
39	BT	55	ASN
43	BX	93	GLU
15	CO	88	ARG
17	CQ	14	LYS
27	DD	239	ARG
30	DG	32	PRO
39	DT	55	ASN
43	DX	2	LYS
50	D4	55	ARG
2	AB	124	SER
11	AK	105	VAL

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Mol	Chain	Res	Type
20	AT	95	ALA
32	BI	107	VAL
35	BP	29	LYS
50	B4	44	THR
2	CB	120	ALA
2	CB	234	PRO
3	CC	156	ARG
7	CG	55	GLY
18	CR	25	THR
20	CT	102	GLY
30	DG	50	ALA
2	AB	202	PRO
2	CB	202	PRO
2	CB	232	PRO
20	CT	100	ILE
35	DP	29	LYS
43	BX	94	GLY
11	CK	105	VAL
7	AG	17	VAL
10	CJ	91	PRO
21	CU	23	PRO
7	CG	80	VAL
13	CM	4	ILE
36	DQ	27	VAL
32	BI	131	LYS

5.3.2 Protein sidechains (i)

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%)	165 (86%)	27 (14%)	3 3
2	CB	187/220 (85%)	160 (86%)	27 (14%)	3 2
3	AC	143/188 (76%)	126 (88%)	17 (12%)	5 5
3	CC	140/188 (74%)	115 (82%)	25 (18%)	2 1
4	AD	170/181 (94%)	155 (91%)	15 (9%)	9 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	CD	173/181 (96%)	158 (91%)	15 (9%)	9 13
5	AE	113/123 (92%)	104 (92%)	9 (8%)	11 15
5	CE	114/123 (93%)	105 (92%)	9 (8%)	11 16
6	AF	83/90 (92%)	78 (94%)	5 (6%)	17 26
6	CF	85/90 (94%)	80 (94%)	5 (6%)	18 27
7	AG	119/127 (94%)	107 (90%)	12 (10%)	7 8
7	CG	120/127 (94%)	108 (90%)	12 (10%)	7 9
8	AH	114/119 (96%)	100 (88%)	14 (12%)	4 4
8	CH	114/119 (96%)	99 (87%)	15 (13%)	4 4
9	AI	90/99 (91%)	78 (87%)	12 (13%)	4 4
9	CI	89/99 (90%)	71 (80%)	18 (20%)	1 1
10	AJ	66/92 (72%)	60 (91%)	6 (9%)	9 11
10	CJ	69/92 (75%)	67 (97%)	2 (3%)	37 55
11	AK	82/99 (83%)	77 (94%)	5 (6%)	17 25
11	CK	83/99 (84%)	79 (95%)	4 (5%)	23 35
12	AL	97/109 (89%)	93 (96%)	4 (4%)	27 41
12	CL	97/109 (89%)	92 (95%)	5 (5%)	21 32
13	AM	93/101 (92%)	80 (86%)	13 (14%)	3 3
13	CM	92/101 (91%)	79 (86%)	13 (14%)	3 3
14	AN	49/50 (98%)	41 (84%)	8 (16%)	2 2
14	CN	49/50 (98%)	42 (86%)	7 (14%)	3 3
15	AO	78/80 (98%)	68 (87%)	10 (13%)	4 4
15	CO	78/80 (98%)	69 (88%)	9 (12%)	5 6
16	AP	69/74 (93%)	60 (87%)	9 (13%)	4 4
16	CP	68/74 (92%)	62 (91%)	6 (9%)	9 12
17	AQ	94/97 (97%)	90 (96%)	4 (4%)	26 39
17	CQ	94/97 (97%)	85 (90%)	9 (10%)	8 9
18	AR	59/77 (77%)	54 (92%)	5 (8%)	10 13
18	CR	59/77 (77%)	52 (88%)	7 (12%)	5 5
19	AS	69/80 (86%)	65 (94%)	4 (6%)	18 27
19	CS	67/80 (84%)	57 (85%)	10 (15%)	3 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	AT	70/82 (85%)	63 (90%)	7 (10%)	7 9
20	CT	70/82 (85%)	63 (90%)	7 (10%)	7 9
21	AU	18/22 (82%)	15 (83%)	3 (17%)	2 2
21	CU	18/22 (82%)	15 (83%)	3 (17%)	2 2
27	BD	215/218 (99%)	193 (90%)	22 (10%)	7 8
27	DD	215/218 (99%)	195 (91%)	20 (9%)	8 10
28	BE	164/166 (99%)	142 (87%)	22 (13%)	4 3
28	DE	164/166 (99%)	142 (87%)	22 (13%)	4 3
29	BF	160/166 (96%)	137 (86%)	23 (14%)	3 2
29	DF	159/166 (96%)	138 (87%)	21 (13%)	4 4
30	BG	143/156 (92%)	126 (88%)	17 (12%)	5 5
30	DG	142/156 (91%)	125 (88%)	17 (12%)	5 5
31	BH	144/148 (97%)	133 (92%)	11 (8%)	12 17
31	DH	144/148 (97%)	128 (89%)	16 (11%)	6 6
32	BI	110/124 (89%)	89 (81%)	21 (19%)	1 1
32	DI	104/124 (84%)	90 (86%)	14 (14%)	4 3
33	BN	118/119 (99%)	102 (86%)	16 (14%)	3 3
33	DN	118/119 (99%)	105 (89%)	13 (11%)	6 6
34	BO	100/100 (100%)	94 (94%)	6 (6%)	17 26
34	DO	100/100 (100%)	93 (93%)	7 (7%)	14 19
35	BP	115/116 (99%)	102 (89%)	13 (11%)	5 6
35	DP	115/116 (99%)	98 (85%)	17 (15%)	3 2
36	BQ	111/111 (100%)	97 (87%)	14 (13%)	4 4
36	DQ	111/111 (100%)	98 (88%)	13 (12%)	5 6
37	BR	101/101 (100%)	82 (81%)	19 (19%)	1 1
37	DR	101/101 (100%)	83 (82%)	18 (18%)	2 1
38	BS	87/88 (99%)	77 (88%)	10 (12%)	5 6
38	DS	85/88 (97%)	75 (88%)	10 (12%)	5 5
39	BT	115/127 (91%)	105 (91%)	10 (9%)	9 13
39	DT	113/127 (89%)	104 (92%)	9 (8%)	11 15
40	BU	93/94 (99%)	86 (92%)	7 (8%)	12 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	DU	93/94 (99%)	85 (91%)	8 (9%)	10 13
41	BV	80/82 (98%)	67 (84%)	13 (16%)	2 2
41	DV	80/82 (98%)	68 (85%)	12 (15%)	3 2
42	BW	90/92 (98%)	82 (91%)	8 (9%)	9 12
42	DW	90/92 (98%)	84 (93%)	6 (7%)	15 21
43	BX	77/78 (99%)	70 (91%)	7 (9%)	9 11
43	DX	77/78 (99%)	67 (87%)	10 (13%)	4 4
44	BY	85/91 (93%)	76 (89%)	9 (11%)	6 7
44	DY	85/91 (93%)	80 (94%)	5 (6%)	18 27
45	BZ	145/179 (81%)	125 (86%)	20 (14%)	3 3
45	DZ	145/179 (81%)	126 (87%)	19 (13%)	4 4
46	B0	65/67 (97%)	61 (94%)	4 (6%)	16 24
46	D0	65/67 (97%)	62 (95%)	3 (5%)	24 36
47	B1	80/83 (96%)	74 (92%)	6 (8%)	12 17
47	D1	80/83 (96%)	71 (89%)	9 (11%)	5 6
48	B2	65/67 (97%)	58 (89%)	7 (11%)	6 7
48	D2	65/67 (97%)	61 (94%)	4 (6%)	16 24
49	B3	51/52 (98%)	47 (92%)	4 (8%)	11 16
49	D3	50/52 (96%)	44 (88%)	6 (12%)	5 5
50	B4	60/63 (95%)	50 (83%)	10 (17%)	2 2
50	D4	53/63 (84%)	46 (87%)	7 (13%)	4 4
51	B5	50/52 (96%)	46 (92%)	4 (8%)	11 15
51	D5	50/52 (96%)	45 (90%)	5 (10%)	7 9
52	B6	51/52 (98%)	44 (86%)	7 (14%)	3 3
52	D6	50/52 (96%)	45 (90%)	5 (10%)	7 9
53	B7	41/42 (98%)	38 (93%)	3 (7%)	13 18
53	D7	41/42 (98%)	39 (95%)	2 (5%)	22 34
54	B8	53/55 (96%)	48 (91%)	5 (9%)	8 10
54	D8	54/55 (98%)	47 (87%)	7 (13%)	4 4
55	B9	34/34 (100%)	33 (97%)	1 (3%)	37 55
55	D9	34/34 (100%)	34 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9320/10066 (93%)	8299 (89%)	1021 (11%)	6 6

All (1021) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	7	VAL
2	AB	8	LYS
2	AB	11	LEU
2	AB	17	PHE
2	AB	21	ARG
2	AB	64	ARG
2	AB	76	GLN
2	AB	80	ILE
2	AB	94	ASN
2	AB	112	VAL
2	AB	114	ARG
2	AB	127	ILE
2	AB	144	ARG
2	AB	145	LEU
2	AB	155	LEU
2	AB	157	ARG
2	AB	169	LYS
2	AB	179	LYS
2	AB	185	ILE
2	AB	187	LEU
2	AB	189	ASP
2	AB	196	LEU
2	AB	200	ILE
2	AB	209	ARG
2	AB	213	LEU
2	AB	217	ARG
2	AB	221	LEU
3	AC	3	ASN
3	AC	8	ILE
3	AC	14	ILE
3	AC	15	THR
3	AC	21	ARG
3	AC	28	GLN
3	AC	37	GLN
3	AC	40	ARG
3	AC	89	GLU
3	AC	115	LEU

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Mol	Chain	Res	Type
3	AC	119	ARG
3	AC	131	ARG
3	AC	150	LYS
3	AC	164	ARG
3	AC	178	LEU
3	AC	195	VAL
3	AC	196	LEU
4	AD	5	ILE
4	AD	15	GLU
4	AD	19	LEU
4	AD	31	CYS
4	AD	49	ARG
4	AD	58	LEU
4	AD	115	ARG
4	AD	119	GLN
4	AD	127	THR
4	AD	135	LEU
4	AD	140	VAL
4	AD	150	GLU
4	AD	157	LEU
4	AD	158	ILE
4	AD	168	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	73	ASN
5	AE	91	LEU
5	AE	151	LEU
6	AF	36	ARG
6	AF	70	ASP
6	AF	74	ASP
6	AF	75	LEU
6	AF	82	ARG
7	AG	8	GLU
7	AG	13	GLN
7	AG	50	ILE
7	AG	51	GLN
7	AG	52	GLU
7	AG	72	ARG

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Mol	Chain	Res	Type
7	AG	79	ARG
7	AG	104	LEU
7	AG	113	GLU
7	AG	114	ARG
7	AG	138	LYS
7	AG	155	ARG
8	AH	2	LEU
8	AH	26	VAL
8	AH	39	LEU
8	AH	51	VAL
8	AH	52	ASP
8	AH	60	ARG
8	AH	63	LEU
8	AH	75	ARG
8	AH	78	GLN
8	AH	91	ARG
8	AH	95	VAL
8	AH	97	VAL
8	AH	112	LEU
8	AH	127	LEU
9	AI	3	GLN
9	AI	14	VAL
9	AI	23	ASN
9	AI	27	THR
9	AI	65	VAL
9	AI	81	ILE
9	AI	86	VAL
9	AI	87	GLN
9	AI	89	ASN
9	AI	108	VAL
9	AI	127	LYS
9	AI	128	ARG
10	AJ	5	ARG
10	AJ	23	ILE
10	AJ	55	LYS
10	AJ	70	ARG
10	AJ	84	GLN
10	AJ	92	THR
11	AK	31	THR
11	AK	48	ILE
11	AK	96	ARG
11	AK	104	GLN

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Mol	Chain	Res	Type
11	AK	114	VAL
12	AL	24	VAL
12	AL	33	ARG
12	AL	53	ARG
12	AL	60	LEU
13	AM	3	ARG
13	AM	4	ILE
13	AM	15	VAL
13	AM	19	LEU
13	AM	27	LYS
13	AM	43	THR
13	AM	56	LEU
13	AM	70	LEU
13	AM	73	GLU
13	AM	78	ILE
13	AM	102	ARG
13	AM	110	ARG
13	AM	121	LYS
14	AN	3	ARG
14	AN	6	LEU
14	AN	7	ILE
14	AN	15	LYS
14	AN	18	VAL
14	AN	23	ARG
14	AN	33	VAL
14	AN	50	LYS
15	AO	3	ILE
15	AO	22	THR
15	AO	24	SER
15	AO	26	GLU
15	AO	39	LEU
15	AO	41	GLU
15	AO	47	LYS
15	AO	64	ARG
15	AO	76	GLU
15	AO	84	LYS
16	AP	2	VAL
16	AP	19	ILE
16	AP	20	VAL
16	AP	21	VAL
16	AP	27	LYS
16	AP	50	LYS

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Mol	Chain	Res	Type
16	AP	54	GLU
16	AP	60	LEU
16	AP	62	VAL
17	AQ	9	VAL
17	AQ	35	VAL
17	AQ	74	LEU
17	AQ	83	ASP
18	AR	31	LEU
18	AR	32	ARG
18	AR	37	VAL
18	AR	46	GLU
18	AR	76	LEU
19	AS	28	LYS
19	AS	37	ARG
19	AS	41	VAL
19	AS	65	ASN
20	AT	8	ARG
20	AT	13	LEU
20	AT	30	LYS
20	AT	45	GLN
20	AT	56	MET
20	AT	62	LEU
20	AT	74	LYS
21	AU	7	ARG
21	AU	9	ARG
21	AU	10	ARG
27	BD	3	VAL
27	BD	12	SER
27	BD	54	ARG
27	BD	61	LEU
27	BD	71	ASP
27	BD	94	LEU
27	BD	99	ASP
27	BD	106	ILE
27	BD	113	VAL
27	BD	116	GLN
27	BD	126	GLN
27	BD	138	VAL
27	BD	142	VAL
27	BD	193	VAL
27	BD	211	ARG
27	BD	217	ARG

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Mol	Chain	Res	Type
27	BD	221	VAL
27	BD	229	VAL
27	BD	242	ARG
27	BD	257	LEU
27	BD	259	THR
27	BD	260	ARG
28	BE	9	VAL
28	BE	12	THR
28	BE	21	VAL
28	BE	24	THR
28	BE	33	VAL
28	BE	34	VAL
28	BE	40	GLU
28	BE	49	LEU
28	BE	73	GLU
28	BE	75	VAL
28	BE	77	ILE
28	BE	78	LEU
28	BE	82	ARG
28	BE	97	LYS
28	BE	111	ARG
28	BE	116	VAL
28	BE	119	ARG
28	BE	144	ARG
28	BE	154	LYS
28	BE	163	GLU
28	BE	175	VAL
28	BE	181	LEU
29	BF	19	GLU
29	BF	20	LEU
29	BF	23	ASP
29	BF	27	GLU
29	BF	28	ILE
29	BF	33	LEU
29	BF	38	ARG
29	BF	53	THR
29	BF	57	VAL
29	BF	88	VAL
29	BF	106	ARG
29	BF	110	LEU
29	BF	125	LEU
29	BF	132	VAL

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Mol	Chain	Res	Type
29	BF	140	LEU
29	BF	158	THR
29	BF	170	LEU
29	BF	175	THR
29	BF	183	VAL
29	BF	192	LEU
29	BF	195	ASP
29	BF	200	GLU
29	BF	201	VAL
30	BG	5	VAL
30	BG	31	VAL
30	BG	43	LEU
30	BG	45	GLU
30	BG	60	LEU
30	BG	70	VAL
30	BG	78	SER
30	BG	81	LYS
30	BG	82	LEU
30	BG	91	ARG
30	BG	135	LEU
30	BG	140	ILE
30	BG	143	GLU
30	BG	148	MET
30	BG	159	VAL
30	BG	170	ARG
30	BG	175	LEU
31	BH	15	VAL
31	BH	41	MET
31	BH	45	VAL
31	BH	59	ARG
31	BH	62	LYS
31	BH	69	ARG
31	BH	71	LEU
31	BH	116	GLU
31	BH	119	GLU
31	BH	130	ARG
31	BH	139	GLN
32	BI	5	LEU
32	BI	10	GLU
32	BI	15	VAL
32	BI	20	ASP
32	BI	38	LEU

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Mol	Chain	Res	Type
32	BI	43	ASN
32	BI	44	LEU
32	BI	47	LEU
32	BI	50	ARG
32	BI	57	ARG
32	BI	60	GLU
32	BI	66	GLU
32	BI	77	LEU
32	BI	87	LYS
32	BI	92	VAL
32	BI	101	LEU
32	BI	109	ILE
32	BI	127	VAL
32	BI	140	LEU
32	BI	142	VAL
32	BI	144	VAL
33	BN	5	VAL
33	BN	15	LEU
33	BN	28	THR
33	BN	33	LEU
33	BN	34	LEU
33	BN	46	VAL
33	BN	48	MET
33	BN	61	ARG
33	BN	62	VAL
33	BN	68	GLU
33	BN	73	THR
33	BN	87	LEU
33	BN	97	ARG
33	BN	99	LEU
33	BN	120	LEU
33	BN	133	GLN
34	BO	8	LEU
34	BO	10	VAL
34	BO	23	ARG
34	BO	24	VAL
34	BO	26	LYS
34	BO	108	GLU
35	BP	1	MET
35	BP	21	ARG
35	BP	55	ARG
35	BP	59	LEU

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Mol	Chain	Res	Type
35	BP	65	ARG
35	BP	68	GLN
35	BP	70	GLN
35	BP	83	VAL
35	BP	106	LEU
35	BP	112	LEU
35	BP	125	VAL
35	BP	135	LEU
35	BP	147	LEU
36	BQ	2	LEU
36	BQ	7	MET
36	BQ	8	LYS
36	BQ	16	ARG
36	BQ	21	THR
36	BQ	35	VAL
36	BQ	42	ILE
36	BQ	45	GLN
36	BQ	54	MET
36	BQ	59	ARG
36	BQ	60	ARG
36	BQ	75	THR
36	BQ	109	VAL
36	BQ	110	THR
37	BR	1	MET
37	BR	6	SER
37	BR	15	SER
37	BR	18	LEU
37	BR	24	GLN
37	BR	28	LEU
37	BR	29	LEU
37	BR	36	THR
37	BR	44	LEU
37	BR	54	LEU
37	BR	60	LEU
37	BR	65	LEU
37	BR	67	LEU
37	BR	75	LEU
37	BR	79	LEU
37	BR	100	LEU
37	BR	102	GLU
37	BR	111	LEU
37	BR	114	VAL

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Mol	Chain	Res	Type
38	BS	14	VAL
38	BS	20	ARG
38	BS	46	VAL
38	BS	49	VAL
38	BS	50	SER
38	BS	57	LYS
38	BS	59	LYS
38	BS	69	VAL
38	BS	78	LEU
38	BS	110	LEU
39	BT	6	LEU
39	BT	16	ARG
39	BT	28	VAL
39	BT	36	GLU
39	BT	49	VAL
39	BT	53	ARG
39	BT	89	VAL
39	BT	96	ARG
39	BT	113	LYS
39	BT	118	ARG
40	BU	8	VAL
40	BU	36	ARG
40	BU	74	LEU
40	BU	83	LEU
40	BU	93	LYS
40	BU	95	LEU
40	BU	104	GLN
41	BV	18	LEU
41	BV	28	GLU
41	BV	32	THR
41	BV	43	GLU
41	BV	46	VAL
41	BV	51	VAL
41	BV	52	VAL
41	BV	61	VAL
41	BV	62	LEU
41	BV	72	VAL
41	BV	79	VAL
41	BV	95	LEU
41	BV	100	ARG
42	BW	4	LYS
42	BW	11	ARG

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Mol	Chain	Res	Type
42	BW	17	VAL
42	BW	19	LEU
42	BW	51	LEU
42	BW	52	GLU
42	BW	100	THR
42	BW	107	LEU
43	BX	23	GLU
43	BX	35	THR
43	BX	57	LEU
43	BX	65	ARG
43	BX	66	LEU
43	BX	76	ARG
43	BX	92	LEU
44	BY	7	VAL
44	BY	23	ARG
44	BY	40	GLU
44	BY	55	TYR
44	BY	72	VAL
44	BY	73	ARG
44	BY	85	VAL
44	BY	90	LEU
44	BY	99	CYS
45	BZ	5	LEU
45	BZ	6	LYS
45	BZ	18	LEU
45	BZ	33	LEU
45	BZ	41	LEU
45	BZ	42	VAL
45	BZ	61	LEU
45	BZ	91	LEU
45	BZ	96	VAL
45	BZ	100	VAL
45	BZ	111	VAL
45	BZ	117	LEU
45	BZ	132	ASN
45	BZ	135	GLU
45	BZ	136	PHE
45	BZ	153	SER
45	BZ	154	ASP
45	BZ	155	LEU
45	BZ	161	VAL
45	BZ	171	ILE

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Mol	Chain	Res	Type
46	B0	20	ARG
46	B0	36	ILE
46	B0	49	LYS
46	B0	82	ARG
47	B1	3	LYS
47	B1	40	ARG
47	B1	59	THR
47	B1	75	GLU
47	B1	78	LYS
47	B1	95	LEU
48	B2	19	VAL
48	B2	30	ARG
48	B2	32	LEU
48	B2	40	SER
48	B2	52	ASP
48	B2	64	LEU
48	B2	70	GLN
49	B3	8	LEU
49	B3	23	LEU
49	B3	54	VAL
49	B3	60	GLU
50	B4	33	VAL
50	B4	34	GLU
50	B4	37	SER
50	B4	46	GLN
50	B4	49	PHE
50	B4	50	VAL
50	B4	58	ARG
50	B4	63	TYR
50	B4	67	TYR
50	B4	68	ARG
51	B5	6	VAL
51	B5	29	THR
51	B5	40	LYS
51	B5	55	ARG
52	B6	4	GLU
52	B6	9	LEU
52	B6	14	THR
52	B6	28	ARG
52	B6	38	LYS
52	B6	48	VAL
52	B6	52	VAL

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Mol	Chain	Res	Type
53	B7	24	THR
53	B7	41	ARG
53	B7	43	THR
54	B8	13	ARG
54	B8	14	VAL
54	B8	23	VAL
54	B8	30	ARG
54	B8	32	LEU
55	B9	17	ILE
2	CB	8	LYS
2	CB	11	LEU
2	CB	23	ARG
2	CB	47	THR
2	CB	48	MET
2	CB	74	LYS
2	CB	76	GLN
2	CB	80	ILE
2	CB	81	VAL
2	CB	94	ASN
2	CB	96	ARG
2	CB	115	LEU
2	CB	126	GLU
2	CB	128	GLU
2	CB	155	LEU
2	CB	169	LYS
2	CB	175	ARG
2	CB	179	LYS
2	CB	185	ILE
2	CB	187	LEU
2	CB	189	ASP
2	CB	196	LEU
2	CB	200	ILE
2	CB	213	LEU
2	CB	217	ARG
2	CB	222	ILE
2	CB	224	GLN
3	CC	3	ASN
3	CC	15	THR
3	CC	21	ARG
3	CC	26	LYS
3	CC	28	GLN
3	CC	30	ARG

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Mol	Chain	Res	Type
3	CC	40	ARG
3	CC	54	ARG
3	CC	57	ILE
3	CC	85	ARG
3	CC	89	GLU
3	CC	104	GLN
3	CC	105	GLU
3	CC	115	LEU
3	CC	118	GLN
3	CC	119	ARG
3	CC	131	ARG
3	CC	151	VAL
3	CC	152	ILE
3	CC	162	GLN
3	CC	178	LEU
3	CC	192	THR
3	CC	195	VAL
3	CC	196	LEU
3	CC	202	ILE
4	CD	19	LEU
4	CD	31	CYS
4	CD	34	GLU
4	CD	58	LEU
4	CD	61	LYS
4	CD	96	LEU
4	CD	108	LEU
4	CD	119	GLN
4	CD	135	LEU
4	CD	141	ARG
4	CD	150	GLU
4	CD	155	LEU
4	CD	157	LEU
4	CD	170	VAL
4	CD	194	LEU
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	64	ARG
5	CE	75	THR

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Mol	Chain	Res	Type
5	CE	79	GLU
6	CF	10	LEU
6	CF	28	ARG
6	CF	36	ARG
6	CF	70	ASP
6	CF	75	LEU
7	CG	10	ARG
7	CG	11	GLN
7	CG	32	ARG
7	CG	51	GLN
7	CG	52	GLU
7	CG	73	MET
7	CG	86	GLN
7	CG	104	LEU
7	CG	113	GLU
7	CG	114	ARG
7	CG	138	LYS
7	CG	155	ARG
8	CH	2	LEU
8	CH	26	VAL
8	CH	29	SER
8	CH	39	LEU
8	CH	51	VAL
8	CH	60	ARG
8	CH	63	LEU
8	CH	75	ARG
8	CH	78	GLN
8	CH	84	ARG
8	CH	91	ARG
8	CH	95	VAL
8	CH	97	VAL
8	CH	112	LEU
8	CH	127	LEU
9	CI	3	GLN
9	CI	7	THR
9	CI	14	VAL
9	CI	17	VAL
9	CI	23	ASN
9	CI	27	THR
9	CI	50	LEU
9	CI	56	LEU
9	CI	64	THR

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Mol	Chain	Res	Type
9	CI	65	VAL
9	CI	81	ILE
9	CI	87	GLN
9	CI	89	ASN
9	CI	102	LEU
9	CI	108	VAL
9	CI	113	LYS
9	CI	127	LYS
9	CI	128	ARG
10	CJ	21	GLN
10	CJ	67	THR
11	CK	14	VAL
11	CK	93	GLN
11	CK	104	GLN
11	CK	114	VAL
12	CL	24	VAL
12	CL	33	ARG
12	CL	50	SER
12	CL	53	ARG
12	CL	79	GLU
13	CM	3	ARG
13	CM	4	ILE
13	CM	15	VAL
13	CM	19	LEU
13	CM	47	ASP
13	CM	56	LEU
13	CM	70	LEU
13	CM	78	ILE
13	CM	98	VAL
13	CM	102	ARG
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	15	LYS
14	CN	23	ARG
14	CN	33	VAL
15	CO	3	ILE
15	CO	5	LYS

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Mol	Chain	Res	Type
15	CO	7	GLU
15	CO	26	GLU
15	CO	38	ARG
15	CO	39	LEU
15	CO	41	GLU
15	CO	54	ARG
15	CO	64	ARG
16	CP	2	VAL
16	CP	20	VAL
16	CP	21	VAL
16	CP	27	LYS
16	CP	62	VAL
16	CP	67	THR
17	CQ	6	LEU
17	CQ	9	VAL
17	CQ	14	LYS
17	CQ	35	VAL
17	CQ	36	ILE
17	CQ	52	LYS
17	CQ	74	LEU
17	CQ	83	ASP
17	CQ	96	GLU
18	CR	26	LEU
18	CR	32	ARG
18	CR	37	VAL
18	CR	41	LYS
18	CR	42	ARG
18	CR	46	GLU
18	CR	76	LEU
19	CS	16	LEU
19	CS	27	GLU
19	CS	28	LYS
19	CS	30	LEU
19	CS	41	VAL
19	CS	56	GLN
19	CS	65	ASN
19	CS	71	LEU
19	CS	77	THR
19	CS	78	ARG
20	CT	30	LYS
20	CT	36	LEU
20	CT	45	GLN

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Mol	Chain	Res	Type
20	CT	56	MET
20	CT	62	LEU
20	CT	80	ARG
20	CT	99	LEU
21	CU	7	ARG
21	CU	10	ARG
21	CU	24	ARG
27	DD	54	ARG
27	DD	61	LEU
27	DD	71	ASP
27	DD	78	LYS
27	DD	94	LEU
27	DD	99	ASP
27	DD	103	ARG
27	DD	106	ILE
27	DD	109	ASP
27	DD	113	VAL
27	DD	116	GLN
27	DD	138	VAL
27	DD	142	VAL
27	DD	155	LEU
27	DD	193	VAL
27	DD	211	ARG
27	DD	221	VAL
27	DD	257	LEU
27	DD	259	THR
27	DD	260	ARG
28	DE	9	VAL
28	DE	12	THR
28	DE	21	VAL
28	DE	24	THR
28	DE	33	VAL
28	DE	34	VAL
28	DE	38	THR
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
28	DE	116	VAL

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Mol	Chain	Res	Type
28	DE	119	ARG
28	DE	134	ILE
28	DE	144	ARG
28	DE	154	LYS
28	DE	163	GLU
28	DE	175	VAL
28	DE	181	LEU
29	DF	19	GLU
29	DF	20	LEU
29	DF	27	GLU
29	DF	33	LEU
29	DF	38	ARG
29	DF	53	THR
29	DF	57	VAL
29	DF	70	THR
29	DF	82	ILE
29	DF	88	VAL
29	DF	106	ARG
29	DF	110	LEU
29	DF	132	VAL
29	DF	140	LEU
29	DF	158	THR
29	DF	170	LEU
29	DF	175	THR
29	DF	183	VAL
29	DF	192	LEU
29	DF	200	GLU
29	DF	201	VAL
30	DG	5	VAL
30	DG	16	ARG
30	DG	31	VAL
30	DG	43	LEU
30	DG	45	GLU
30	DG	47	LYS
30	DG	49	ASP
30	DG	60	LEU
30	DG	70	VAL
30	DG	91	ARG
30	DG	115	ARG
30	DG	136	ARG
30	DG	140	ILE
30	DG	143	GLU

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Mol	Chain	Res	Type
30	DG	148	MET
30	DG	170	ARG
30	DG	175	LEU
31	DH	3	ARG
31	DH	15	VAL
31	DH	33	LEU
31	DH	34	GLU
31	DH	62	LYS
31	DH	63	SER
31	DH	69	ARG
31	DH	71	LEU
31	DH	72	ILE
31	DH	95	ARG
31	DH	105	LEU
31	DH	106	THR
31	DH	124	GLU
31	DH	136	ILE
31	DH	139	GLN
31	DH	175	LYS
32	DI	5	LEU
32	DI	9	LEU
32	DI	15	VAL
32	DI	20	ASP
32	DI	38	LEU
32	DI	43	ASN
32	DI	44	LEU
32	DI	47	LEU
32	DI	61	ARG
32	DI	73	GLU
32	DI	77	LEU
32	DI	92	VAL
32	DI	127	VAL
32	DI	140	LEU
33	DN	15	LEU
33	DN	28	THR
33	DN	33	LEU
33	DN	34	LEU
33	DN	46	VAL
33	DN	58	ASP
33	DN	61	ARG
33	DN	62	VAL
33	DN	85	ILE

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Mol	Chain	Res	Type
33	DN	87	LEU
33	DN	97	ARG
33	DN	99	LEU
33	DN	120	LEU
34	DO	8	LEU
34	DO	9	GLU
34	DO	10	VAL
34	DO	23	ARG
34	DO	24	VAL
34	DO	69	ILE
34	DO	108	GLU
35	DP	1	MET
35	DP	2	LYS
35	DP	15	ARG
35	DP	21	ARG
35	DP	45	LEU
35	DP	50	ARG
35	DP	55	ARG
35	DP	65	ARG
35	DP	68	GLN
35	DP	77	ARG
35	DP	83	VAL
35	DP	95	VAL
35	DP	99	LEU
35	DP	106	LEU
35	DP	112	LEU
35	DP	135	LEU
35	DP	147	LEU
36	DQ	1	MET
36	DQ	5	ARG
36	DQ	16	ARG
36	DQ	21	THR
36	DQ	45	GLN
36	DQ	48	GLU
36	DQ	54	MET
36	DQ	56	ARG
36	DQ	60	ARG
36	DQ	75	THR
36	DQ	109	VAL
36	DQ	110	THR
36	DQ	112	GLU
37	DR	1	MET

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Mol	Chain	Res	Type
37	DR	6	SER
37	DR	18	LEU
37	DR	24	GLN
37	DR	28	LEU
37	DR	29	LEU
37	DR	36	THR
37	DR	44	LEU
37	DR	54	LEU
37	DR	60	LEU
37	DR	65	LEU
37	DR	67	LEU
37	DR	75	LEU
37	DR	78	LYS
37	DR	79	LEU
37	DR	100	LEU
37	DR	102	GLU
37	DR	114	VAL
38	DS	14	VAL
38	DS	33	LYS
38	DS	46	VAL
38	DS	50	SER
38	DS	67	ARG
38	DS	68	GLN
38	DS	75	GLU
38	DS	80	LEU
38	DS	110	LEU
38	DS	111	GLU
39	DT	1	MET
39	DT	16	ARG
39	DT	17	THR
39	DT	28	VAL
39	DT	38	ASN
39	DT	49	VAL
39	DT	89	VAL
39	DT	96	ARG
39	DT	113	LYS
40	DU	36	ARG
40	DU	74	LEU
40	DU	83	LEU
40	DU	92	ARG
40	DU	93	LYS
40	DU	95	LEU

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Mol	Chain	Res	Type
40	DU	104	GLN
40	DU	108	GLU
41	DV	15	GLU
41	DV	18	LEU
41	DV	28	GLU
41	DV	32	THR
41	DV	46	VAL
41	DV	51	VAL
41	DV	52	VAL
41	DV	61	VAL
41	DV	62	LEU
41	DV	79	VAL
41	DV	85	LYS
41	DV	95	LEU
42	DW	4	LYS
42	DW	11	ARG
42	DW	17	VAL
42	DW	51	LEU
42	DW	100	THR
42	DW	107	LEU
43	DX	1	MET
43	DX	23	GLU
43	DX	35	THR
43	DX	52	VAL
43	DX	57	LEU
43	DX	65	ARG
43	DX	70	LEU
43	DX	76	ARG
43	DX	88	LYS
43	DX	92	LEU
44	DY	7	VAL
44	DY	40	GLU
44	DY	72	VAL
44	DY	85	VAL
44	DY	99	CYS
45	DZ	5	LEU
45	DZ	18	LEU
45	DZ	33	LEU
45	DZ	41	LEU
45	DZ	42	VAL
45	DZ	61	LEU
45	DZ	96	VAL

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Mol	Chain	Res	Type
45	DZ	97	GLU
45	DZ	100	VAL
45	DZ	111	VAL
45	DZ	117	LEU
45	DZ	119	GLU
45	DZ	121	HIS
45	DZ	131	ARG
45	DZ	146	ILE
45	DZ	153	SER
45	DZ	154	ASP
45	DZ	155	LEU
45	DZ	161	VAL
46	D0	20	ARG
46	D0	24	LYS
46	D0	49	LYS
47	D1	3	LYS
47	D1	4	VAL
47	D1	32	LYS
47	D1	40	ARG
47	D1	59	THR
47	D1	76	ARG
47	D1	89	GLU
47	D1	95	LEU
47	D1	97	LEU
48	D2	19	VAL
48	D2	32	LEU
48	D2	64	LEU
48	D2	70	GLN
49	D3	8	LEU
49	D3	23	LEU
49	D3	24	LYS
49	D3	31	LEU
49	D3	44	ARG
49	D3	54	VAL
50	D4	5	ILE
50	D4	33	VAL
50	D4	34	GLU
50	D4	50	VAL
50	D4	56	VAL
50	D4	58	ARG
50	D4	68	ARG
51	D5	6	VAL

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Mol	Chain	Res	Type
51	D5	29	THR
51	D5	40	LYS
51	D5	48	GLU
51	D5	59	GLU
52	D6	9	LEU
52	D6	14	THR
52	D6	28	ARG
52	D6	48	VAL
52	D6	52	VAL
53	D7	1	MET
53	D7	43	THR
54	D8	14	VAL
54	D8	23	VAL
54	D8	26	LYS
54	D8	30	ARG
54	D8	32	LEU
54	D8	37	SER
54	D8	41	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (158) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	16	HIS
2	AB	19	HIS
2	AB	40	HIS
2	AB	94	ASN
2	AB	135	GLN
3	AC	6	HIS
3	AC	28	GLN
3	AC	98	ASN
3	AC	102	ASN
3	AC	104	GLN
3	AC	136	GLN
3	AC	162	GLN
3	AC	181	ASN
4	AD	45	GLN
4	AD	77	ASN
5	AE	38	GLN
5	AE	56	GLN
5	AE	65	ASN
5	AE	141	GLN
6	AF	100	ASN

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Mol	Chain	Res	Type
7	AG	28	ASN
7	AG	51	GLN
7	AG	64	GLN
7	AG	97	GLN
7	AG	106	GLN
8	AH	78	GLN
9	AI	23	ASN
10	AJ	56	HIS
11	AK	99	GLN
11	AK	104	GLN
11	AK	116	HIS
12	AL	78	GLN
12	AL	99	HIS
15	AO	28	GLN
17	AQ	93	GLN
19	AS	23	ASN
19	AS	65	ASN
19	AS	69	HIS
19	AS	83	HIS
20	AT	42	GLN
20	AT	45	GLN
20	AT	75	ASN
27	BD	87	ASN
27	BD	112	GLN
27	BD	164	GLN
27	BD	253	GLN
28	BE	85	ASN
28	BE	143	ASN
29	BF	8	GLN
29	BF	69	HIS
29	BF	169	ASN
29	BF	203	GLN
30	BG	26	GLN
32	BI	43	ASN
32	BI	74	ASN
35	BP	38	GLN
35	BP	70	GLN
36	BQ	12	GLN
36	BQ	45	GLN
36	BQ	57	HIS
36	BQ	123	HIS
37	BR	31	HIS

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Mol	Chain	Res	Type
37	BR	71	GLN
39	BT	43	GLN
39	BT	84	GLN
39	BT	123	GLN
40	BU	94	ASN
40	BU	104	GLN
42	BW	60	ASN
43	BX	31	HIS
43	BX	82	GLN
44	BY	6	HIS
44	BY	43	ASN
45	BZ	55	HIS
45	BZ	118	GLN
49	B3	32	GLN
50	B4	46	GLN
54	B8	35	GLN
55	B9	36	GLN
2	CB	135	GLN
2	CB	224	GLN
3	CC	6	HIS
3	CC	28	GLN
3	CC	37	GLN
3	CC	69	HIS
3	CC	104	GLN
3	CC	108	ASN
3	CC	123	GLN
3	CC	136	GLN
3	CC	181	ASN
4	CD	45	GLN
4	CD	77	ASN
4	CD	125	HIS
4	CD	160	GLN
4	CD	201	GLN
5	CE	38	GLN
5	CE	56	GLN
5	CE	73	ASN
5	CE	141	GLN
6	CF	64	GLN
6	CF	73	ASN
6	CF	94	GLN
6	CF	100	ASN
7	CG	28	ASN

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Mol	Chain	Res	Type
7	CG	51	GLN
7	CG	97	GLN
7	CG	148	ASN
9	CI	23	ASN
9	CI	31	GLN
9	CI	58	HIS
9	CI	124	GLN
10	CJ	13	HIS
10	CJ	21	GLN
11	CK	93	GLN
11	CK	104	GLN
11	CK	116	HIS
12	CL	78	GLN
12	CL	99	HIS
13	CM	40	ASN
15	CO	28	GLN
19	CS	23	ASN
19	CS	65	ASN
19	CS	69	HIS
19	CS	83	HIS
20	CT	16	HIS
27	DD	164	GLN
27	DD	253	GLN
28	DE	85	ASN
29	DF	40	GLN
29	DF	69	HIS
29	DF	169	ASN
29	DF	203	GLN
30	DG	26	GLN
30	DG	40	ASN
30	DG	41	GLN
30	DG	132	ASN
32	DI	105	HIS
33	DN	94	HIS
33	DN	101	HIS
33	DN	133	GLN
34	DO	89	ASN
35	DP	38	GLN
36	DQ	45	GLN
37	DR	13	HIS
37	DR	71	GLN
38	DS	68	GLN

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Mol	Chain	Res	Type
39	DT	123	GLN
41	DV	64	HIS
41	DV	89	GLN
42	DW	60	ASN
43	DX	31	HIS
43	DX	82	GLN
44	DY	92	ASN
45	DZ	34	ASN
45	DZ	55	HIS
49	D3	32	GLN
50	D4	60	GLN
55	D9	36	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	310 (20%)	21 (1%)
1	CA	1501/1521 (98%)	312 (20%)	23 (1%)
22	AV	12/24 (50%)	3 (25%)	0
22	CV	12/24 (50%)	3 (25%)	0
23	AW	72/76 (94%)	30 (41%)	2 (2%)
23	AY	72/76 (94%)	34 (47%)	1 (1%)
23	CW	69/76 (90%)	30 (43%)	3 (4%)
23	CY	70/76 (92%)	29 (41%)	0
24	AX	75/77 (97%)	18 (24%)	1 (1%)
24	CX	75/77 (97%)	19 (25%)	0
25	BA	2811/2915 (96%)	434 (15%)	27 (0%)
25	DA	2791/2915 (95%)	502 (17%)	33 (1%)
26	BB	119/121 (98%)	13 (10%)	0
26	DB	119/121 (98%)	17 (14%)	0
All	All	9293/9620 (96%)	1754 (18%)	111 (1%)

All (1754) 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

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Mol	Chain	Res	Type
1	AA	48	C
1	AA	51	A
1	AA	54	C
1	AA	61	G
1	AA	65	U
1	AA	70	G
1	AA	73	G
1	AA	78	G
1	AA	79	G
1	AA	96	U
1	AA	97	G
1	AA	98	G
1	AA	111	G
1	AA	115	G
1	AA	116	A
1	AA	121	C
1	AA	129(A)	G
1	AA	131	C
1	AA	145	G
1	AA	146	G
1	AA	155	C
1	AA	156	G
1	AA	163	C
1	AA	166	G
1	AA	171	A
1	AA	174	C
1	AA	180	U
1	AA	182	U
1	AA	189(C)	C
1	AA	189(E)	U
1	AA	189(F)	U
1	AA	189(I)	G
1	AA	189(J)	G
1	AA	189(K)	U
1	AA	190	U
1	AA	194	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

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Mol	Chain	Res	Type
1	AA	216	G
1	AA	217	C
1	AA	220	G
1	AA	247	G
1	AA	251	G
1	AA	253	U
1	AA	258	G
1	AA	262	A
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	329	A
1	AA	332	G
1	AA	341	C
1	AA	346	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	382	A
1	AA	384	G
1	AA	388	G
1	AA	397	A
1	AA	398	C
1	AA	406	G
1	AA	412	A
1	AA	413	G
1	AA	424	G
1	AA	429	U
1	AA	430	A
1	AA	439	A
1	AA	442	C
1	AA	443	C
1	AA	449	C

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Mol	Chain	Res	Type
1	AA	452	A
1	AA	455	C
1	AA	457	C
1	AA	461	A
1	AA	470	C
1	AA	475	G
1	AA	477	A
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	513	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	560	U
1	AA	561	U
1	AA	572	A
1	AA	573	A
1	AA	576	G
1	AA	577	G
1	AA	581	G
1	AA	590	C
1	AA	596	C
1	AA	619	U
1	AA	630	G
1	AA	653	A
1	AA	657	G
1	AA	660	G
1	AA	665	A
1	AA	671	G
1	AA	673	G

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Mol	Chain	Res	Type
1	AA	687	A
1	AA	688	G
1	AA	693	G
1	AA	695	A
1	AA	703	G
1	AA	723	U
1	AA	731	G
1	AA	733	A
1	AA	749	C
1	AA	752	G
1	AA	755	G
1	AA	773	G
1	AA	774	G
1	AA	777	A
1	AA	792	A
1	AA	793	U
1	AA	794	A
1	AA	815	A
1	AA	817	C
1	AA	821	G
1	AA	827	U
1	AA	828	A
1	AA	829	G
1	AA	833	U
1	AA	834	C
1	AA	840	C
1	AA	841	U
1	AA	848	C
1	AA	851	G
1	AA	853	G
1	AA	859	A
1	AA	874	G
1	AA	902	G
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	934	C
1	AA	960	U
1	AA	961	U
1	AA	968	A
1	AA	969	A
1	AA	971	G

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Mol	Chain	Res	Type
1	AA	972	C
1	AA	974	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	991	U
1	AA	992	U
1	AA	993	G
1	AA	996	A
1	AA	997	U
1	AA	998	G
1	AA	1003	G
1	AA	1004	A
1	AA	1005	A
1	AA	1006	C
1	AA	1008	C
1	AA	1014	A
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(A)	G
1	AA	1030(C)	G
1	AA	1030(D)	A
1	AA	1031	G
1	AA	1033	G
1	AA	1035	A
1	AA	1036	G
1	AA	1037	C
1	AA	1039	C
1	AA	1054	C
1	AA	1060	C
1	AA	1065	U
1	AA	1066	C
1	AA	1068	G
1	AA	1076	C

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Mol	Chain	Res	Type
1	AA	1081	G
1	AA	1088	G
1	AA	1089	G
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1104	G
1	AA	1108	G
1	AA	1110	A
1	AA	1122	U
1	AA	1123	A
1	AA	1124	G
1	AA	1125	U
1	AA	1126	U
1	AA	1130	A
1	AA	1132	C
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	1145	C
1	AA	1146	A
1	AA	1152	A
1	AA	1154	G
1	AA	1157	A
1	AA	1158	C
1	AA	1159	U
1	AA	1175	G
1	AA	1183	A
1	AA	1184	G
1	AA	1191	A
1	AA	1196	U
1	AA	1197	G
1	AA	1201	A
1	AA	1202	G
1	AA	1212	U
1	AA	1213	A
1	AA	1227	A
1	AA	1228	C

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Mol	Chain	Res	Type
1	AA	1236	A
1	AA	1238	A
1	AA	1250	A
1	AA	1255	G
1	AA	1256	A
1	AA	1257	U
1	AA	1258	G
1	AA	1260	C
1	AA	1263	C
1	AA	1270	C
1	AA	1272	G
1	AA	1273	G
1	AA	1278	U
1	AA	1279	A
1	AA	1280	A
1	AA	1281	U
1	AA	1286	A
1	AA	1287	A
1	AA	1297	C
1	AA	1299	A
1	AA	1300	G
1	AA	1302	U
1	AA	1317	C
1	AA	1319	A
1	AA	1320	C
1	AA	1338	G
1	AA	1340	A
1	AA	1346	A
1	AA	1347	G
1	AA	1358	U
1	AA	1363	C
1	AA	1370	G
1	AA	1397	C
1	AA	1419	G
1	AA	1442	G
1	AA	1442(A)	G
1	AA	1442(B)	A
1	AA	1446	U
1	AA	1447	A
1	AA	1452	C
1	AA	1456	G
1	AA	1492	A

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Mol	Chain	Res	Type
1	AA	1493	A
1	AA	1503	A
1	AA	1504	G
1	AA	1506	U
1	AA	1517	G
1	AA	1520	G
1	AA	1529	G
1	AA	1530	G
1	AA	1531	A
1	AA	1532	U
22	AV	13	A
22	AV	14	A
22	AV	24	A
23	AW	2	C
23	AW	3	C
23	AW	6	G
23	AW	8	4SU
23	AW	11	C
23	AW	13	C
23	AW	14	A
23	AW	19	G
23	AW	20	U
23	AW	21	A
23	AW	22	G
23	AW	23	A
23	AW	26	A
23	AW	34	G
23	AW	42	C
23	AW	44	G
23	AW	45	U
23	AW	46	7MG
23	AW	47	U
23	AW	48	C
23	AW	49	C
23	AW	61	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
23	AW	75	C

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Mol	Chain	Res	Type
23	AW	76	A
24	AX	3	C
24	AX	9	G
24	AX	18	G
24	AX	19	G
24	AX	20	U
24	AX	21	A
24	AX	31	G
24	AX	42	G
24	AX	47	U
24	AX	48	C
24	AX	60	U
24	AX	61	C
24	AX	62	C
24	AX	65	C
24	AX	67	C
24	AX	68	C
24	AX	70	G
24	AX	76	A
23	AY	2	C
23	AY	3	C
23	AY	5	G
23	AY	9	A
23	AY	13	C
23	AY	14	A
23	AY	15	G
23	AY	19	G
23	AY	20	U
23	AY	21	A
23	AY	22	G
23	AY	30	G
23	AY	31	A
23	AY	33	U
23	AY	34	G
23	AY	35	A
23	AY	37	MIA
23	AY	39	PSU
23	AY	44	G
23	AY	45	U
23	AY	46	7MG
23	AY	47	U
23	AY	48	C

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Mol	Chain	Res	Type
23	AY	49	C
23	AY	51	U
23	AY	53	G
23	AY	56	C
23	AY	57	G
23	AY	58	A
23	AY	62	C
23	AY	65	G
23	AY	67	C
23	AY	70	G
23	AY	73	A
25	BA	11	G
25	BA	12	U
25	BA	13	A
25	BA	34	C
25	BA	45	C
25	BA	54	G
25	BA	60	G
25	BA	63	A
25	BA	70	A
25	BA	71	U
25	BA	73	A
25	BA	74	G
25	BA	82	G
25	BA	83	A
25	BA	94	G
25	BA	95	G
25	BA	116	A
25	BA	117	A
25	BA	118	U
25	BA	170	A
25	BA	185	A
25	BA	188	A
25	BA	194	G
25	BA	203	G
25	BA	204	G
25	BA	205	A
25	BA	210	A
25	BA	211	A
25	BA	212	A
25	BA	218	A
25	BA	219	U

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Mol	Chain	Res	Type
25	BA	222	A
25	BA	237	G
25	BA	256	C
25	BA	265	U
25	BA	269	G
25	BA	271	U
25	BA	272	U
25	BA	273	G
25	BA	274	U
25	BA	275	C
25	BA	276	C
25	BA	279	G
25	BA	289	G
25	BA	294	C
25	BA	303	C
25	BA	307	A
25	BA	335	A
25	BA	353	G
25	BA	354	A
25	BA	376	G
25	BA	387	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	433	G
25	BA	438	G
25	BA	448	U
25	BA	455	A
25	BA	469	A
25	BA	470	C
25	BA	474	U
25	BA	477	C
25	BA	481	C
25	BA	482	C
25	BA	496	A
25	BA	497	A
25	BA	507	G
25	BA	526	A
25	BA	529	U

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Mol	Chain	Res	Type
25	BA	530	A
25	BA	534	C
25	BA	553	A
25	BA	555	G
25	BA	556	C
25	BA	557	A
25	BA	558	G
25	BA	569	G
25	BA	573	G
25	BA	585	U
25	BA	586	G
25	BA	596	G
25	BA	598	A
25	BA	609	A
25	BA	626	A
25	BA	627	G
25	BA	630	U
25	BA	638	U
25	BA	639	G
25	BA	640	A
25	BA	641	G
25	BA	652	A
25	BA	662	A
25	BA	670	C
25	BA	671	A
25	BA	678	A
25	BA	693	G
25	BA	694	G
25	BA	697	C
25	BA	698	G
25	BA	716	G
25	BA	724	A
25	BA	733	G
25	BA	777	C
25	BA	795	G
25	BA	796	C
25	BA	811	A
25	BA	812	G
25	BA	822	G
25	BA	823	G
25	BA	829	A
25	BA	830	A

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Mol	Chain	Res	Type
25	BA	831	A
25	BA	832	G
25	BA	836	A
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	908	A
25	BA	913	A
25	BA	924	U
25	BA	926	G
25	BA	927	G
25	BA	929	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	938	G
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	998	A
25	BA	1004	A
25	BA	1006	C
25	BA	1019	G
25	BA	1020	C
25	BA	1029	A

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Mol	Chain	Res	Type
25	BA	1042	A
25	BA	1051	C
25	BA	1058	U
25	BA	1059	C
25	BA	1068	G
25	BA	1072	U
25	BA	1079	U
25	BA	1084	C
25	BA	1087	C
25	BA	1088	G
25	BA	1091	A
25	BA	1092	A
25	BA	1093	G
25	BA	1097	G
25	BA	1153	G
25	BA	1154	U
25	BA	1156	G
25	BA	1158	G
25	BA	1174	A
25	BA	1180	C
25	BA	1181	G
25	BA	1184	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
25	BA	1250	U
25	BA	1255	A
25	BA	1256	U
25	BA	1263	C
25	BA	1265	A
25	BA	1299	A
25	BA	1302	G
25	BA	1317	G
25	BA	1318	A
25	BA	1346	U
25	BA	1347	A
25	BA	1349	G
25	BA	1360	C

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Mol	Chain	Res	Type
25	BA	1365	G
25	BA	1398	U
25	BA	1405	A
25	BA	1406	A
25	BA	1411	A
25	BA	1416	C
25	BA	1426	G
25	BA	1430	A
25	BA	1431	G
25	BA	1462	G
25	BA	1463	C
25	BA	1466	U
25	BA	1467	G
25	BA	1474	C
25	BA	1483	C
25	BA	1491	A
25	BA	1496	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	1525	G
25	BA	1529	G
25	BA	1539	C
25	BA	1540	A
25	BA	1553	A
25	BA	1554	A
25	BA	1555	C
25	BA	1556	A
25	BA	1578	C
25	BA	1589	A
25	BA	1605	A
25	BA	1613	A
25	BA	1616	A
25	BA	1625	U
25	BA	1628	G
25	BA	1629	C
25	BA	1631	C
25	BA	1632	A
25	BA	1654	A

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Mol	Chain	Res	Type
25	BA	1655	A
25	BA	1656	A
25	BA	1695	C
25	BA	1701	A
25	BA	1708	G
25	BA	1721	G
25	BA	1743	G
25	BA	1747	A
25	BA	1748	A
25	BA	1766	G
25	BA	1767	A
25	BA	1787	G
25	BA	1794	G
25	BA	1795	G
25	BA	1804	A
25	BA	1811	A
25	BA	1813	C
25	BA	1822	A
25	BA	1831	C
25	BA	1847	G
25	BA	1848	G
25	BA	1860	A
25	BA	1878	A
25	BA	1879	A
25	BA	1892	G
25	BA	1899	A
25	BA	1900	G
25	BA	1911	A
25	BA	1922	A
25	BA	1928	G
25	BA	1937	U
25	BA	1941	A
25	BA	1949	A
25	BA	1951	G
25	BA	1952	G
25	BA	1953	U
25	BA	1959	A
25	BA	1960	A
25	BA	1977	U
25	BA	1985	U
25	BA	1987	C
25	BA	1989	C

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Mol	Chain	Res	Type
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	2061	C
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	2118	U
25	BA	2120	U
25	BA	2132	G
25	BA	2135	U
25	BA	2138	G
25	BA	2141	A
25	BA	2142	G
25	BA	2144	U
25	BA	2147	G
25	BA	2149	G
25	BA	2151	C
25	BA	2153	G
25	BA	2154	U
25	BA	2155	G
25	BA	2156	A
25	BA	2157	A
25	BA	2158	C
25	BA	2164	C
25	BA	2165	C
25	BA	2168	C
25	BA	2170	G
25	BA	2175	G
25	BA	2179	G

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Mol	Chain	Res	Type
25	BA	2180	A
25	BA	2181	G
25	BA	2182	G
25	BA	2188	G
25	BA	2189	U
25	BA	2190	G
25	BA	2193	A
25	BA	2194	U
25	BA	2195	A
25	BA	2196	C
25	BA	2197	C
25	BA	2200	C
25	BA	2203	G
25	BA	2204	G
25	BA	2206	G
25	BA	2207	C
25	BA	2208	G
25	BA	2210	C
25	BA	2212	G
25	BA	2214	G
25	BA	2220	A
25	BA	2221	A
25	BA	2227	G
25	BA	2228	G
25	BA	2229	A
25	BA	2230	U
25	BA	2237	A
25	BA	2250	G
25	BA	2251	G
25	BA	2280	A
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	2332	A
25	BA	2337	G
25	BA	2346	G
25	BA	2348	A
25	BA	2355	C
25	BA	2359	C

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Mol	Chain	Res	Type
25	BA	2366	G
25	BA	2373	A
25	BA	2395	G
25	BA	2397	C
25	BA	2418	U
25	BA	2419	G
25	BA	2435	U
25	BA	2436	C
25	BA	2437	A
25	BA	2441	G
25	BA	2442	A
25	BA	2446	A
25	BA	2447	A
25	BA	2451	A
25	BA	2453	C
25	BA	2460	A
25	BA	2461	U
25	BA	2480	G
25	BA	2481	A
25	BA	2486	C
25	BA	2488	A
25	BA	2490	A
25	BA	2514	G
25	BA	2517	G
25	BA	2530	A
25	BA	2541	G
25	BA	2561	G
25	BA	2566	U
25	BA	2578	A
25	BA	2579	G
25	BA	2585	C
25	BA	2590	G
25	BA	2614	A
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	2666	A
25	BA	2682	A
25	BA	2701	U

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Mol	Chain	Res	Type
25	BA	2702	C
25	BA	2703	C
25	BA	2715	C
25	BA	2725	A
25	BA	2726	A
25	BA	2727	G
25	BA	2739	U
25	BA	2746	A
25	BA	2771	A
25	BA	2777	A
25	BA	2778	A
25	BA	2782	C
25	BA	2791	A
25	BA	2803	A
25	BA	2813	G
25	BA	2828	G
25	BA	2830	A
25	BA	2831	A
25	BA	2845	A
25	BA	2846	U
25	BA	2882	G
25	BA	2890	C
25	BA	2901	A
25	BA	2902	G
25	BA	2903	G
26	BB	2	C
26	BB	7	G
26	BB	15	A
26	BB	20	C
26	BB	25	A
26	BB	42	C
26	BB	56	G
26	BB	73	A
26	BB	75	G
26	BB	85	G
26	BB	98	G
26	BB	106	G
26	BB	110	G
1	CA	5	U
1	CA	6	G
1	CA	9	G
1	CA	22	G

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Mol	Chain	Res	Type
1	CA	32	A
1	CA	39	G
1	CA	47	C
1	CA	48	C
1	CA	51	A
1	CA	54	C
1	CA	65	U
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	96	U
1	CA	97	G
1	CA	98	G
1	CA	111	G
1	CA	112	G
1	CA	115	G
1	CA	116	A
1	CA	121	C
1	CA	129(A)	G
1	CA	131	C
1	CA	143	A
1	CA	155	C
1	CA	156	G
1	CA	163	C
1	CA	166	G
1	CA	171	A
1	CA	174	C
1	CA	180	U
1	CA	182	U
1	CA	189(C)	C
1	CA	189(E)	U
1	CA	189(F)	U
1	CA	189(I)	G
1	CA	189(K)	U
1	CA	190	U
1	CA	194	C
1	CA	195	A
1	CA	197	A

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Mol	Chain	Res	Type
1	CA	201	C
1	CA	202	U
1	CA	203	U
1	CA	204	U
1	CA	216	G
1	CA	220	G
1	CA	247	G
1	CA	251	G
1	CA	253	U
1	CA	258	G
1	CA	262	A
1	CA	266	G
1	CA	267	C
1	CA	289	G
1	CA	301	G
1	CA	321	A
1	CA	328	C
1	CA	329	A
1	CA	332	G
1	CA	341	C
1	CA	343	U
1	CA	344	A
1	CA	346	G
1	CA	350	G
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	382	A
1	CA	384	G
1	CA	388	G
1	CA	397	A
1	CA	398	C
1	CA	406	G
1	CA	412	A
1	CA	413	G
1	CA	424	G
1	CA	429	U
1	CA	430	A

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Mol	Chain	Res	Type
1	CA	439	A
1	CA	442	C
1	CA	443	C
1	CA	449	C
1	CA	452	A
1	CA	455	C
1	CA	457	C
1	CA	461	A
1	CA	470	C
1	CA	475	G
1	CA	477	A
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	513	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	560	U
1	CA	561	U
1	CA	572	A
1	CA	573	A
1	CA	576	G
1	CA	577	G
1	CA	581	G
1	CA	590	C
1	CA	596	C
1	CA	619	U
1	CA	630	G
1	CA	653	A
1	CA	657	G
1	CA	660	G

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Mol	Chain	Res	Type
1	CA	665	A
1	CA	671	G
1	CA	673	G
1	CA	687	A
1	CA	688	G
1	CA	693	G
1	CA	695	A
1	CA	702	A
1	CA	723	U
1	CA	731	G
1	CA	749	C
1	CA	752	G
1	CA	755	G
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	817	C
1	CA	821	G
1	CA	827	U
1	CA	828	A
1	CA	829	G
1	CA	833	U
1	CA	834	C
1	CA	840	C
1	CA	841	U
1	CA	848	C
1	CA	851	G
1	CA	853	G
1	CA	859	A
1	CA	874	G
1	CA	902	G
1	CA	914	A
1	CA	926	G
1	CA	927	G
1	CA	932	C
1	CA	934	C
1	CA	960	U
1	CA	961	U

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Mol	Chain	Res	Type
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	991	U
1	CA	992	U
1	CA	993	G
1	CA	996	A
1	CA	997	U
1	CA	998	G
1	CA	1002	G
1	CA	1003	G
1	CA	1004	A
1	CA	1005	A
1	CA	1006	C
1	CA	1014	A
1	CA	1020	U
1	CA	1021	G
1	CA	1022	G
1	CA	1023	G
1	CA	1024	G
1	CA	1025	U
1	CA	1026	G
1	CA	1027	C
1	CA	1028	C
1	CA	1029	C
1	CA	1030(A)	G
1	CA	1030(C)	G
1	CA	1030(D)	A
1	CA	1031	G
1	CA	1033	G
1	CA	1035	A
1	CA	1037	C
1	CA	1039	C
1	CA	1041	A
1	CA	1054	C
1	CA	1060	C
1	CA	1065	U

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Mol	Chain	Res	Type
1	CA	1066	C
1	CA	1068	G
1	CA	1076	C
1	CA	1081	G
1	CA	1088	G
1	CA	1089	G
1	CA	1094	G
1	CA	1095	U
1	CA	1101	A
1	CA	1104	G
1	CA	1108	G
1	CA	1110	A
1	CA	1117	G
1	CA	1122	U
1	CA	1125	U
1	CA	1126	U
1	CA	1129	C
1	CA	1130	A
1	CA	1132	C
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	1145	C
1	CA	1146	A
1	CA	1152	A
1	CA	1154	G
1	CA	1157	A
1	CA	1158	C
1	CA	1159	U
1	CA	1175	G
1	CA	1182	G
1	CA	1183	A
1	CA	1184	G
1	CA	1191	A
1	CA	1196	U
1	CA	1197	G
1	CA	1201	A
1	CA	1202	G

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Mol	Chain	Res	Type
1	CA	1212	U
1	CA	1213	A
1	CA	1227	A
1	CA	1228	C
1	CA	1236	A
1	CA	1238	A
1	CA	1250	A
1	CA	1256	A
1	CA	1257	U
1	CA	1258	G
1	CA	1260	C
1	CA	1263	C
1	CA	1270	C
1	CA	1272	G
1	CA	1273	G
1	CA	1278	U
1	CA	1279	A
1	CA	1280	A
1	CA	1281	U
1	CA	1286	A
1	CA	1287	A
1	CA	1297	C
1	CA	1299	A
1	CA	1300	G
1	CA	1305	G
1	CA	1317	C
1	CA	1319	A
1	CA	1320	C
1	CA	1338	G
1	CA	1340	A
1	CA	1346	A
1	CA	1347	G
1	CA	1353	G
1	CA	1358	U
1	CA	1363	C
1	CA	1370	G
1	CA	1397	C
1	CA	1419	G
1	CA	1442	G
1	CA	1442(A)	G
1	CA	1442(B)	A
1	CA	1446	U

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Mol	Chain	Res	Type
1	CA	1447	A
1	CA	1452	C
1	CA	1456	G
1	CA	1492	A
1	CA	1493	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
22	CV	14	A
22	CV	24	A
23	CW	3	C
23	CW	5	G
23	CW	6	G
23	CW	7	A
23	CW	8	4SU
23	CW	9	A
23	CW	12	U
23	CW	13	C
23	CW	14	A
23	CW	19	G
23	CW	22	G
23	CW	25	C
23	CW	27	G
23	CW	28	G
23	CW	44	G
23	CW	46	7MG
23	CW	47	U
23	CW	48	C
23	CW	59	U
23	CW	61	C
23	CW	62	C
23	CW	63	G
23	CW	64	A
23	CW	66	U
23	CW	67	C

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Mol	Chain	Res	Type
23	CW	70	G
23	CW	73	A
23	CW	74	C
23	CW	75	C
23	CW	76	A
24	CX	3	C
24	CX	9	G
24	CX	13	C
24	CX	18	G
24	CX	19	G
24	CX	20	U
24	CX	21	A
24	CX	31	G
24	CX	42	G
24	CX	47	U
24	CX	48	C
24	CX	60	U
24	CX	61	C
24	CX	62	C
24	CX	65	C
24	CX	67	C
24	CX	68	C
24	CX	70	G
24	CX	76	A
23	CY	2	C
23	CY	3	C
23	CY	8	4SU
23	CY	13	C
23	CY	14	A
23	CY	15	G
23	CY	19	G
23	CY	22	G
23	CY	30	G
23	CY	31	A
23	CY	33	U
23	CY	34	G
23	CY	35	A
23	CY	37	MIA
23	CY	39	PSU
23	CY	45	U
23	CY	46	7MG
23	CY	47	U

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Mol	Chain	Res	Type
23	CY	49	C
23	CY	51	U
23	CY	52	G
23	CY	56	C
23	CY	57	G
23	CY	58	A
23	CY	62	C
23	CY	65	G
23	CY	67	C
23	CY	70	G
23	CY	73	A
25	DA	11	G
25	DA	12	U
25	DA	15	G
25	DA	34	C
25	DA	35	G
25	DA	45	C
25	DA	59	U
25	DA	71	A
25	DA	74	A
25	DA	75	G
25	DA	84	A
25	DA	95	G
25	DA	118	A
25	DA	119	A
25	DA	120	U
25	DA	141	A
25	DA	154(A)	C
25	DA	157	U
25	DA	173	G
25	DA	181	A
25	DA	182	A
25	DA	196	A
25	DA	199	A
25	DA	205	G
25	DA	213	A
25	DA	214	G
25	DA	215	G
25	DA	216	A
25	DA	221	A
25	DA	222	A
25	DA	229	A

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Mol	Chain	Res	Type
25	DA	230	U
25	DA	233	A
25	DA	248	G
25	DA	269	U
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	271(S)	G
25	DA	272(A)	U
25	DA	272(B)	G
25	DA	274	G
25	DA	277	C
25	DA	278	A
25	DA	283	A
25	DA	292	C
25	DA	311	A
25	DA	312	G
25	DA	327	G
25	DA	329	G
25	DA	330	A
25	DA	342	G
25	DA	352	G
25	DA	363	G
25	DA	380	U
25	DA	386	G
25	DA	396	G
25	DA	405	U
25	DA	411	G
25	DA	412	A
25	DA	418	G
25	DA	422	A
25	DA	428	A
25	DA	442	G
25	DA	443	A
25	DA	444	C
25	DA	455	C
25	DA	457	A
25	DA	481	G
25	DA	494	G

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Mol	Chain	Res	Type
25	DA	504	U
25	DA	505	A
25	DA	507	A
25	DA	508	G
25	DA	509	C
25	DA	530	G
25	DA	531	C
25	DA	532	A
25	DA	533	G
25	DA	545	G
25	DA	555	U
25	DA	556	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	599	G
25	DA	603	A
25	DA	604	G
25	DA	607	U
25	DA	614(B)	G
25	DA	615	G
25	DA	627	A
25	DA	637	A
25	DA	645	C
25	DA	652(B)	A
25	DA	652(C)	G
25	DA	653	A
25	DA	655	A
25	DA	669	G
25	DA	686	G
25	DA	701	G
25	DA	730	C
25	DA	752	A
25	DA	753	C
25	DA	774	A
25	DA	775	G
25	DA	776	G
25	DA	782	A
25	DA	784	A

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Mol	Chain	Res	Type
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	849	A
25	DA	857	C
25	DA	859	G
25	DA	866	A
25	DA	874	G
25	DA	878	A
25	DA	879	G
25	DA	882	G
25	DA	884	C
25	DA	886	C
25	DA	887	A
25	DA	888	C
25	DA	889	C
25	DA	890	A
25	DA	893	C
25	DA	895	U
25	DA	896	A
25	DA	897	C
25	DA	900	A
25	DA	901	A
25	DA	903	C
25	DA	907	U
25	DA	910	A
25	DA	915	C
25	DA	917	A
25	DA	932	G
25	DA	938	G
25	DA	941	A
25	DA	945	A
25	DA	946	G
25	DA	953	A
25	DA	958	U
25	DA	959	A
25	DA	961	C

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Mol	Chain	Res	Type
25	DA	974	G
25	DA	975	C
25	DA	983	A
25	DA	996	A
25	DA	1003	G
25	DA	1006	C
25	DA	1012	U
25	DA	1013	C
25	DA	1017	G
25	DA	1022	G
25	DA	1025	G
25	DA	1026	U
25	DA	1027	A
25	DA	1033	U
25	DA	1038	C
25	DA	1039	G
25	DA	1040	C
25	DA	1042	G
25	DA	1043	C
25	DA	1113	U
25	DA	1116	C
25	DA	1128	A
25	DA	1129	A
25	DA	1130	U
25	DA	1135	C
25	DA	1136	G
25	DA	1138	G
25	DA	1139	G
25	DA	1142	U
25	DA	1143	A
25	DA	1144	G
25	DA	1168	G
25	DA	1170	G
25	DA	1171	G
25	DA	1188	U
25	DA	1206	G
25	DA	1211	U
25	DA	1219	G
25	DA	1220	A
25	DA	1229	G
25	DA	1237	A
25	DA	1241	A

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Mol	Chain	Res	Type
25	DA	1244	G
25	DA	1248	G
25	DA	1253	A
25	DA	1256	G
25	DA	1271	G
25	DA	1272	A
25	DA	1284	A
25	DA	1286	A
25	DA	1287	A
25	DA	1300	U
25	DA	1301	A
25	DA	1303	G
25	DA	1305	C
25	DA	1314	C
25	DA	1345	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	1408	C
25	DA	1416	G
25	DA	1417	C
25	DA	1419	A
25	DA	1420	U
25	DA	1421	G
25	DA	1428	C
25	DA	1435	G
25	DA	1437	C
25	DA	1445	A
25	DA	1449	A
25	DA	1450	G
25	DA	1459	G
25	DA	1461	G
25	DA	1467	C
25	DA	1471	A
25	DA	1482	G
25	DA	1487	G
25	DA	1490	A
25	DA	1493	C

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Mol	Chain	Res	Type
25	DA	1494	A
25	DA	1496	A
25	DA	1497	U
25	DA	1505	C
25	DA	1508	A
25	DA	1509	C
25	DA	1509(A)	A
25	DA	1531	C
25	DA	1533	G
25	DA	1541	G
25	DA	1542	A
25	DA	1545	A
25	DA	1547	C
25	DA	1558	A
25	DA	1559	G
25	DA	1566	A
25	DA	1569	A
25	DA	1578	U
25	DA	1580	A
25	DA	1583	A
25	DA	1584	C
25	DA	1586	A
25	DA	1598	C
25	DA	1608	A
25	DA	1610	A
25	DA	1616	A
25	DA	1639	U
25	DA	1640	C
25	DA	1648	C
25	DA	1654	A
25	DA	1664	A
25	DA	1674	G
25	DA	1696	G
25	DA	1700	A
25	DA	1701	A
25	DA	1721	G
25	DA	1722	A
25	DA	1740	G
25	DA	1756	G
25	DA	1762	A
25	DA	1763	G
25	DA	1764	G

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Mol	Chain	Res	Type
25	DA	1773	A
25	DA	1780	A
25	DA	1782	C
25	DA	1791	A
25	DA	1797	C
25	DA	1800	C
25	DA	1801	G
25	DA	1816	G
25	DA	1829	A
25	DA	1835	G
25	DA	1847	A
25	DA	1848	A
25	DA	1877	A
25	DA	1878	G
25	DA	1896	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	1937	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	1995	U
25	DA	1996	C
25	DA	1997	G
25	DA	2005	A
25	DA	2023	G
25	DA	2031	A
25	DA	2032	G
25	DA	2033	A
25	DA	2043	C
25	DA	2046	G
25	DA	2055	C
25	DA	2056	G

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Mol	Chain	Res	Type
25	DA	2060	A
25	DA	2061	G
25	DA	2062	A
25	DA	2069	G
25	DA	2070	G
25	DA	2082	A
25	DA	2099	U
25	DA	2103	C
25	DA	2107	C
25	DA	2110	G
25	DA	2111	C
25	DA	2113	U
25	DA	2115	G
25	DA	2116	G
25	DA	2117	A
25	DA	2119	A
25	DA	2122	U
25	DA	2124	G
25	DA	2126	A
25	DA	2127	G
25	DA	2129	C
25	DA	2132	U
25	DA	2133	G
25	DA	2134	A
25	DA	2135	A
25	DA	2136	C
25	DA	2137	C
25	DA	2141	G
25	DA	2142	C
25	DA	2145	C
25	DA	2146	C
25	DA	2148	G
25	DA	2153	G
25	DA	2154	G
25	DA	2156	G
25	DA	2157	G
25	DA	2158	A
25	DA	2159	G
25	DA	2163	C
25	DA	2164	C
25	DA	2165	G
25	DA	2166	G

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Mol	Chain	Res	Type
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	2176	A
25	DA	2177	C
25	DA	2178	C
25	DA	2180	U
25	DA	2188	C
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	2268	A
25	DA	2272	U
25	DA	2275	C
25	DA	2279	G
25	DA	2283	C
25	DA	2287	A
25	DA	2289	G
25	DA	2302	G
25	DA	2303	G
25	DA	2305	A
25	DA	2308	G
25	DA	2312	U
25	DA	2318	G
25	DA	2319	G
25	DA	2320	A
25	DA	2325	G
25	DA	2327	A
25	DA	2334	G
25	DA	2336	A
25	DA	2343	C
25	DA	2347	C
25	DA	2350	C

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Mol	Chain	Res	Type
25	DA	2354	G
25	DA	2355	C
25	DA	2376	A
25	DA	2383	G
25	DA	2385	C
25	DA	2393	A
25	DA	2406	U
25	DA	2410	G
25	DA	2414	G
25	DA	2422	A
25	DA	2423	U
25	DA	2425	A
25	DA	2428	G
25	DA	2429	G
25	DA	2430	A
25	DA	2431	U
25	DA	2434	A
25	DA	2435	A
25	DA	2439	A
25	DA	2441	C
25	DA	2448	A
25	DA	2453	A
25	DA	2469	A
25	DA	2474	C
25	DA	2476	A
25	DA	2478	A
25	DA	2487	G
25	DA	2490	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	2529	G
25	DA	2554	U
25	DA	2556	C
25	DA	2566	A
25	DA	2567	G
25	DA	2573	C
25	DA	2602	A
25	DA	2611	U

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Mol	Chain	Res	Type
25	DA	2612	C
25	DA	2615	U
25	DA	2629	A
25	DA	2630	G
25	DA	2647	U
25	DA	2652	C
25	DA	2654	A
25	DA	2663	G
25	DA	2681	C
25	DA	2689	U
25	DA	2690	C
25	DA	2691	C
25	DA	2702	U
25	DA	2703	C
25	DA	2712(A)	A
25	DA	2713	A
25	DA	2726	U
25	DA	2733	A
25	DA	2744	G
25	DA	2748	A
25	DA	2751	G
25	DA	2752	C
25	DA	2754	U
25	DA	2757	A
25	DA	2758	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	2808	U
25	DA	2818	G
25	DA	2820	A
25	DA	2821	A
25	DA	2833	G
25	DA	2835	A
25	DA	2872	G

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Mol	Chain	Res	Type
25	DA	2873	A
25	DA	2876	G
25	DA	2879	C
25	DA	2880	C
25	DA	2892	A
25	DA	2894	G
25	DA	2895	U
25	DA	2896	C
25	DA	2897	U
26	DB	2	C
26	DB	5	C
26	DB	7	G
26	DB	8	U
26	DB	15	A
26	DB	20	C
26	DB	25	A
26	DB	42	C
26	DB	56	G
26	DB	73	A
26	DB	75	G
26	DB	85	G
26	DB	98	G
26	DB	106	G
26	DB	108	U
26	DB	110	G
26	DB	112	U

All (111) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	97	G
1	AA	115	G
1	AA	266	G
1	AA	429	U
1	AA	509	A
1	AA	532	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

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Mol	Chain	Res	Type
1	AA	1036	G
1	AA	1065	U
1	AA	1067	A
1	AA	1190	G
1	AA	1201	A
1	AA	1285	A
1	AA	1299	A
1	AA	1442	G
1	AA	1492	A
23	AW	13	C
23	AW	22	G
24	AX	47	U
23	AY	44	G
25	BA	70	A
25	BA	184	A
25	BA	185	A
25	BA	270	C
25	BA	271	U
25	BA	273	G
25	BA	288	U
25	BA	302	A
25	BA	732	A
25	BA	793	A
25	BA	795	G
25	BA	811	A
25	BA	1019	G
25	BA	1188	A
25	BA	1219	A
25	BA	1220	U
25	BA	1221	G
25	BA	1255	A
25	BA	1346	U
25	BA	1425	A
25	BA	1466	U
25	BA	1700	G
25	BA	1793	A
25	BA	2014	G
25	BA	2203	G
25	BA	2418	U
25	BA	2701	U
1	CA	65	U
1	CA	115	G

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Mol	Chain	Res	Type
1	CA	266	G
1	CA	429	U
1	CA	509	A
1	CA	532	A
1	CA	560	U
1	CA	687	A
1	CA	748	C
1	CA	913	A
1	CA	991	U
1	CA	992	U
1	CA	1064	G
1	CA	1065	U
1	CA	1067	A
1	CA	1128	C
1	CA	1183	A
1	CA	1190	G
1	CA	1201	A
1	CA	1212	U
1	CA	1256	A
1	CA	1442	G
1	CA	1492	A
23	CW	4	C
23	CW	13	C
23	CW	75	C
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	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	1026	U
25	DA	1210	A
25	DA	1240	U
25	DA	1300	U
25	DA	1420	U

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Mol	Chain	Res	Type
25	DA	1427	A
25	DA	1493	C
25	DA	1530	C
25	DA	1558	A
25	DA	1653	G
25	DA	1663	C
25	DA	1913	A
25	DA	1992	G
25	DA	2110	G
25	DA	2116	G
25	DA	2335	A
25	DA	2406	U
25	DA	2430	A
25	DA	2689	U
25	DA	2756	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	AW	8	23	18,21,22	1.81	6 (33%)	25,30,33	1.84	6 (24%)
23	PSU	AW	39	23	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
23	7MG	AW	46	23	23,26,27	1.34	3 (13%)	27,39,42	2.64	7 (25%)
23	MIA	CW	37	23	21,24,32	1.55	4 (19%)	30,35,47	2.15	8 (26%)
24	4SU	CX	8	24	18,21,22	1.97	4 (22%)	25,30,33	1.34	4 (16%)
24	4SU	AX	8	24	18,21,22	2.28	6 (33%)	25,30,33	1.74	7 (28%)
23	PSU	AY	55	23	18,21,22	1.29	2 (11%)	21,30,33	2.06	6 (28%)
23	PSU	CY	55	23	18,21,22	1.40	2 (11%)	21,30,33	2.11	3 (14%)
23	PSU	AW	55	23	18,21,22	1.41	2 (11%)	21,30,33	2.03	3 (14%)
23	MIA	AW	37	23	28,31,32	2.35	6 (21%)	38,44,47	2.67	13 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	5MU	CX	54	24	19,22,23	1.38	6 (31%)	27,32,35	2.11	8 (29%)
23	PSU	CW	32	23	18,21,22	1.37	4 (22%)	21,30,33	1.99	4 (19%)
24	PSU	CX	55	24	18,21,22	1.36	2 (11%)	21,30,33	1.99	6 (28%)
23	7MG	CW	46	23	23,26,27	1.33	4 (17%)	27,39,42	2.66	6 (22%)
23	PSU	AW	32	56,23	18,21,22	1.39	3 (16%)	21,30,33	1.83	4 (19%)
23	PSU	CW	39	23	18,21,22	1.41	2 (11%)	21,30,33	1.64	3 (14%)
23	4SU	CY	8	23	18,21,22	1.76	4 (22%)	25,30,33	2.27	4 (16%)
23	4SU	CW	8	56,23	18,21,22	1.69	5 (27%)	25,30,33	2.01	4 (16%)
23	5MU	CY	54	23	19,22,23	1.50	5 (26%)	27,32,35	1.95	9 (33%)
23	4SU	AY	8	23	18,21,22	1.80	7 (38%)	25,30,33	1.57	5 (20%)
23	5MU	AY	54	23	19,22,23	1.47	5 (26%)	27,32,35	1.63	6 (22%)
23	7MG	CY	46	23	23,26,27	1.39	4 (17%)	27,39,42	2.63	7 (25%)
24	5MU	AX	54	56,24	19,22,23	1.44	6 (31%)	27,32,35	2.05	6 (22%)
23	7MG	AY	46	23	23,26,27	1.39	4 (17%)	27,39,42	2.61	6 (22%)
23	5MU	AW	54	23	19,22,23	1.46	5 (26%)	27,32,35	1.71	5 (18%)
24	5MC	AX	32	24	19,22,23	1.68	3 (15%)	26,32,35	1.24	2 (7%)
23	5MU	CW	54	23	19,22,23	1.33	5 (26%)	27,32,35	1.98	7 (25%)
24	5MC	CX	32	24	19,22,23	1.63	3 (15%)	26,32,35	1.30	3 (11%)
23	MIA	AY	37	23	21,24,32	1.64	4 (19%)	30,35,47	1.94	7 (23%)
23	PSU	CW	55	23	18,21,22	1.41	2 (11%)	21,30,33	2.10	3 (14%)
24	PSU	AX	55	24	18,21,22	1.35	2 (11%)	21,30,33	1.98	4 (19%)
23	PSU	AY	39	23	18,21,22	1.50	3 (16%)	21,30,33	1.68	4 (19%)
23	PSU	CY	39	23	18,21,22	1.46	3 (16%)	21,30,33	1.96	3 (14%)
23	PSU	CY	32	23	18,21,22	1.37	2 (11%)	21,30,33	1.91	3 (14%)
23	PSU	AY	32	23	18,21,22	1.35	2 (11%)	21,30,33	2.06	4 (19%)
23	MIA	CY	37	23	21,24,32	1.64	3 (14%)	30,35,47	2.03	8 (26%)

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	AW	8	23	-	0/7/25/26	0/2/2/2
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	AW	46	23	-	3/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	MIA	CW	37	23	-	0/7/25/34	0/3/3/3
24	4SU	CX	8	24	-	0/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/7/25/26	0/2/2/2
23	PSU	AY	55	23	-	1/7/25/26	0/2/2/2
23	PSU	CY	55	23	-	3/7/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
23	MIA	AW	37	23	-	1/15/33/34	0/3/3/3
24	5MU	CX	54	24	-	0/7/25/26	0/2/2/2
23	PSU	CW	32	23	-	4/7/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2
23	7MG	CW	46	23	-	2/7/37/38	0/3/3/3
23	PSU	AW	32	56,23	-	0/7/25/26	0/2/2/2
23	PSU	CW	39	23	-	0/7/25/26	0/2/2/2
23	4SU	CY	8	23	-	2/7/25/26	0/2/2/2
23	4SU	CW	8	56,23	-	0/7/25/26	0/2/2/2
23	5MU	CY	54	23	-	1/7/25/26	0/2/2/2
23	4SU	AY	8	23	-	1/7/25/26	0/2/2/2
23	5MU	AY	54	23	-	0/7/25/26	0/2/2/2
23	7MG	CY	46	23	-	2/7/37/38	0/3/3/3
24	5MU	AX	54	56,24	-	0/7/25/26	0/2/2/2
23	7MG	AY	46	23	-	3/7/37/38	0/3/3/3
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/7/25/26	0/2/2/2
23	5MU	CW	54	23	-	0/7/25/26	0/2/2/2
24	5MC	CX	32	24	-	0/7/25/26	0/2/2/2
23	MIA	AY	37	23	-	1/7/25/34	0/3/3/3
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
23	PSU	AY	39	23	-	2/7/25/26	0/2/2/2
23	PSU	CY	39	23	-	2/7/25/26	0/2/2/2
23	PSU	CY	32	23	-	1/7/25/26	0/2/2/2
23	PSU	AY	32	23	-	0/7/25/26	0/2/2/2
23	MIA	CY	37	23	-	3/7/25/34	0/3/3/3

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C2-S10	-7.49	1.69	1.75
23	AW	37	MIA	C13-C14	6.84	1.52	1.32
24	AX	32	5MC	C5-C4	5.98	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	8	4SU	C4-N3	-5.87	1.31	1.37
24	CX	32	5MC	C5-C4	5.67	1.48	1.44
23	CY	37	MIA	C5-C4	5.25	1.48	1.39
23	AY	37	MIA	C5-C4	5.23	1.48	1.39
23	CY	8	4SU	C4-S4	-4.93	1.60	1.68
23	CW	37	MIA	C5-C4	4.75	1.47	1.39
23	AW	8	4SU	C4-S4	-4.67	1.60	1.68
23	AW	37	MIA	C5-C4	4.61	1.47	1.39
24	AX	8	4SU	C4-S4	-4.48	1.60	1.68
23	CW	8	4SU	C4-S4	-4.48	1.60	1.68
24	CX	8	4SU	C4-N3	-4.44	1.33	1.37
23	AY	8	4SU	C4-S4	-4.39	1.60	1.68
24	CX	8	4SU	C4-S4	-4.31	1.61	1.68
23	CW	55	PSU	C6-C5	4.16	1.39	1.35
24	AX	8	4SU	C2-N3	-4.10	1.30	1.38
23	AW	55	PSU	C6-C5	4.05	1.39	1.35
23	AY	39	PSU	C6-C5	4.03	1.39	1.35
23	CY	32	PSU	C6-C5	4.01	1.39	1.35
24	CX	55	PSU	C6-C5	3.73	1.39	1.35
23	CW	39	PSU	C6-C5	3.72	1.39	1.35
23	CY	39	PSU	C6-C5	3.72	1.39	1.35
23	AY	46	7MG	C5-C4	3.70	1.49	1.37
23	AY	32	PSU	C6-C5	3.70	1.39	1.35
23	AY	55	PSU	C6-C5	3.69	1.39	1.35
23	CY	55	PSU	C6-C5	3.54	1.39	1.35
23	AW	39	PSU	C6-C5	3.53	1.39	1.35
23	CY	46	7MG	C5-C4	3.44	1.48	1.37
23	AW	46	7MG	C5-C4	3.40	1.48	1.37
23	AY	8	4SU	C4-N3	-3.39	1.34	1.37
23	AW	32	PSU	C6-C5	3.39	1.39	1.35
23	CW	46	7MG	C5-C4	3.35	1.47	1.37
24	CX	8	4SU	C5-C4	-3.34	1.38	1.42
23	CY	46	7MG	C4-N9	-3.23	1.33	1.37
23	CW	32	PSU	C6-C5	3.21	1.38	1.35
24	CX	32	5MC	C6-C5	3.16	1.39	1.34
23	AW	8	4SU	C4-N3	-3.10	1.34	1.37
24	AX	55	PSU	C6-C5	3.09	1.38	1.35
24	AX	8	4SU	C5-C4	-3.07	1.38	1.42
24	CX	8	4SU	C2-N3	-2.97	1.32	1.38
23	CY	54	5MU	C6-C5	2.93	1.39	1.34
23	CY	37	MIA	C5-C6	2.91	1.49	1.41
23	AY	37	MIA	C5-C6	2.91	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CY	54	5MU	C2-N1	2.89	1.43	1.38
23	CY	8	4SU	C5-C4	-2.89	1.39	1.42
23	AW	8	4SU	C5-C4	-2.88	1.39	1.42
23	CW	8	4SU	C4-N3	-2.87	1.34	1.37
23	AW	54	5MU	C4-N3	-2.82	1.33	1.38
23	AW	54	5MU	C6-C5	2.80	1.39	1.34
23	AY	54	5MU	C6-C5	2.80	1.39	1.34
24	AX	54	5MU	C4-N3	-2.77	1.33	1.38
23	AW	46	7MG	C4-N9	-2.76	1.34	1.37
23	AW	32	PSU	C4-N3	-2.75	1.33	1.38
23	AY	54	5MU	C4-N3	-2.73	1.33	1.38
24	AX	32	5MC	C6-C5	2.72	1.39	1.34
24	AX	32	5MC	C6-N1	-2.70	1.33	1.38
24	AX	54	5MU	C6-C5	2.69	1.39	1.34
23	CW	37	MIA	C5-C6	2.68	1.48	1.41
24	CX	54	5MU	C6-C5	2.68	1.39	1.34
23	CW	39	PSU	C4-N3	-2.67	1.33	1.38
24	CX	54	5MU	C4-C5	2.65	1.49	1.44
23	CY	54	5MU	C4-C5	2.65	1.49	1.44
23	CW	54	5MU	C6-C5	2.65	1.38	1.34
23	CW	46	7MG	C4-N9	-2.64	1.34	1.37
23	AY	8	4SU	C5-C4	-2.60	1.39	1.42
24	CX	55	PSU	C4-N3	-2.59	1.34	1.38
23	CY	55	PSU	C4-N3	-2.56	1.34	1.38
23	AW	37	MIA	C5-N7	-2.54	1.34	1.39
23	CW	32	PSU	C4-N3	-2.53	1.34	1.38
24	AX	55	PSU	C4-N3	-2.53	1.34	1.38
23	AY	39	PSU	C4-N3	-2.53	1.34	1.38
23	CW	55	PSU	C4-N3	-2.49	1.34	1.38
23	CW	8	4SU	C2-N1	2.49	1.42	1.38
23	CY	54	5MU	C4-N3	-2.49	1.34	1.38
23	AY	46	7MG	C8-N9	2.48	1.47	1.45
23	AW	39	PSU	C4-N3	-2.48	1.34	1.38
23	CY	39	PSU	C4-N3	-2.48	1.34	1.38
23	AY	54	5MU	C4-C5	2.48	1.48	1.44
23	AW	55	PSU	C4-N3	-2.48	1.34	1.38
23	CW	54	5MU	C4-C5	2.47	1.48	1.44
24	CX	54	5MU	C4-N3	-2.45	1.34	1.38
23	CW	37	MIA	C5-N7	-2.44	1.34	1.39
23	CY	8	4SU	C2-N1	2.44	1.42	1.38
23	AY	37	MIA	C8-N7	2.43	1.36	1.31
23	CY	37	MIA	C8-N7	2.42	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CY	8	4SU	C4-N3	-2.42	1.35	1.37
23	AY	32	PSU	C4-N3	-2.41	1.34	1.38
23	CY	46	7MG	C6-N1	-2.40	1.34	1.38
23	AW	54	5MU	C2-N1	2.38	1.42	1.38
23	AY	46	7MG	C4-N9	-2.38	1.34	1.37
24	AX	54	5MU	C4-C5	2.38	1.48	1.44
23	AW	37	MIA	C5-C6	2.36	1.47	1.41
23	AW	54	5MU	C4-C5	2.36	1.48	1.44
23	AY	54	5MU	C2-N1	2.36	1.42	1.38
23	AY	55	PSU	C4-N3	-2.35	1.34	1.38
23	CY	32	PSU	C4-N3	-2.33	1.34	1.38
23	AY	39	PSU	O4'-C1'	-2.33	1.40	1.43
23	AW	8	4SU	C2-N1	2.33	1.42	1.38
23	AY	46	7MG	C6-N1	-2.32	1.34	1.38
23	AW	54	5MU	C2-N3	-2.32	1.33	1.38
23	CW	37	MIA	C8-N7	2.31	1.36	1.31
24	AX	54	5MU	C2-N3	-2.30	1.34	1.38
23	AY	8	4SU	C2-N1	2.30	1.42	1.38
23	AW	46	7MG	C6-N1	-2.25	1.34	1.38
24	AX	8	4SU	O2-C2	2.24	1.27	1.23
23	AW	37	MIA	C8-N7	2.24	1.36	1.31
23	CW	54	5MU	C2-N1	2.24	1.42	1.38
23	CW	46	7MG	C6-N1	-2.23	1.34	1.38
23	CW	32	PSU	C4-C5	2.20	1.50	1.44
23	CW	46	7MG	C8-N9	2.18	1.47	1.45
24	CX	32	5MC	C6-N1	-2.16	1.34	1.38
23	AY	8	4SU	C2-N3	-2.12	1.34	1.38
23	CY	39	PSU	O4'-C1'	-2.12	1.40	1.43
23	AW	8	4SU	C2-N3	-2.11	1.34	1.38
23	CY	54	5MU	C2-N3	-2.10	1.34	1.38
24	AX	54	5MU	C2-N1	2.08	1.41	1.38
23	AW	32	PSU	C2-N3	-2.07	1.34	1.37
23	AY	8	4SU	O2-C2	2.07	1.26	1.23
23	CW	54	5MU	C4-N3	-2.07	1.35	1.38
24	AX	54	5MU	C6-N1	-2.06	1.34	1.38
24	AX	8	4SU	C6-C5	2.05	1.39	1.35
23	CW	8	4SU	C5-C4	-2.05	1.40	1.42
24	CX	54	5MU	C2-N1	2.05	1.41	1.38
24	CX	54	5MU	C2-N3	-2.05	1.34	1.38
23	AY	37	MIA	C5-N7	-2.03	1.35	1.39
23	CW	8	4SU	C6-C5	2.03	1.39	1.35
24	CX	54	5MU	C6-N1	-2.03	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AY	54	5MU	C2-N3	-2.03	1.34	1.38
23	AY	8	4SU	C6-C5	2.01	1.39	1.35
23	CY	46	7MG	C8-N9	2.01	1.47	1.45
23	CW	32	PSU	C2-N3	-2.01	1.34	1.37
23	AW	8	4SU	O2-C2	2.00	1.26	1.23
23	CW	54	5MU	C6-N1	-2.00	1.34	1.38

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AY	46	7MG	N9-C4-N3	9.30	139.09	125.46
23	AW	46	7MG	N9-C4-N3	9.21	138.96	125.46
23	CW	46	7MG	N9-C4-N3	9.01	138.66	125.46
23	CY	46	7MG	N9-C4-N3	8.82	138.38	125.46
23	AW	37	MIA	C12-C13-C14	-8.27	112.17	127.01
23	AW	37	MIA	C5-C4-N3	-7.69	119.08	127.18
23	CW	55	PSU	N1-C2-N3	6.62	122.15	115.17
23	AY	32	PSU	N1-C2-N3	6.44	121.96	115.17
23	CY	55	PSU	N1-C2-N3	6.44	121.96	115.17
23	CW	37	MIA	C5-C4-N3	-6.29	118.06	126.72
23	AW	55	PSU	N1-C2-N3	6.24	121.75	115.17
23	AW	37	MIA	N3-C4-N9	6.24	134.91	126.99
23	CY	39	PSU	N1-C2-N3	6.17	121.68	115.17
24	AX	55	PSU	N1-C2-N3	6.14	121.65	115.17
23	AW	39	PSU	N1-C2-N3	6.14	121.64	115.17
23	AY	55	PSU	N1-C2-N3	6.05	121.55	115.17
23	CY	8	4SU	C5-C4-N3	5.97	120.30	114.75
23	CW	8	4SU	C4-N3-C2	-5.96	121.60	127.31
23	CY	32	PSU	N1-C2-N3	5.93	121.42	115.17
23	CY	8	4SU	C4-N3-C2	-5.90	121.66	127.31
23	CW	46	7MG	C5-C4-N3	-5.83	117.19	128.13
23	AW	32	PSU	N1-C2-N3	5.83	121.31	115.17
24	CX	55	PSU	N1-C2-N3	5.76	121.24	115.17
23	CW	32	PSU	N1-C2-N3	5.73	121.21	115.17
23	AY	37	MIA	C5-C4-N3	-5.54	119.08	126.72
23	CY	37	MIA	C5-C4-N3	-5.52	119.11	126.72
23	AW	46	7MG	C5-C4-N3	-5.39	118.01	128.13
23	AY	46	7MG	C5-C4-N3	-5.37	118.04	128.13
23	CY	8	4SU	C5-C4-S4	-5.30	118.26	124.31
23	AW	8	4SU	C5-C4-N3	5.27	119.65	114.75
23	AW	46	7MG	N9-C8-N7	-5.27	95.92	103.37
23	CY	46	7MG	N9-C8-N7	-5.23	95.96	103.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AY	39	PSU	N1-C2-N3	5.16	120.61	115.17
23	CY	46	7MG	C5-C4-N3	-5.12	118.53	128.13
24	CX	54	5MU	N3-C2-N1	5.08	121.51	114.89
23	CW	39	PSU	N1-C2-N3	5.05	120.50	115.17
24	CX	54	5MU	C4-N3-C2	-5.02	120.76	127.34
23	CW	37	MIA	N3-C4-N9	4.92	135.53	127.17
24	AX	54	5MU	C4-N3-C2	-4.92	120.89	127.34
23	CW	8	4SU	C5-C4-N3	4.90	119.31	114.75
23	CW	46	7MG	N9-C8-N7	-4.89	96.45	103.37
23	CY	37	MIA	N3-C4-N9	4.82	135.37	127.17
23	CW	46	7MG	C2-N3-C4	4.76	120.50	112.30
24	AX	54	5MU	C5-C4-N3	4.75	119.46	115.32
23	AY	46	7MG	N9-C8-N7	-4.71	96.71	103.37
24	AX	54	5MU	N3-C2-N1	4.60	120.88	114.89
23	CY	55	PSU	O2-C2-N1	-4.54	118.10	122.79
23	CW	54	5MU	C4-N3-C2	-4.48	121.46	127.34
23	AY	37	MIA	N3-C4-N9	4.48	134.78	127.17
23	CY	46	7MG	C2-N3-C4	4.40	119.87	112.30
23	CW	54	5MU	O4-C4-C5	-4.39	119.89	124.92
24	CX	55	PSU	C4-N3-C2	-4.37	120.35	126.37
23	AW	46	7MG	C2-N3-C4	4.36	119.80	112.30
24	CX	54	5MU	C5-C4-N3	4.34	119.09	115.32
23	CY	54	5MU	C5-C4-N3	4.30	119.06	115.32
23	AW	8	4SU	C4-N3-C2	-4.28	123.21	127.31
23	CY	39	PSU	O2-C2-N1	-4.26	118.40	122.79
23	AW	54	5MU	N3-C2-N1	4.24	120.41	114.89
23	AY	32	PSU	C4-N3-C2	-4.24	120.53	126.37
23	CY	54	5MU	C4-N3-C2	-4.23	121.79	127.34
23	CW	54	5MU	C5-C4-N3	4.23	119.00	115.32
23	AY	46	7MG	C2-N3-C4	4.23	119.58	112.30
23	CY	54	5MU	N3-C2-N1	4.22	120.38	114.89
23	AY	55	PSU	C4-N3-C2	-4.22	120.56	126.37
23	CW	54	5MU	N3-C2-N1	4.16	120.31	114.89
23	AY	8	4SU	C5-C4-N3	4.14	118.60	114.75
23	AW	39	PSU	C4-N3-C2	-4.13	120.68	126.37
23	AW	37	MIA	C15-C14-C13	-4.07	110.44	122.66
23	CY	55	PSU	C4-N3-C2	-4.06	120.78	126.37
23	CW	55	PSU	C4-N3-C2	-4.04	120.81	126.37
24	AX	8	4SU	C6-C5-C4	-4.03	116.46	119.95
23	AW	55	PSU	C4-N3-C2	-4.03	120.82	126.37
23	CW	37	MIA	C2-N3-C4	4.01	121.62	111.83
23	CW	8	4SU	N3-C2-N1	4.01	120.11	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	CW	37	MIA	N3-C2-N1	-3.98	122.55	128.58
24	AX	32	5MC	C5-C6-N1	-3.97	119.00	123.31
23	AW	37	MIA	C16-C14-C13	-3.95	110.80	122.66
24	AX	55	PSU	C4-N3-C2	-3.95	120.93	126.37
24	AX	8	4SU	O2-C2-N1	3.90	127.87	122.80
23	AW	54	5MU	C4-N3-C2	-3.80	122.36	127.34
24	AX	54	5MU	C5-C6-N1	-3.79	119.20	123.31
23	CW	32	PSU	C4-N3-C2	-3.77	121.17	126.37
24	CX	54	5MU	O4-C4-C5	-3.77	120.61	124.92
24	AX	54	5MU	O4-C4-C5	-3.74	120.64	124.92
23	CY	32	PSU	C4-N3-C2	-3.74	121.22	126.37
23	AW	54	5MU	C5-C4-N3	3.71	118.55	115.32
23	CW	55	PSU	O2-C2-N1	-3.65	119.02	122.79
24	AX	55	PSU	O2-C2-N1	-3.64	119.03	122.79
23	CW	37	MIA	C4-C5-N7	-3.61	106.45	110.58
23	AY	37	MIA	C2-N3-C4	3.60	120.63	111.83
23	AY	32	PSU	O2-C2-N1	-3.60	119.08	122.79
23	AW	8	4SU	C5-C4-S4	-3.58	120.21	124.31
23	AW	32	PSU	C4-N3-C2	-3.57	121.46	126.37
23	AY	54	5MU	C5-C4-N3	3.56	118.42	115.32
23	CY	37	MIA	C2-N3-C4	3.56	120.52	111.83
23	AY	54	5MU	N3-C2-N1	3.53	119.49	114.89
23	AY	8	4SU	C4-N3-C2	-3.52	123.94	127.31
23	CY	54	5MU	O4-C4-C5	-3.52	120.89	124.92
23	AW	39	PSU	O2-C2-N1	-3.51	119.17	122.79
23	AY	37	MIA	N3-C2-N1	-3.49	123.30	128.58
23	CY	37	MIA	N3-C2-N1	-3.48	123.32	128.58
23	CY	39	PSU	C4-N3-C2	-3.47	121.60	126.37
24	CX	32	5MC	C5-C6-N1	-3.45	119.57	123.31
23	CW	32	PSU	C6-C5-C4	-3.40	115.88	118.17
24	AX	8	4SU	S4-C4-N3	-3.40	116.65	120.20
24	CX	8	4SU	C6-C5-C4	-3.38	117.02	119.95
23	AY	55	PSU	O2-C2-N1	-3.36	119.32	122.79
23	AY	54	5MU	C4-N3-C2	-3.36	122.94	127.34
23	CY	8	4SU	N3-C2-N1	3.30	119.19	114.89
23	AW	37	MIA	N6-C6-N1	3.30	122.75	118.33
24	CX	32	5MC	C5-C4-N3	-3.25	118.42	121.75
23	AY	37	MIA	C4-C5-N7	-3.23	106.89	110.58
23	AW	37	MIA	C2-N3-C4	3.22	120.73	112.29
23	CY	32	PSU	O2-C2-N1	-3.21	119.48	122.79
23	CW	8	4SU	C5-C4-S4	-3.17	120.68	124.31
23	CY	37	MIA	C4-N9-C8	3.17	109.06	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	CY	37	MIA	C4-C5-N7	-3.13	107.00	110.58
24	CX	8	4SU	C1'-N1-C2	3.08	123.12	117.59
23	AW	54	5MU	O4-C4-C5	-3.06	121.41	124.92
23	AW	55	PSU	O2-C2-N1	-3.02	119.68	122.79
24	CX	54	5MU	C5-C6-N1	-3.00	120.05	123.31
23	AY	8	4SU	C1'-N1-C2	3.00	122.98	117.59
23	AW	37	MIA	C4-C5-N7	-2.98	107.17	110.58
23	CW	46	7MG	C5-C6-N1	2.97	116.17	110.94
23	CW	39	PSU	C4-N3-C2	-2.97	122.28	126.37
24	CX	32	5MC	O2-C2-N3	-2.91	117.73	122.33
23	AY	54	5MU	O4-C4-C5	-2.88	121.62	124.92
23	CY	54	5MU	C5-C6-N1	-2.88	120.19	123.31
24	AX	32	5MC	C5-C4-N3	-2.85	118.83	121.75
24	CX	54	5MU	O2-C2-N1	-2.84	119.10	122.80
23	CW	32	PSU	O2-C2-N1	-2.82	119.88	122.79
24	CX	54	5MU	C5M-C5-C4	2.82	121.79	118.78
24	AX	8	4SU	C5-C4-N3	2.79	117.35	114.75
23	CW	37	MIA	C5-N7-C8	2.78	107.82	103.45
23	AY	39	PSU	C6-C5-C4	-2.78	116.30	118.17
23	AW	54	5MU	C5-C6-N1	-2.74	120.34	123.31
23	AY	8	4SU	N3-C2-N1	2.73	118.45	114.89
23	AW	8	4SU	C1'-N1-C2	2.73	122.50	117.59
23	AY	46	7MG	C5-C4-N9	-2.71	102.86	106.33
23	CW	54	5MU	C5M-C5-C4	2.63	121.59	118.78
23	AY	39	PSU	C4-N3-C2	-2.62	122.76	126.37
24	CX	8	4SU	C5-C4-N3	2.59	117.16	114.75
23	AY	54	5MU	C5-C6-N1	-2.59	120.51	123.31
23	AW	46	7MG	C5-C4-N9	-2.58	103.03	106.33
23	AW	8	4SU	N3-C2-N1	2.57	118.24	114.89
23	AW	37	MIA	C6-C5-N7	2.56	135.22	132.43
23	CY	46	7MG	C5-C4-N9	-2.56	103.06	106.33
23	CY	54	5MU	C1'-N1-C2	2.53	122.14	117.59
24	AX	54	5MU	O2-C2-N1	-2.53	119.50	122.80
23	CW	54	5MU	C5-C6-N1	-2.52	120.58	123.31
23	AW	37	MIA	C2-N1-C6	2.52	122.32	117.54
23	AW	46	7MG	C5-C6-N1	2.51	115.35	110.94
23	CY	46	7MG	O4'-C1'-N9	-2.47	105.93	109.30
23	AW	37	MIA	C4-N9-C8	2.44	108.30	105.74
23	CY	37	MIA	C5-N7-C8	2.43	107.27	103.45
23	CY	54	5MU	C1'-N1-C6	-2.42	117.16	121.15
24	AX	8	4SU	O2-C2-N3	-2.42	117.03	121.49
23	CW	39	PSU	O2-C2-N1	-2.40	120.32	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	CY	54	5MU	C5M-C5-C4	2.40	121.34	118.78
24	AX	8	4SU	C1'-N1-C2	2.39	121.88	117.59
23	AY	54	5MU	C5M-C5-C4	2.38	121.33	118.78
23	AY	37	MIA	C4-N9-C8	2.37	108.23	105.74
23	AY	39	PSU	O2-C2-N1	-2.33	120.39	122.79
23	AY	55	PSU	C5-C6-N1	-2.31	118.94	122.14
24	CX	55	PSU	C5-C6-N1	-2.29	118.96	122.14
23	AW	37	MIA	C5-N7-C8	2.29	107.05	103.45
23	AY	37	MIA	C5-N7-C8	2.29	107.05	103.45
23	CW	54	5MU	O2-C2-N1	-2.27	119.84	122.80
23	CY	46	7MG	C5-C6-N1	2.27	114.93	110.94
23	AW	37	MIA	N3-C2-N1	-2.26	122.87	127.00
24	CX	55	PSU	C6-C5-C4	-2.26	116.65	118.17
23	CW	46	7MG	O6-C6-C5	-2.24	122.12	127.62
23	AY	8	4SU	C5-C4-S4	-2.20	121.79	124.31
23	AY	55	PSU	O4-C4-C5	-2.19	118.57	124.01
23	CW	37	MIA	C4-N9-C8	2.18	108.03	105.74
23	CY	54	5MU	O2-C2-N3	-2.17	117.49	121.49
23	AW	32	PSU	O2-C2-N1	-2.16	120.56	122.79
23	AY	46	7MG	C5-C6-N1	2.15	114.72	110.94
24	CX	55	PSU	O2-C2-N3	-2.11	118.12	121.86
24	CX	8	4SU	C6-N1-C2	-2.10	118.44	121.00
23	AW	32	PSU	O2-C2-N3	-2.10	118.12	121.86
23	AW	8	4SU	C6-C5-C4	-2.10	118.13	119.95
23	AY	32	PSU	C5-C6-N1	-2.10	119.22	122.14
23	AY	55	PSU	O4'-C1'-C2'	2.08	108.03	105.15
24	CX	55	PSU	O2-C2-N1	-2.08	120.64	122.79
24	AX	55	PSU	C5-C6-N1	-2.07	119.26	122.14
23	CW	37	MIA	C2-N1-C6	2.07	122.13	118.73
24	CX	54	5MU	C5M-C5-C6	-2.06	120.06	122.85
23	AW	46	7MG	O6-C6-C5	-2.06	122.57	127.62
24	AX	8	4SU	C4-N3-C2	2.05	129.28	127.31
23	CY	37	MIA	C2-N1-C6	2.04	122.08	118.73
23	AW	39	PSU	C5-C6-N1	-2.01	119.36	122.14

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AW	37	MIA	C12-C13-C14-C16
23	AY	46	7MG	C4'-C5'-O5'-P
23	CW	32	PSU	C2'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
23	CW	32	PSU	C2'-C1'-C5-C6
23	CY	55	PSU	C2'-C1'-C5-C4
23	AY	39	PSU	C3'-C4'-C5'-O5'
23	CY	37	MIA	C3'-C4'-C5'-O5'
23	CY	39	PSU	C3'-C4'-C5'-O5'
23	CY	46	7MG	O4'-C4'-C5'-O5'
23	AY	39	PSU	O4'-C4'-C5'-O5'
23	CY	39	PSU	O4'-C4'-C5'-O5'
23	CY	8	4SU	O4'-C4'-C5'-O5'
23	CY	37	MIA	O4'-C4'-C5'-O5'
23	CY	46	7MG	C3'-C4'-C5'-O5'
23	CW	46	7MG	C2'-C1'-N9-C8
23	AY	46	7MG	C2'-C1'-N9-C8
23	AW	46	7MG	C3'-C4'-C5'-O5'
23	CY	55	PSU	C3'-C4'-C5'-O5'
23	AW	46	7MG	O4'-C4'-C5'-O5'
23	AY	37	MIA	C4'-C5'-O5'-P
23	AY	55	PSU	O4'-C1'-C5-C4
23	CW	32	PSU	O4'-C1'-C5-C4
23	CY	55	PSU	O4'-C1'-C5-C4
23	CY	37	MIA	C4'-C5'-O5'-P
23	CY	32	PSU	O4'-C4'-C5'-O5'
23	CY	8	4SU	C3'-C4'-C5'-O5'
23	CW	32	PSU	O4'-C1'-C5-C6
23	AY	46	7MG	O4'-C1'-N9-C8
23	CW	46	7MG	O4'-C1'-N9-C8
23	CY	54	5MU	C2'-C1'-N1-C2
23	AW	46	7MG	C4'-C5'-O5'-P
23	AY	8	4SU	C2'-C1'-N1-C2

There are no ring outliers.

18 monomers are involved in 30 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	32	PSU	1	0
23	CW	39	PSU	2	0
23	CY	8	4SU	4	0
23	CW	8	4SU	1	0
23	AY	8	4SU	1	0
23	AY	54	5MU	2	0
23	CY	46	7MG	1	0
23	AY	46	7MG	1	0
23	CY	39	PSU	2	0
23	CY	37	MIA	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2152 ligands modelled in this entry, 2148 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	$\#\|Z\| > 2$
58	SF4	CD	501	4	0,12,12	-	-	-		
57	PCY	CA	3178	-	34,42,42	1.70	4 (11%)	41,65,65	1.17	4 (9%)
58	SF4	AD	501	4	0,12,12	-	-	-		
57	PCY	AA	3231	-	34,42,42	1.73	5 (14%)	41,65,65	1.44	7 (17%)

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
58	SF4	CD	501	4	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PCY	CA	3178	-	-	8/33/67/67	0/3/3/3
58	SF4	AD	501	4	-	-	0/6/5/5
57	PCY	AA	3231	-	-	5/33/67/67	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	AA	3231	PCY	C34-C30	-5.60	1.40	1.51
57	CA	3178	PCY	C34-C30	-5.56	1.40	1.51
57	CA	3178	PCY	C28-C32	-5.50	1.39	1.49
57	AA	3231	PCY	C28-C32	-5.35	1.39	1.49
57	AA	3231	PCY	C27-C23	-4.14	1.40	1.50
57	CA	3178	PCY	C27-C23	-3.71	1.41	1.50
57	CA	3178	PCY	C22-N20	-3.14	1.33	1.39
57	AA	3231	PCY	C22-N20	-2.86	1.34	1.39
57	AA	3231	PCY	C17-N20	2.32	1.48	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	AA	3231	PCY	C18-O21-C23	-4.84	107.00	116.55
57	CA	3178	PCY	C18-O21-C23	-3.69	109.27	116.55
57	AA	3231	PCY	O21-C23-C27	3.04	119.12	112.35
57	AA	3231	PCY	O21-C18-C15	2.78	112.92	107.79
57	AA	3231	PCY	O36-C31-C27	-2.29	116.91	121.14
57	CA	3178	PCY	C38-C32-C28	-2.19	115.07	119.21
57	AA	3231	PCY	C34-C30-C35	-2.18	116.08	120.28
57	AA	3231	PCY	C34-C30-C27	2.17	124.53	121.67
57	AA	3231	PCY	C30-C27-C23	2.17	126.64	120.47
57	CA	3178	PCY	C34-C30-C35	-2.05	116.32	120.28
57	CA	3178	PCY	C10-N4-C9	2.03	122.35	115.87

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	AA	3231	PCY	N2-C3-C6-C11
57	AA	3231	PCY	C7-C3-C6-C11
57	AA	3231	PCY	C7-C15-C18-O21
57	AA	3231	PCY	C17-C15-C18-O21
57	AA	3231	PCY	O19-C15-C18-O21

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Mol	Chain	Res	Type	Atoms
57	CA	3178	PCY	N2-C3-C6-C11
57	CA	3178	PCY	N2-C3-C6-O12
57	CA	3178	PCY	C7-C3-C6-C11
57	CA	3178	PCY	C7-C3-C6-O12
57	CA	3178	PCY	O26-C23-C27-C30
57	CA	3178	PCY	O21-C23-C27-C30
57	CA	3178	PCY	O26-C23-C27-C31
57	CA	3178	PCY	O21-C23-C27-C31

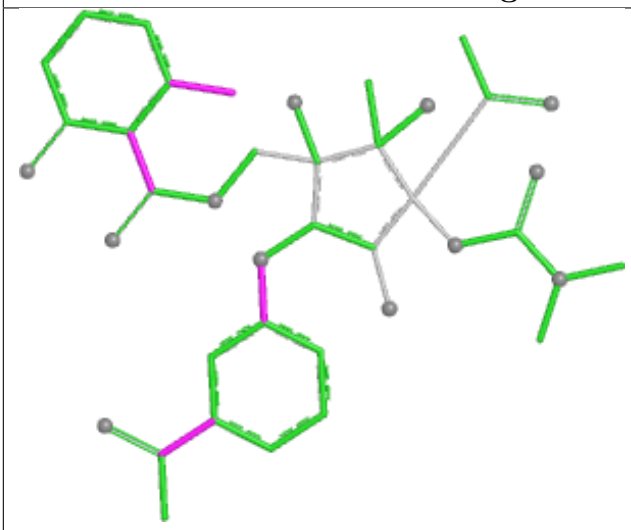
There are no ring outliers.

2 monomers are involved in 16 short contacts:

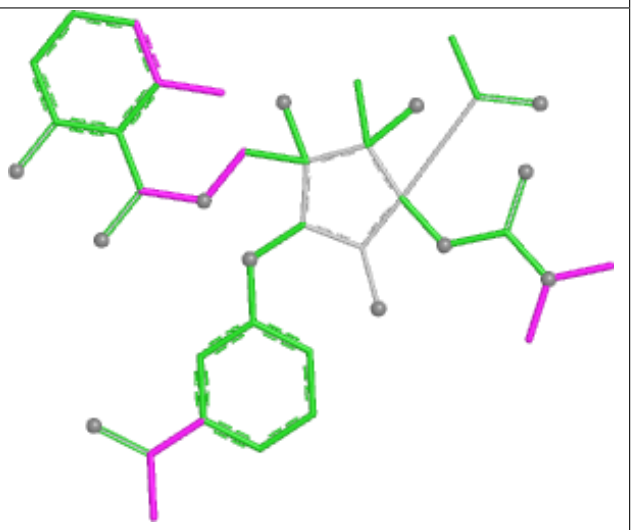
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	CA	3178	PCY	9	0
57	AA	3231	PCY	7	0

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 then 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.

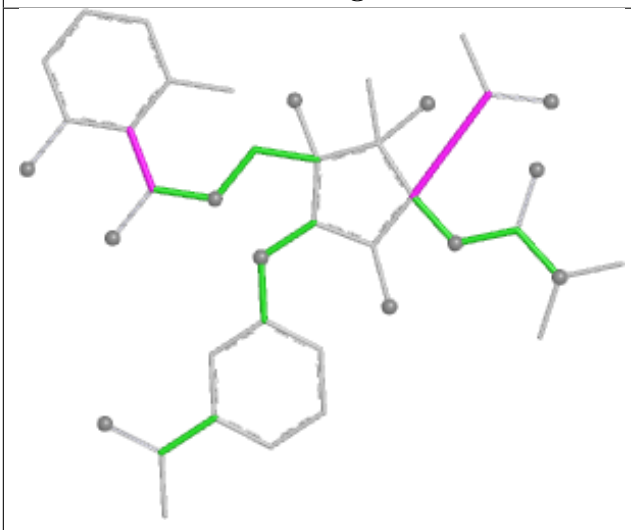
Ligand PCY CA 3178



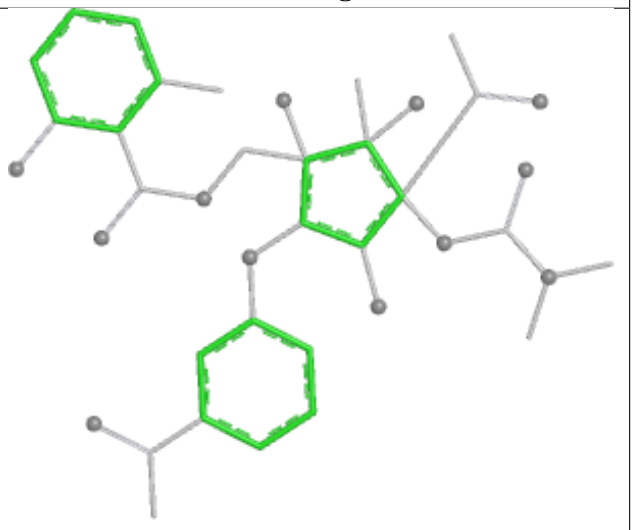
Bond lengths



Bond angles

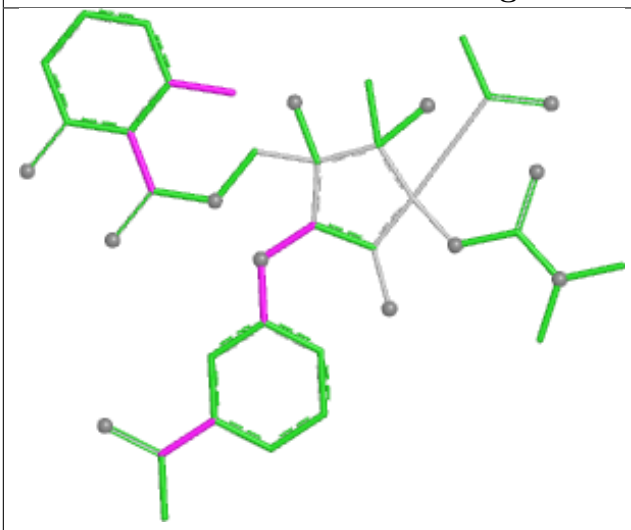


Torsions

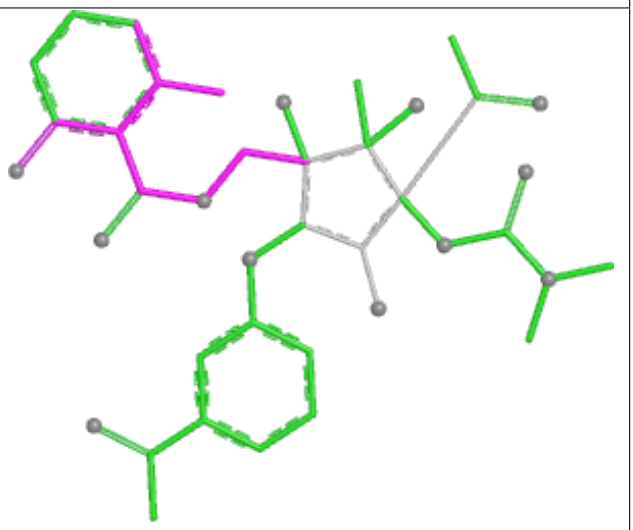


Rings

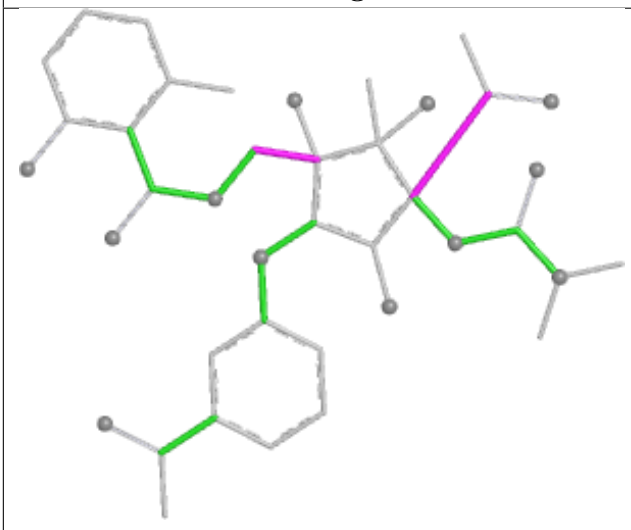
Ligand PCY AA 3231



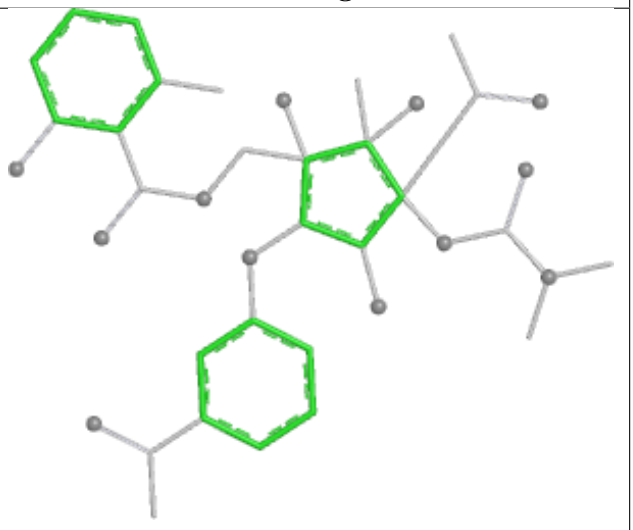
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1498/1521 (98%)	0.43	45 (3%) 52 54	40, 67, 92, 106	0
1	CA	1503/1521 (98%)	0.51	62 (4%) 41 42	43, 69, 92, 106	0
2	AB	231/256 (90%)	1.32	43 (18%) 3 2	63, 80, 90, 94	0
2	CB	231/256 (90%)	1.72	71 (30%) 1 0	64, 82, 89, 96	0
3	AC	206/239 (86%)	1.20	24 (11%) 9 8	61, 74, 84, 92	0
3	CC	206/239 (86%)	1.55	52 (25%) 1 1	64, 76, 86, 92	0
4	AD	208/209 (99%)	1.40	43 (20%) 2 2	56, 68, 79, 87	0
4	CD	208/209 (99%)	1.06	22 (10%) 11 11	57, 68, 78, 87	0
5	AE	148/162 (91%)	1.11	9 (6%) 27 26	56, 67, 77, 91	0
5	CE	148/162 (91%)	1.08	18 (12%) 8 7	57, 69, 79, 92	0
6	AF	100/101 (99%)	1.00	7 (7%) 22 21	53, 66, 76, 82	0
6	CF	100/101 (99%)	0.80	1 (1%) 79 80	54, 66, 76, 82	0
7	AG	155/156 (99%)	1.17	14 (9%) 15 14	61, 71, 83, 93	0
7	CG	155/156 (99%)	1.48	33 (21%) 2 2	62, 73, 84, 96	0
8	AH	137/138 (99%)	1.27	19 (13%) 6 5	57, 69, 75, 83	0
8	CH	137/138 (99%)	1.00	7 (5%) 33 33	58, 71, 77, 84	0
9	AI	127/128 (99%)	1.51	31 (24%) 2 1	56, 78, 85, 90	0
9	CI	127/128 (99%)	2.16	67 (52%) 0 0	62, 79, 86, 89	0
10	AJ	97/105 (92%)	1.60	27 (27%) 1 1	57, 78, 90, 91	0
10	CJ	96/105 (91%)	2.31	53 (55%) 0 0	60, 80, 91, 93	0
11	AK	114/129 (88%)	1.08	12 (10%) 11 11	47, 66, 80, 83	0
11	CK	114/129 (88%)	1.12	15 (13%) 7 6	47, 67, 79, 83	0
12	AL	122/132 (92%)	0.80	8 (6%) 24 24	42, 56, 69, 75	0
12	CL	122/132 (92%)	0.78	6 (4%) 35 34	45, 58, 71, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	123/126 (97%)	0.98	14 (11%) 10 9	42, 63, 75, 80	0
13	CM	122/126 (96%)	1.88	48 (39%) 1 0	66, 79, 86, 90	0
14	AN	60/61 (98%)	1.42	10 (16%) 4 3	60, 70, 77, 81	0
14	CN	60/61 (98%)	2.37	33 (55%) 0 0	64, 73, 80, 83	0
15	AO	88/89 (98%)	1.26	10 (11%) 10 9	50, 66, 76, 82	0
15	CO	88/89 (98%)	0.90	6 (6%) 23 22	53, 68, 77, 82	0
16	AP	82/88 (93%)	1.64	26 (31%) 1 0	52, 68, 76, 80	0
16	CP	82/88 (93%)	1.15	8 (9%) 13 12	51, 68, 76, 79	0
17	AQ	99/105 (94%)	1.19	5 (5%) 33 33	55, 68, 77, 79	0
17	CQ	99/105 (94%)	1.09	8 (8%) 18 17	57, 69, 77, 80	0
18	AR	68/88 (77%)	0.97	3 (4%) 39 39	58, 66, 76, 80	0
18	CR	68/88 (77%)	0.85	3 (4%) 39 39	59, 68, 77, 80	0
19	AS	83/93 (89%)	1.28	12 (14%) 6 5	63, 73, 81, 91	0
19	CS	83/93 (89%)	1.78	28 (33%) 1 0	66, 76, 84, 92	0
20	AT	96/106 (90%)	1.06	9 (9%) 14 13	57, 68, 80, 86	0
20	CT	96/106 (90%)	1.31	16 (16%) 4 3	58, 68, 82, 87	0
21	AU	23/27 (85%)	1.23	5 (21%) 2 2	63, 66, 72, 75	0
21	CU	23/27 (85%)	1.74	7 (30%) 1 0	65, 68, 74, 77	0
22	AV	13/24 (54%)	0.98	2 (15%) 5 4	52, 64, 82, 98	0
22	CV	13/24 (54%)	1.07	3 (23%) 2 1	56, 67, 85, 99	0
23	AW	67/76 (88%)	0.81	7 (10%) 11 11	47, 84, 97, 104	0
23	AY	67/76 (88%)	1.65	18 (26%) 1 1	38, 97, 101, 104	0
23	CW	65/76 (85%)	1.23	11 (16%) 4 3	68, 91, 102, 104	0
23	CY	66/76 (86%)	1.82	23 (34%) 1 0	43, 97, 101, 104	0
24	AX	72/77 (93%)	0.69	5 (6%) 23 22	39, 68, 85, 93	0
24	CX	72/77 (93%)	0.52	2 (2%) 55 56	43, 71, 86, 94	0
25	BA	2819/2915 (96%)	-0.20	112 (3%) 42 43	23, 42, 88, 104	0
25	DA	2800/2915 (96%)	-0.10	81 (2%) 53 55	27, 47, 89, 108	0
26	BB	120/121 (99%)	0.08	0 100 100	35, 56, 70, 86	0
26	DB	120/121 (99%)	0.51	3 (2%) 58 59	42, 62, 73, 87	0
27	BD	275/276 (99%)	0.22	7 (2%) 58 59	23, 40, 55, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
27	DD	275/276 (99%)	0.31	11 (4%) 42 43	26, 42, 56, 77	0
28	BE	204/206 (99%)	0.40	4 (1%) 65 65	22, 47, 66, 76	0
28	DE	204/206 (99%)	0.50	8 (3%) 43 44	28, 50, 67, 77	0
29	BF	203/210 (96%)	0.50	7 (3%) 48 49	23, 49, 73, 88	0
29	DF	203/210 (96%)	0.61	8 (3%) 43 44	27, 55, 75, 88	0
30	BG	181/182 (99%)	1.19	27 (14%) 5 5	44, 64, 78, 90	0
30	DG	181/182 (99%)	1.19	24 (13%) 7 6	50, 67, 80, 90	0
31	BH	174/180 (96%)	1.33	30 (17%) 4 3	51, 65, 76, 85	0
31	DH	174/180 (96%)	1.38	27 (15%) 5 4	57, 70, 80, 86	0
32	BI	146/148 (98%)	1.18	12 (8%) 17 17	50, 71, 82, 86	0
32	DI	146/148 (98%)	1.08	13 (8%) 15 14	53, 71, 82, 85	0
33	BN	140/140 (100%)	0.64	4 (2%) 53 55	32, 47, 68, 75	0
33	DN	140/140 (100%)	0.72	3 (2%) 63 64	36, 52, 70, 76	0
34	BO	122/122 (100%)	0.01	2 (1%) 70 71	25, 38, 59, 65	0
34	DO	122/122 (100%)	0.71	3 (2%) 58 59	47, 59, 74, 79	0
35	BP	149/150 (99%)	0.62	8 (5%) 31 31	24, 55, 74, 81	0
35	DP	149/150 (99%)	0.74	7 (4%) 36 36	29, 59, 76, 82	0
36	BQ	141/141 (100%)	0.52	0 100 100	31, 50, 66, 77	0
36	DQ	141/141 (100%)	0.92	8 (5%) 29 29	38, 54, 69, 80	0
37	BR	118/118 (100%)	-0.13	0 100 100	21, 32, 50, 58	0
37	DR	118/118 (100%)	0.49	2 (1%) 69 69	38, 53, 64, 74	0
38	BS	110/112 (98%)	0.17	0 100 100	32, 48, 64, 67	0
38	DS	110/112 (98%)	1.13	9 (8%) 17 17	58, 69, 80, 85	0
39	BT	131/146 (89%)	0.11	6 (4%) 37 38	31, 42, 68, 89	0
39	DT	131/146 (89%)	0.99	10 (7%) 20 19	51, 64, 78, 84	0
40	BU	116/118 (98%)	-0.45	1 (0%) 81 83	17, 28, 47, 65	0
40	DU	116/118 (98%)	0.76	4 (3%) 48 49	40, 62, 76, 82	0
41	BV	101/101 (100%)	-0.20	0 100 100	15, 35, 54, 67	0
41	DV	101/101 (100%)	1.21	9 (8%) 15 14	39, 74, 81, 88	0
42	BW	112/113 (99%)	-0.40	2 (1%) 67 68	17, 28, 53, 79	0
42	DW	112/113 (99%)	0.43	1 (0%) 81 83	38, 51, 68, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
43	BX	95/96 (98%)	-0.05	1 (1%) 78 79	21, 35, 60, 75	0
43	DX	95/96 (98%)	1.01	12 (12%) 8 7	38, 56, 76, 85	0
44	BY	107/110 (97%)	0.13	3 (2%) 55 56	30, 46, 65, 83	0
44	DY	107/110 (97%)	1.46	24 (22%) 2 2	57, 71, 83, 86	0
45	BZ	171/206 (83%)	1.29	38 (22%) 2 2	35, 67, 94, 105	0
45	DZ	174/206 (84%)	1.97	66 (37%) 1 0	65, 83, 97, 103	0
46	B0	83/85 (97%)	-0.04	5 (6%) 27 27	20, 36, 57, 76	0
46	D0	83/85 (97%)	1.37	13 (15%) 5 4	44, 64, 74, 79	0
47	B1	97/98 (98%)	0.29	2 (2%) 63 64	24, 45, 70, 73	0
47	D1	97/98 (98%)	0.74	8 (8%) 17 17	37, 56, 75, 86	0
48	B2	70/72 (97%)	0.19	1 (1%) 73 74	30, 45, 58, 78	0
48	D2	70/72 (97%)	1.09	6 (8%) 16 15	53, 66, 78, 82	0
49	B3	59/60 (98%)	-0.17	2 (3%) 48 49	19, 31, 58, 75	0
49	D3	59/60 (98%)	1.16	6 (10%) 12 11	54, 66, 78, 88	0
50	B4	69/71 (97%)	1.17	11 (15%) 5 4	51, 70, 89, 99	0
50	D4	69/71 (97%)	1.63	17 (24%) 2 1	72, 82, 92, 93	0
51	B5	59/60 (98%)	-0.42	1 (1%) 69 69	17, 27, 43, 54	0
51	D5	59/60 (98%)	0.41	1 (1%) 69 69	35, 50, 66, 74	0
52	B6	53/54 (98%)	-0.02	1 (1%) 66 66	28, 39, 56, 67	0
52	D6	53/54 (98%)	0.78	3 (5%) 29 29	48, 59, 71, 76	0
53	B7	48/49 (97%)	-0.20	2 (4%) 40 41	18, 26, 62, 72	0
53	D7	48/49 (97%)	0.31	3 (6%) 26 25	30, 41, 61, 78	0
54	B8	64/65 (98%)	-0.36	0 100 100	19, 31, 40, 63	0
54	D8	64/65 (98%)	0.83	4 (6%) 26 25	44, 54, 65, 71	0
55	B9	37/37 (100%)	0.50	1 (2%) 56 57	26, 47, 63, 70	0
55	D9	37/37 (100%)	1.12	4 (10%) 11 10	45, 57, 68, 75	0
All	All	20900/21748 (96%)	0.56	1699 (8%) 18 17	15, 61, 87, 108	0

All (1699) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	CG	82	GLY	7.9
1	AA	1532	U	7.2

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Mol	Chain	Res	Type	RSRZ
13	CM	123	ALA	7.1
14	AN	2	ALA	6.7
7	AG	82	GLY	6.6
31	BH	2	SER	6.6
45	DZ	111	VAL	6.6
45	DZ	116	VAL	6.6
45	DZ	115	GLY	6.5
2	CB	237	ALA	6.4
13	AM	123	ALA	6.4
45	BZ	108	PRO	6.3
45	BZ	115	GLY	6.0
45	DZ	114	GLY	6.0
45	DZ	113	ALA	5.9
45	BZ	144	LEU	5.9
47	B1	2	SER	5.8
25	BA	2806	G	5.4
7	AG	79	ARG	5.4
25	BA	1221	G	5.4
19	CS	13	ASP	5.3
7	AG	80	VAL	5.3
14	CN	2	ALA	5.3
45	BZ	109	ALA	5.3
50	D4	49	PHE	5.2
7	CG	16	LEU	5.2
14	CN	39	LEU	5.1
11	CK	14	VAL	5.1
45	DZ	112	ARG	5.1
15	AO	87	ILE	5.1
10	AJ	4	ILE	5.0
2	CB	123	ALA	4.9
25	BA	932	C	4.9
9	CI	102	LEU	4.9
19	CS	9	VAL	4.9
32	BI	106	GLY	4.8
45	BZ	143	GLY	4.8
7	CG	81	GLY	4.8
46	D0	2	ALA	4.7
13	AM	124	PRO	4.7
45	DZ	144	LEU	4.7
11	AK	14	VAL	4.7
45	BZ	116	VAL	4.7
10	CJ	100	THR	4.7

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Mol	Chain	Res	Type	RSRZ
25	DA	883	G	4.7
7	CG	85	TYR	4.7
27	BD	276	LYS	4.7
9	CI	9	ARG	4.7
23	AW	1	G	4.7
44	DY	1	MET	4.6
28	DE	204	ALA	4.6
13	CM	6	GLY	4.6
27	DD	262	ARG	4.6
25	BA	942	A	4.6
43	DX	95	LEU	4.6
25	BA	931	C	4.5
23	CY	15	G	4.5
10	CJ	63	PHE	4.5
45	BZ	111	VAL	4.5
13	CM	124	PRO	4.5
23	CW	72	C	4.5
50	B4	49	PHE	4.4
2	CB	165	VAL	4.4
1	CA	1149	C	4.4
25	BA	2803	A	4.4
2	CB	236	TYR	4.4
50	D4	56	VAL	4.4
10	CJ	78	ASN	4.4
14	CN	18	VAL	4.3
25	BA	2180	A	4.3
43	DX	92	LEU	4.3
19	AS	13	ASP	4.3
13	CM	121	LYS	4.3
7	CG	84	ASN	4.3
23	CY	18	G	4.3
35	BP	15	ARG	4.3
1	CA	1030(B)	C	4.3
4	AD	194	LEU	4.3
46	D0	7	LEU	4.3
25	BA	934	A	4.2
9	CI	11	LYS	4.2
10	CJ	10	GLY	4.2
23	CY	34	G	4.2
33	BN	9	VAL	4.2
10	CJ	40	LEU	4.2
17	AQ	98	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
30	BG	80	PHE	4.2
14	CN	34	TYR	4.2
22	CV	12	A	4.2
2	AB	237	ALA	4.2
7	AG	83	ALA	4.2
45	DZ	149	SER	4.1
9	AI	2	GLU	4.1
14	CN	38	GLY	4.1
45	BZ	114	GLY	4.1
45	DZ	168	GLU	4.1
13	CM	64	TRP	4.1
25	BA	271	U	4.1
39	BT	130	ALA	4.1
23	AW	71	G	4.1
9	CI	28	VAL	4.1
25	BA	2814	C	4.1
7	AG	85	TYR	4.1
2	CB	161	ALA	4.0
9	CI	44	VAL	4.0
25	BA	2816	G	4.0
1	AA	1503	A	4.0
45	BZ	1	MET	4.0
23	CY	36	A	4.0
50	B4	54	GLY	4.0
50	D4	66	SER	4.0
2	AB	50	GLU	4.0
10	CJ	55	LYS	4.0
45	DZ	170	THR	4.0
4	AD	201	GLN	4.0
45	BZ	113	ALA	3.9
44	DY	107	ASP	3.9
45	DZ	117	LEU	3.9
45	BZ	136	PHE	3.9
10	CJ	88	LEU	3.9
23	CW	71	G	3.9
43	DX	94	GLY	3.9
10	CJ	74	ILE	3.9
47	D1	2	SER	3.9
1	CA	1002	G	3.9
15	CO	60	VAL	3.9
25	DA	2116	G	3.9
25	BA	2815	C	3.9

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Mol	Chain	Res	Type	RSRZ
30	BG	146	TYR	3.9
43	DX	91	ALA	3.9
7	AG	84	ASN	3.9
45	BZ	117	LEU	3.9
45	DZ	109	ALA	3.8
45	DZ	147	GLY	3.8
13	CM	102	ARG	3.8
14	CN	44	LEU	3.8
10	CJ	41	PRO	3.8
23	AY	36	A	3.8
6	AF	46	ARG	3.8
25	BA	2168	C	3.8
17	AQ	36	ILE	3.8
2	AB	7	VAL	3.8
7	CG	83	ALA	3.8
39	DT	131	ALA	3.8
39	BT	38	ASN	3.8
25	BA	944	C	3.8
10	CJ	90	LEU	3.8
30	BG	48	GLU	3.8
10	AJ	33	GLN	3.8
9	CI	126	SER	3.8
7	CG	156	TRP	3.8
2	AB	12	GLU	3.8
44	DY	5	MET	3.8
2	CB	11	LEU	3.7
16	AP	68	ASP	3.7
38	DS	3	ARG	3.7
45	DZ	166	SER	3.7
11	CK	13	GLN	3.7
13	CM	4	ILE	3.7
3	CC	48	TYR	3.7
1	CA	1030(D)	A	3.7
10	CJ	87	THR	3.7
50	B4	50	VAL	3.7
13	AM	2	ALA	3.7
5	CE	23	GLY	3.7
10	CJ	23	ILE	3.7
10	CJ	86	MET	3.7
9	CI	4	TYR	3.7
45	DZ	164	ALA	3.6
9	CI	8	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
12	CL	95	GLY	3.6
30	BG	42	GLY	3.6
45	BZ	110	GLY	3.6
8	AH	2	LEU	3.6
3	CC	182	ILE	3.6
26	DB	1	U	3.6
2	CB	97	TRP	3.6
14	CN	13	THR	3.6
45	BZ	157	LEU	3.6
11	CK	117	ASN	3.6
23	AY	34	G	3.6
50	D4	67	TYR	3.6
1	AA	1030(A)	G	3.6
14	CN	25	VAL	3.6
25	BA	2181	G	3.6
11	CK	89	ALA	3.6
16	CP	82	GLN	3.6
25	DA	896	A	3.6
45	BZ	118	GLN	3.6
30	DG	53	LEU	3.6
2	CB	41	ILE	3.6
25	BA	943	C	3.5
25	DA	884	C	3.5
25	BA	2154	U	3.5
2	CB	31	TYR	3.5
2	CB	33	TYR	3.5
1	AA	630	G	3.5
10	CJ	65	LEU	3.5
18	CR	66	LEU	3.5
25	DA	882	G	3.5
27	DD	2	ALA	3.5
45	DZ	57	ILE	3.5
10	CJ	76	ASN	3.5
30	BG	49	ASP	3.5
13	CM	120	LYS	3.5
13	CM	15	VAL	3.5
45	DZ	174	VAL	3.5
11	CK	25	TYR	3.5
9	AI	47	LEU	3.5
16	CP	48	TRP	3.5
20	CT	47	GLY	3.5
20	CT	97	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	AA	1003	G	3.5
2	CB	17	PHE	3.5
23	CW	3	C	3.5
13	CM	101	GLN	3.5
19	CS	80	TYR	3.5
45	DZ	99	TYR	3.5
2	CB	154	LEU	3.5
46	D0	84	LEU	3.5
44	DY	80	GLY	3.5
46	B0	6	GLY	3.5
23	CW	70	G	3.5
25	DA	2159	G	3.5
45	DZ	157	LEU	3.5
9	CI	106	ALA	3.5
10	CJ	47	PHE	3.5
20	CT	74	LYS	3.5
1	AA	1447	A	3.4
1	CA	1001	A	3.4
25	BA	2153	G	3.4
25	BA	2163	G	3.4
3	CC	76	VAL	3.4
9	CI	7	THR	3.4
45	DZ	107	THR	3.4
20	CT	103	GLY	3.4
45	DZ	108	PRO	3.4
2	AB	127	ILE	3.4
9	CI	125	TYR	3.4
50	D4	59	PHE	3.4
11	CK	126	ARG	3.4
30	BG	26	GLN	3.4
4	AD	188	LEU	3.4
19	CS	2	PRO	3.4
19	AS	40	ILE	3.4
1	AA	1027	C	3.4
25	BA	2167	C	3.4
10	CJ	77	PRO	3.4
9	CI	69	GLY	3.4
39	DT	130	ALA	3.4
14	CN	35	ARG	3.4
50	B4	59	PHE	3.4
23	AW	72	C	3.4
25	BA	2183	C	3.4

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Mol	Chain	Res	Type	RSRZ
3	AC	18	TRP	3.4
14	CN	61	TRP	3.4
29	BF	89	VAL	3.4
30	BG	82	LEU	3.4
10	CJ	35	SER	3.4
4	AD	110	PHE	3.3
1	AA	163	C	3.3
25	DA	2139	C	3.3
4	AD	88	VAL	3.3
9	CI	17	VAL	3.3
19	AS	71	LEU	3.3
31	BH	44	VAL	3.3
9	CI	42	ARG	3.3
19	AS	84	GLY	3.3
23	AW	73	A	3.3
9	CI	61	ALA	3.3
16	AP	19	ILE	3.3
45	DZ	136	PHE	3.3
23	CY	19	G	3.3
2	CB	155	LEU	3.3
19	AS	9	VAL	3.3
14	CN	55	GLY	3.3
46	B0	3	HIS	3.3
30	BG	35	GLU	3.3
3	AC	65	ALA	3.3
5	CE	17	ALA	3.3
11	AK	75	TYR	3.3
10	CJ	33	GLN	3.3
23	CY	22	G	3.3
7	CG	80	VAL	3.3
10	CJ	56	HIS	3.3
12	CL	18	VAL	3.3
31	BH	17	VAL	3.3
3	AC	39	ILE	3.3
10	AJ	86	MET	3.3
30	BG	52	ILE	3.3
2	AB	236	TYR	3.3
16	AP	49	LEU	3.3
25	BA	930	G	3.3
49	D3	60	GLU	3.3
16	AP	69	THR	3.3
25	BA	2807	C	3.3

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Mol	Chain	Res	Type	RSRZ
4	AD	173	TRP	3.3
23	AY	35	A	3.2
23	CW	76	A	3.2
23	CY	21	A	3.2
1	AA	204	U	3.2
10	CJ	34	VAL	3.2
9	CI	64	THR	3.2
1	CA	1030	C	3.2
25	BA	34	C	3.2
25	BA	935	C	3.2
25	DA	2117	A	3.2
50	D4	65	ASP	3.2
2	CB	10	LEU	3.2
9	CI	2	GLU	3.2
1	AA	841	U	3.2
9	CI	14	VAL	3.2
1	AA	1030(B)	C	3.2
1	AA	1031	G	3.2
25	BA	929	G	3.2
25	DA	2155	G	3.2
2	CB	158	LEU	3.2
10	CJ	85	LEU	3.2
31	DH	173	PRO	3.2
32	BI	117	GLU	3.2
46	D0	3	HIS	3.2
12	AL	18	VAL	3.2
19	AS	48	THR	3.2
14	CN	3	ARG	3.2
25	DA	885	C	3.2
23	AY	15	G	3.2
2	AB	232	PRO	3.2
10	CJ	71	LEU	3.2
3	AC	184	TYR	3.2
3	CC	198	VAL	3.2
39	BT	37	GLY	3.2
41	DV	63	GLY	3.2
1	AA	1446	U	3.2
9	CI	103	THR	3.2
31	BH	3	ARG	3.1
17	CQ	100	LYS	3.1
45	DZ	16	SER	3.1
25	BA	936	C	3.1

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Mol	Chain	Res	Type	RSRZ
49	B3	2	PRO	3.1
50	D4	57	GLU	3.1
9	CI	56	LEU	3.1
9	CI	79	LEU	3.1
9	CI	80	GLY	3.1
14	CN	33	VAL	3.1
45	BZ	106	GLY	3.1
18	AR	25	THR	3.1
45	DZ	171	ILE	3.1
13	AM	122	LYS	3.1
2	CB	131	PRO	3.1
25	BA	2160	C	3.1
25	DA	2145	C	3.1
15	AO	86	GLY	3.1
19	CS	68	GLY	3.1
23	AY	18	G	3.1
25	BA	2805	G	3.1
7	CG	78	ARG	3.1
25	BA	945	A	3.1
25	BA	2195	A	3.1
25	DA	2158	A	3.1
30	BG	50	ALA	3.1
45	DZ	172	ALA	3.1
16	AP	50	LYS	3.1
53	B7	48	LYS	3.1
2	AB	125	PRO	3.1
11	CK	125	PHE	3.1
14	CN	37	PHE	3.1
3	CC	207	VAL	3.1
10	CJ	38	ILE	3.1
9	CI	5	TYR	3.1
13	CM	59	TYR	3.1
50	D4	63	TYR	3.1
45	DZ	118	GLN	3.1
1	AA	1023	G	3.1
13	CM	27	LYS	3.1
13	CM	30	ALA	3.1
25	BA	2146	G	3.1
25	BA	2155	G	3.1
23	AY	47	U	3.1
10	AJ	77	PRO	3.1
30	DG	17	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
31	DH	168	PRO	3.1
45	DZ	92	SER	3.1
42	BW	112	GLY	3.1
25	BA	1555	C	3.1
16	AP	82	GLN	3.0
7	CG	7	ALA	3.0
39	DT	109	GLU	3.0
1	CA	1257	U	3.0
25	BA	273	G	3.0
25	DA	2115	G	3.0
3	CC	178	LEU	3.0
30	BG	53	LEU	3.0
32	BI	75	LEU	3.0
45	DZ	52	SER	3.0
4	AD	87	GLY	3.0
10	AJ	36	GLY	3.0
16	AP	59	TRP	3.0
45	DZ	143	GLY	3.0
31	DH	92	ILE	3.0
53	D7	46	VAL	3.0
45	BZ	107	THR	3.0
1	CA	1038	C	3.0
9	CI	15	ALA	3.0
23	CW	2	C	3.0
25	DA	888	C	3.0
11	CK	75	TYR	3.0
24	AX	47	U	3.0
3	AC	204	LEU	3.0
13	CM	90	LEU	3.0
32	DI	68	LEU	3.0
2	AB	195	ASP	3.0
1	CA	1003	G	3.0
25	BA	926	G	3.0
25	DA	2160	G	3.0
45	BZ	149	SER	3.0
5	CE	22	GLY	3.0
31	DH	174	GLY	3.0
2	AB	229	VAL	3.0
11	AK	13	GLN	3.0
11	AK	42	TRP	3.0
33	BN	131	GLN	3.0
3	AC	100	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
5	AE	10	MET	3.0
14	CN	5	ALA	3.0
39	DT	1	MET	3.0
2	CB	92	TYR	3.0
9	CI	114	TYR	3.0
44	DY	55	TYR	3.0
45	DZ	167	PRO	3.0
15	AO	88	ARG	3.0
14	CN	16	PHE	3.0
13	CM	122	LYS	3.0
1	AA	1033	G	3.0
1	AA	1034	G	3.0
25	BA	2902	G	3.0
9	AI	30	GLY	3.0
29	BF	208	GLY	3.0
31	BH	66	GLY	3.0
9	CI	27	THR	3.0
13	AM	5	ALA	3.0
25	BA	2164	C	3.0
25	BA	2905	C	3.0
45	BZ	150	LEU	3.0
1	AA	1025	U	3.0
1	AA	1531	A	3.0
25	DA	229	A	3.0
10	CJ	36	GLY	3.0
2	AB	15	VAL	2.9
25	DA	1171	G	2.9
47	D1	83	GLU	2.9
3	CC	65	ALA	2.9
13	CM	33	ALA	2.9
44	DY	65	ALA	2.9
20	CT	98	PRO	2.9
30	DG	12	TYR	2.9
41	DV	85	LYS	2.9
46	D0	4	LYS	2.9
50	B4	63	TYR	2.9
1	CA	1043	C	2.9
25	BA	270	C	2.9
9	AI	126	SER	2.9
23	CW	73	A	2.9
3	CC	2	GLY	2.9
13	CM	119	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	CB	39	ILE	2.9
10	CJ	75	ILE	2.9
4	AD	170	VAL	2.9
5	CE	51	VAL	2.9
31	DH	169	VAL	2.9
10	AJ	32	ALA	2.9
14	CN	10	ALA	2.9
25	BA	2147	G	2.9
25	DA	171	G	2.9
25	DA	2125	G	2.9
9	CI	19	LEU	2.9
7	CG	154	TYR	2.9
43	DX	69	TYR	2.9
11	AK	117	ASN	2.9
46	B0	8	GLY	2.9
2	CB	143	GLU	2.9
31	BH	18	GLU	2.9
28	BE	77	ILE	2.9
2	AB	230	VAL	2.9
31	BH	35	VAL	2.9
7	AG	2	ALA	2.9
10	CJ	37	PRO	2.9
19	CS	24	ALA	2.9
27	BD	275	LYS	2.9
31	BH	13	LYS	2.9
45	DZ	150	LEU	2.9
52	D6	11	LEU	2.9
1	AA	1032	G	2.9
1	AA	1036	G	2.9
1	CA	1034	G	2.9
25	BA	2813	G	2.9
9	AI	125	TYR	2.9
3	AC	205	GLY	2.9
4	CD	167	GLY	2.9
2	CB	208	ILE	2.9
9	CI	74	ILE	2.9
25	BA	2186	C	2.9
10	CJ	68	HIS	2.9
23	CY	14	A	2.9
25	BA	1219	A	2.9
25	BA	2157	A	2.9
25	BA	2901	A	2.9

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Mol	Chain	Res	Type	RSRZ
30	BG	83	ARG	2.9
9	AI	64	THR	2.9
10	CJ	42	THR	2.9
9	CI	36	TYR	2.9
14	CN	21	TYR	2.9
25	DA	2166	G	2.9
4	AD	179	GLU	2.9
2	CB	66	GLY	2.9
30	DG	42	GLY	2.9
7	CG	5	ARG	2.8
27	DD	275	LYS	2.8
30	BG	182	LYS	2.8
46	D0	5	LYS	2.8
33	BN	5	VAL	2.8
50	B4	56	VAL	2.8
25	DA	1536	C	2.8
25	DA	2136	C	2.8
10	AJ	87	THR	2.8
2	CB	34	ALA	2.8
23	CY	35	A	2.8
39	BT	131	ALA	2.8
45	DZ	173	ALA	2.8
32	DI	38	LEU	2.8
2	AB	97	TRP	2.8
10	AJ	73	ASP	2.8
7	CG	26	PHE	2.8
13	CM	50	GLU	2.8
19	CS	10	PHE	2.8
27	BD	28	GLU	2.8
32	DI	135	GLU	2.8
21	AU	18	TYR	2.8
9	CI	10	ARG	2.8
27	BD	38	LYS	2.8
27	DD	38	LYS	2.8
41	DV	86	GLY	2.8
25	DA	2133	G	2.8
45	BZ	142	SER	2.8
3	CC	195	VAL	2.8
16	AP	2	VAL	2.8
19	CS	41	VAL	2.8
33	DN	9	VAL	2.8
9	CI	91	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
4	AD	49	ARG	2.8
3	CC	185	GLY	2.8
9	CI	62	TYR	2.8
9	CI	92	TYR	2.8
14	CN	51	GLY	2.8
45	DZ	121	HIS	2.8
30	BG	88	ILE	2.8
45	DZ	142	SER	2.8
13	CM	60	VAL	2.8
28	DE	59	VAL	2.8
29	DF	6	VAL	2.8
1	CA	1030(A)	G	2.8
25	BA	2182	G	2.8
25	DA	2802	G	2.8
1	CA	1020	U	2.8
2	CB	67	THR	2.8
25	BA	2135	U	2.8
20	AT	10	LEU	2.8
25	BA	933	C	2.8
26	DB	88	C	2.8
25	BA	2139	A	2.8
26	DB	120	A	2.8
3	CC	190	ARG	2.8
9	CI	105	ASP	2.8
9	AI	8	GLY	2.8
13	CM	100	GLY	2.8
19	CS	8	GLY	2.8
50	B4	4	GLY	2.8
50	B4	45	GLY	2.8
3	CC	193	TYR	2.8
6	AF	19	LEU	2.8
7	CG	12	LEU	2.8
10	AJ	100	THR	2.8
15	AO	57	LEU	2.8
20	AT	43	LEU	2.8
30	DG	161	THR	2.8
25	BA	924	U	2.8
25	BA	2906	U	2.8
25	DA	2144	U	2.8
25	DA	2150	U	2.8
24	AX	46	G	2.8
25	DA	2154	G	2.8

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Mol	Chain	Res	Type	RSRZ
1	AA	48	C	2.8
7	CG	4	ARG	2.8
54	D8	29	LYS	2.8
1	CA	1035	A	2.8
25	BA	2191	A	2.8
25	DA	2119	A	2.8
9	AI	105	ASP	2.8
2	AB	19	HIS	2.8
12	CL	63	GLY	2.7
2	CB	223	ILE	2.7
30	DG	52	ILE	2.7
21	CU	14	TRP	2.7
4	AD	189	PRO	2.7
8	AH	137	VAL	2.7
9	CI	109	VAL	2.7
10	CJ	49	VAL	2.7
7	AG	16	LEU	2.7
9	CI	52	ALA	2.7
16	CP	69	THR	2.7
45	DZ	125	LEU	2.7
30	DG	50	ALA	2.7
25	DA	2130	U	2.7
46	D0	24	LYS	2.7
48	D2	11	GLU	2.7
25	BA	2184	G	2.7
25	BA	2817	G	2.7
1	CA	1116	C	2.7
11	CK	36	ASP	2.7
16	AP	78	GLY	2.7
2	CB	32	ILE	2.7
2	CB	127	ILE	2.7
2	CB	222	ILE	2.7
3	CC	39	ILE	2.7
8	AH	80	ILE	2.7
14	CN	14	PRO	2.7
2	CB	81	VAL	2.7
13	CM	7	VAL	2.7
45	BZ	99	TYR	2.7
50	D4	50	VAL	2.7
4	AD	155	LEU	2.7
30	DG	139	LEU	2.7
13	CM	104	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
25	BA	1985	U	2.7
19	CS	14	HIS	2.7
19	CS	84	GLY	2.7
25	DA	2156	G	2.7
2	CB	55	PHE	2.7
2	CB	57	PHE	2.7
25	DA	652(B)	A	2.7
25	DA	2134	A	2.7
3	CC	77	ILE	2.7
9	CI	81	ILE	2.7
45	DZ	146	ILE	2.7
10	AJ	72	VAL	2.7
45	DZ	42	VAL	2.7
2	AB	11	LEU	2.7
2	CB	121	LEU	2.7
6	AF	63	TYR	2.7
19	CS	5	LEU	2.7
7	CG	65	ALA	2.7
9	CI	66	ARG	2.7
14	CN	12	ARG	2.7
29	BF	17	ARG	2.7
5	AE	20	GLN	2.7
1	AA	1257	U	2.7
3	CC	194	GLY	2.7
20	AT	69	GLY	2.7
31	DH	14	GLY	2.7
41	DV	30	GLY	2.7
46	D0	76	GLY	2.7
45	DZ	159	PRO	2.7
55	B9	17	ILE	2.7
1	CA	1001(A)	G	2.7
1	CA	1054	C	2.7
1	CA	1286	A	2.7
23	AY	19	G	2.7
23	CW	19	G	2.7
23	CY	1	G	2.7
23	AY	13	C	2.7
23	CW	4	C	2.7
25	DA	1847	A	2.7
2	CB	215	LEU	2.7
3	AC	66	VAL	2.7
20	AT	13	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
20	AT	62	LEU	2.7
30	BG	76	SER	2.7
19	AS	80	TYR	2.7
52	B6	4	GLU	2.7
10	AJ	10	GLY	2.6
28	DE	71	GLY	2.6
13	AM	39	ILE	2.6
21	CU	23	PRO	2.6
30	DG	20	ILE	2.6
31	DH	175	LYS	2.6
32	BI	109	ILE	2.6
45	BZ	104	PHE	2.6
53	D7	48	LYS	2.6
4	CD	132	ARG	2.6
13	CM	29	ARG	2.6
30	BG	51	ARG	2.6
45	BZ	112	ARG	2.6
7	CG	38	LEU	2.6
9	CI	99	LEU	2.6
19	CS	11	VAL	2.6
19	CS	16	LEU	2.6
25	BA	2162	C	2.6
25	BA	2179	G	2.6
25	DA	897	C	2.6
25	DA	2138	C	2.6
25	DA	2146	C	2.6
45	DZ	169	GLU	2.6
8	AH	28	ALA	2.6
10	CJ	32	ALA	2.6
44	DY	57	GLN	2.6
3	AC	2	GLY	2.6
5	AE	23	GLY	2.6
20	AT	103	GLY	2.6
31	DH	91	GLY	2.6
2	CB	234	PRO	2.6
45	BZ	146	ILE	2.6
55	D9	17	ILE	2.6
5	CE	18	ARG	2.6
31	BH	6	ARG	2.6
38	DS	61	ASN	2.6
3	CC	75	VAL	2.6
32	DI	41	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
25	BA	2141	A	2.6
45	BZ	166	SER	2.6
9	AI	13	ALA	2.6
16	AP	45	THR	2.6
37	DR	101	ALA	2.6
45	BZ	170	THR	2.6
1	AA	1030(C)	G	2.6
4	CD	20	TYR	2.6
25	DA	892	G	2.6
42	BW	111	HIS	2.6
2	AB	18	GLY	2.6
9	CI	100	GLY	2.6
4	AD	73	ARG	2.6
8	AH	84	ARG	2.6
9	CI	49	PRO	2.6
10	CJ	79	ARG	2.6
13	AM	102	ARG	2.6
14	CN	7	ILE	2.6
14	CN	42	ILE	2.6
16	AP	4	ILE	2.6
31	DH	151	ILE	2.6
38	DS	20	ARG	2.6
43	DX	68	ARG	2.6
2	CB	69	LEU	2.6
9	AI	56	LEU	2.6
46	B0	7	LEU	2.6
32	BI	107	VAL	2.6
11	AK	89	ALA	2.6
44	DY	78	ALA	2.6
1	CA	1503	A	2.6
23	CY	23	A	2.6
25	DA	2135	A	2.6
1	AA	1397	C	2.6
1	CA	630	G	2.6
1	CA	998	G	2.6
23	AY	1	G	2.6
25	DA	2151	G	2.6
11	CK	49	GLY	2.6
2	CB	185	ILE	2.6
1	CA	1532	U	2.6
9	CI	18	PHE	2.6
17	AQ	27	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	AB	187	LEU	2.6
4	CD	188	LEU	2.6
10	AJ	88	LEU	2.6
45	BZ	2	GLU	2.6
7	CG	37	ASN	2.6
6	AF	16	GLN	2.6
7	CG	66	VAL	2.6
13	CM	18	ALA	2.6
29	BF	15	SER	2.6
1	AA	1030(D)	A	2.6
20	CT	8	ARG	2.5
25	BA	2159	C	2.5
5	CE	74	GLY	2.5
31	BH	21	PRO	2.5
31	BH	174	GLY	2.5
39	BT	107	ASP	2.5
45	DZ	98	MET	2.5
48	D2	1	MET	2.5
1	CA	1190	G	2.5
10	AJ	75	ILE	2.5
23	CY	24	G	2.5
25	DA	2157	G	2.5
25	DA	2319	G	2.5
6	AF	60	PHE	2.5
9	AI	59	PHE	2.5
2	CB	61	LEU	2.5
8	AH	112	LEU	2.5
32	BI	140	LEU	2.5
2	CB	94	ASN	2.5
2	CB	164	VAL	2.5
2	AB	16	HIS	2.5
10	CJ	62	HIS	2.5
12	AL	126	LYS	2.5
13	CM	76	ALA	2.5
14	CN	20	ALA	2.5
35	BP	12	ALA	2.5
41	DV	92	THR	2.5
15	AO	68	ARG	2.5
1	CA	1004	A	2.5
1	CA	1005	A	2.5
16	AP	38	TYR	2.5
25	BA	302	A	2.5

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Mol	Chain	Res	Type	RSRZ
25	BA	572	A	2.5
25	DA	2114	A	2.5
44	BY	1	MET	2.5
1	AA	1028	C	2.5
2	AB	228	GLY	2.5
5	AE	85	GLY	2.5
10	CJ	58	ASP	2.5
25	BA	2165	C	2.5
40	DU	73	GLY	2.5
45	DZ	148	ASP	2.5
2	AB	200	ILE	2.5
13	CM	39	ILE	2.5
15	AO	3	ILE	2.5
2	AB	9	GLU	2.5
8	CH	2	LEU	2.5
10	CJ	54	PHE	2.5
1	CA	1031	G	2.5
13	AM	90	LEU	2.5
14	CN	6	LEU	2.5
25	BA	927	G	2.5
25	DA	1533	G	2.5
25	DA	2206	G	2.5
45	DZ	155	LEU	2.5
9	CI	86	VAL	2.5
11	AK	106	LYS	2.5
19	CS	19	VAL	2.5
30	DG	182	LYS	2.5
46	B0	5	LYS	2.5
2	AB	13	ALA	2.5
32	BI	146	ALA	2.5
43	DX	35	THR	2.5
2	AB	53	ARG	2.5
14	CN	29	ARG	2.5
21	CU	9	ARG	2.5
31	BH	42	ARG	2.5
54	D8	4	MET	2.5
1	CA	977	A	2.5
1	CA	983	A	2.5
19	AS	8	GLY	2.5
47	D1	28	GLY	2.5
3	CC	157	ILE	2.5
10	CJ	6	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
25	DA	2137	C	2.5
54	D8	34	TRP	2.5
2	CB	152	PHE	2.5
3	CC	47	LEU	2.5
9	CI	96	LEU	2.5
14	AN	16	PHE	2.5
16	AP	74	LEU	2.5
30	BG	139	LEU	2.5
31	BH	171	LEU	2.5
4	AD	86	LYS	2.5
13	CM	92	HIS	2.5
3	AC	98	ASN	2.5
14	AN	33	VAL	2.5
25	BA	2818	U	2.5
1	AA	1001(A)	G	2.5
1	CA	1030(C)	G	2.5
1	CA	1033	G	2.5
23	AY	24	G	2.5
25	DA	2207	G	2.5
25	DA	2793	G	2.5
3	CC	60	ALA	2.5
7	CG	2	ALA	2.5
13	CM	28	ALA	2.5
49	D3	29	ARG	2.5
8	CH	67	PRO	2.5
3	CC	25	GLY	2.5
4	AD	180	GLY	2.5
4	CD	192	GLU	2.5
12	AL	14	GLY	2.5
20	CT	101	GLY	2.5
29	DF	131	GLY	2.5
8	AH	134	ILE	2.5
20	AT	55	ILE	2.5
27	BD	71	ASP	2.5
2	CB	51	LEU	2.5
4	CD	78	LEU	2.5
43	BX	95	LEU	2.5
44	DY	34	LYS	2.5
16	AP	80	PHE	2.5
2	CB	136	VAL	2.5
3	AC	76	VAL	2.5
4	CD	198	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
7	CG	21	VAL	2.5
8	CH	51	VAL	2.5
3	AC	190	ARG	2.5
14	AN	3	ARG	2.5
9	AI	119	ALA	2.5
18	CR	60	ALA	2.5
14	CN	22	THR	2.5
17	AQ	99	SER	2.5
25	BA	162	G	2.5
25	DA	2165	G	2.5
31	DH	10	PRO	2.4
5	CE	114	GLY	2.4
7	AG	8	GLU	2.4
35	BP	82	GLY	2.4
38	DS	109	GLY	2.4
55	D9	21	GLY	2.4
8	CH	48	TYR	2.4
9	CI	75	ASP	2.4
9	CI	97	LYS	2.4
11	CK	59	TYR	2.4
19	CS	52	TYR	2.4
31	DH	25	LYS	2.4
47	D1	78	LYS	2.4
2	CB	145	LEU	2.4
3	AC	47	LEU	2.4
4	CD	194	LEU	2.4
35	BP	148	LEU	2.4
3	CC	186	PHE	2.4
9	CI	101	PHE	2.4
10	CJ	13	HIS	2.4
19	CS	81	ARG	2.4
3	AC	151	VAL	2.4
3	CC	99	VAL	2.4
9	AI	65	VAL	2.4
17	CQ	9	VAL	2.4
31	DH	79	VAL	2.4
1	CA	1150	U	2.4
4	AD	195	ALA	2.4
9	AI	15	ALA	2.4
9	CI	119	ALA	2.4
10	CJ	27	ALA	2.4
17	CQ	82	MET	2.4

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Mol	Chain	Res	Type	RSRZ
18	AR	20	ALA	2.4
18	CR	20	ALA	2.4
30	BG	2	PRO	2.4
48	D2	66	GLU	2.4
1	CA	1117	G	2.4
1	CA	1202	G	2.4
4	CD	87	GLY	2.4
19	CS	46	GLY	2.4
20	CT	96	GLY	2.4
25	BA	694	G	2.4
25	DA	2112	G	2.4
45	DZ	160	GLY	2.4
46	D0	42	GLY	2.4
9	CI	63	ILE	2.4
11	AK	36	ASP	2.4
2	CB	102	LEU	2.4
18	AR	31	LEU	2.4
20	CT	62	LEU	2.4
30	DG	146	TYR	2.4
31	DH	88	LEU	2.4
50	D4	25	TYR	2.4
4	CD	73	ARG	2.4
4	CD	115	ARG	2.4
10	AJ	63	PHE	2.4
53	D7	47	ARG	2.4
1	AA	1005	A	2.4
25	BA	1091	A	2.4
25	BA	1878	A	2.4
25	BA	2136	A	2.4
25	DA	2126	A	2.4
5	AE	67	VAL	2.4
13	CM	40	ASN	2.4
20	CT	26	ASN	2.4
1	CA	1019	C	2.4
4	CD	48	ALA	2.4
11	AK	15	ALA	2.4
23	CY	13	C	2.4
1	AA	65	U	2.4
1	CA	1126	U	2.4
4	AD	89	THR	2.4
3	AC	206	GLU	2.4
9	CI	110	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
16	AP	41	PRO	2.4
30	DG	2	PRO	2.4
13	CM	65	LYS	2.4
14	CN	11	LYS	2.4
27	DD	276	LYS	2.4
30	DG	30	GLU	2.4
35	DP	76	LYS	2.4
9	CI	57	GLY	2.4
12	AL	95	GLY	2.4
13	CM	68	GLY	2.4
29	BF	16	GLY	2.4
29	BF	131	GLY	2.4
2	AB	222	ILE	2.4
1	CA	976	G	2.4
2	AB	221	LEU	2.4
15	CO	9	GLN	2.4
25	BA	2178	G	2.4
25	BA	2187	G	2.4
25	DA	2148	G	2.4
47	B1	82	LEU	2.4
13	CM	87	TYR	2.4
10	AJ	47	PHE	2.4
4	AD	165	MET	2.4
13	CM	53	VAL	2.4
17	CQ	23	VAL	2.4
31	DH	76	VAL	2.4
45	BZ	141	VAL	2.4
51	B5	60	VAL	2.4
1	AA	1035	A	2.4
22	AV	13	A	2.4
29	DF	160	ASN	2.4
3	CC	100	ALA	2.4
2	CB	47	THR	2.4
8	AH	3	THR	2.4
9	CI	98	PRO	2.4
14	CN	17	LYS	2.4
28	BE	73	GLU	2.4
31	BH	32	GLU	2.4
43	DX	33	LYS	2.4
50	D4	52	THR	2.4
1	AA	343	U	2.4
1	AA	1029	C	2.4

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Mol	Chain	Res	Type	RSRZ
1	AA	1030	C	2.4
1	CA	1045	C	2.4
23	AY	12	U	2.4
25	BA	2152	U	2.4
25	DA	886	C	2.4
28	DE	74	PRO	2.4
45	DZ	129	SER	2.4
7	AG	81	GLY	2.4
4	AD	191	ARG	2.4
6	AF	14	LEU	2.4
10	AJ	85	LEU	2.4
10	CJ	46	ARG	2.4
10	CJ	70	ARG	2.4
14	AN	35	ARG	2.4
30	DG	136	ARG	2.4
30	DG	147	ASP	2.4
38	DS	17	ARG	2.4
45	BZ	125	LEU	2.4
53	B7	47	ARG	2.4
1	CA	973	G	2.4
1	CA	1385	G	2.4
2	CB	148	TYR	2.4
25	DA	2127	G	2.4
36	DQ	104	PHE	2.4
10	CJ	44	VAL	2.4
13	CM	54	VAL	2.4
31	DH	45	VAL	2.4
40	DU	90	VAL	2.4
44	DY	3	VAL	2.4
45	DZ	90	VAL	2.4
10	CJ	69	ASN	2.4
3	AC	53	ALA	2.4
22	AV	12	A	2.4
22	CV	14	A	2.4
25	BA	937	A	2.4
25	BA	2812	A	2.4
27	BD	2	ALA	2.4
2	CB	126	GLU	2.4
9	AI	90	PRO	2.3
10	CJ	48	THR	2.3
14	AN	14	PRO	2.3
32	DI	137	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
44	DY	82	PRO	2.3
23	AW	20	U	2.3
25	BA	941	U	2.3
2	AB	227	GLY	2.3
9	CI	115	GLY	2.3
23	AY	67	C	2.3
24	AX	69	C	2.3
2	CB	80	ILE	2.3
4	AD	131	ARG	2.3
14	CN	23	ARG	2.3
30	DG	115	ARG	2.3
35	BP	79	ARG	2.3
45	DZ	81	ARG	2.3
45	DZ	103	ARG	2.3
13	CM	70	LEU	2.3
29	DF	12	LEU	2.3
30	BG	3	LEU	2.3
45	BZ	151	HIS	2.3
45	BZ	155	LEU	2.3
48	B2	70	GLN	2.3
28	BE	1	MET	2.3
2	AB	28	PHE	2.3
28	DE	151	TYR	2.3
44	DY	35	TYR	2.3
45	DZ	9	TYR	2.3
45	DZ	89	PHE	2.3
9	CI	26	VAL	2.3
20	AT	74	LYS	2.3
1	CA	1032	G	2.3
4	AD	154	ASN	2.3
10	AJ	76	ASN	2.3
23	AW	70	G	2.3
25	BA	11	G	2.3
25	BA	1152	G	2.3
25	DA	881	G	2.3
10	AJ	83	GLU	2.3
12	AL	94	PRO	2.3
1	CA	1041	A	2.3
7	CG	3	ARG	2.3
7	CG	115	ARG	2.3
9	AI	128	ARG	2.3
13	AM	26	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
29	DF	16	GLY	2.3
31	BH	14	GLY	2.3
31	DH	48	GLY	2.3
49	B3	55	ARG	2.3
1	CA	1148	U	2.3
9	CI	124	GLN	2.3
25	DA	2132	U	2.3
20	AT	100	ILE	2.3
40	BU	117	GLN	2.3
3	AC	87	LEU	2.3
10	AJ	90	LEU	2.3
32	DI	75	LEU	2.3
44	DY	44	ILE	2.3
44	DY	75	ILE	2.3
45	DZ	163	LEU	2.3
1	CA	999	C	2.3
23	AW	2	C	2.3
25	BA	670	C	2.3
25	BA	940	C	2.3
45	DZ	1	MET	2.3
11	CK	124	LYS	2.3
14	CN	40	CYS	2.3
36	DQ	22	LYS	2.3
50	D4	38	LYS	2.3
3	AC	207	VAL	2.3
3	CC	23	TYR	2.3
7	CG	151	TYR	2.3
8	AH	53	VAL	2.3
10	CJ	72	VAL	2.3
45	BZ	161	VAL	2.3
7	CG	40	ALA	2.3
31	BH	168	PRO	2.3
33	DN	44	PRO	2.3
1	AA	104	G	2.3
1	CA	1024	G	2.3
13	AM	49	THR	2.3
13	CM	49	THR	2.3
9	AI	9	ARG	2.3
10	AJ	79	ARG	2.3
1	CA	1183	A	2.3
3	CC	41	GLY	2.3
19	CS	34	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
38	DS	45	GLY	2.3
2	CB	42	ILE	2.3
4	AD	96	LEU	2.3
4	CD	5	ILE	2.3
4	CD	19	LEU	2.3
20	CT	100	ILE	2.3
31	DH	7	LEU	2.3
31	DH	103	LEU	2.3
40	DU	88	ILE	2.3
44	DY	61	ILE	2.3
45	BZ	171	ILE	2.3
45	DZ	120	ILE	2.3
25	BA	12	U	2.3
25	BA	1220	U	2.3
25	DA	2167	U	2.3
25	DA	1509	C	2.3
25	DA	2789	C	2.3
50	B4	69	LYS	2.3
9	AI	33	PHE	2.3
16	AP	9	PHE	2.3
2	AB	126	GLU	2.3
2	CB	93	VAL	2.3
16	AP	21	VAL	2.3
45	DZ	119	GLU	2.3
30	BG	25	TYR	2.3
49	D3	59	VAL	2.3
54	D8	64	TYR	2.3
2	CB	88	ALA	2.3
3	CC	129	ALA	2.3
4	CD	154	ASN	2.3
9	AI	46	ALA	2.3
13	CM	72	ALA	2.3
31	BH	20	ALA	2.3
31	DH	39	PRO	2.3
32	DI	146	ALA	2.3
34	DO	29	ASN	2.3
13	CM	110	ARG	2.3
39	DT	111	ARG	2.3
50	B4	55	ARG	2.3
12	AL	6	THR	2.3
16	AP	22	THR	2.3
21	CU	17	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	CC	31	HIS	2.3
5	CE	20	GLN	2.3
7	AG	110	GLN	2.3
15	CO	61	GLY	2.3
19	AS	4	SER	2.3
1	AA	607	A	2.3
3	CC	18	TRP	2.3
9	AI	74	ILE	2.3
20	CT	99	LEU	2.3
25	BA	569	G	2.3
25	BA	2188	G	2.3
35	DP	1	MET	2.3
45	DZ	28	MET	2.3
2	AB	27	LYS	2.3
25	BA	9	U	2.3
17	CQ	96	GLU	2.3
25	BA	696	C	2.3
25	BA	2197	C	2.3
30	DG	48	GLU	2.3
3	CC	88	ARG	2.3
5	AE	96	PRO	2.3
5	CE	133	TYR	2.3
16	AP	75	ARG	2.3
31	DH	112	PRO	2.3
9	AI	76	ALA	2.2
9	CI	13	ALA	2.2
9	CI	45	ALA	2.2
9	CI	82	ALA	2.2
11	CK	74	ALA	2.2
43	DX	18	TYR	2.3
50	B4	67	TYR	2.3
2	CB	16	HIS	2.2
9	CI	39	GLY	2.2
11	CK	102	GLY	2.2
35	BP	116	GLY	2.2
36	DQ	33	GLY	2.2
46	D0	80	HIS	2.2
2	AB	39	ILE	2.2
3	CC	202	ILE	2.2
8	AH	111	ILE	2.2
10	AJ	74	ILE	2.2
10	CJ	82	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
12	AL	17	LYS	2.2
13	AM	27	LYS	2.2
19	CS	15	LEU	2.2
30	BG	43	LEU	2.2
38	DS	58	LEU	2.2
44	DY	46	LYS	2.2
46	D0	37	LEU	2.2
1	CA	1044	A	2.2
27	DD	200	ASP	2.2
39	DT	124	ASP	2.2
1	CA	1036	G	2.2
23	AY	53	G	2.2
25	BA	2173	G	2.2
25	BA	2174	G	2.2
23	CY	45	U	2.2
25	DA	2118	U	2.2
2	CB	12	GLU	2.2
10	AJ	64	GLU	2.2
31	BH	34	GLU	2.2
9	AI	18	PHE	2.2
36	DQ	65	PHE	2.2
1	CA	1260	C	2.2
3	CC	68	VAL	2.2
3	CC	151	VAL	2.2
4	AD	3	ARG	2.2
4	AD	139	ARG	2.2
5	CE	25	ARG	2.2
7	CG	155	ARG	2.2
9	AI	14	VAL	2.2
10	AJ	66	ARG	2.2
13	CM	41	PRO	2.2
14	AN	23	ARG	2.2
19	CS	58	VAL	2.2
27	BD	262	ARG	2.2
28	BE	72	VAL	2.2
31	BH	113	VAL	2.2
39	BT	125	ARG	2.2
5	AE	48	ALA	2.2
9	CI	94	ALA	2.2
13	CM	51	ALA	2.2
52	D6	20	ASN	2.2
4	AD	138	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
11	AK	104	GLN	2.2
48	D2	43	GLN	2.2
4	CD	2	GLY	2.2
9	CI	67	GLY	2.2
10	CJ	31	GLY	2.2
12	CL	126	LYS	2.2
14	AN	51	GLY	2.2
21	AU	2	GLY	2.2
21	CU	11	GLY	2.2
37	DR	7	GLY	2.2
2	CB	118	LEU	2.2
4	CD	196	LEU	2.2
5	CE	53	LEU	2.2
5	CE	71	LEU	2.2
9	AI	19	LEU	2.2
13	CM	34	LEU	2.2
19	CS	71	LEU	2.2
29	DF	196	LEU	2.2
8	CH	29	SER	2.2
45	DZ	137	ILE	2.2
2	AB	193	ASP	2.2
4	AD	53	ASP	2.2
9	AI	32	ASP	2.2
16	CP	59	TRP	2.2
3	CC	19	GLU	2.2
5	CE	50	GLU	2.2
44	BY	91	GLU	2.2
1	AA	1026	G	2.2
4	AD	118	ARG	2.2
7	CG	32	ARG	2.2
10	CJ	5	ARG	2.2
23	AY	22	G	2.2
23	CY	5	G	2.2
24	CX	2	G	2.2
24	CX	70	G	2.2
25	DA	10	G	2.2
25	DA	879	G	2.2
25	DA	880	G	2.2
8	AH	31	PHE	2.2
15	AO	19	PRO	2.2
36	DQ	109	VAL	2.2
45	DZ	96	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
45	DZ	128	VAL	2.2
50	D4	29	PRO	2.2
55	D9	3	VAL	2.2
2	CB	225	ALA	2.2
9	CI	46	ALA	2.2
14	CN	30	ALA	2.2
25	DA	2140	C	2.2
34	BO	89	ASN	2.2
3	CC	107	GLN	2.2
16	AP	17	TYR	2.2
19	AS	83	HIS	2.2
32	DI	129	THR	2.2
36	DQ	113	GLN	2.2
38	DS	33	LYS	2.2
2	CB	48	MET	2.2
2	AB	196	LEU	2.2
4	AD	2	GLY	2.2
4	AD	108	LEU	2.2
4	AD	202	LEU	2.2
9	CI	50	LEU	2.2
30	DG	119	GLY	2.2
31	BH	5	GLY	2.2
38	DS	24	LEU	2.2
44	DY	25	GLY	2.2
44	DY	104	GLY	2.2
21	CU	13	ILE	2.2
30	BG	77	ILE	2.2
16	AP	23	ASP	2.2
29	BF	23	ASP	2.2
42	DW	63	ASP	2.2
29	DF	161	GLU	2.2
45	DZ	2	GLU	2.2
2	CB	36	ARG	2.2
2	CB	130	ARG	2.2
5	CE	24	ARG	2.2
13	CM	88	ARG	2.2
16	AP	25	ARG	2.2
47	D1	26	ARG	2.2
23	AY	20	U	2.2
25	BA	1072	U	2.2
25	DA	899	A	2.2
9	CI	21	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
31	DH	123	PHE	2.2
39	DT	57	PHE	2.2
43	DX	21	PHE	2.2
8	AH	61	VAL	2.2
13	AM	117	VAL	2.2
55	D9	16	VAL	2.2
1	CA	485	G	2.2
23	CY	57	G	2.2
24	AX	2	G	2.2
25	DA	2149	G	2.2
4	CD	195	ALA	2.2
43	DX	22	ALA	2.2
44	DY	6	HIS	2.2
3	CC	196	LEU	2.2
4	AD	162	LEU	2.2
8	AH	47	GLY	2.2
9	AI	102	LEU	2.2
19	AS	82	GLY	2.2
19	CS	22	LEU	2.2
24	AX	67	C	2.2
25	BA	939	C	2.2
25	BA	2129	C	2.2
25	BA	2158	C	2.2
25	DA	2111	C	2.2
30	DG	25	TYR	2.2
35	DP	93	GLY	2.2
45	DZ	110	GLY	2.2
2	AB	182	ILE	2.2
3	AC	124	ILE	2.2
14	AN	7	ILE	2.2
31	BH	4	ILE	2.2
2	CB	192	SER	2.2
27	DD	22	SER	2.2
8	AH	54	ASP	2.2
45	BZ	145	GLU	2.2
5	AE	18	ARG	2.2
8	CH	30	ARG	2.2
15	CO	68	ARG	2.2
21	AU	24	ARG	2.2
32	DI	103	ARG	2.2
50	D4	48	ARG	2.2
19	CS	59	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
30	DG	29	TRP	2.2
1	AA	160	A	2.1
3	CC	4	LYS	2.2
13	CM	31	LYS	2.2
15	AO	5	LYS	2.2
17	CQ	14	LYS	2.2
25	BA	1554	A	2.1
25	BA	2172	U	2.2
27	DD	15	PHE	2.2
30	DG	180	PHE	2.2
45	DZ	104	PHE	2.2
2	AB	93	VAL	2.1
16	AP	51	VAL	2.1
31	BH	24	VAL	2.1
31	BH	37	VAL	2.1
31	DH	114	VAL	2.1
32	BI	127	VAL	2.1
2	AB	120	ALA	2.1
2	CB	40	HIS	2.1
2	CB	77	ALA	2.1
19	CS	47	HIS	2.1
3	CC	162	GLN	2.1
3	CC	170	GLN	2.1
34	DO	51	ALA	2.1
1	AA	1024	G	2.1
1	CA	1127	G	2.1
8	CH	10	LEU	2.1
13	CM	105	THR	2.1
14	CN	47	LEU	2.1
25	BA	938	G	2.1
25	BA	2177	G	2.1
25	BA	2190	G	2.1
25	DA	545	G	2.1
25	DA	2893	G	2.1
31	DH	171	LEU	2.1
32	BI	72	LEU	2.1
50	D4	44	THR	2.1
2	AB	31	TYR	2.1
4	AD	70	ILE	2.1
10	AJ	82	ILE	2.1
11	AK	25	TYR	2.1
19	CS	31	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
30	BG	140	ILE	2.1
23	AY	48	C	2.1
25	BA	2130	C	2.1
25	DA	2128	C	2.1
2	AB	30	ARG	2.1
15	AO	64	ARG	2.1
30	DG	54	GLU	2.1
50	D4	30	GLU	2.1
6	AF	55	ASP	2.1
39	DT	107	ASP	2.1
2	CB	91	PRO	2.1
4	AD	169	LYS	2.1
9	AI	21	PRO	2.1
10	AJ	80	LYS	2.1
10	CJ	91	PRO	2.1
3	CC	128	PHE	2.1
14	AN	18	VAL	2.1
45	DZ	141	VAL	2.1
4	AD	181	MET	2.1
23	CY	60	U	2.1
25	DA	12	U	2.1
25	DA	157	U	2.1
25	DA	1026	U	2.1
25	DA	2113	U	2.1
2	AB	207	ALA	2.1
16	AP	70	ALA	2.1
25	BA	2198	A	2.1
3	CC	32	LEU	2.1
7	CG	130	GLY	2.1
8	AH	59	LEU	2.1
31	DH	82	GLY	2.1
35	DP	44	GLY	2.1
41	DV	17	GLY	2.1
45	BZ	160	GLY	2.1
2	AB	214	ILE	2.1
3	CC	57	ILE	2.1
3	CC	124	ILE	2.1
5	AE	11	ILE	2.1
7	AG	50	ILE	2.1
17	CQ	90	ILE	2.1
31	BH	92	ILE	2.1
32	DI	109	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	AA	346	G	2.1
2	AB	231	GLU	2.1
9	AI	88	TYR	2.1
10	AJ	29	ARG	2.1
12	CL	64	TYR	2.1
16	CP	26	ARG	2.1
17	CQ	49	GLU	2.1
20	CT	86	ARG	2.1
32	BI	57	ARG	2.1
25	BA	269	G	2.1
25	BA	299	G	2.1
25	BA	2176	G	2.1
45	BZ	135	GLU	2.1
1	CA	1244	C	2.1
4	CD	71	SER	2.1
5	CE	5	ASP	2.1
10	CJ	19	SER	2.1
10	CJ	59	SER	2.1
25	BA	2210	C	2.1
25	DA	2164	C	2.1
30	BG	156	ASP	2.1
31	BH	25	LYS	2.1
47	D1	48	LYS	2.1
10	CJ	39	PRO	2.1
41	DV	50	PRO	2.1
16	CP	9	PHE	2.1
4	AD	104	VAL	2.1
7	AG	86	GLN	2.1
11	CK	105	VAL	2.1
27	DD	112	GLN	2.1
32	BI	136	VAL	2.1
33	DN	5	VAL	2.1
1	CA	981	U	2.1
3	AC	50	ALA	2.1
3	CC	92	ALA	2.1
8	AH	138	TRP	2.1
21	AU	14	TRP	2.1
49	D3	21	ALA	2.1
1	AA	1286	A	2.1
2	CB	138	LEU	2.1
4	AD	157	LEU	2.1
10	CJ	15	THR	2.1

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Mol	Chain	Res	Type	RSRZ
15	AO	89	GLY	2.1
16	CP	74	LEU	2.1
25	BA	554	A	2.1
25	DA	2173	A	2.1
45	BZ	163	LEU	2.1
15	CO	4	THR	2.1
21	CU	24	ARG	2.1
3	CC	134	ILE	2.1
4	AD	5	ILE	2.1
13	AM	25	ILE	2.1
15	CO	3	ILE	2.1
39	DT	52	ILE	2.1
45	DZ	133	ILE	2.1
4	AD	68	TYR	2.1
4	AD	207	TYR	2.1
12	AL	64	TYR	2.1
49	D3	15	TYR	2.1
50	D4	43	TYR	2.1
10	AJ	57	LYS	2.1
28	DE	69	LYS	2.1
52	D6	53	LYS	2.1
34	DO	28	SER	2.1
23	CY	6	G	2.1
23	CY	53	G	2.1
23	CY	69	G	2.1
1	AA	91	C	2.1
1	CA	1006	C	2.1
1	CA	1007	C	2.1
25	BA	2185	C	2.1
25	DA	2175	C	2.1
2	CB	83	MET	2.1
3	AC	10	PHE	2.1
8	AH	70	GLN	2.1
4	CD	88	VAL	2.1
7	CG	69	VAL	2.1
8	AH	93	VAL	2.1
11	AK	125	PHE	2.1
27	DD	18	VAL	2.1
31	DH	49	VAL	2.1
45	DZ	139	VAL	2.1
28	DE	131	ALA	2.1
29	DF	130	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
31	DH	156	ALA	2.1
1	CA	1000	U	2.1
2	AB	24	TRP	2.1
2	CB	137	ARG	2.1
4	CD	21	LEU	2.1
7	CG	103	TRP	2.1
3	AC	96	GLY	2.1
9	CI	111	ARG	2.1
23	CY	33	U	2.1
23	CY	59	U	2.1
25	BA	2194	U	2.1
25	DA	2172	U	2.1
44	DY	50	ARG	2.1
44	DY	106	LEU	2.1
2	AB	129	GLU	2.1
4	AD	80	GLU	2.1
30	BG	54	GLU	2.1
41	DV	32	THR	2.1
45	DZ	145	GLU	2.1
1	AA	1001	A	2.1
3	CC	5	ILE	2.1
4	AD	204	ILE	2.1
25	BA	702	A	2.1
25	DA	887	A	2.1
35	BP	75	ILE	2.1
13	CM	46	LYS	2.1
30	BG	75	LYS	2.1
6	CF	55	ASP	2.1
10	CJ	73	ASP	2.1
35	DP	110	TYR	2.1
17	AQ	28	PRO	2.1
21	AU	23	PRO	2.1
31	BH	36	PRO	2.1
32	DI	8	PRO	2.1
5	CE	10	MET	2.1
23	CW	15	G	2.0
25	BA	2903	G	2.0
9	AI	37	PHE	2.0
28	DE	72	VAL	2.0
30	DG	80	PHE	2.0
35	DP	146	VAL	2.0
41	DV	51	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
45	BZ	165	VAL	2.0
46	D0	57	PHE	2.0
46	D0	79	VAL	2.0
51	D5	60	VAL	2.0
3	CC	187	ALA	2.0
4	AD	47	ARG	2.0
5	CE	146	ALA	2.0
7	AG	127	ALA	2.0
7	CG	79	ARG	2.0
9	AI	10	ARG	2.0
19	CS	3	ARG	2.0
30	BG	136	ARG	2.0
30	DG	83	ARG	2.0
33	BN	115	ARG	2.0
44	DY	48	ALA	2.0
45	DZ	4	ARG	2.0
3	CC	12	LEU	2.0
48	D2	10	LEU	2.0
49	D3	23	LEU	2.0
2	CB	65	GLY	2.0
3	AC	19	GLU	2.0
4	CD	69	GLY	2.0
32	DI	16	GLY	2.0
47	D1	31	GLY	2.0
1	CA	992	U	2.0
3	CC	8	ILE	2.0
7	CG	42	ILE	2.0
9	CI	78	LYS	2.0
12	CL	61	THR	2.0
13	AM	4	ILE	2.0
16	CP	45	THR	2.0
19	AS	79	THR	2.0
19	CS	48	THR	2.0
23	AY	45	U	2.0
23	CW	45	U	2.0
32	BI	79	ILE	2.0
39	DT	102	ILE	2.0
22	CV	24	A	2.0
2	CB	232	PRO	2.0
2	AB	48	MET	2.0
3	AC	49	SER	2.0
5	CE	70	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
20	CT	82	SER	2.0
31	BH	112	PRO	2.0
31	DH	21	PRO	2.0
16	AP	1	MET	2.0
31	BH	41	MET	2.0
7	CG	86	GLN	2.0
1	AA	345	C	2.0
1	CA	962	C	2.0
2	CB	7	VAL	2.0
2	CB	144	ARG	2.0
2	CB	226	ARG	2.0
3	CC	86	VAL	2.0
9	AI	26	VAL	2.0
9	CI	65	VAL	2.0
13	CM	17	VAL	2.0
13	CM	98	VAL	2.0
16	AP	79	VAL	2.0
23	AY	56	C	2.0
25	DA	2794	C	2.0
31	BH	23	ARG	2.0
35	BP	83	VAL	2.0
43	DX	81	VAL	2.0
44	DY	89	PHE	2.0
48	D2	25	VAL	2.0
1	AA	78	G	2.0
1	AA	1002	G	2.0
1	CA	1154	G	2.0
25	BA	1218	G	2.0
25	DA	271(M)	G	2.0
25	DA	2153	G	2.0
4	AD	78	LEU	2.0
36	DQ	53	ALA	2.0
45	DZ	67	LEU	2.0
2	CB	38	GLY	2.0
3	CC	51	GLY	2.0
3	CC	72	LYS	2.0
27	DD	238	GLY	2.0
44	BY	92	ASN	2.0
44	DY	95	LYS	2.0
2	CB	200	ILE	2.0
8	AH	24	THR	2.0
20	CT	63	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
35	DP	75	ILE	2.0
36	DQ	75	THR	2.0
40	DU	62	ILE	2.0
1	CA	1040	U	2.0
1	CA	1281	U	2.0
23	CY	47	U	2.0
1	CA	969	A	2.0
1	CA	1250	A	2.0
3	CC	62	ASP	2.0
25	BA	925	A	2.0
25	BA	946	A	2.0
34	BO	112	MET	2.0
13	CM	23	TYR	2.0
20	CT	11	SER	2.0
31	BH	63	SER	2.0
32	DI	130	TYR	2.0
47	D1	86	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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	PSU	CY	55	20/21	0.64	0.15	92,98,105,119	0
23	MIA	CY	37	22/30	0.65	0.19	82,93,117,140	0
23	7MG	AY	46	24/25	0.66	0.17	80,94,107,121	0
23	PSU	AY	55	20/21	0.69	0.17	93,99,105,118	0
23	4SU	AY	8	20/21	0.70	0.15	92,98,108,126	0
23	7MG	CY	46	24/25	0.71	0.17	86,95,102,125	0
23	5MU	CY	54	21/22	0.72	0.19	78,92,113,136	0
23	5MU	AY	54	21/22	0.73	0.16	81,91,102,125	0
23	7MG	AW	46	24/25	0.73	0.14	70,83,111,120	0
23	4SU	CY	8	20/21	0.73	0.16	83,99,114,124	0
23	PSU	CY	32	20/21	0.73	0.16	83,92,99,105	0
23	7MG	CW	46	24/25	0.75	0.14	85,98,110,126	0
23	MIA	AY	37	22/30	0.76	0.14	72,87,104,128	0
23	4SU	CW	8	20/21	0.78	0.12	88,94,105,122	0
23	PSU	CY	39	20/21	0.80	0.14	80,88,99,111	0
23	PSU	AY	32	20/21	0.81	0.15	83,91,98,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	4SU	AW	8	20/21	0.83	0.13	73,85,96,105	0
23	PSU	CW	55	20/21	0.84	0.12	61,83,94,94	0
23	PSU	AY	39	20/21	0.84	0.14	77,86,97,100	0
23	PSU	CW	32	20/21	0.85	0.15	70,85,92,95	0
24	5MU	CX	54	21/22	0.87	0.13	71,80,88,94	0
24	PSU	CX	55	20/21	0.87	0.12	63,69,89,97	0
24	4SU	CX	8	20/21	0.87	0.12	54,78,85,86	0
23	5MU	CW	54	21/22	0.89	0.11	60,72,84,86	0
24	5MC	CX	32	21/22	0.90	0.16	66,71,81,83	0
24	5MU	AX	54	21/22	0.91	0.12	58,65,74,81	0
24	PSU	AX	55	20/21	0.92	0.10	60,67,93,94	0
23	MIA	CW	37	22/30	0.92	0.09	55,66,75,81	0
23	PSU	AW	32	20/21	0.93	0.10	50,60,69,69	0
23	PSU	AW	55	20/21	0.93	0.08	50,70,80,81	0
24	5MC	AX	32	21/22	0.95	0.13	48,54,58,72	0
23	PSU	CW	39	20/21	0.95	0.08	63,72,81,82	0
23	5MU	AW	54	21/22	0.95	0.07	42,58,69,76	0
24	4SU	AX	8	20/21	0.95	0.10	51,64,80,88	0
23	MIA	AW	37	29/30	0.96	0.11	40,49,63,75	0
23	PSU	AW	39	20/21	0.96	0.08	49,59,65,65	0

6.3 Carbohydrates (i)

There are no oligosaccharides 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(Å^2)	Q<0.9
56	MG	CA	3121	1/1	0.51	0.26	75,75,75,75	0
56	MG	DA	3607	1/1	0.61	0.28	53,53,53,53	0
56	MG	CJ	5001	1/1	0.62	0.23	76,76,76,76	0
56	MG	DA	3565	1/1	0.63	0.20	70,70,70,70	0
56	MG	BA	3367	1/1	0.64	0.31	53,53,53,53	0
56	MG	B8	101	1/1	0.64	0.14	42,42,42,42	0
56	MG	BA	3470	1/1	0.68	0.19	48,48,48,48	0
56	MG	AA	3204	1/1	0.68	0.27	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3571	1/1	0.69	0.13	66,66,66,66	0
56	MG	BA	3548	1/1	0.69	0.26	48,48,48,48	0
56	MG	BA	3726	1/1	0.70	0.19	70,70,70,70	0
56	MG	BA	3221	1/1	0.70	0.16	54,54,54,54	0
56	MG	BA	3692	1/1	0.71	0.23	57,57,57,57	0
56	MG	DA	3241	1/1	0.72	0.17	50,50,50,50	0
56	MG	AA	3190	1/1	0.72	0.21	65,65,65,65	0
56	MG	DA	3580	1/1	0.72	0.22	64,64,64,64	0
56	MG	BA	3553	1/1	0.72	0.16	42,42,42,42	0
56	MG	AA	3198	1/1	0.73	0.24	70,70,70,70	0
56	MG	DA	3002	1/1	0.73	0.16	68,68,68,68	0
56	MG	BA	3728	1/1	0.73	0.15	72,72,72,72	0
56	MG	BA	3333	1/1	0.74	0.16	61,61,61,61	0
56	MG	AA	3192	1/1	0.74	0.30	69,69,69,69	0
56	MG	DA	3521	1/1	0.74	0.14	51,51,51,51	0
56	MG	DA	3547	1/1	0.75	0.17	65,65,65,65	0
56	MG	BA	3720	1/1	0.75	0.14	46,46,46,46	0
56	MG	BA	3585	1/1	0.75	0.25	55,55,55,55	0
56	MG	BA	3105	1/1	0.75	0.33	69,69,69,69	0
56	MG	DA	3466	1/1	0.76	0.17	62,62,62,62	0
56	MG	BA	3605	1/1	0.76	0.14	61,61,61,61	0
56	MG	BA	3618	1/1	0.76	0.21	63,63,63,63	0
56	MG	BA	3637	1/1	0.76	0.17	59,59,59,59	0
56	MG	BA	3079	1/1	0.76	0.19	57,57,57,57	0
56	MG	DA	3404	1/1	0.76	0.15	51,51,51,51	0
56	MG	DA	3508	1/1	0.77	0.14	59,59,59,59	0
56	MG	BA	3435	1/1	0.77	0.16	57,57,57,57	0
56	MG	DA	3538	1/1	0.77	0.12	56,56,56,56	0
56	MG	DA	3066	1/1	0.77	0.19	65,65,65,65	0
56	MG	BA	3725	1/1	0.77	0.28	67,67,67,67	0
56	MG	BE	307	1/1	0.77	0.21	70,70,70,70	0
56	MG	CX	3006	1/1	0.77	0.21	70,70,70,70	0
56	MG	AA	3095	1/1	0.78	0.28	68,68,68,68	0
56	MG	DA	3408	1/1	0.78	0.19	48,48,48,48	0
56	MG	AA	3069	1/1	0.78	0.31	67,67,67,67	0
56	MG	BA	3527	1/1	0.78	0.14	52,52,52,52	0
56	MG	BA	3531	1/1	0.78	0.26	61,61,61,61	0
56	MG	BA	3639	1/1	0.79	0.29	59,59,59,59	0
56	MG	CA	3122	1/1	0.79	0.19	70,70,70,70	0
56	MG	CA	3169	1/1	0.79	0.21	65,65,65,65	0
56	MG	BA	3753	1/1	0.79	0.15	44,44,44,44	0
56	MG	BB	3018	1/1	0.79	0.18	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3516	1/1	0.79	0.21	65,65,65,65	0
56	MG	B1	102	1/1	0.79	0.26	68,68,68,68	0
56	MG	BA	3712	1/1	0.79	0.18	64,64,64,64	0
56	MG	DA	3312	1/1	0.79	0.14	52,52,52,52	0
56	MG	DA	3583	1/1	0.79	0.13	60,60,60,60	0
56	MG	DA	3401	1/1	0.79	0.10	36,36,36,36	0
56	MG	BA	3431	1/1	0.80	0.18	55,55,55,55	0
56	MG	BA	3503	1/1	0.80	0.18	58,58,58,58	0
56	MG	CA	3060	1/1	0.80	0.35	68,68,68,68	0
56	MG	CA	3070	1/1	0.80	0.17	71,71,71,71	0
56	MG	BA	3734	1/1	0.80	0.23	60,60,60,60	0
56	MG	DA	3549	1/1	0.80	0.19	57,57,57,57	0
56	MG	DA	3323	1/1	0.80	0.19	53,53,53,53	0
56	MG	BA	3204	1/1	0.80	0.35	66,66,66,66	0
56	MG	DA	3581	1/1	0.80	0.23	63,63,63,63	0
56	MG	BA	3633	1/1	0.80	0.15	45,45,45,45	0
56	MG	DA	3596	1/1	0.80	0.28	63,63,63,63	0
56	MG	BA	3442	1/1	0.80	0.13	59,59,59,59	0
56	MG	DA	3505	1/1	0.81	0.12	66,66,66,66	0
56	MG	AA	3222	1/1	0.81	0.25	67,67,67,67	0
56	MG	DA	3286	1/1	0.81	0.14	64,64,64,64	0
56	MG	BA	3760	1/1	0.81	0.26	68,68,68,68	0
56	MG	DA	3319	1/1	0.81	0.19	43,43,43,43	0
56	MG	CA	3012	1/1	0.81	0.26	68,68,68,68	0
56	MG	DA	3556	1/1	0.81	0.15	64,64,64,64	0
56	MG	DA	3564	1/1	0.81	0.18	53,53,53,53	0
56	MG	DA	3393	1/1	0.81	0.14	52,52,52,52	0
56	MG	BB	3005	1/1	0.81	0.25	64,64,64,64	0
56	MG	BA	3358	1/1	0.81	0.20	64,64,64,64	0
56	MG	BA	3291	1/1	0.81	0.18	71,71,71,71	0
56	MG	DA	3424	1/1	0.81	0.19	63,63,63,63	0
56	MG	DA	3102	1/1	0.81	0.13	57,57,57,57	0
56	MG	DB	3001	1/1	0.81	0.19	73,73,73,73	0
56	MG	BA	3625	1/1	0.82	0.17	57,57,57,57	0
56	MG	BA	3298	1/1	0.82	0.28	68,68,68,68	0
56	MG	CA	3140	1/1	0.82	0.29	79,79,79,79	0
56	MG	BA	3743	1/1	0.82	0.10	21,21,21,21	0
56	MG	AW	3005	1/1	0.82	0.25	68,68,68,68	0
56	MG	BA	3638	1/1	0.82	0.13	38,38,38,38	0
56	MG	CA	3027	1/1	0.82	0.34	70,70,70,70	0
56	MG	DA	3041	1/1	0.82	0.13	55,55,55,55	0
56	MG	BA	3825	1/1	0.82	0.21	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3420	1/1	0.82	0.13	46,46,46,46	0
56	MG	AA	3033	1/1	0.82	0.18	57,57,57,57	0
56	MG	DA	3436	1/1	0.82	0.11	54,54,54,54	0
56	MG	DA	3155	1/1	0.82	0.21	40,40,40,40	0
56	MG	DA	3199	1/1	0.82	0.23	52,52,52,52	0
56	MG	BA	3511	1/1	0.83	0.17	54,54,54,54	0
56	MG	DA	3528	1/1	0.83	0.18	57,57,57,57	0
56	MG	DA	3028	1/1	0.83	0.20	70,70,70,70	0
56	MG	DA	3400	1/1	0.83	0.17	39,39,39,39	0
56	MG	CA	3051	1/1	0.83	0.18	66,66,66,66	0
56	MG	BA	3831	1/1	0.83	0.51	52,52,52,52	0
56	MG	AA	3139	1/1	0.83	0.19	58,58,58,58	0
56	MG	AA	3125	1/1	0.83	0.13	71,71,71,71	0
56	MG	BA	3685	1/1	0.83	0.14	59,59,59,59	0
56	MG	BA	3449	1/1	0.83	0.27	60,60,60,60	0
56	MG	DA	3452	1/1	0.83	0.21	61,61,61,61	0
56	MG	BA	3409	1/1	0.83	0.22	62,62,62,62	0
56	MG	CA	3007	1/1	0.83	0.21	69,69,69,69	0
56	MG	BA	3347	1/1	0.83	0.14	48,48,48,48	0
60	K	CX	3001	1/1	0.83	0.18	74,74,74,74	0
56	MG	BA	3683	1/1	0.84	0.18	61,61,61,61	0
56	MG	BA	3446	1/1	0.84	0.18	52,52,52,52	0
56	MG	AA	3183	1/1	0.84	0.16	71,71,71,71	0
56	MG	DA	3460	1/1	0.84	0.25	65,65,65,65	0
56	MG	BA	3699	1/1	0.84	0.18	42,42,42,42	0
56	MG	DA	3504	1/1	0.84	0.17	60,60,60,60	0
56	MG	BA	3464	1/1	0.84	0.21	56,56,56,56	0
56	MG	BA	3716	1/1	0.84	0.15	54,54,54,54	0
56	MG	BA	3593	1/1	0.84	0.15	42,42,42,42	0
56	MG	BA	3224	1/1	0.84	0.20	64,64,64,64	0
56	MG	BA	3606	1/1	0.84	0.12	34,34,34,34	0
56	MG	DA	3540	1/1	0.84	0.13	67,67,67,67	0
56	MG	DA	3542	1/1	0.84	0.13	63,63,63,63	0
56	MG	DA	3297	1/1	0.84	0.13	66,66,66,66	0
56	MG	DA	3300	1/1	0.84	0.22	60,60,60,60	0
56	MG	CA	3054	1/1	0.84	0.31	71,71,71,71	0
56	MG	BA	3249	1/1	0.84	0.29	74,74,74,74	0
56	MG	AA	3038	1/1	0.84	0.16	51,51,51,51	0
56	MG	DA	3568	1/1	0.84	0.15	54,54,54,54	0
56	MG	DA	3347	1/1	0.84	0.10	44,44,44,44	0
56	MG	BA	3740	1/1	0.84	0.17	51,51,51,51	0
56	MG	AA	3210	1/1	0.84	0.20	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3315	1/1	0.84	0.16	56,56,56,56	0
56	MG	DA	3605	1/1	0.84	0.12	52,52,52,52	0
56	MG	BA	3439	1/1	0.84	0.20	58,58,58,58	0
56	MG	DA	3614	1/1	0.84	0.12	50,50,50,50	0
56	MG	AA	3098	1/1	0.84	0.23	68,68,68,68	0
56	MG	BA	3681	1/1	0.84	0.18	53,53,53,53	0
56	MG	BA	3030	1/1	0.85	0.12	50,50,50,50	0
56	MG	AA	3213	1/1	0.85	0.11	69,69,69,69	0
56	MG	DA	3105	1/1	0.85	0.19	60,60,60,60	0
56	MG	BA	3101	1/1	0.85	0.18	60,60,60,60	0
56	MG	BA	3311	1/1	0.85	0.12	37,37,37,37	0
56	MG	CA	3036	1/1	0.85	0.09	60,60,60,60	0
56	MG	AA	3216	1/1	0.85	0.18	72,72,72,72	0
56	MG	BA	3320	1/1	0.85	0.18	60,60,60,60	0
56	MG	BA	3186	1/1	0.85	0.23	51,51,51,51	0
56	MG	BA	3746	1/1	0.85	0.12	25,25,25,25	0
56	MG	CA	3103	1/1	0.85	0.15	75,75,75,75	0
56	MG	AA	3134	1/1	0.85	0.17	69,69,69,69	0
56	MG	DA	3342	1/1	0.85	0.14	56,56,56,56	0
56	MG	DA	3562	1/1	0.85	0.14	58,58,58,58	0
56	MG	BA	3689	1/1	0.85	0.18	57,57,57,57	0
56	MG	DA	3359	1/1	0.85	0.19	57,57,57,57	0
56	MG	CA	3125	1/1	0.85	0.11	64,64,64,64	0
56	MG	AN	502	1/1	0.85	0.10	52,52,52,52	0
56	MG	BA	3490	1/1	0.85	0.09	44,44,44,44	0
56	MG	BA	3708	1/1	0.85	0.32	63,63,63,63	0
56	MG	BA	3492	1/1	0.85	0.14	55,55,55,55	0
56	MG	DA	3598	1/1	0.85	0.19	63,63,63,63	0
56	MG	BB	3020	1/1	0.85	0.14	54,54,54,54	0
56	MG	AA	3082	1/1	0.85	0.29	68,68,68,68	0
56	MG	DA	3434	1/1	0.85	0.20	51,51,51,51	0
56	MG	DA	3632	1/1	0.85	0.15	58,58,58,58	0
56	MG	DA	3645	1/1	0.85	0.10	44,44,44,44	0
56	MG	BA	3718	1/1	0.85	0.12	46,46,46,46	0
56	MG	DB	3005	1/1	0.85	0.28	64,64,64,64	0
57	PCY	CA	3178	40/40	0.85	0.19	58,78,89,91	0
56	MG	DA	3051	1/1	0.85	0.15	56,56,56,56	0
56	MG	CA	3067	1/1	0.86	0.31	79,79,79,79	0
56	MG	BA	3577	1/1	0.86	0.18	60,60,60,60	0
56	MG	AA	3024	1/1	0.86	0.14	58,58,58,58	0
56	MG	CA	3109	1/1	0.86	0.23	68,68,68,68	0
56	MG	AX	3003	1/1	0.86	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3594	1/1	0.86	0.12	24,24,24,24	0
56	MG	DA	3454	1/1	0.86	0.14	54,54,54,54	0
56	MG	DA	3457	1/1	0.86	0.09	47,47,47,47	0
56	MG	BA	3595	1/1	0.86	0.15	32,32,32,32	0
56	MG	AY	3002	1/1	0.86	0.14	68,68,68,68	0
56	MG	DA	3468	1/1	0.86	0.14	44,44,44,44	0
56	MG	BA	3028	1/1	0.86	0.17	59,59,59,59	0
56	MG	BA	3617	1/1	0.86	0.20	64,64,64,64	0
56	MG	AA	3153	1/1	0.86	0.15	55,55,55,55	0
56	MG	DA	3518	1/1	0.86	0.14	50,50,50,50	0
56	MG	AA	3176	1/1	0.86	0.17	54,54,54,54	0
56	MG	BA	3089	1/1	0.86	0.16	45,45,45,45	0
56	MG	DA	3536	1/1	0.86	0.11	54,54,54,54	0
56	MG	BA	3787	1/1	0.86	0.20	59,59,59,59	0
56	MG	BA	3472	1/1	0.86	0.16	70,70,70,70	0
56	MG	AA	3073	1/1	0.86	0.26	58,58,58,58	0
56	MG	AA	3062	1/1	0.86	0.14	60,60,60,60	0
56	MG	BA	3651	1/1	0.86	0.18	56,56,56,56	0
56	MG	BA	3659	1/1	0.86	0.15	53,53,53,53	0
56	MG	DA	3163	1/1	0.86	0.16	49,49,49,49	0
56	MG	BB	3022	1/1	0.86	0.18	62,62,62,62	0
56	MG	BE	305	1/1	0.86	0.17	59,59,59,59	0
56	MG	BA	3357	1/1	0.86	0.12	46,46,46,46	0
56	MG	BA	3114	1/1	0.86	0.12	52,52,52,52	0
56	MG	AA	3094	1/1	0.86	0.21	44,44,44,44	0
56	MG	BA	3523	1/1	0.86	0.13	64,64,64,64	0
56	MG	BA	3370	1/1	0.86	0.16	60,60,60,60	0
56	MG	BA	3393	1/1	0.86	0.12	54,54,54,54	0
56	MG	CA	3028	1/1	0.86	0.13	60,60,60,60	0
56	MG	BA	3706	1/1	0.86	0.10	50,50,50,50	0
56	MG	BA	3404	1/1	0.86	0.12	36,36,36,36	0
56	MG	DA	3365	1/1	0.86	0.21	57,57,57,57	0
56	MG	CA	3053	1/1	0.86	0.18	74,74,74,74	0
56	MG	DA	3398	1/1	0.86	0.17	57,57,57,57	0
56	MG	AA	3194	1/1	0.86	0.17	58,58,58,58	0
56	MG	DB	3007	1/1	0.86	0.14	59,59,59,59	0
56	MG	CA	3056	1/1	0.86	0.20	60,60,60,60	0
56	MG	AW	3001	1/1	0.86	0.12	55,55,55,55	0
56	MG	DA	3410	1/1	0.87	0.12	62,62,62,62	0
56	MG	BA	3115	1/1	0.87	0.12	67,67,67,67	0
56	MG	BA	3701	1/1	0.87	0.14	51,51,51,51	0
56	MG	DA	3428	1/1	0.87	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3433	1/1	0.87	0.18	61,61,61,61	0
56	MG	AA	3003	1/1	0.87	0.14	66,66,66,66	0
56	MG	BA	3200	1/1	0.87	0.24	56,56,56,56	0
56	MG	DA	3451	1/1	0.87	0.14	56,56,56,56	0
56	MG	DA	3014	1/1	0.87	0.12	50,50,50,50	0
56	MG	AA	3068	1/1	0.87	0.17	60,60,60,60	0
56	MG	BR	202	1/1	0.87	0.23	53,53,53,53	0
56	MG	BR	203	1/1	0.87	0.14	44,44,44,44	0
56	MG	DA	3064	1/1	0.87	0.20	64,64,64,64	0
56	MG	BY	502	1/1	0.87	0.20	50,50,50,50	0
56	MG	DA	3079	1/1	0.87	0.08	48,48,48,48	0
56	MG	BA	3491	1/1	0.87	0.17	47,47,47,47	0
56	MG	AA	3145	1/1	0.87	0.18	58,58,58,58	0
56	MG	DA	3513	1/1	0.87	0.14	50,50,50,50	0
56	MG	DA	3117	1/1	0.87	0.23	60,60,60,60	0
56	MG	DA	3127	1/1	0.87	0.12	38,38,38,38	0
56	MG	DA	3144	1/1	0.87	0.17	63,63,63,63	0
56	MG	BA	3031	1/1	0.87	0.23	56,56,56,56	0
56	MG	AA	3150	1/1	0.87	0.23	55,55,55,55	0
56	MG	DA	3182	1/1	0.87	0.17	64,64,64,64	0
56	MG	BA	3278	1/1	0.87	0.20	55,55,55,55	0
56	MG	AA	3100	1/1	0.87	0.15	68,68,68,68	0
56	MG	DA	3243	1/1	0.87	0.13	54,54,54,54	0
56	MG	DA	3260	1/1	0.87	0.10	41,41,41,41	0
56	MG	BA	3729	1/1	0.87	0.15	52,52,52,52	0
56	MG	BA	3433	1/1	0.87	0.15	57,57,57,57	0
56	MG	BA	3095	1/1	0.87	0.16	53,53,53,53	0
56	MG	DA	3303	1/1	0.87	0.12	42,42,42,42	0
56	MG	BA	3652	1/1	0.87	0.12	46,46,46,46	0
56	MG	BA	3438	1/1	0.87	0.09	47,47,47,47	0
56	MG	BA	3672	1/1	0.87	0.17	61,61,61,61	0
56	MG	DA	3584	1/1	0.87	0.24	58,58,58,58	0
56	MG	BA	3758	1/1	0.87	0.10	34,34,34,34	0
56	MG	AA	3156	1/1	0.87	0.14	52,52,52,52	0
56	MG	CA	3090	1/1	0.87	0.19	62,62,62,62	0
56	MG	BA	3784	1/1	0.87	0.23	52,52,52,52	0
56	MG	DA	3610	1/1	0.87	0.16	48,48,48,48	0
56	MG	DA	3387	1/1	0.87	0.15	56,56,56,56	0
56	MG	AA	3042	1/1	0.87	0.13	57,57,57,57	0
56	MG	DA	3642	1/1	0.87	0.14	49,49,49,49	0
56	MG	BA	3113	1/1	0.87	0.28	58,58,58,58	0
56	MG	DA	3674	1/1	0.87	0.18	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AX	3010	1/1	0.87	0.17	62,62,62,62	0
56	MG	BA	3838	1/1	0.87	0.15	50,50,50,50	0
56	MG	CA	3133	1/1	0.87	0.13	65,65,65,65	0
56	MG	DB	3008	1/1	0.87	0.14	68,68,68,68	0
56	MG	DF	301	1/1	0.87	0.08	47,47,47,47	0
56	MG	DA	3405	1/1	0.87	0.15	52,52,52,52	0
56	MG	BA	3457	1/1	0.87	0.13	44,44,44,44	0
56	MG	AX	3007	1/1	0.88	0.28	72,72,72,72	0
56	MG	CA	3059	1/1	0.88	0.38	67,67,67,67	0
56	MG	BA	3588	1/1	0.88	0.08	47,47,47,47	0
56	MG	BA	3441	1/1	0.88	0.22	46,46,46,46	0
56	MG	AA	3209	1/1	0.88	0.16	51,51,51,51	0
56	MG	CA	3072	1/1	0.88	0.19	62,62,62,62	0
56	MG	CA	3083	1/1	0.88	0.09	58,58,58,58	0
56	MG	CA	3085	1/1	0.88	0.32	71,71,71,71	0
56	MG	AA	3174	1/1	0.88	0.17	60,60,60,60	0
56	MG	BA	3603	1/1	0.88	0.10	54,54,54,54	0
56	MG	DA	3415	1/1	0.88	0.12	50,50,50,50	0
56	MG	DA	3419	1/1	0.88	0.12	44,44,44,44	0
56	MG	BA	3181	1/1	0.88	0.11	41,41,41,41	0
56	MG	DA	3421	1/1	0.88	0.11	53,53,53,53	0
56	MG	CA	3113	1/1	0.88	0.10	55,55,55,55	0
56	MG	BA	3023	1/1	0.88	0.22	55,55,55,55	0
56	MG	BA	3356	1/1	0.88	0.15	55,55,55,55	0
56	MG	BA	3199	1/1	0.88	0.15	53,53,53,53	0
56	MG	CA	3126	1/1	0.88	0.18	72,72,72,72	0
56	MG	AA	3067	1/1	0.88	0.20	59,59,59,59	0
56	MG	BA	3626	1/1	0.88	0.10	49,49,49,49	0
56	MG	CA	3151	1/1	0.88	0.18	65,65,65,65	0
56	MG	CA	3158	1/1	0.88	0.15	53,53,53,53	0
56	MG	BA	3769	1/1	0.88	0.10	56,56,56,56	0
56	MG	CA	3177	1/1	0.88	0.16	62,62,62,62	0
56	MG	BA	3773	1/1	0.88	0.17	49,49,49,49	0
56	MG	DA	3493	1/1	0.88	0.15	58,58,58,58	0
56	MG	DA	3500	1/1	0.88	0.09	45,45,45,45	0
56	MG	CX	3002	1/1	0.88	0.13	81,81,81,81	0
56	MG	BA	3779	1/1	0.88	0.14	59,59,59,59	0
56	MG	BA	3478	1/1	0.88	0.13	59,59,59,59	0
56	MG	BA	3483	1/1	0.88	0.10	38,38,38,38	0
56	MG	BA	3797	1/1	0.88	0.13	52,52,52,52	0
56	MG	AA	3017	1/1	0.88	0.13	62,62,62,62	0
56	MG	AA	3221	1/1	0.88	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3376	1/1	0.88	0.12	34,34,34,34	0
56	MG	DA	3065	1/1	0.88	0.12	56,56,56,56	0
56	MG	AA	3084	1/1	0.88	0.10	49,49,49,49	0
56	MG	DA	3072	1/1	0.88	0.15	36,36,36,36	0
56	MG	BA	3654	1/1	0.88	0.17	55,55,55,55	0
56	MG	BA	3401	1/1	0.88	0.13	48,48,48,48	0
56	MG	AA	3109	1/1	0.88	0.26	64,64,64,64	0
56	MG	BA	3676	1/1	0.88	0.22	53,53,53,53	0
56	MG	BA	3680	1/1	0.88	0.11	52,52,52,52	0
56	MG	BO	5001	1/1	0.88	0.09	55,55,55,55	0
56	MG	BA	3254	1/1	0.88	0.09	30,30,30,30	0
56	MG	DA	3569	1/1	0.88	0.13	57,57,57,57	0
56	MG	BA	3413	1/1	0.88	0.14	41,41,41,41	0
56	MG	BX	101	1/1	0.88	0.15	65,65,65,65	0
56	MG	DA	3184	1/1	0.88	0.18	49,49,49,49	0
56	MG	BA	3429	1/1	0.88	0.13	47,47,47,47	0
56	MG	DA	3589	1/1	0.88	0.09	63,63,63,63	0
56	MG	BA	3534	1/1	0.88	0.14	31,31,31,31	0
56	MG	BA	3539	1/1	0.88	0.12	23,23,23,23	0
56	MG	DA	3604	1/1	0.88	0.17	57,57,57,57	0
56	MG	DA	3244	1/1	0.88	0.10	48,48,48,48	0
56	MG	CA	3005	1/1	0.88	0.12	58,58,58,58	0
56	MG	BA	3693	1/1	0.88	0.15	70,70,70,70	0
56	MG	BA	3547	1/1	0.88	0.15	41,41,41,41	0
56	MG	DA	3615	1/1	0.88	0.12	47,47,47,47	0
56	MG	CA	3026	1/1	0.88	0.17	64,64,64,64	0
56	MG	DA	3636	1/1	0.88	0.11	56,56,56,56	0
56	MG	AA	3120	1/1	0.88	0.21	59,59,59,59	0
56	MG	DA	3310	1/1	0.88	0.11	55,55,55,55	0
56	MG	BA	3290	1/1	0.88	0.24	58,58,58,58	0
56	MG	CA	3034	1/1	0.88	0.14	61,61,61,61	0
56	MG	BA	3560	1/1	0.88	0.14	35,35,35,35	0
56	MG	DA	3325	1/1	0.88	0.15	57,57,57,57	0
56	MG	BA	3563	1/1	0.88	0.12	60,60,60,60	0
56	MG	AA	3155	1/1	0.88	0.13	53,53,53,53	0
56	MG	D8	5001	1/1	0.88	0.23	55,55,55,55	0
56	MG	DA	3354	1/1	0.88	0.15	46,46,46,46	0
56	MG	AA	3040	1/1	0.88	0.26	59,59,59,59	0
56	MG	CA	3163	1/1	0.89	0.16	53,53,53,53	0
56	MG	AA	3046	1/1	0.89	0.18	56,56,56,56	0
56	MG	BA	3392	1/1	0.89	0.11	46,46,46,46	0
56	MG	BA	3241	1/1	0.89	0.16	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3136	1/1	0.89	0.11	53,53,53,53	0
56	MG	BA	3504	1/1	0.89	0.17	58,58,58,58	0
56	MG	DA	3422	1/1	0.89	0.21	43,43,43,43	0
56	MG	DA	3423	1/1	0.89	0.14	51,51,51,51	0
56	MG	AA	3050	1/1	0.89	0.28	70,70,70,70	0
56	MG	BA	3408	1/1	0.89	0.12	55,55,55,55	0
56	MG	DA	3432	1/1	0.89	0.12	56,56,56,56	0
56	MG	BA	3635	1/1	0.89	0.17	62,62,62,62	0
56	MG	DA	3039	1/1	0.89	0.18	56,56,56,56	0
56	MG	B9	502	1/1	0.89	0.18	57,57,57,57	0
56	MG	BA	3275	1/1	0.89	0.11	46,46,46,46	0
56	MG	AA	3162	1/1	0.89	0.24	59,59,59,59	0
56	MG	DA	3453	1/1	0.89	0.12	45,45,45,45	0
56	MG	AA	3203	1/1	0.89	0.19	57,57,57,57	0
56	MG	CA	3025	1/1	0.89	0.21	61,61,61,61	0
56	MG	BA	3111	1/1	0.89	0.17	47,47,47,47	0
56	MG	AX	3006	1/1	0.89	0.20	74,74,74,74	0
56	MG	BA	3544	1/1	0.89	0.13	35,35,35,35	0
56	MG	DA	3487	1/1	0.89	0.22	65,65,65,65	0
56	MG	CA	3029	1/1	0.89	0.25	61,61,61,61	0
56	MG	DA	3110	1/1	0.89	0.10	50,50,50,50	0
56	MG	BA	3755	1/1	0.89	0.10	52,52,52,52	0
56	MG	AA	3165	1/1	0.89	0.16	60,60,60,60	0
56	MG	CA	3046	1/1	0.89	0.17	56,56,56,56	0
56	MG	DA	3509	1/1	0.89	0.09	53,53,53,53	0
56	MG	BA	3663	1/1	0.89	0.11	50,50,50,50	0
56	MG	BA	3761	1/1	0.89	0.14	54,54,54,54	0
56	MG	BA	3763	1/1	0.89	0.23	34,34,34,34	0
56	MG	BA	3313	1/1	0.89	0.12	46,46,46,46	0
56	MG	DA	3197	1/1	0.89	0.09	48,48,48,48	0
56	MG	AA	3205	1/1	0.89	0.08	51,51,51,51	0
56	MG	DA	3213	1/1	0.89	0.14	61,61,61,61	0
56	MG	DA	3238	1/1	0.89	0.21	61,61,61,61	0
56	MG	BA	3778	1/1	0.89	0.12	35,35,35,35	0
56	MG	BA	3170	1/1	0.89	0.12	48,48,48,48	0
56	MG	BA	3322	1/1	0.89	0.10	32,32,32,32	0
56	MG	DA	3248	1/1	0.89	0.15	33,33,33,33	0
56	MG	BA	3171	1/1	0.89	0.21	53,53,53,53	0
56	MG	DA	3284	1/1	0.89	0.13	40,40,40,40	0
56	MG	BA	3794	1/1	0.89	0.13	33,33,33,33	0
56	MG	DA	3293	1/1	0.89	0.13	60,60,60,60	0
56	MG	CA	3084	1/1	0.89	0.41	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3143	1/1	0.89	0.21	73,73,73,73	0
56	MG	BA	3802	1/1	0.89	0.15	56,56,56,56	0
56	MG	CA	3092	1/1	0.89	0.12	44,44,44,44	0
56	MG	AA	3096	1/1	0.89	0.24	48,48,48,48	0
56	MG	CA	3107	1/1	0.89	0.21	66,66,66,66	0
56	MG	DA	3320	1/1	0.89	0.09	40,40,40,40	0
56	MG	DA	3600	1/1	0.89	0.09	53,53,53,53	0
56	MG	BA	3828	1/1	0.89	0.12	37,37,37,37	0
56	MG	AA	3179	1/1	0.89	0.14	79,79,79,79	0
56	MG	CA	3120	1/1	0.89	0.13	64,64,64,64	0
56	MG	AA	3182	1/1	0.89	0.18	52,52,52,52	0
56	MG	BB	3001	1/1	0.89	0.20	50,50,50,50	0
56	MG	BA	3364	1/1	0.89	0.11	42,42,42,42	0
56	MG	DA	3620	1/1	0.89	0.16	62,62,62,62	0
56	MG	BB	3012	1/1	0.89	0.09	59,59,59,59	0
56	MG	DA	3633	1/1	0.89	0.14	61,61,61,61	0
56	MG	DA	3366	1/1	0.89	0.11	50,50,50,50	0
56	MG	DA	3639	1/1	0.89	0.11	64,64,64,64	0
56	MG	DA	3370	1/1	0.89	0.08	46,46,46,46	0
56	MG	DA	3380	1/1	0.89	0.09	55,55,55,55	0
56	MG	DA	3649	1/1	0.89	0.12	64,64,64,64	0
56	MG	DA	3672	1/1	0.89	0.13	52,52,52,52	0
56	MG	CA	3128	1/1	0.89	0.14	63,63,63,63	0
56	MG	AA	3032	1/1	0.89	0.25	75,75,75,75	0
56	MG	DB	3002	1/1	0.89	0.15	56,56,56,56	0
56	MG	DA	3395	1/1	0.89	0.10	42,42,42,42	0
56	MG	BA	3702	1/1	0.89	0.10	51,51,51,51	0
56	MG	CA	3143	1/1	0.89	0.19	62,62,62,62	0
56	MG	BA	3704	1/1	0.89	0.13	55,55,55,55	0
56	MG	DA	3402	1/1	0.89	0.26	65,65,65,65	0
56	MG	CA	3154	1/1	0.89	0.24	62,62,62,62	0
56	MG	BA	3067	1/1	0.89	0.18	49,49,49,49	0
56	MG	AA	3103	1/1	0.90	0.24	59,59,59,59	0
56	MG	DA	3403	1/1	0.90	0.17	57,57,57,57	0
56	MG	BA	3586	1/1	0.90	0.14	65,65,65,65	0
56	MG	BW	201	1/1	0.90	0.10	46,46,46,46	0
56	MG	BA	3116	1/1	0.90	0.07	29,29,29,29	0
56	MG	AX	3009	1/1	0.90	0.14	71,71,71,71	0
56	MG	BA	3451	1/1	0.90	0.09	64,64,64,64	0
56	MG	DA	3005	1/1	0.90	0.18	58,58,58,58	0
56	MG	AA	3140	1/1	0.90	0.12	71,71,71,71	0
56	MG	AA	3141	1/1	0.90	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3020	1/1	0.90	0.14	61,61,61,61	0
56	MG	BA	3193	1/1	0.90	0.20	57,57,57,57	0
56	MG	BA	3608	1/1	0.90	0.23	60,60,60,60	0
56	MG	CA	3016	1/1	0.90	0.11	61,61,61,61	0
56	MG	CA	3020	1/1	0.90	0.22	73,73,73,73	0
56	MG	BA	3477	1/1	0.90	0.10	55,55,55,55	0
56	MG	AA	3027	1/1	0.90	0.24	54,54,54,54	0
56	MG	BA	3481	1/1	0.90	0.13	45,45,45,45	0
56	MG	DA	3448	1/1	0.90	0.08	41,41,41,41	0
56	MG	DA	3098	1/1	0.90	0.11	43,43,43,43	0
56	MG	BA	3748	1/1	0.90	0.10	63,63,63,63	0
56	MG	DA	3103	1/1	0.90	0.14	50,50,50,50	0
56	MG	BA	3482	1/1	0.90	0.13	59,59,59,59	0
56	MG	AA	3116	1/1	0.90	0.14	61,61,61,61	0
56	MG	BA	3486	1/1	0.90	0.21	48,48,48,48	0
56	MG	AA	3218	1/1	0.90	0.23	53,53,53,53	0
56	MG	DA	3131	1/1	0.90	0.18	52,52,52,52	0
56	MG	DA	3135	1/1	0.90	0.13	50,50,50,50	0
56	MG	BA	3220	1/1	0.90	0.20	55,55,55,55	0
56	MG	DA	3497	1/1	0.90	0.38	51,51,51,51	0
56	MG	BA	3762	1/1	0.90	0.19	40,40,40,40	0
56	MG	BA	3371	1/1	0.90	0.12	54,54,54,54	0
56	MG	CA	3055	1/1	0.90	0.10	53,53,53,53	0
56	MG	BA	3768	1/1	0.90	0.10	56,56,56,56	0
56	MG	AA	3020	1/1	0.90	0.17	59,59,59,59	0
56	MG	BA	3044	1/1	0.90	0.20	49,49,49,49	0
56	MG	DA	3516	1/1	0.90	0.14	59,59,59,59	0
56	MG	DA	3201	1/1	0.90	0.26	52,52,52,52	0
56	MG	DA	3206	1/1	0.90	0.09	39,39,39,39	0
56	MG	AA	3022	1/1	0.90	0.15	55,55,55,55	0
56	MG	DA	3534	1/1	0.90	0.16	74,74,74,74	0
56	MG	CA	3068	1/1	0.90	0.28	55,55,55,55	0
56	MG	DA	3537	1/1	0.90	0.11	55,55,55,55	0
56	MG	BA	3658	1/1	0.90	0.13	45,45,45,45	0
56	MG	AA	3223	1/1	0.90	0.29	59,59,59,59	0
56	MG	AA	3127	1/1	0.90	0.10	48,48,48,48	0
56	MG	BA	3270	1/1	0.90	0.21	57,57,57,57	0
56	MG	DA	3250	1/1	0.90	0.15	61,61,61,61	0
56	MG	BA	3795	1/1	0.90	0.11	53,53,53,53	0
56	MG	DA	3557	1/1	0.90	0.10	34,34,34,34	0
56	MG	DA	3263	1/1	0.90	0.16	61,61,61,61	0
56	MG	DA	3272	1/1	0.90	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3282	1/1	0.90	0.09	42,42,42,42	0
56	MG	DA	3566	1/1	0.90	0.08	48,48,48,48	0
56	MG	BA	3274	1/1	0.90	0.15	49,49,49,49	0
56	MG	BA	3679	1/1	0.90	0.15	61,61,61,61	0
56	MG	DA	3579	1/1	0.90	0.09	55,55,55,55	0
56	MG	DA	3288	1/1	0.90	0.18	61,61,61,61	0
56	MG	CA	3102	1/1	0.90	0.13	54,54,54,54	0
56	MG	BA	3808	1/1	0.90	0.15	34,34,34,34	0
56	MG	AA	3130	1/1	0.90	0.08	43,43,43,43	0
56	MG	BA	3427	1/1	0.90	0.12	32,32,32,32	0
56	MG	DA	3591	1/1	0.90	0.09	56,56,56,56	0
56	MG	BA	3428	1/1	0.90	0.11	38,38,38,38	0
56	MG	DA	3597	1/1	0.90	0.08	51,51,51,51	0
56	MG	BA	3277	1/1	0.90	0.20	54,54,54,54	0
56	MG	DA	3317	1/1	0.90	0.11	55,55,55,55	0
56	MG	AW	3002	1/1	0.90	0.12	69,69,69,69	0
56	MG	BB	3004	1/1	0.90	0.10	47,47,47,47	0
56	MG	CA	3124	1/1	0.90	0.09	79,79,79,79	0
56	MG	BA	3102	1/1	0.90	0.22	54,54,54,54	0
56	MG	DA	3327	1/1	0.90	0.14	59,59,59,59	0
56	MG	BB	3009	1/1	0.90	0.22	58,58,58,58	0
56	MG	AA	3202	1/1	0.90	0.11	57,57,57,57	0
56	MG	DA	3628	1/1	0.90	0.09	56,56,56,56	0
56	MG	DA	3631	1/1	0.90	0.14	56,56,56,56	0
56	MG	DA	3349	1/1	0.90	0.08	44,44,44,44	0
56	MG	AX	3002	1/1	0.90	0.11	53,53,53,53	0
56	MG	DA	3635	1/1	0.90	0.11	52,52,52,52	0
56	MG	DA	3357	1/1	0.90	0.08	44,44,44,44	0
56	MG	CA	3136	1/1	0.90	0.17	65,65,65,65	0
56	MG	CA	3139	1/1	0.90	0.10	61,61,61,61	0
56	MG	BA	3700	1/1	0.90	0.14	54,54,54,54	0
56	MG	BA	3567	1/1	0.90	0.13	50,50,50,50	0
56	MG	DA	3650	1/1	0.90	0.12	44,44,44,44	0
56	MG	DA	3655	1/1	0.90	0.14	57,57,57,57	0
56	MG	DA	3657	1/1	0.90	0.16	67,67,67,67	0
56	MG	DA	3378	1/1	0.90	0.10	45,45,45,45	0
56	MG	CA	3147	1/1	0.90	0.18	72,72,72,72	0
56	MG	DA	3386	1/1	0.90	0.12	48,48,48,48	0
56	MG	CA	3150	1/1	0.90	0.21	62,62,62,62	0
56	MG	AA	3019	1/1	0.90	0.09	48,48,48,48	0
56	MG	AA	3102	1/1	0.90	0.19	51,51,51,51	0
56	MG	DA	3396	1/1	0.90	0.13	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3397	1/1	0.90	0.09	49,49,49,49	0
56	MG	DR	5001	1/1	0.90	0.12	58,58,58,58	0
56	MG	CA	3156	1/1	0.90	0.15	68,68,68,68	0
56	MG	BA	3583	1/1	0.90	0.09	45,45,45,45	0
56	MG	BQ	3005	1/1	0.90	0.18	50,50,50,50	0
56	MG	DA	3335	1/1	0.91	0.12	32,32,32,32	0
56	MG	DA	3338	1/1	0.91	0.07	40,40,40,40	0
56	MG	DA	3341	1/1	0.91	0.11	31,31,31,31	0
56	MG	BA	3634	1/1	0.91	0.11	64,64,64,64	0
56	MG	DA	3343	1/1	0.91	0.12	40,40,40,40	0
56	MG	AA	3079	1/1	0.91	0.14	47,47,47,47	0
56	MG	CA	3105	1/1	0.91	0.08	49,49,49,49	0
56	MG	BA	3363	1/1	0.91	0.12	50,50,50,50	0
56	MG	DA	3355	1/1	0.91	0.11	50,50,50,50	0
56	MG	AA	3101	1/1	0.91	0.11	54,54,54,54	0
56	MG	CA	3111	1/1	0.91	0.19	61,61,61,61	0
56	MG	BA	3365	1/1	0.91	0.11	49,49,49,49	0
56	MG	BA	3647	1/1	0.91	0.08	45,45,45,45	0
56	MG	BA	3798	1/1	0.91	0.12	61,61,61,61	0
56	MG	BA	3799	1/1	0.91	0.14	47,47,47,47	0
56	MG	AA	3188	1/1	0.91	0.13	56,56,56,56	0
56	MG	DA	3385	1/1	0.91	0.14	55,55,55,55	0
56	MG	BA	3804	1/1	0.91	0.09	58,58,58,58	0
56	MG	AA	3080	1/1	0.91	0.09	47,47,47,47	0
56	MG	BA	3818	1/1	0.91	0.13	32,32,32,32	0
56	MG	BA	3060	1/1	0.91	0.11	56,56,56,56	0
56	MG	BA	3229	1/1	0.91	0.20	51,51,51,51	0
56	MG	CA	3137	1/1	0.91	0.11	52,52,52,52	0
56	MG	BA	3508	1/1	0.91	0.08	54,54,54,54	0
56	MG	BA	3382	1/1	0.91	0.09	55,55,55,55	0
56	MG	BA	3670	1/1	0.91	0.10	47,47,47,47	0
56	MG	BA	3512	1/1	0.91	0.11	27,27,27,27	0
56	MG	CA	3148	1/1	0.91	0.17	67,67,67,67	0
56	MG	BA	3233	1/1	0.91	0.18	48,48,48,48	0
56	MG	BA	3678	1/1	0.91	0.09	58,58,58,58	0
56	MG	BB	3011	1/1	0.91	0.08	59,59,59,59	0
56	MG	BA	3519	1/1	0.91	0.08	44,44,44,44	0
56	MG	DA	3412	1/1	0.91	0.17	63,63,63,63	0
56	MG	BA	3520	1/1	0.91	0.23	47,47,47,47	0
56	MG	DA	3418	1/1	0.91	0.11	37,37,37,37	0
56	MG	CA	3160	1/1	0.91	0.25	65,65,65,65	0
56	MG	CA	3162	1/1	0.91	0.23	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3237	1/1	0.91	0.14	36,36,36,36	0
56	MG	BA	3524	1/1	0.91	0.16	53,53,53,53	0
56	MG	CA	3171	1/1	0.91	0.19	63,63,63,63	0
56	MG	CA	3172	1/1	0.91	0.19	64,64,64,64	0
56	MG	CA	3173	1/1	0.91	0.19	69,69,69,69	0
56	MG	BE	304	1/1	0.91	0.20	40,40,40,40	0
56	MG	CE	201	1/1	0.91	0.19	50,50,50,50	0
56	MG	AA	3228	1/1	0.91	0.13	68,68,68,68	0
56	MG	CV	3001	1/1	0.91	0.18	58,58,58,58	0
56	MG	DA	3442	1/1	0.91	0.12	44,44,44,44	0
56	MG	DA	3445	1/1	0.91	0.11	72,72,72,72	0
56	MG	DA	3446	1/1	0.91	0.20	47,47,47,47	0
56	MG	BA	3686	1/1	0.91	0.12	30,30,30,30	0
56	MG	BF	305	1/1	0.91	0.14	47,47,47,47	0
56	MG	BA	3688	1/1	0.91	0.12	45,45,45,45	0
56	MG	AA	3229	1/1	0.91	0.30	62,62,62,62	0
56	MG	DA	3010	1/1	0.91	0.08	43,43,43,43	0
56	MG	DA	3456	1/1	0.91	0.19	49,49,49,49	0
56	MG	BA	3690	1/1	0.91	0.14	63,63,63,63	0
56	MG	BA	3532	1/1	0.91	0.20	49,49,49,49	0
56	MG	DA	3029	1/1	0.91	0.09	51,51,51,51	0
56	MG	AK	201	1/1	0.91	0.13	61,61,61,61	0
56	MG	DA	3477	1/1	0.91	0.10	55,55,55,55	0
56	MG	DA	3040	1/1	0.91	0.14	53,53,53,53	0
56	MG	BA	3268	1/1	0.91	0.27	58,58,58,58	0
56	MG	DA	3043	1/1	0.91	0.15	48,48,48,48	0
56	MG	DA	3044	1/1	0.91	0.11	58,58,58,58	0
56	MG	BA	3543	1/1	0.91	0.11	26,26,26,26	0
56	MG	DA	3063	1/1	0.91	0.19	46,46,46,46	0
56	MG	AA	3004	1/1	0.91	0.13	67,67,67,67	0
56	MG	B4	502	1/1	0.91	0.23	72,72,72,72	0
56	MG	DA	3512	1/1	0.91	0.12	46,46,46,46	0
56	MG	BA	3424	1/1	0.91	0.14	24,24,24,24	0
56	MG	BA	3273	1/1	0.91	0.20	53,53,53,53	0
56	MG	CA	3001	1/1	0.91	0.23	73,73,73,73	0
56	MG	DA	3081	1/1	0.91	0.13	45,45,45,45	0
56	MG	BA	3705	1/1	0.91	0.12	54,54,54,54	0
56	MG	DA	3099	1/1	0.91	0.09	60,60,60,60	0
56	MG	DA	3535	1/1	0.91	0.12	54,54,54,54	0
56	MG	DA	3101	1/1	0.91	0.11	53,53,53,53	0
56	MG	AV	101	1/1	0.91	0.17	59,59,59,59	0
56	MG	CA	3010	1/1	0.91	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3557	1/1	0.91	0.16	56,56,56,56	0
56	MG	DA	3109	1/1	0.91	0.22	66,66,66,66	0
56	MG	CA	3015	1/1	0.91	0.16	58,58,58,58	0
56	MG	DA	3548	1/1	0.91	0.20	65,65,65,65	0
56	MG	AA	3025	1/1	0.91	0.16	43,43,43,43	0
56	MG	BA	3714	1/1	0.91	0.09	47,47,47,47	0
56	MG	CA	3023	1/1	0.91	0.29	55,55,55,55	0
56	MG	DA	3560	1/1	0.91	0.12	34,34,34,34	0
56	MG	CA	3024	1/1	0.91	0.19	63,63,63,63	0
56	MG	BA	3430	1/1	0.91	0.11	32,32,32,32	0
56	MG	DA	3153	1/1	0.91	0.12	44,44,44,44	0
56	MG	AA	3085	1/1	0.91	0.15	55,55,55,55	0
56	MG	BA	3432	1/1	0.91	0.16	52,52,52,52	0
56	MG	DA	3169	1/1	0.91	0.17	49,49,49,49	0
56	MG	DA	3575	1/1	0.91	0.07	47,47,47,47	0
56	MG	DA	3178	1/1	0.91	0.09	54,54,54,54	0
56	MG	DA	3181	1/1	0.91	0.14	45,45,45,45	0
56	MG	AA	3088	1/1	0.91	0.22	56,56,56,56	0
56	MG	DA	3582	1/1	0.91	0.08	39,39,39,39	0
56	MG	BA	3112	1/1	0.91	0.08	57,57,57,57	0
56	MG	DA	3186	1/1	0.91	0.10	40,40,40,40	0
56	MG	DA	3588	1/1	0.91	0.12	39,39,39,39	0
56	MG	DA	3195	1/1	0.91	0.11	57,57,57,57	0
56	MG	CA	3032	1/1	0.91	0.21	52,52,52,52	0
56	MG	CA	3033	1/1	0.91	0.18	56,56,56,56	0
56	MG	BA	3436	1/1	0.91	0.08	46,46,46,46	0
56	MG	AA	3091	1/1	0.91	0.26	70,70,70,70	0
56	MG	DA	3207	1/1	0.91	0.16	57,57,57,57	0
56	MG	CA	3037	1/1	0.91	0.19	55,55,55,55	0
56	MG	DA	3220	1/1	0.91	0.10	46,46,46,46	0
56	MG	DA	3223	1/1	0.91	0.15	54,54,54,54	0
56	MG	DA	3229	1/1	0.91	0.07	55,55,55,55	0
56	MG	DA	3611	1/1	0.91	0.14	55,55,55,55	0
56	MG	BA	3292	1/1	0.91	0.07	42,42,42,42	0
56	MG	CA	3049	1/1	0.91	0.16	68,68,68,68	0
56	MG	AA	3044	1/1	0.91	0.35	71,71,71,71	0
56	MG	BA	3309	1/1	0.91	0.09	55,55,55,55	0
56	MG	DA	3247	1/1	0.91	0.27	57,57,57,57	0
56	MG	AA	3034	1/1	0.91	0.22	48,48,48,48	0
56	MG	AA	3207	1/1	0.91	0.13	68,68,68,68	0
56	MG	BA	3604	1/1	0.91	0.17	72,72,72,72	0
56	MG	CA	3058	1/1	0.91	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3158	1/1	0.91	0.25	44,44,44,44	0
56	MG	DA	3277	1/1	0.91	0.18	56,56,56,56	0
56	MG	DA	3643	1/1	0.91	0.13	60,60,60,60	0
56	MG	DA	3278	1/1	0.91	0.16	53,53,53,53	0
56	MG	BA	3317	1/1	0.91	0.12	64,64,64,64	0
56	MG	CA	3061	1/1	0.91	0.26	56,56,56,56	0
56	MG	CA	3063	1/1	0.91	0.13	59,59,59,59	0
56	MG	CA	3064	1/1	0.91	0.14	57,57,57,57	0
56	MG	DA	3667	1/1	0.91	0.34	73,73,73,73	0
56	MG	AA	3011	1/1	0.91	0.07	64,64,64,64	0
56	MG	BA	3612	1/1	0.91	0.13	62,62,62,62	0
56	MG	AA	3076	1/1	0.91	0.20	55,55,55,55	0
56	MG	AA	3212	1/1	0.91	0.16	59,59,59,59	0
56	MG	DB	3003	1/1	0.91	0.20	68,68,68,68	0
56	MG	BA	3619	1/1	0.91	0.16	51,51,51,51	0
56	MG	AA	3099	1/1	0.91	0.34	63,63,63,63	0
56	MG	BA	3770	1/1	0.91	0.16	37,37,37,37	0
56	MG	DE	301	1/1	0.91	0.25	45,45,45,45	0
56	MG	DE	304	1/1	0.91	0.12	47,47,47,47	0
56	MG	CA	3086	1/1	0.91	0.22	61,61,61,61	0
56	MG	DG	3001	1/1	0.91	0.11	56,56,56,56	0
56	MG	BA	3022	1/1	0.91	0.09	40,40,40,40	0
56	MG	DW	3002	1/1	0.91	0.21	65,65,65,65	0
56	MG	DW	3003	1/1	0.91	0.14	47,47,47,47	0
56	MG	AA	3181	1/1	0.91	0.13	75,75,75,75	0
56	MG	CA	3094	1/1	0.91	0.22	72,72,72,72	0
56	MG	CA	3101	1/1	0.91	0.17	54,54,54,54	0
56	MG	CA	3022	1/1	0.92	0.11	53,53,53,53	0
56	MG	BA	3747	1/1	0.92	0.10	42,42,42,42	0
56	MG	DA	3012	1/1	0.92	0.09	39,39,39,39	0
56	MG	BA	3192	1/1	0.92	0.11	48,48,48,48	0
56	MG	DA	3020	1/1	0.92	0.13	50,50,50,50	0
56	MG	DA	3027	1/1	0.92	0.15	53,53,53,53	0
56	MG	BA	3752	1/1	0.92	0.09	19,19,19,19	0
56	MG	BA	3005	1/1	0.92	0.17	51,51,51,51	0
56	MG	DA	3034	1/1	0.92	0.14	43,43,43,43	0
56	MG	DA	3037	1/1	0.92	0.08	54,54,54,54	0
56	MG	BA	3197	1/1	0.92	0.12	36,36,36,36	0
56	MG	BA	3757	1/1	0.92	0.07	25,25,25,25	0
56	MG	BA	3630	1/1	0.92	0.09	30,30,30,30	0
56	MG	DA	3406	1/1	0.92	0.08	40,40,40,40	0
56	MG	BA	3359	1/1	0.92	0.08	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3360	1/1	0.92	0.09	50,50,50,50	0
56	MG	DA	3411	1/1	0.92	0.13	46,46,46,46	0
56	MG	DA	3046	1/1	0.92	0.36	57,57,57,57	0
56	MG	DA	3047	1/1	0.92	0.17	49,49,49,49	0
56	MG	BA	3007	1/1	0.92	0.10	51,51,51,51	0
56	MG	DA	3056	1/1	0.92	0.16	44,44,44,44	0
56	MG	BA	3636	1/1	0.92	0.10	53,53,53,53	0
56	MG	BA	3765	1/1	0.92	0.11	33,33,33,33	0
56	MG	CA	3044	1/1	0.92	0.22	55,55,55,55	0
56	MG	AA	3167	1/1	0.92	0.20	47,47,47,47	0
56	MG	DA	3068	1/1	0.92	0.10	58,58,58,58	0
56	MG	DA	3426	1/1	0.92	0.10	41,41,41,41	0
56	MG	BA	3203	1/1	0.92	0.09	39,39,39,39	0
56	MG	DA	3078	1/1	0.92	0.07	45,45,45,45	0
56	MG	AA	3169	1/1	0.92	0.12	64,64,64,64	0
56	MG	BA	3645	1/1	0.92	0.12	32,32,32,32	0
56	MG	DA	3087	1/1	0.92	0.17	49,49,49,49	0
56	MG	DA	3093	1/1	0.92	0.13	57,57,57,57	0
56	MG	DA	3096	1/1	0.92	0.11	51,51,51,51	0
56	MG	BA	3775	1/1	0.92	0.09	43,43,43,43	0
56	MG	BA	3369	1/1	0.92	0.11	55,55,55,55	0
56	MG	DA	3449	1/1	0.92	0.12	47,47,47,47	0
56	MG	BA	3648	1/1	0.92	0.17	53,53,53,53	0
56	MG	CA	3057	1/1	0.92	0.29	58,58,58,58	0
56	MG	BA	3781	1/1	0.92	0.15	52,52,52,52	0
56	MG	AA	3055	1/1	0.92	0.26	58,58,58,58	0
56	MG	DA	3106	1/1	0.92	0.28	61,61,61,61	0
56	MG	BA	3510	1/1	0.92	0.08	48,48,48,48	0
56	MG	AA	3057	1/1	0.92	0.21	61,61,61,61	0
56	MG	DA	3463	1/1	0.92	0.12	37,37,37,37	0
56	MG	BA	3656	1/1	0.92	0.12	45,45,45,45	0
56	MG	DA	3118	1/1	0.92	0.20	52,52,52,52	0
56	MG	DA	3469	1/1	0.92	0.12	54,54,54,54	0
56	MG	AA	3002	1/1	0.92	0.10	62,62,62,62	0
56	MG	BA	3227	1/1	0.92	0.10	57,57,57,57	0
56	MG	DA	3132	1/1	0.92	0.19	41,41,41,41	0
56	MG	BA	3385	1/1	0.92	0.10	39,39,39,39	0
56	MG	DA	3138	1/1	0.92	0.26	59,59,59,59	0
56	MG	DA	3143	1/1	0.92	0.20	50,50,50,50	0
56	MG	BA	3666	1/1	0.92	0.16	58,58,58,58	0
56	MG	DA	3145	1/1	0.92	0.31	49,49,49,49	0
56	MG	AA	3030	1/1	0.92	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3511	1/1	0.92	0.10	45,45,45,45	0
56	MG	CA	3076	1/1	0.92	0.20	56,56,56,56	0
56	MG	BA	3807	1/1	0.92	0.10	67,67,67,67	0
56	MG	DA	3515	1/1	0.92	0.11	57,57,57,57	0
56	MG	AA	3014	1/1	0.92	0.08	69,69,69,69	0
56	MG	BA	3812	1/1	0.92	0.09	52,52,52,52	0
56	MG	AA	3005	1/1	0.92	0.10	53,53,53,53	0
56	MG	DA	3523	1/1	0.92	0.10	57,57,57,57	0
56	MG	BA	3525	1/1	0.92	0.11	52,52,52,52	0
56	MG	DA	3533	1/1	0.92	0.21	53,53,53,53	0
56	MG	BA	3403	1/1	0.92	0.14	31,31,31,31	0
56	MG	DA	3185	1/1	0.92	0.23	54,54,54,54	0
56	MG	BA	3066	1/1	0.92	0.21	51,51,51,51	0
56	MG	DA	3188	1/1	0.92	0.19	50,50,50,50	0
56	MG	DA	3190	1/1	0.92	0.08	45,45,45,45	0
56	MG	DA	3191	1/1	0.92	0.08	44,44,44,44	0
56	MG	CA	3097	1/1	0.92	0.19	57,57,57,57	0
56	MG	DA	3545	1/1	0.92	0.09	37,37,37,37	0
56	MG	CA	3100	1/1	0.92	0.11	62,62,62,62	0
56	MG	AA	3187	1/1	0.92	0.12	62,62,62,62	0
56	MG	BA	3070	1/1	0.92	0.19	55,55,55,55	0
56	MG	DA	3204	1/1	0.92	0.12	51,51,51,51	0
56	MG	BA	3262	1/1	0.92	0.15	47,47,47,47	0
56	MG	AA	3230	1/1	0.92	0.18	68,68,68,68	0
56	MG	DA	3561	1/1	0.92	0.08	48,48,48,48	0
56	MG	DA	3211	1/1	0.92	0.09	48,48,48,48	0
56	MG	AA	3110	1/1	0.92	0.21	61,61,61,61	0
56	MG	DA	3216	1/1	0.92	0.16	46,46,46,46	0
56	MG	AA	3112	1/1	0.92	0.10	57,57,57,57	0
56	MG	CA	3110	1/1	0.92	0.11	48,48,48,48	0
56	MG	DA	3226	1/1	0.92	0.16	54,54,54,54	0
56	MG	DA	3574	1/1	0.92	0.09	51,51,51,51	0
56	MG	BA	3096	1/1	0.92	0.08	41,41,41,41	0
56	MG	DA	3235	1/1	0.92	0.24	61,61,61,61	0
56	MG	BA	3099	1/1	0.92	0.16	50,50,50,50	0
56	MG	AA	3148	1/1	0.92	0.20	63,63,63,63	0
56	MG	AA	3113	1/1	0.92	0.13	59,59,59,59	0
56	MG	BD	305	1/1	0.92	0.10	37,37,37,37	0
56	MG	CA	3123	1/1	0.92	0.14	80,80,80,80	0
56	MG	DA	3587	1/1	0.92	0.08	61,61,61,61	0
56	MG	BA	3284	1/1	0.92	0.23	51,51,51,51	0
56	MG	AA	3195	1/1	0.92	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3251	1/1	0.92	0.09	51,51,51,51	0
56	MG	DA	3594	1/1	0.92	0.07	44,44,44,44	0
56	MG	DA	3595	1/1	0.92	0.12	61,61,61,61	0
56	MG	AA	3071	1/1	0.92	0.32	62,62,62,62	0
56	MG	BA	3576	1/1	0.92	0.12	48,48,48,48	0
56	MG	CA	3132	1/1	0.92	0.21	70,70,70,70	0
56	MG	BF	306	1/1	0.92	0.16	40,40,40,40	0
56	MG	DA	3601	1/1	0.92	0.13	54,54,54,54	0
56	MG	CA	3134	1/1	0.92	0.23	70,70,70,70	0
56	MG	DA	3279	1/1	0.92	0.08	48,48,48,48	0
56	MG	DA	3280	1/1	0.92	0.07	43,43,43,43	0
56	MG	DA	3609	1/1	0.92	0.10	60,60,60,60	0
56	MG	BF	311	1/1	0.92	0.08	43,43,43,43	0
56	MG	AA	3010	1/1	0.92	0.20	59,59,59,59	0
56	MG	DA	3612	1/1	0.92	0.14	56,56,56,56	0
56	MG	AA	3121	1/1	0.92	0.17	66,66,66,66	0
56	MG	DA	3287	1/1	0.92	0.13	47,47,47,47	0
56	MG	DA	3618	1/1	0.92	0.14	54,54,54,54	0
56	MG	AX	3004	1/1	0.92	0.23	70,70,70,70	0
56	MG	CA	3141	1/1	0.92	0.18	49,49,49,49	0
56	MG	AA	3158	1/1	0.92	0.14	59,59,59,59	0
56	MG	CA	3145	1/1	0.92	0.13	63,63,63,63	0
56	MG	DA	3302	1/1	0.92	0.07	33,33,33,33	0
56	MG	CA	3146	1/1	0.92	0.10	69,69,69,69	0
56	MG	AA	3159	1/1	0.92	0.09	59,59,59,59	0
56	MG	BA	3447	1/1	0.92	0.14	26,26,26,26	0
56	MG	CA	3149	1/1	0.92	0.17	65,65,65,65	0
56	MG	BA	3133	1/1	0.92	0.22	47,47,47,47	0
56	MG	B0	101	1/1	0.92	0.11	39,39,39,39	0
56	MG	DA	3648	1/1	0.92	0.18	60,60,60,60	0
56	MG	AA	3047	1/1	0.92	0.08	47,47,47,47	0
56	MG	DA	3324	1/1	0.92	0.11	39,39,39,39	0
56	MG	DA	3653	1/1	0.92	0.18	58,58,58,58	0
56	MG	BA	3724	1/1	0.92	0.16	44,44,44,44	0
56	MG	B5	105	1/1	0.92	0.07	49,49,49,49	0
56	MG	DA	3658	1/1	0.92	0.08	37,37,37,37	0
56	MG	DA	3663	1/1	0.92	0.19	60,60,60,60	0
56	MG	B6	101	1/1	0.92	0.12	48,48,48,48	0
56	MG	CA	3161	1/1	0.92	0.15	70,70,70,70	0
56	MG	BA	3452	1/1	0.92	0.12	27,27,27,27	0
56	MG	AA	3037	1/1	0.92	0.12	44,44,44,44	0
56	MG	CA	3165	1/1	0.92	0.13	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3727	1/1	0.92	0.14	39,39,39,39	0
56	MG	BA	3459	1/1	0.92	0.13	48,48,48,48	0
56	MG	AA	3166	1/1	0.92	0.08	65,65,65,65	0
56	MG	BA	3467	1/1	0.92	0.15	39,39,39,39	0
56	MG	DB	3010	1/1	0.92	0.11	55,55,55,55	0
56	MG	CA	3011	1/1	0.92	0.16	63,63,63,63	0
56	MG	DE	303	1/1	0.92	0.14	44,44,44,44	0
56	MG	BA	3328	1/1	0.92	0.12	60,60,60,60	0
56	MG	CA	3013	1/1	0.92	0.16	63,63,63,63	0
56	MG	BA	3742	1/1	0.92	0.08	51,51,51,51	0
56	MG	DA	3367	1/1	0.92	0.08	51,51,51,51	0
56	MG	DV	3002	1/1	0.92	0.26	57,57,57,57	0
56	MG	AY	3003	1/1	0.92	0.08	48,48,48,48	0
56	MG	DA	3377	1/1	0.92	0.07	42,42,42,42	0
56	MG	CX	3004	1/1	0.92	0.16	54,54,54,54	0
57	PCY	AA	3231	40/40	0.92	0.13	45,69,81,87	0
56	MG	CA	3019	1/1	0.92	0.22	58,58,58,58	0
56	MG	BA	3002	1/1	0.92	0.18	62,62,62,62	0
56	MG	BA	3783	1/1	0.93	0.13	53,53,53,53	0
56	MG	BA	3198	1/1	0.93	0.18	55,55,55,55	0
56	MG	BA	3352	1/1	0.93	0.09	29,29,29,29	0
56	MG	BA	3641	1/1	0.93	0.10	49,49,49,49	0
56	MG	BA	3643	1/1	0.93	0.07	30,30,30,30	0
56	MG	BA	3796	1/1	0.93	0.09	40,40,40,40	0
56	MG	DA	3086	1/1	0.93	0.14	62,62,62,62	0
56	MG	CA	3066	1/1	0.93	0.20	66,66,66,66	0
56	MG	DA	3091	1/1	0.93	0.10	43,43,43,43	0
56	MG	DA	3092	1/1	0.93	0.14	48,48,48,48	0
56	MG	DA	3413	1/1	0.93	0.14	36,36,36,36	0
56	MG	BA	3354	1/1	0.93	0.11	31,31,31,31	0
56	MG	DA	3416	1/1	0.93	0.15	40,40,40,40	0
56	MG	AA	3168	1/1	0.93	0.09	62,62,62,62	0
56	MG	DA	3097	1/1	0.93	0.18	43,43,43,43	0
56	MG	BA	3057	1/1	0.93	0.20	53,53,53,53	0
56	MG	AA	3072	1/1	0.93	0.20	68,68,68,68	0
56	MG	CA	3073	1/1	0.93	0.13	48,48,48,48	0
56	MG	BA	3064	1/1	0.93	0.29	61,61,61,61	0
56	MG	CA	3079	1/1	0.93	0.24	54,54,54,54	0
56	MG	BA	3806	1/1	0.93	0.14	51,51,51,51	0
56	MG	BA	3218	1/1	0.93	0.10	44,44,44,44	0
56	MG	DA	3429	1/1	0.93	0.10	40,40,40,40	0
56	MG	BA	3655	1/1	0.93	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3810	1/1	0.93	0.17	50,50,50,50	0
56	MG	CA	3088	1/1	0.93	0.29	53,53,53,53	0
56	MG	BA	3811	1/1	0.93	0.27	38,38,38,38	0
56	MG	DA	3119	1/1	0.93	0.30	62,62,62,62	0
56	MG	AA	3170	1/1	0.93	0.14	57,57,57,57	0
56	MG	BA	3493	1/1	0.93	0.07	46,46,46,46	0
56	MG	CA	3095	1/1	0.93	0.15	61,61,61,61	0
56	MG	BA	3820	1/1	0.93	0.11	45,45,45,45	0
56	MG	AW	3003	1/1	0.93	0.30	59,59,59,59	0
56	MG	DA	3142	1/1	0.93	0.10	45,45,45,45	0
56	MG	AW	3004	1/1	0.93	0.07	51,51,51,51	0
56	MG	BA	3366	1/1	0.93	0.09	45,45,45,45	0
56	MG	BA	3833	1/1	0.93	0.08	43,43,43,43	0
56	MG	DA	3150	1/1	0.93	0.08	41,41,41,41	0
56	MG	DA	3458	1/1	0.93	0.09	42,42,42,42	0
56	MG	AA	3172	1/1	0.93	0.09	47,47,47,47	0
56	MG	DA	3154	1/1	0.93	0.22	52,52,52,52	0
56	MG	BA	3228	1/1	0.93	0.11	50,50,50,50	0
56	MG	DA	3159	1/1	0.93	0.08	41,41,41,41	0
56	MG	AA	3086	1/1	0.93	0.18	52,52,52,52	0
56	MG	DA	3474	1/1	0.93	0.08	53,53,53,53	0
56	MG	BA	3230	1/1	0.93	0.13	62,62,62,62	0
56	MG	DA	3485	1/1	0.93	0.08	44,44,44,44	0
56	MG	DA	3486	1/1	0.93	0.13	44,44,44,44	0
56	MG	BA	3374	1/1	0.93	0.06	37,37,37,37	0
56	MG	BA	3093	1/1	0.93	0.11	38,38,38,38	0
56	MG	CA	3114	1/1	0.93	0.17	56,56,56,56	0
56	MG	DA	3499	1/1	0.93	0.16	60,60,60,60	0
56	MG	BA	3522	1/1	0.93	0.15	36,36,36,36	0
56	MG	DA	3502	1/1	0.93	0.11	64,64,64,64	0
56	MG	BB	3014	1/1	0.93	0.17	69,69,69,69	0
56	MG	BA	3377	1/1	0.93	0.07	30,30,30,30	0
56	MG	DA	3507	1/1	0.93	0.16	60,60,60,60	0
56	MG	DA	3187	1/1	0.93	0.12	56,56,56,56	0
56	MG	BB	3019	1/1	0.93	0.10	49,49,49,49	0
56	MG	DA	3510	1/1	0.93	0.10	50,50,50,50	0
56	MG	BA	3235	1/1	0.93	0.13	37,37,37,37	0
56	MG	BB	3021	1/1	0.93	0.13	54,54,54,54	0
56	MG	DA	3192	1/1	0.93	0.15	51,51,51,51	0
56	MG	AA	3175	1/1	0.93	0.11	54,54,54,54	0
56	MG	DA	3196	1/1	0.93	0.10	53,53,53,53	0
56	MG	CA	3127	1/1	0.93	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3390	1/1	0.93	0.16	52,52,52,52	0
56	MG	DA	3200	1/1	0.93	0.19	43,43,43,43	0
56	MG	DA	3527	1/1	0.93	0.18	53,53,53,53	0
56	MG	BA	3530	1/1	0.93	0.09	51,51,51,51	0
56	MG	DA	3531	1/1	0.93	0.10	54,54,54,54	0
56	MG	AA	3149	1/1	0.93	0.06	41,41,41,41	0
56	MG	BA	3244	1/1	0.93	0.10	63,63,63,63	0
56	MG	BA	3396	1/1	0.93	0.18	55,55,55,55	0
56	MG	BA	3535	1/1	0.93	0.08	18,18,18,18	0
56	MG	BA	3397	1/1	0.93	0.15	53,53,53,53	0
56	MG	BN	3001	1/1	0.93	0.20	51,51,51,51	0
56	MG	DA	3217	1/1	0.93	0.17	50,50,50,50	0
56	MG	DA	3218	1/1	0.93	0.13	47,47,47,47	0
56	MG	BA	3541	1/1	0.93	0.07	29,29,29,29	0
56	MG	AA	3051	1/1	0.93	0.22	62,62,62,62	0
56	MG	DA	3224	1/1	0.93	0.21	48,48,48,48	0
56	MG	CA	3144	1/1	0.93	0.14	59,59,59,59	0
56	MG	BA	3252	1/1	0.93	0.08	45,45,45,45	0
56	MG	AA	3211	1/1	0.93	0.13	59,59,59,59	0
56	MG	DA	3558	1/1	0.93	0.12	34,34,34,34	0
56	MG	BA	3256	1/1	0.93	0.11	49,49,49,49	0
56	MG	DA	3239	1/1	0.93	0.12	54,54,54,54	0
56	MG	DA	3240	1/1	0.93	0.12	51,51,51,51	0
56	MG	BA	3260	1/1	0.93	0.32	57,57,57,57	0
56	MG	BA	3711	1/1	0.93	0.09	45,45,45,45	0
56	MG	AA	3180	1/1	0.93	0.09	57,57,57,57	0
56	MG	BA	3558	1/1	0.93	0.08	29,29,29,29	0
56	MG	CA	3152	1/1	0.93	0.16	79,79,79,79	0
56	MG	DA	3573	1/1	0.93	0.12	46,46,46,46	0
56	MG	B3	101	1/1	0.93	0.15	48,48,48,48	0
56	MG	CA	3155	1/1	0.93	0.14	50,50,50,50	0
56	MG	DA	3256	1/1	0.93	0.09	47,47,47,47	0
56	MG	BA	3715	1/1	0.93	0.10	53,53,53,53	0
56	MG	DA	3262	1/1	0.93	0.07	43,43,43,43	0
56	MG	CA	3157	1/1	0.93	0.27	64,64,64,64	0
56	MG	DA	3268	1/1	0.93	0.10	60,60,60,60	0
56	MG	DA	3271	1/1	0.93	0.08	47,47,47,47	0
56	MG	BA	3559	1/1	0.93	0.08	30,30,30,30	0
56	MG	DA	3276	1/1	0.93	0.07	33,33,33,33	0
56	MG	BA	3414	1/1	0.93	0.08	29,29,29,29	0
56	MG	DA	3590	1/1	0.93	0.13	60,60,60,60	0
56	MG	B7	102	1/1	0.93	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3066	1/1	0.93	0.07	44,44,44,44	0
56	MG	AX	3011	1/1	0.93	0.12	50,50,50,50	0
56	MG	AA	3106	1/1	0.93	0.20	51,51,51,51	0
56	MG	CA	3167	1/1	0.93	0.09	48,48,48,48	0
56	MG	CA	3168	1/1	0.93	0.11	72,72,72,72	0
56	MG	BA	3575	1/1	0.93	0.09	64,64,64,64	0
56	MG	AA	3018	1/1	0.93	0.06	51,51,51,51	0
56	MG	AA	3185	1/1	0.93	0.23	53,53,53,53	0
56	MG	BA	3578	1/1	0.93	0.14	47,47,47,47	0
56	MG	DA	3298	1/1	0.93	0.05	33,33,33,33	0
56	MG	BA	3004	1/1	0.93	0.10	36,36,36,36	0
56	MG	BA	3739	1/1	0.93	0.14	46,46,46,46	0
56	MG	AA	3028	1/1	0.93	0.23	56,56,56,56	0
56	MG	DA	3305	1/1	0.93	0.06	28,28,28,28	0
56	MG	DA	3306	1/1	0.93	0.08	42,42,42,42	0
56	MG	DA	3309	1/1	0.93	0.07	42,42,42,42	0
56	MG	DA	3616	1/1	0.93	0.07	45,45,45,45	0
56	MG	DA	3617	1/1	0.93	0.11	53,53,53,53	0
56	MG	BA	3130	1/1	0.93	0.09	48,48,48,48	0
56	MG	DA	3619	1/1	0.93	0.10	58,58,58,58	0
56	MG	BA	3434	1/1	0.93	0.07	34,34,34,34	0
56	MG	DA	3627	1/1	0.93	0.07	48,48,48,48	0
56	MG	BA	3289	1/1	0.93	0.18	55,55,55,55	0
56	MG	AA	3111	1/1	0.93	0.20	52,52,52,52	0
56	MG	DA	3001	1/1	0.93	0.11	58,58,58,58	0
56	MG	BA	3136	1/1	0.93	0.14	58,58,58,58	0
56	MG	BA	3017	1/1	0.93	0.09	50,50,50,50	0
56	MG	DA	3006	1/1	0.93	0.10	43,43,43,43	0
56	MG	DA	3007	1/1	0.93	0.13	54,54,54,54	0
56	MG	DA	3332	1/1	0.93	0.09	41,41,41,41	0
56	MG	DA	3333	1/1	0.93	0.08	50,50,50,50	0
56	MG	BA	3167	1/1	0.93	0.11	50,50,50,50	0
56	MG	DA	3646	1/1	0.93	0.10	49,49,49,49	0
56	MG	AA	3189	1/1	0.93	0.13	59,59,59,59	0
56	MG	BA	3756	1/1	0.93	0.10	27,27,27,27	0
56	MG	DA	3019	1/1	0.93	0.13	57,57,57,57	0
56	MG	BA	3444	1/1	0.93	0.10	48,48,48,48	0
56	MG	BA	3021	1/1	0.93	0.15	60,60,60,60	0
56	MG	BA	3176	1/1	0.93	0.21	55,55,55,55	0
56	MG	AA	3081	1/1	0.93	0.25	58,58,58,58	0
56	MG	AA	3058	1/1	0.93	0.26	57,57,57,57	0
56	MG	DA	3665	1/1	0.93	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3666	1/1	0.93	0.27	41,41,41,41	0
56	MG	BA	3190	1/1	0.93	0.17	45,45,45,45	0
56	MG	BA	3620	1/1	0.93	0.08	47,47,47,47	0
56	MG	DA	3361	1/1	0.93	0.21	55,55,55,55	0
56	MG	CA	3043	1/1	0.93	0.19	54,54,54,54	0
56	MG	AE	3001	1/1	0.93	0.07	66,66,66,66	0
56	MG	CA	3045	1/1	0.93	0.27	58,58,58,58	0
56	MG	DB	3004	1/1	0.93	0.11	51,51,51,51	0
56	MG	BA	3323	1/1	0.93	0.12	39,39,39,39	0
56	MG	DA	3371	1/1	0.93	0.16	55,55,55,55	0
56	MG	BA	3463	1/1	0.93	0.09	37,37,37,37	0
56	MG	AA	3142	1/1	0.93	0.09	62,62,62,62	0
56	MG	DB	3011	1/1	0.93	0.14	52,52,52,52	0
56	MG	DA	3379	1/1	0.93	0.13	59,59,59,59	0
56	MG	AA	3059	1/1	0.93	0.25	59,59,59,59	0
56	MG	DA	3381	1/1	0.93	0.17	60,60,60,60	0
56	MG	DA	3053	1/1	0.93	0.09	45,45,45,45	0
56	MG	BA	3339	1/1	0.93	0.11	40,40,40,40	0
56	MG	DQ	3003	1/1	0.93	0.08	58,58,58,58	0
56	MG	DA	3057	1/1	0.93	0.09	47,47,47,47	0
56	MG	DU	3002	1/1	0.93	0.09	50,50,50,50	0
56	MG	DA	3060	1/1	0.93	0.09	47,47,47,47	0
56	MG	DA	3061	1/1	0.93	0.15	56,56,56,56	0
56	MG	DA	3062	1/1	0.93	0.16	53,53,53,53	0
56	MG	BA	3471	1/1	0.93	0.07	45,45,45,45	0
56	MG	BA	3346	1/1	0.93	0.05	32,32,32,32	0
56	MG	DA	3399	1/1	0.93	0.13	47,47,47,47	0
56	MG	BA	3782	1/1	0.93	0.08	51,51,51,51	0
56	MG	BA	3206	1/1	0.94	0.10	29,29,29,29	0
56	MG	BA	3698	1/1	0.94	0.09	48,48,48,48	0
56	MG	BA	3215	1/1	0.94	0.13	45,45,45,45	0
56	MG	DA	3383	1/1	0.94	0.07	37,37,37,37	0
56	MG	DA	3384	1/1	0.94	0.08	52,52,52,52	0
56	MG	BA	3514	1/1	0.94	0.10	41,41,41,41	0
56	MG	CA	3002	1/1	0.94	0.08	51,51,51,51	0
56	MG	CA	3004	1/1	0.94	0.09	71,71,71,71	0
56	MG	DA	3389	1/1	0.94	0.11	53,53,53,53	0
56	MG	BA	3515	1/1	0.94	0.07	20,20,20,20	0
56	MG	BA	3087	1/1	0.94	0.14	37,37,37,37	0
56	MG	CA	3009	1/1	0.94	0.17	50,50,50,50	0
56	MG	BA	3219	1/1	0.94	0.09	29,29,29,29	0
56	MG	BA	3361	1/1	0.94	0.12	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3041	1/1	0.94	0.24	52,52,52,52	0
56	MG	BA	3707	1/1	0.94	0.13	66,66,66,66	0
56	MG	AA	3087	1/1	0.94	0.24	52,52,52,52	0
56	MG	DA	3059	1/1	0.94	0.20	53,53,53,53	0
56	MG	BA	3709	1/1	0.94	0.23	44,44,44,44	0
56	MG	AA	3215	1/1	0.94	0.21	57,57,57,57	0
56	MG	AA	3184	1/1	0.94	0.11	55,55,55,55	0
56	MG	AA	3128	1/1	0.94	0.09	41,41,41,41	0
56	MG	DA	3407	1/1	0.94	0.06	46,46,46,46	0
56	MG	AX	3013	1/1	0.94	0.13	39,39,39,39	0
56	MG	AA	3105	1/1	0.94	0.09	49,49,49,49	0
56	MG	BA	3103	1/1	0.94	0.12	48,48,48,48	0
56	MG	DA	3067	1/1	0.94	0.08	49,49,49,49	0
56	MG	BA	3234	1/1	0.94	0.12	48,48,48,48	0
56	MG	DA	3414	1/1	0.94	0.14	41,41,41,41	0
56	MG	BA	3723	1/1	0.94	0.11	47,47,47,47	0
56	MG	DA	3074	1/1	0.94	0.15	50,50,50,50	0
56	MG	AA	3131	1/1	0.94	0.25	63,63,63,63	0
56	MG	BA	3236	1/1	0.94	0.14	43,43,43,43	0
56	MG	BA	3380	1/1	0.94	0.09	60,60,60,60	0
56	MG	DA	3085	1/1	0.94	0.10	52,52,52,52	0
56	MG	AA	3048	1/1	0.94	0.09	51,51,51,51	0
56	MG	AA	3226	1/1	0.94	0.27	58,58,58,58	0
56	MG	DA	3089	1/1	0.94	0.10	46,46,46,46	0
56	MG	DA	3090	1/1	0.94	0.09	45,45,45,45	0
56	MG	DA	3427	1/1	0.94	0.06	38,38,38,38	0
56	MG	CA	3035	1/1	0.94	0.13	60,60,60,60	0
56	MG	BA	3386	1/1	0.94	0.09	42,42,42,42	0
56	MG	AA	3060	1/1	0.94	0.25	59,59,59,59	0
56	MG	DA	3094	1/1	0.94	0.09	52,52,52,52	0
56	MG	BA	3248	1/1	0.94	0.08	45,45,45,45	0
56	MG	DA	3435	1/1	0.94	0.07	44,44,44,44	0
56	MG	BA	3554	1/1	0.94	0.13	37,37,37,37	0
56	MG	DA	3440	1/1	0.94	0.07	39,39,39,39	0
56	MG	AA	3061	1/1	0.94	0.11	54,54,54,54	0
56	MG	BA	3394	1/1	0.94	0.11	52,52,52,52	0
56	MG	BA	3744	1/1	0.94	0.06	20,20,20,20	0
56	MG	CA	3050	1/1	0.94	0.20	60,60,60,60	0
56	MG	BA	3251	1/1	0.94	0.10	52,52,52,52	0
56	MG	BA	3015	1/1	0.94	0.12	47,47,47,47	0
56	MG	BA	3561	1/1	0.94	0.06	27,27,27,27	0
56	MG	BA	3751	1/1	0.94	0.11	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3562	1/1	0.94	0.12	35,35,35,35	0
56	MG	DA	3113	1/1	0.94	0.20	44,44,44,44	0
56	MG	BA	3399	1/1	0.94	0.06	25,25,25,25	0
56	MG	BA	3754	1/1	0.94	0.18	60,60,60,60	0
56	MG	DA	3459	1/1	0.94	0.07	57,57,57,57	0
56	MG	BA	3564	1/1	0.94	0.07	41,41,41,41	0
56	MG	DA	3461	1/1	0.94	0.07	56,56,56,56	0
56	MG	DA	3462	1/1	0.94	0.14	43,43,43,43	0
56	MG	DA	3124	1/1	0.94	0.09	34,34,34,34	0
56	MG	DA	3464	1/1	0.94	0.06	44,44,44,44	0
56	MG	BA	3253	1/1	0.94	0.11	40,40,40,40	0
56	MG	DA	3467	1/1	0.94	0.18	43,43,43,43	0
56	MG	BA	3402	1/1	0.94	0.08	30,30,30,30	0
56	MG	AA	3016	1/1	0.94	0.15	46,46,46,46	0
56	MG	DA	3133	1/1	0.94	0.12	40,40,40,40	0
56	MG	BA	3255	1/1	0.94	0.28	58,58,58,58	0
56	MG	DA	3483	1/1	0.94	0.10	48,48,48,48	0
56	MG	DA	3484	1/1	0.94	0.08	45,45,45,45	0
56	MG	BA	3117	1/1	0.94	0.25	42,42,42,42	0
56	MG	DA	3139	1/1	0.94	0.05	40,40,40,40	0
56	MG	BA	3259	1/1	0.94	0.16	52,52,52,52	0
56	MG	DA	3488	1/1	0.94	0.10	37,37,37,37	0
56	MG	DA	3491	1/1	0.94	0.08	45,45,45,45	0
56	MG	BA	3581	1/1	0.94	0.06	38,38,38,38	0
56	MG	CA	3069	1/1	0.94	0.23	68,68,68,68	0
56	MG	BA	3582	1/1	0.94	0.11	44,44,44,44	0
56	MG	CA	3071	1/1	0.94	0.07	50,50,50,50	0
56	MG	DA	3152	1/1	0.94	0.14	42,42,42,42	0
56	MG	DA	3503	1/1	0.94	0.07	37,37,37,37	0
56	MG	BA	3410	1/1	0.94	0.09	46,46,46,46	0
56	MG	BA	3584	1/1	0.94	0.08	27,27,27,27	0
56	MG	CA	3074	1/1	0.94	0.32	55,55,55,55	0
56	MG	BA	3119	1/1	0.94	0.11	36,36,36,36	0
56	MG	DA	3160	1/1	0.94	0.21	59,59,59,59	0
56	MG	CA	3078	1/1	0.94	0.15	48,48,48,48	0
56	MG	DA	3168	1/1	0.94	0.17	53,53,53,53	0
56	MG	AD	502	1/1	0.94	0.28	56,56,56,56	0
56	MG	DA	3170	1/1	0.94	0.06	50,50,50,50	0
56	MG	DA	3171	1/1	0.94	0.17	38,38,38,38	0
56	MG	DA	3172	1/1	0.94	0.09	51,51,51,51	0
56	MG	DA	3174	1/1	0.94	0.12	48,48,48,48	0
56	MG	CA	3082	1/1	0.94	0.24	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3422	1/1	0.94	0.08	32,32,32,32	0
56	MG	DA	3526	1/1	0.94	0.10	47,47,47,47	0
56	MG	BA	3777	1/1	0.94	0.07	49,49,49,49	0
56	MG	DA	3183	1/1	0.94	0.27	58,58,58,58	0
56	MG	BA	3591	1/1	0.94	0.12	23,23,23,23	0
56	MG	BA	3592	1/1	0.94	0.10	29,29,29,29	0
56	MG	BA	3266	1/1	0.94	0.32	64,64,64,64	0
56	MG	CA	3089	1/1	0.94	0.07	58,58,58,58	0
56	MG	BA	3131	1/1	0.94	0.08	38,38,38,38	0
56	MG	CA	3091	1/1	0.94	0.13	48,48,48,48	0
56	MG	BA	3269	1/1	0.94	0.25	53,53,53,53	0
56	MG	DA	3539	1/1	0.94	0.06	46,46,46,46	0
56	MG	CA	3093	1/1	0.94	0.07	34,34,34,34	0
56	MG	DA	3541	1/1	0.94	0.07	54,54,54,54	0
56	MG	BA	3596	1/1	0.94	0.13	45,45,45,45	0
56	MG	BA	3601	1/1	0.94	0.07	42,42,42,42	0
56	MG	AA	3063	1/1	0.94	0.12	63,63,63,63	0
56	MG	CA	3098	1/1	0.94	0.12	43,43,43,43	0
56	MG	CA	3099	1/1	0.94	0.13	62,62,62,62	0
56	MG	AA	3197	1/1	0.94	0.12	56,56,56,56	0
56	MG	BA	3138	1/1	0.94	0.10	48,48,48,48	0
56	MG	BA	3140	1/1	0.94	0.11	46,46,46,46	0
56	MG	BA	3149	1/1	0.94	0.11	53,53,53,53	0
56	MG	DA	3210	1/1	0.94	0.11	44,44,44,44	0
56	MG	BA	3150	1/1	0.94	0.08	48,48,48,48	0
56	MG	BA	3616	1/1	0.94	0.11	53,53,53,53	0
56	MG	BA	3279	1/1	0.94	0.07	43,43,43,43	0
56	MG	BA	3280	1/1	0.94	0.08	49,49,49,49	0
56	MG	DA	3567	1/1	0.94	0.08	46,46,46,46	0
56	MG	BA	3152	1/1	0.94	0.08	43,43,43,43	0
56	MG	DA	3219	1/1	0.94	0.18	54,54,54,54	0
56	MG	DA	3571	1/1	0.94	0.12	57,57,57,57	0
56	MG	BA	3287	1/1	0.94	0.27	54,54,54,54	0
56	MG	DA	3221	1/1	0.94	0.12	49,49,49,49	0
56	MG	BA	3156	1/1	0.94	0.08	41,41,41,41	0
56	MG	DA	3577	1/1	0.94	0.07	49,49,49,49	0
56	MG	CA	3119	1/1	0.94	0.15	58,58,58,58	0
56	MG	DA	3225	1/1	0.94	0.15	54,54,54,54	0
56	MG	AA	3039	1/1	0.94	0.14	61,61,61,61	0
56	MG	BA	3628	1/1	0.94	0.10	30,30,30,30	0
56	MG	DA	3231	1/1	0.94	0.14	57,57,57,57	0
56	MG	DA	3234	1/1	0.94	0.09	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3815	1/1	0.94	0.18	50,50,50,50	0
56	MG	BA	3166	1/1	0.94	0.08	40,40,40,40	0
56	MG	AA	3114	1/1	0.94	0.13	51,51,51,51	0
56	MG	BA	3824	1/1	0.94	0.08	43,43,43,43	0
56	MG	BA	3293	1/1	0.94	0.20	52,52,52,52	0
56	MG	DA	3592	1/1	0.94	0.10	52,52,52,52	0
56	MG	BA	3448	1/1	0.94	0.09	28,28,28,28	0
56	MG	BA	3295	1/1	0.94	0.08	42,42,42,42	0
56	MG	DA	3245	1/1	0.94	0.12	62,62,62,62	0
56	MG	AA	3054	1/1	0.94	0.25	52,52,52,52	0
56	MG	AA	3147	1/1	0.94	0.09	55,55,55,55	0
56	MG	BA	3453	1/1	0.94	0.10	42,42,42,42	0
56	MG	CA	3135	1/1	0.94	0.12	53,53,53,53	0
56	MG	DA	3602	1/1	0.94	0.12	51,51,51,51	0
56	MG	BB	3002	1/1	0.94	0.19	52,52,52,52	0
56	MG	BB	3003	1/1	0.94	0.07	40,40,40,40	0
56	MG	BA	3455	1/1	0.94	0.12	39,39,39,39	0
56	MG	AA	3119	1/1	0.94	0.09	58,58,58,58	0
56	MG	BB	3008	1/1	0.94	0.21	54,54,54,54	0
56	MG	BA	3180	1/1	0.94	0.10	58,58,58,58	0
56	MG	BA	3052	1/1	0.94	0.10	43,43,43,43	0
56	MG	DA	3613	1/1	0.94	0.10	50,50,50,50	0
56	MG	AA	3206	1/1	0.94	0.12	47,47,47,47	0
56	MG	BA	3650	1/1	0.94	0.09	57,57,57,57	0
56	MG	BA	3319	1/1	0.94	0.11	20,20,20,20	0
56	MG	BA	3469	1/1	0.94	0.14	37,37,37,37	0
56	MG	BA	3059	1/1	0.94	0.07	55,55,55,55	0
56	MG	AA	3177	1/1	0.94	0.20	57,57,57,57	0
56	MG	BA	3063	1/1	0.94	0.09	47,47,47,47	0
56	MG	DA	3623	1/1	0.94	0.09	70,70,70,70	0
56	MG	DA	3625	1/1	0.94	0.09	53,53,53,53	0
56	MG	BD	301	1/1	0.94	0.18	49,49,49,49	0
56	MG	BD	303	1/1	0.94	0.25	44,44,44,44	0
56	MG	DA	3630	1/1	0.94	0.14	49,49,49,49	0
56	MG	BA	3473	1/1	0.94	0.09	57,57,57,57	0
56	MG	DA	3289	1/1	0.94	0.10	42,42,42,42	0
56	MG	BA	3475	1/1	0.94	0.15	53,53,53,53	0
56	MG	BA	3661	1/1	0.94	0.10	53,53,53,53	0
56	MG	BA	3662	1/1	0.94	0.12	50,50,50,50	0
56	MG	BF	302	1/1	0.94	0.06	39,39,39,39	0
56	MG	DA	3301	1/1	0.94	0.13	48,48,48,48	0
56	MG	BA	3476	1/1	0.94	0.07	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3644	1/1	0.94	0.14	55,55,55,55	0
56	MG	BA	3325	1/1	0.94	0.12	56,56,56,56	0
56	MG	BA	3668	1/1	0.94	0.08	56,56,56,56	0
56	MG	CA	3164	1/1	0.94	0.10	54,54,54,54	0
56	MG	BA	3326	1/1	0.94	0.10	38,38,38,38	0
56	MG	BN	3002	1/1	0.94	0.07	46,46,46,46	0
56	MG	BN	3005	1/1	0.94	0.21	51,51,51,51	0
56	MG	DA	3654	1/1	0.94	0.09	55,55,55,55	0
56	MG	BA	3196	1/1	0.94	0.21	51,51,51,51	0
56	MG	BP	201	1/1	0.94	0.38	41,41,41,41	0
56	MG	AW	3006	1/1	0.94	0.16	50,50,50,50	0
56	MG	DA	3661	1/1	0.94	0.15	42,42,42,42	0
56	MG	BR	201	1/1	0.94	0.14	44,44,44,44	0
56	MG	DA	3664	1/1	0.94	0.10	38,38,38,38	0
56	MG	AW	3007	1/1	0.94	0.10	64,64,64,64	0
56	MG	BA	3340	1/1	0.94	0.09	45,45,45,45	0
56	MG	CE	202	1/1	0.94	0.11	66,66,66,66	0
56	MG	DA	3671	1/1	0.94	0.13	59,59,59,59	0
56	MG	BU	201	1/1	0.94	0.09	39,39,39,39	0
56	MG	CT	3001	1/1	0.94	0.08	47,47,47,47	0
56	MG	BA	3488	1/1	0.94	0.09	50,50,50,50	0
56	MG	CW	3001	1/1	0.94	0.20	63,63,63,63	0
56	MG	AA	3045	1/1	0.94	0.26	59,59,59,59	0
56	MG	BX	102	1/1	0.94	0.17	41,41,41,41	0
56	MG	CX	3005	1/1	0.94	0.23	58,58,58,58	0
56	MG	DB	3006	1/1	0.94	0.21	62,62,62,62	0
56	MG	BA	3068	1/1	0.94	0.18	51,51,51,51	0
56	MG	BZ	3001	1/1	0.94	0.20	52,52,52,52	0
56	MG	DA	3351	1/1	0.94	0.06	39,39,39,39	0
56	MG	DA	3353	1/1	0.94	0.09	37,37,37,37	0
56	MG	DD	307	1/1	0.94	0.11	56,56,56,56	0
56	MG	BA	3348	1/1	0.94	0.12	54,54,54,54	0
56	MG	B0	102	1/1	0.94	0.13	68,68,68,68	0
56	MG	B0	103	1/1	0.94	0.07	54,54,54,54	0
56	MG	BA	3349	1/1	0.94	0.11	34,34,34,34	0
56	MG	DA	3360	1/1	0.94	0.09	51,51,51,51	0
56	MG	DN	5001	1/1	0.94	0.06	62,62,62,62	0
56	MG	DA	3009	1/1	0.94	0.07	38,38,38,38	0
56	MG	B2	3001	1/1	0.94	0.10	45,45,45,45	0
56	MG	BA	3351	1/1	0.94	0.08	34,34,34,34	0
56	MG	BA	3201	1/1	0.94	0.09	40,40,40,40	0
56	MG	DA	3369	1/1	0.94	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	B5	103	1/1	0.94	0.09	44,44,44,44	0
56	MG	AA	3021	1/1	0.94	0.09	45,45,45,45	0
56	MG	DA	3372	1/1	0.94	0.06	47,47,47,47	0
56	MG	AA	3123	1/1	0.94	0.16	57,57,57,57	0
56	MG	B6	102	1/1	0.94	0.27	55,55,55,55	0
56	MG	DA	3167	1/1	0.95	0.14	47,47,47,47	0
56	MG	BN	3004	1/1	0.95	0.24	50,50,50,50	0
56	MG	BA	3240	1/1	0.95	0.12	45,45,45,45	0
56	MG	BA	3062	1/1	0.95	0.30	57,57,57,57	0
56	MG	DA	3438	1/1	0.95	0.13	60,60,60,60	0
56	MG	BA	3139	1/1	0.95	0.10	61,61,61,61	0
56	MG	CA	3129	1/1	0.95	0.19	61,61,61,61	0
56	MG	DA	3443	1/1	0.95	0.07	51,51,51,51	0
56	MG	BQ	3003	1/1	0.95	0.11	54,54,54,54	0
56	MG	DA	3176	1/1	0.95	0.09	52,52,52,52	0
56	MG	DA	3177	1/1	0.95	0.09	54,54,54,54	0
56	MG	BQ	3004	1/1	0.95	0.13	35,35,35,35	0
56	MG	DA	3179	1/1	0.95	0.05	46,46,46,46	0
56	MG	BA	3717	1/1	0.95	0.12	58,58,58,58	0
56	MG	AX	3012	1/1	0.95	0.14	59,59,59,59	0
56	MG	BA	3719	1/1	0.95	0.07	42,42,42,42	0
56	MG	BA	3456	1/1	0.95	0.16	41,41,41,41	0
56	MG	BA	3141	1/1	0.95	0.06	38,38,38,38	0
56	MG	BU	208	1/1	0.95	0.14	41,41,41,41	0
56	MG	BA	3143	1/1	0.95	0.13	42,42,42,42	0
56	MG	CA	3142	1/1	0.95	0.16	61,61,61,61	0
56	MG	AA	3036	1/1	0.95	0.16	52,52,52,52	0
56	MG	AY	3001	1/1	0.95	0.24	70,70,70,70	0
56	MG	BA	3465	1/1	0.95	0.09	42,42,42,42	0
56	MG	DA	3194	1/1	0.95	0.15	35,35,35,35	0
56	MG	DA	3465	1/1	0.95	0.12	55,55,55,55	0
56	MG	AA	3007	1/1	0.95	0.25	65,65,65,65	0
56	MG	BA	3362	1/1	0.95	0.09	19,19,19,19	0
56	MG	BA	3733	1/1	0.95	0.14	41,41,41,41	0
56	MG	BA	3153	1/1	0.95	0.07	39,39,39,39	0
56	MG	DA	3470	1/1	0.95	0.10	42,42,42,42	0
56	MG	DA	3471	1/1	0.95	0.10	50,50,50,50	0
56	MG	B1	101	1/1	0.95	0.24	44,44,44,44	0
56	MG	BA	3736	1/1	0.95	0.10	56,56,56,56	0
56	MG	DA	3480	1/1	0.95	0.07	48,48,48,48	0
56	MG	DA	3481	1/1	0.95	0.06	30,30,30,30	0
56	MG	DA	3482	1/1	0.95	0.09	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3203	1/1	0.95	0.13	37,37,37,37	0
56	MG	BA	3738	1/1	0.95	0.14	58,58,58,58	0
56	MG	BA	3597	1/1	0.95	0.07	44,44,44,44	0
56	MG	BA	3598	1/1	0.95	0.07	47,47,47,47	0
56	MG	DA	3209	1/1	0.95	0.07	52,52,52,52	0
56	MG	BA	3741	1/1	0.95	0.06	28,28,28,28	0
56	MG	BA	3599	1/1	0.95	0.12	23,23,23,23	0
56	MG	BA	3600	1/1	0.95	0.11	56,56,56,56	0
56	MG	DA	3496	1/1	0.95	0.09	48,48,48,48	0
56	MG	DA	3214	1/1	0.95	0.09	47,47,47,47	0
56	MG	DA	3498	1/1	0.95	0.13	57,57,57,57	0
56	MG	CA	3159	1/1	0.95	0.14	57,57,57,57	0
56	MG	AA	3052	1/1	0.95	0.34	68,68,68,68	0
56	MG	DA	3501	1/1	0.95	0.21	59,59,59,59	0
56	MG	BA	3602	1/1	0.95	0.17	46,46,46,46	0
56	MG	AA	3164	1/1	0.95	0.19	50,50,50,50	0
56	MG	BA	3073	1/1	0.95	0.13	41,41,41,41	0
56	MG	BA	3749	1/1	0.95	0.15	45,45,45,45	0
56	MG	DA	3506	1/1	0.95	0.07	48,48,48,48	0
56	MG	DA	3222	1/1	0.95	0.14	54,54,54,54	0
56	MG	AA	3208	1/1	0.95	0.07	45,45,45,45	0
56	MG	CA	3003	1/1	0.95	0.23	58,58,58,58	0
56	MG	BA	3264	1/1	0.95	0.08	39,39,39,39	0
56	MG	BA	3169	1/1	0.95	0.16	47,47,47,47	0
56	MG	DA	3227	1/1	0.95	0.12	38,38,38,38	0
56	MG	CA	3170	1/1	0.95	0.13	64,64,64,64	0
56	MG	DA	3514	1/1	0.95	0.09	41,41,41,41	0
56	MG	CA	3006	1/1	0.95	0.24	53,53,53,53	0
56	MG	DA	3232	1/1	0.95	0.13	53,53,53,53	0
56	MG	BA	3610	1/1	0.95	0.12	64,64,64,64	0
56	MG	CA	3008	1/1	0.95	0.06	50,50,50,50	0
56	MG	CA	3174	1/1	0.95	0.11	46,46,46,46	0
56	MG	CA	3176	1/1	0.95	0.08	43,43,43,43	0
56	MG	BA	3081	1/1	0.95	0.19	49,49,49,49	0
56	MG	BA	3613	1/1	0.95	0.08	45,45,45,45	0
56	MG	DA	3529	1/1	0.95	0.07	41,41,41,41	0
56	MG	DA	3530	1/1	0.95	0.09	55,55,55,55	0
56	MG	BA	3082	1/1	0.95	0.09	59,59,59,59	0
56	MG	DA	3532	1/1	0.95	0.11	57,57,57,57	0
56	MG	BA	3375	1/1	0.95	0.06	35,35,35,35	0
56	MG	BA	3759	1/1	0.95	0.06	9,9,9,9	0
56	MG	CA	3014	1/1	0.95	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3172	1/1	0.95	0.13	45,45,45,45	0
56	MG	BA	3085	1/1	0.95	0.06	31,31,31,31	0
56	MG	CX	3003	1/1	0.95	0.24	50,50,50,50	0
56	MG	DA	3253	1/1	0.95	0.10	38,38,38,38	0
56	MG	BA	3379	1/1	0.95	0.13	45,45,45,45	0
56	MG	BA	3622	1/1	0.95	0.07	31,31,31,31	0
56	MG	BA	3764	1/1	0.95	0.11	58,58,58,58	0
56	MG	DA	3543	1/1	0.95	0.05	55,55,55,55	0
56	MG	CY	3001	1/1	0.95	0.23	58,58,58,58	0
56	MG	DA	3546	1/1	0.95	0.09	53,53,53,53	0
56	MG	DA	3266	1/1	0.95	0.07	47,47,47,47	0
56	MG	DA	3267	1/1	0.95	0.09	38,38,38,38	0
56	MG	BA	3623	1/1	0.95	0.09	52,52,52,52	0
56	MG	DA	3555	1/1	0.95	0.08	54,54,54,54	0
56	MG	DA	3270	1/1	0.95	0.09	49,49,49,49	0
56	MG	BA	3766	1/1	0.95	0.07	31,31,31,31	0
56	MG	BA	3767	1/1	0.95	0.16	29,29,29,29	0
56	MG	DA	3559	1/1	0.95	0.09	48,48,48,48	0
56	MG	DA	3273	1/1	0.95	0.06	45,45,45,45	0
56	MG	AA	3144	1/1	0.95	0.06	50,50,50,50	0
56	MG	BA	3006	1/1	0.95	0.09	52,52,52,52	0
56	MG	AA	3097	1/1	0.95	0.11	50,50,50,50	0
56	MG	BA	3094	1/1	0.95	0.06	43,43,43,43	0
56	MG	CA	3031	1/1	0.95	0.08	53,53,53,53	0
56	MG	BA	3496	1/1	0.95	0.13	39,39,39,39	0
56	MG	DA	3283	1/1	0.95	0.16	46,46,46,46	0
56	MG	BA	3388	1/1	0.95	0.07	52,52,52,52	0
56	MG	BA	3191	1/1	0.95	0.15	40,40,40,40	0
56	MG	BA	3505	1/1	0.95	0.08	54,54,54,54	0
56	MG	AA	3186	1/1	0.95	0.11	52,52,52,52	0
56	MG	BA	3509	1/1	0.95	0.07	39,39,39,39	0
56	MG	DA	3031	1/1	0.95	0.20	51,51,51,51	0
56	MG	DA	3578	1/1	0.95	0.10	55,55,55,55	0
56	MG	DA	3295	1/1	0.95	0.11	58,58,58,58	0
56	MG	CA	3038	1/1	0.95	0.13	46,46,46,46	0
56	MG	CA	3039	1/1	0.95	0.17	50,50,50,50	0
56	MG	DA	3038	1/1	0.95	0.13	47,47,47,47	0
56	MG	CA	3040	1/1	0.95	0.16	58,58,58,58	0
56	MG	CA	3041	1/1	0.95	0.14	58,58,58,58	0
56	MG	DA	3585	1/1	0.95	0.06	51,51,51,51	0
56	MG	BA	3281	1/1	0.95	0.07	49,49,49,49	0
56	MG	BA	3283	1/1	0.95	0.10	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3785	1/1	0.95	0.11	41,41,41,41	0
56	MG	DA	3045	1/1	0.95	0.09	47,47,47,47	0
56	MG	AA	3146	1/1	0.95	0.08	53,53,53,53	0
56	MG	CA	3048	1/1	0.95	0.24	52,52,52,52	0
56	MG	DA	3593	1/1	0.95	0.07	39,39,39,39	0
56	MG	DA	3048	1/1	0.95	0.07	45,45,45,45	0
56	MG	AA	3115	1/1	0.95	0.08	51,51,51,51	0
56	MG	BA	3100	1/1	0.95	0.08	45,45,45,45	0
56	MG	DA	3321	1/1	0.95	0.09	35,35,35,35	0
56	MG	DA	3054	1/1	0.95	0.07	43,43,43,43	0
56	MG	DA	3599	1/1	0.95	0.28	38,38,38,38	0
56	MG	DA	3055	1/1	0.95	0.10	36,36,36,36	0
56	MG	AA	3074	1/1	0.95	0.09	47,47,47,47	0
56	MG	BA	3649	1/1	0.95	0.07	43,43,43,43	0
56	MG	DA	3603	1/1	0.95	0.11	52,52,52,52	0
56	MG	DA	3328	1/1	0.95	0.08	47,47,47,47	0
56	MG	DA	3058	1/1	0.95	0.09	46,46,46,46	0
56	MG	AA	3108	1/1	0.95	0.16	55,55,55,55	0
56	MG	AA	3135	1/1	0.95	0.12	65,65,65,65	0
56	MG	BA	3521	1/1	0.95	0.09	36,36,36,36	0
56	MG	DA	3340	1/1	0.95	0.11	42,42,42,42	0
56	MG	BA	3653	1/1	0.95	0.19	49,49,49,49	0
56	MG	AA	3152	1/1	0.95	0.13	45,45,45,45	0
56	MG	BA	3202	1/1	0.95	0.09	46,46,46,46	0
56	MG	BA	3106	1/1	0.95	0.21	50,50,50,50	0
56	MG	BA	3300	1/1	0.95	0.17	22,22,22,22	0
56	MG	BA	3411	1/1	0.95	0.07	36,36,36,36	0
56	MG	BA	3302	1/1	0.95	0.10	35,35,35,35	0
56	MG	DA	3070	1/1	0.95	0.08	48,48,48,48	0
56	MG	CA	3065	1/1	0.95	0.15	65,65,65,65	0
56	MG	BA	3109	1/1	0.95	0.08	42,42,42,42	0
56	MG	DA	3076	1/1	0.95	0.11	43,43,43,43	0
56	MG	DA	3626	1/1	0.95	0.06	54,54,54,54	0
56	MG	DA	3077	1/1	0.95	0.09	43,43,43,43	0
56	MG	BA	3416	1/1	0.95	0.06	21,21,21,21	0
56	MG	DA	3629	1/1	0.95	0.08	52,52,52,52	0
56	MG	DA	3362	1/1	0.95	0.10	43,43,43,43	0
56	MG	BA	3533	1/1	0.95	0.12	50,50,50,50	0
56	MG	BA	3822	1/1	0.95	0.09	21,21,21,21	0
56	MG	DA	3084	1/1	0.95	0.10	27,27,27,27	0
56	MG	DA	3634	1/1	0.95	0.12	53,53,53,53	0
56	MG	BA	3823	1/1	0.95	0.09	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3418	1/1	0.95	0.07	32,32,32,32	0
56	MG	BA	3110	1/1	0.95	0.06	41,41,41,41	0
56	MG	BA	3826	1/1	0.95	0.17	33,33,33,33	0
56	MG	BA	3538	1/1	0.95	0.13	45,45,45,45	0
56	MG	CA	3075	1/1	0.95	0.10	44,44,44,44	0
56	MG	BA	3829	1/1	0.95	0.24	45,45,45,45	0
56	MG	BA	3673	1/1	0.95	0.14	47,47,47,47	0
56	MG	BA	3423	1/1	0.95	0.06	23,23,23,23	0
56	MG	CA	3081	1/1	0.95	0.21	58,58,58,58	0
56	MG	BA	3677	1/1	0.95	0.05	62,62,62,62	0
56	MG	DA	3652	1/1	0.95	0.09	49,49,49,49	0
56	MG	BA	3540	1/1	0.95	0.11	44,44,44,44	0
56	MG	BA	3029	1/1	0.95	0.12	46,46,46,46	0
56	MG	BA	3314	1/1	0.95	0.07	47,47,47,47	0
56	MG	AA	3089	1/1	0.95	0.28	57,57,57,57	0
56	MG	DA	3392	1/1	0.95	0.08	36,36,36,36	0
56	MG	AA	3154	1/1	0.95	0.11	59,59,59,59	0
56	MG	BB	3006	1/1	0.95	0.10	38,38,38,38	0
56	MG	BA	3032	1/1	0.95	0.11	38,38,38,38	0
56	MG	BA	3552	1/1	0.95	0.11	34,34,34,34	0
56	MG	BA	3038	1/1	0.95	0.22	47,47,47,47	0
56	MG	BA	3223	1/1	0.95	0.07	29,29,29,29	0
56	MG	DA	3668	1/1	0.95	0.17	79,79,79,79	0
56	MG	DA	3115	1/1	0.95	0.16	41,41,41,41	0
56	MG	AA	3029	1/1	0.95	0.15	53,53,53,53	0
56	MG	DA	3673	1/1	0.95	0.09	61,61,61,61	0
56	MG	BA	3047	1/1	0.95	0.05	27,27,27,27	0
56	MG	AX	3008	1/1	0.95	0.28	57,57,57,57	0
56	MG	DA	3122	1/1	0.95	0.08	36,36,36,36	0
56	MG	BA	3695	1/1	0.95	0.14	48,48,48,48	0
56	MG	BA	3124	1/1	0.95	0.12	38,38,38,38	0
56	MG	DA	3129	1/1	0.95	0.05	45,45,45,45	0
56	MG	BA	3128	1/1	0.95	0.13	27,27,27,27	0
56	MG	DA	3409	1/1	0.95	0.08	47,47,47,47	0
56	MG	BA	3055	1/1	0.95	0.14	31,31,31,31	0
56	MG	DB	3009	1/1	0.95	0.15	47,47,47,47	0
56	MG	AA	3201	1/1	0.95	0.06	59,59,59,59	0
56	MG	BA	3341	1/1	0.95	0.12	57,57,57,57	0
56	MG	BD	306	1/1	0.95	0.13	22,22,22,22	0
56	MG	AA	3178	1/1	0.95	0.10	54,54,54,54	0
56	MG	BA	3568	1/1	0.95	0.13	52,52,52,52	0
56	MG	BE	306	1/1	0.95	0.08	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3570	1/1	0.95	0.13	30,30,30,30	0
56	MG	BF	301	1/1	0.95	0.11	38,38,38,38	0
56	MG	DA	3149	1/1	0.95	0.14	48,48,48,48	0
56	MG	BA	3135	1/1	0.95	0.18	35,35,35,35	0
56	MG	CA	3115	1/1	0.95	0.10	62,62,62,62	0
56	MG	DU	3001	1/1	0.95	0.14	50,50,50,50	0
56	MG	AA	3122	1/1	0.95	0.23	60,60,60,60	0
56	MG	BA	3238	1/1	0.95	0.09	43,43,43,43	0
56	MG	BF	307	1/1	0.95	0.08	39,39,39,39	0
56	MG	BA	3710	1/1	0.95	0.06	28,28,28,28	0
56	MG	D7	102	1/1	0.95	0.26	43,43,43,43	0
56	MG	BA	3350	1/1	0.95	0.11	27,27,27,27	0
56	MG	BA	3450	1/1	0.95	0.13	34,34,34,34	0
56	MG	DA	3430	1/1	0.95	0.07	28,28,28,28	0
59	ZN	D4	501	1/1	0.95	0.07	119,119,119,119	0
56	MG	DA	3164	1/1	0.95	0.17	33,33,33,33	0
56	MG	BV	203	1/1	0.96	0.31	32,32,32,32	0
56	MG	BA	3587	1/1	0.96	0.08	44,44,44,44	0
56	MG	BA	3145	1/1	0.96	0.27	32,32,32,32	0
56	MG	BA	3019	1/1	0.96	0.17	42,42,42,42	0
56	MG	BA	3083	1/1	0.96	0.29	47,47,47,47	0
56	MG	BA	3242	1/1	0.96	0.30	42,42,42,42	0
56	MG	BA	3460	1/1	0.96	0.12	35,35,35,35	0
56	MG	BA	3461	1/1	0.96	0.09	31,31,31,31	0
56	MG	CA	3153	1/1	0.96	0.10	61,61,61,61	0
56	MG	BA	3737	1/1	0.96	0.13	36,36,36,36	0
56	MG	AA	3023	1/1	0.96	0.07	37,37,37,37	0
56	MG	AA	3191	1/1	0.96	0.07	48,48,48,48	0
56	MG	BA	3154	1/1	0.96	0.15	29,29,29,29	0
56	MG	BA	3355	1/1	0.96	0.07	24,24,24,24	0
56	MG	DA	3198	1/1	0.96	0.05	51,51,51,51	0
56	MG	BA	3468	1/1	0.96	0.10	49,49,49,49	0
56	MG	B5	102	1/1	0.96	0.24	45,45,45,45	0
56	MG	AA	3214	1/1	0.96	0.08	44,44,44,44	0
56	MG	DA	3202	1/1	0.96	0.19	50,50,50,50	0
56	MG	BA	3090	1/1	0.96	0.16	37,37,37,37	0
56	MG	AA	3118	1/1	0.96	0.16	53,53,53,53	0
56	MG	DA	3205	1/1	0.96	0.11	47,47,47,47	0
56	MG	BA	3025	1/1	0.96	0.06	38,38,38,38	0
56	MG	BA	3027	1/1	0.96	0.14	42,42,42,42	0
56	MG	DA	3478	1/1	0.96	0.08	47,47,47,47	0
56	MG	DA	3208	1/1	0.96	0.06	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3166	1/1	0.96	0.09	66,66,66,66	0
56	MG	AA	3043	1/1	0.96	0.08	26,26,26,26	0
56	MG	BA	3750	1/1	0.96	0.10	49,49,49,49	0
56	MG	BA	3258	1/1	0.96	0.20	41,41,41,41	0
56	MG	AA	3107	1/1	0.96	0.18	51,51,51,51	0
56	MG	AA	3219	1/1	0.96	0.21	65,65,65,65	0
56	MG	BA	3479	1/1	0.96	0.10	37,37,37,37	0
56	MG	BA	3615	1/1	0.96	0.28	35,35,35,35	0
56	MG	DA	3489	1/1	0.96	0.10	37,37,37,37	0
56	MG	DA	3490	1/1	0.96	0.06	39,39,39,39	0
56	MG	BA	3261	1/1	0.96	0.17	44,44,44,44	0
56	MG	CA	3175	1/1	0.96	0.08	39,39,39,39	0
56	MG	DA	3495	1/1	0.96	0.11	62,62,62,62	0
56	MG	BA	3175	1/1	0.96	0.05	35,35,35,35	0
56	MG	AA	3196	1/1	0.96	0.10	32,32,32,32	0
56	MG	BA	3178	1/1	0.96	0.17	38,38,38,38	0
56	MG	BA	3267	1/1	0.96	0.06	37,37,37,37	0
56	MG	CF	3001	1/1	0.96	0.14	38,38,38,38	0
56	MG	BA	3621	1/1	0.96	0.13	52,52,52,52	0
56	MG	BA	3179	1/1	0.96	0.07	39,39,39,39	0
56	MG	DA	3228	1/1	0.96	0.07	42,42,42,42	0
56	MG	BA	3372	1/1	0.96	0.11	24,24,24,24	0
56	MG	BA	3624	1/1	0.96	0.07	29,29,29,29	0
56	MG	CW	3002	1/1	0.96	0.13	74,74,74,74	0
56	MG	DA	3233	1/1	0.96	0.09	43,43,43,43	0
56	MG	BA	3373	1/1	0.96	0.10	38,38,38,38	0
56	MG	AA	3078	1/1	0.96	0.08	48,48,48,48	0
56	MG	DA	3237	1/1	0.96	0.07	51,51,51,51	0
56	MG	CA	3018	1/1	0.96	0.13	45,45,45,45	0
56	MG	BA	3034	1/1	0.96	0.10	28,28,28,28	0
56	MG	BA	3629	1/1	0.96	0.09	56,56,56,56	0
56	MG	BA	3502	1/1	0.96	0.18	45,45,45,45	0
56	MG	BA	3631	1/1	0.96	0.07	43,43,43,43	0
56	MG	BA	3771	1/1	0.96	0.07	41,41,41,41	0
56	MG	DA	3517	1/1	0.96	0.06	47,47,47,47	0
56	MG	BA	3632	1/1	0.96	0.10	55,55,55,55	0
56	MG	BA	3774	1/1	0.96	0.06	43,43,43,43	0
56	MG	BA	3271	1/1	0.96	0.05	26,26,26,26	0
56	MG	DA	3525	1/1	0.96	0.08	41,41,41,41	0
56	MG	AA	3157	1/1	0.96	0.06	46,46,46,46	0
56	MG	AA	3199	1/1	0.96	0.12	59,59,59,59	0
56	MG	BA	3507	1/1	0.96	0.07	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3046	1/1	0.96	0.07	43,43,43,43	0
56	MG	DA	3258	1/1	0.96	0.20	59,59,59,59	0
56	MG	AA	3200	1/1	0.96	0.17	45,45,45,45	0
56	MG	DA	3261	1/1	0.96	0.06	44,44,44,44	0
56	MG	BA	3049	1/1	0.96	0.12	37,37,37,37	0
56	MG	DA	3023	1/1	0.96	0.09	30,30,30,30	0
56	MG	DA	3025	1/1	0.96	0.08	44,44,44,44	0
56	MG	DA	3026	1/1	0.96	0.06	42,42,42,42	0
56	MG	BA	3640	1/1	0.96	0.20	39,39,39,39	0
56	MG	BA	3194	1/1	0.96	0.09	37,37,37,37	0
56	MG	BA	3786	1/1	0.96	0.07	37,37,37,37	0
56	MG	DA	3030	1/1	0.96	0.11	40,40,40,40	0
56	MG	BA	3195	1/1	0.96	0.19	50,50,50,50	0
56	MG	BA	3788	1/1	0.96	0.07	41,41,41,41	0
56	MG	DA	3035	1/1	0.96	0.07	38,38,38,38	0
56	MG	DA	3036	1/1	0.96	0.06	29,29,29,29	0
56	MG	BA	3789	1/1	0.96	0.16	39,39,39,39	0
56	MG	BA	3791	1/1	0.96	0.08	47,47,47,47	0
56	MG	DA	3281	1/1	0.96	0.11	33,33,33,33	0
56	MG	CA	3042	1/1	0.96	0.10	58,58,58,58	0
56	MG	DA	3550	1/1	0.96	0.06	51,51,51,51	0
56	MG	DA	3553	1/1	0.96	0.09	54,54,54,54	0
56	MG	BA	3793	1/1	0.96	0.07	38,38,38,38	0
56	MG	BA	3051	1/1	0.96	0.07	25,25,25,25	0
56	MG	DA	3285	1/1	0.96	0.07	28,28,28,28	0
56	MG	BA	3646	1/1	0.96	0.07	38,38,38,38	0
56	MG	BA	3391	1/1	0.96	0.09	41,41,41,41	0
56	MG	AA	3006	1/1	0.96	0.05	37,37,37,37	0
56	MG	AA	3015	1/1	0.96	0.16	60,60,60,60	0
56	MG	BA	3285	1/1	0.96	0.23	49,49,49,49	0
56	MG	DA	3294	1/1	0.96	0.06	42,42,42,42	0
56	MG	BA	3286	1/1	0.96	0.18	46,46,46,46	0
56	MG	DA	3296	1/1	0.96	0.07	48,48,48,48	0
56	MG	DA	3049	1/1	0.96	0.06	24,24,24,24	0
56	MG	CA	3052	1/1	0.96	0.15	65,65,65,65	0
56	MG	DA	3052	1/1	0.96	0.07	38,38,38,38	0
56	MG	BA	3056	1/1	0.96	0.15	33,33,33,33	0
56	MG	BA	3288	1/1	0.96	0.29	40,40,40,40	0
56	MG	AA	3161	1/1	0.96	0.18	46,46,46,46	0
56	MG	BA	3058	1/1	0.96	0.14	36,36,36,36	0
56	MG	BA	3809	1/1	0.96	0.07	29,29,29,29	0
56	MG	BA	3118	1/1	0.96	0.13	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3124	1/1	0.96	0.08	53,53,53,53	0
56	MG	DA	3311	1/1	0.96	0.09	42,42,42,42	0
56	MG	BA	3406	1/1	0.96	0.06	32,32,32,32	0
56	MG	DA	3314	1/1	0.96	0.06	33,33,33,33	0
56	MG	BA	3407	1/1	0.96	0.09	37,37,37,37	0
56	MG	DA	3318	1/1	0.96	0.08	42,42,42,42	0
56	MG	CA	3062	1/1	0.96	0.18	44,44,44,44	0
56	MG	DA	3586	1/1	0.96	0.08	44,44,44,44	0
56	MG	AA	3064	1/1	0.96	0.07	61,61,61,61	0
56	MG	BA	3126	1/1	0.96	0.08	43,43,43,43	0
56	MG	BA	3209	1/1	0.96	0.12	41,41,41,41	0
56	MG	BA	3667	1/1	0.96	0.08	52,52,52,52	0
56	MG	BA	3536	1/1	0.96	0.12	48,48,48,48	0
56	MG	DA	3326	1/1	0.96	0.09	46,46,46,46	0
56	MG	BA	3669	1/1	0.96	0.06	42,42,42,42	0
56	MG	BA	3213	1/1	0.96	0.06	45,45,45,45	0
56	MG	DA	3330	1/1	0.96	0.06	46,46,46,46	0
56	MG	DA	3071	1/1	0.96	0.13	44,44,44,44	0
56	MG	BA	3671	1/1	0.96	0.09	45,45,45,45	0
56	MG	DA	3073	1/1	0.96	0.15	54,54,54,54	0
56	MG	DA	3336	1/1	0.96	0.06	47,47,47,47	0
56	MG	BA	3214	1/1	0.96	0.08	49,49,49,49	0
56	MG	BA	3303	1/1	0.96	0.13	35,35,35,35	0
56	MG	BA	3832	1/1	0.96	0.05	37,37,37,37	0
56	MG	BA	3674	1/1	0.96	0.07	47,47,47,47	0
56	MG	BA	3308	1/1	0.96	0.08	39,39,39,39	0
56	MG	DA	3080	1/1	0.96	0.16	45,45,45,45	0
56	MG	DA	3606	1/1	0.96	0.09	54,54,54,54	0
56	MG	BA	3127	1/1	0.96	0.09	41,41,41,41	0
56	MG	DA	3608	1/1	0.96	0.09	53,53,53,53	0
56	MG	DA	3083	1/1	0.96	0.06	51,51,51,51	0
56	MG	DA	3352	1/1	0.96	0.07	35,35,35,35	0
56	MG	BA	3001	1/1	0.96	0.15	43,43,43,43	0
56	MG	BA	3545	1/1	0.96	0.12	41,41,41,41	0
56	MG	CA	3080	1/1	0.96	0.23	52,52,52,52	0
56	MG	BA	3546	1/1	0.96	0.14	30,30,30,30	0
56	MG	DA	3358	1/1	0.96	0.16	45,45,45,45	0
56	MG	BA	3312	1/1	0.96	0.11	33,33,33,33	0
56	MG	BA	3682	1/1	0.96	0.14	50,50,50,50	0
56	MG	AK	202	1/1	0.96	0.14	38,38,38,38	0
56	MG	BA	3684	1/1	0.96	0.15	49,49,49,49	0
56	MG	BB	3010	1/1	0.96	0.09	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3621	1/1	0.96	0.09	45,45,45,45	0
56	MG	CA	3087	1/1	0.96	0.17	63,63,63,63	0
56	MG	DA	3624	1/1	0.96	0.07	47,47,47,47	0
56	MG	BA	3550	1/1	0.96	0.13	34,34,34,34	0
56	MG	BA	3551	1/1	0.96	0.07	33,33,33,33	0
56	MG	AA	3126	1/1	0.96	0.07	46,46,46,46	0
56	MG	BA	3132	1/1	0.96	0.06	42,42,42,42	0
56	MG	DA	3100	1/1	0.96	0.05	36,36,36,36	0
56	MG	AA	3090	1/1	0.96	0.29	53,53,53,53	0
56	MG	BA	3318	1/1	0.96	0.07	37,37,37,37	0
56	MG	BA	3134	1/1	0.96	0.13	35,35,35,35	0
56	MG	BA	3694	1/1	0.96	0.08	27,27,27,27	0
56	MG	CA	3096	1/1	0.96	0.15	61,61,61,61	0
56	MG	BA	3225	1/1	0.96	0.10	42,42,42,42	0
56	MG	BD	302	1/1	0.96	0.13	23,23,23,23	0
56	MG	DA	3638	1/1	0.96	0.11	60,60,60,60	0
56	MG	DA	3111	1/1	0.96	0.08	33,33,33,33	0
56	MG	BA	3696	1/1	0.96	0.08	33,33,33,33	0
56	MG	BA	3697	1/1	0.96	0.06	35,35,35,35	0
56	MG	BA	3321	1/1	0.96	0.06	54,54,54,54	0
56	MG	DA	3390	1/1	0.96	0.05	54,54,54,54	0
56	MG	BD	307	1/1	0.96	0.14	35,35,35,35	0
56	MG	DA	3647	1/1	0.96	0.10	47,47,47,47	0
56	MG	BD	308	1/1	0.96	0.07	39,39,39,39	0
56	MG	DA	3121	1/1	0.96	0.08	41,41,41,41	0
56	MG	CA	3104	1/1	0.96	0.14	64,64,64,64	0
56	MG	DA	3123	1/1	0.96	0.13	47,47,47,47	0
56	MG	BE	301	1/1	0.96	0.06	23,23,23,23	0
56	MG	AA	3008	1/1	0.96	0.07	54,54,54,54	0
56	MG	DA	3128	1/1	0.96	0.05	45,45,45,45	0
56	MG	CA	3108	1/1	0.96	0.10	51,51,51,51	0
56	MG	AA	3129	1/1	0.96	0.07	73,73,73,73	0
56	MG	DA	3659	1/1	0.96	0.24	67,67,67,67	0
56	MG	BA	3137	1/1	0.96	0.13	45,45,45,45	0
56	MG	DA	3662	1/1	0.96	0.05	27,27,27,27	0
56	MG	BA	3437	1/1	0.96	0.07	28,28,28,28	0
56	MG	BA	3565	1/1	0.96	0.12	42,42,42,42	0
56	MG	DA	3137	1/1	0.96	0.09	54,54,54,54	0
56	MG	BA	3566	1/1	0.96	0.07	30,30,30,30	0
56	MG	BA	3011	1/1	0.96	0.12	40,40,40,40	0
56	MG	DA	3141	1/1	0.96	0.13	56,56,56,56	0
56	MG	DA	3669	1/1	0.96	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3117	1/1	0.96	0.10	48,48,48,48	0
56	MG	CA	3118	1/1	0.96	0.07	47,47,47,47	0
56	MG	BA	3327	1/1	0.96	0.09	25,25,25,25	0
56	MG	BA	3569	1/1	0.96	0.12	57,57,57,57	0
56	MG	BA	3232	1/1	0.96	0.06	37,37,37,37	0
56	MG	BF	312	1/1	0.96	0.07	47,47,47,47	0
56	MG	BG	201	1/1	0.96	0.11	57,57,57,57	0
56	MG	DA	3417	1/1	0.96	0.10	33,33,33,33	0
56	MG	BG	203	1/1	0.96	0.05	36,36,36,36	0
56	MG	BA	3072	1/1	0.96	0.06	30,30,30,30	0
56	MG	BA	3574	1/1	0.96	0.08	63,63,63,63	0
56	MG	DA	3157	1/1	0.96	0.15	44,44,44,44	0
56	MG	DA	3158	1/1	0.96	0.13	40,40,40,40	0
56	MG	BA	3335	1/1	0.96	0.14	50,50,50,50	0
56	MG	BA	3338	1/1	0.96	0.09	41,41,41,41	0
56	MG	DD	302	1/1	0.96	0.09	49,49,49,49	0
56	MG	DD	303	1/1	0.96	0.12	49,49,49,49	0
56	MG	DA	3425	1/1	0.96	0.07	45,45,45,45	0
56	MG	DA	3161	1/1	0.96	0.21	49,49,49,49	0
56	MG	DE	302	1/1	0.96	0.10	39,39,39,39	0
56	MG	AA	3083	1/1	0.96	0.20	52,52,52,52	0
56	MG	CA	3130	1/1	0.96	0.14	60,60,60,60	0
56	MG	DA	3166	1/1	0.96	0.10	46,46,46,46	0
56	MG	DF	303	1/1	0.96	0.06	46,46,46,46	0
56	MG	DF	305	1/1	0.96	0.18	43,43,43,43	0
56	MG	BA	3016	1/1	0.96	0.12	44,44,44,44	0
56	MG	BA	3579	1/1	0.96	0.05	47,47,47,47	0
56	MG	DQ	3002	1/1	0.96	0.06	42,42,42,42	0
56	MG	AA	3104	1/1	0.96	0.14	50,50,50,50	0
56	MG	BA	3342	1/1	0.96	0.06	51,51,51,51	0
56	MG	BA	3344	1/1	0.96	0.06	37,37,37,37	0
56	MG	BA	3721	1/1	0.96	0.08	47,47,47,47	0
56	MG	DV	3001	1/1	0.96	0.10	71,71,71,71	0
56	MG	DA	3437	1/1	0.96	0.10	39,39,39,39	0
56	MG	BA	3345	1/1	0.96	0.08	44,44,44,44	0
56	MG	DA	3439	1/1	0.96	0.18	50,50,50,50	0
56	MG	D0	102	1/1	0.96	0.12	62,62,62,62	0
56	MG	BA	3144	1/1	0.96	0.06	43,43,43,43	0
56	MG	BU	202	1/1	0.96	0.13	40,40,40,40	0
56	MG	BU	204	1/1	0.96	0.13	38,38,38,38	0
56	MG	BU	206	1/1	0.96	0.27	43,43,43,43	0
56	MG	BA	3454	1/1	0.96	0.07	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3447	1/1	0.96	0.07	35,35,35,35	0
56	MG	DA	3257	1/1	0.97	0.09	34,34,34,34	0
56	MG	BE	308	1/1	0.97	0.04	21,21,21,21	0
56	MG	BA	3500	1/1	0.97	0.05	26,26,26,26	0
56	MG	BA	3732	1/1	0.97	0.26	40,40,40,40	0
56	MG	BF	303	1/1	0.97	0.22	42,42,42,42	0
56	MG	BA	3501	1/1	0.97	0.05	20,20,20,20	0
56	MG	DA	3265	1/1	0.97	0.17	52,52,52,52	0
56	MG	DA	3069	1/1	0.97	0.10	53,53,53,53	0
56	MG	BA	3123	1/1	0.97	0.09	35,35,35,35	0
56	MG	BA	3614	1/1	0.97	0.05	26,26,26,26	0
56	MG	DA	3269	1/1	0.97	0.07	32,32,32,32	0
56	MG	BF	309	1/1	0.97	0.14	30,30,30,30	0
56	MG	BF	310	1/1	0.97	0.22	38,38,38,38	0
56	MG	BA	3398	1/1	0.97	0.06	42,42,42,42	0
56	MG	DA	3075	1/1	0.97	0.11	39,39,39,39	0
56	MG	DA	3274	1/1	0.97	0.07	33,33,33,33	0
56	MG	DA	3275	1/1	0.97	0.06	52,52,52,52	0
56	MG	BA	3033	1/1	0.97	0.06	33,33,33,33	0
56	MG	BA	3316	1/1	0.97	0.08	23,23,23,23	0
56	MG	BA	3506	1/1	0.97	0.12	51,51,51,51	0
56	MG	BA	3125	1/1	0.97	0.07	42,42,42,42	0
56	MG	BA	3246	1/1	0.97	0.09	27,27,27,27	0
56	MG	BA	3247	1/1	0.97	0.04	28,28,28,28	0
56	MG	DA	3082	1/1	0.97	0.16	34,34,34,34	0
56	MG	BA	3182	1/1	0.97	0.12	41,41,41,41	0
56	MG	BA	3745	1/1	0.97	0.08	30,30,30,30	0
56	MG	BA	3184	1/1	0.97	0.17	30,30,30,30	0
56	MG	BP	202	1/1	0.97	0.17	34,34,34,34	0
56	MG	BP	203	1/1	0.97	0.06	32,32,32,32	0
56	MG	DA	3088	1/1	0.97	0.06	42,42,42,42	0
56	MG	BQ	3002	1/1	0.97	0.08	37,37,37,37	0
56	MG	DA	3291	1/1	0.97	0.05	42,42,42,42	0
56	MG	BA	3250	1/1	0.97	0.12	40,40,40,40	0
56	MG	DA	3519	1/1	0.97	0.04	24,24,24,24	0
56	MG	BA	3513	1/1	0.97	0.07	34,34,34,34	0
56	MG	AA	3026	1/1	0.97	0.23	53,53,53,53	0
56	MG	CA	3116	1/1	0.97	0.12	55,55,55,55	0
56	MG	BA	3035	1/1	0.97	0.12	31,31,31,31	0
56	MG	DA	3095	1/1	0.97	0.20	47,47,47,47	0
56	MG	DA	3299	1/1	0.97	0.08	43,43,43,43	0
56	MG	BA	3036	1/1	0.97	0.13	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3517	1/1	0.97	0.08	51,51,51,51	0
56	MG	BA	3518	1/1	0.97	0.10	43,43,43,43	0
56	MG	BA	3084	1/1	0.97	0.16	45,45,45,45	0
56	MG	AA	3220	1/1	0.97	0.05	64,64,64,64	0
56	MG	BA	3329	1/1	0.97	0.06	29,29,29,29	0
56	MG	DA	3308	1/1	0.97	0.10	45,45,45,45	0
56	MG	BA	3417	1/1	0.97	0.13	33,33,33,33	0
56	MG	BA	3086	1/1	0.97	0.09	41,41,41,41	0
56	MG	BV	204	1/1	0.97	0.17	50,50,50,50	0
56	MG	BA	3419	1/1	0.97	0.08	39,39,39,39	0
56	MG	DA	3313	1/1	0.97	0.07	23,23,23,23	0
56	MG	DA	3107	1/1	0.97	0.16	49,49,49,49	0
56	MG	DA	3315	1/1	0.97	0.07	41,41,41,41	0
56	MG	DA	3316	1/1	0.97	0.05	44,44,44,44	0
56	MG	DA	3544	1/1	0.97	0.12	37,37,37,37	0
56	MG	BW	202	1/1	0.97	0.14	49,49,49,49	0
56	MG	BW	203	1/1	0.97	0.16	34,34,34,34	0
56	MG	BA	3420	1/1	0.97	0.06	22,22,22,22	0
56	MG	BA	3421	1/1	0.97	0.09	33,33,33,33	0
56	MG	BA	3528	1/1	0.97	0.05	43,43,43,43	0
56	MG	DA	3322	1/1	0.97	0.13	43,43,43,43	0
56	MG	DA	3552	1/1	0.97	0.06	43,43,43,43	0
56	MG	DA	3116	1/1	0.97	0.15	57,57,57,57	0
56	MG	BA	3529	1/1	0.97	0.07	33,33,33,33	0
56	MG	BA	3642	1/1	0.97	0.10	37,37,37,37	0
56	MG	BA	3334	1/1	0.97	0.10	30,30,30,30	0
56	MG	DA	3120	1/1	0.97	0.15	45,45,45,45	0
56	MG	BA	3644	1/1	0.97	0.04	36,36,36,36	0
56	MG	DA	3329	1/1	0.97	0.04	29,29,29,29	0
56	MG	BA	3257	1/1	0.97	0.17	41,41,41,41	0
56	MG	DA	3331	1/1	0.97	0.08	39,39,39,39	0
56	MG	BA	3040	1/1	0.97	0.05	47,47,47,47	0
56	MG	BA	3042	1/1	0.97	0.18	40,40,40,40	0
56	MG	DA	3125	1/1	0.97	0.12	45,45,45,45	0
56	MG	DA	3126	1/1	0.97	0.12	44,44,44,44	0
56	MG	DA	3337	1/1	0.97	0.05	43,43,43,43	0
56	MG	BA	3043	1/1	0.97	0.21	39,39,39,39	0
56	MG	DA	3570	1/1	0.97	0.05	49,49,49,49	0
56	MG	DA	3339	1/1	0.97	0.07	52,52,52,52	0
56	MG	AA	3092	1/1	0.97	0.13	39,39,39,39	0
56	MG	B5	101	1/1	0.97	0.15	31,31,31,31	0
56	MG	DA	3130	1/1	0.97	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3093	1/1	0.97	0.14	50,50,50,50	0
56	MG	DA	3344	1/1	0.97	0.08	44,44,44,44	0
56	MG	DA	3345	1/1	0.97	0.05	35,35,35,35	0
56	MG	DA	3346	1/1	0.97	0.05	35,35,35,35	0
56	MG	BA	3537	1/1	0.97	0.07	49,49,49,49	0
56	MG	DA	3348	1/1	0.97	0.05	38,38,38,38	0
56	MG	BA	3343	1/1	0.97	0.08	33,33,33,33	0
56	MG	DA	3350	1/1	0.97	0.10	29,29,29,29	0
56	MG	DA	3134	1/1	0.97	0.09	49,49,49,49	0
56	MG	BA	3263	1/1	0.97	0.19	32,32,32,32	0
56	MG	DA	3136	1/1	0.97	0.16	44,44,44,44	0
56	MG	BA	3008	1/1	0.97	0.14	27,27,27,27	0
56	MG	AA	3065	1/1	0.97	0.14	58,58,58,58	0
56	MG	BA	3780	1/1	0.97	0.06	41,41,41,41	0
56	MG	B8	103	1/1	0.97	0.14	48,48,48,48	0
56	MG	BA	3542	1/1	0.97	0.09	48,48,48,48	0
56	MG	BA	3657	1/1	0.97	0.18	47,47,47,47	0
56	MG	BA	3097	1/1	0.97	0.15	52,52,52,52	0
56	MG	BA	3098	1/1	0.97	0.14	26,26,26,26	0
56	MG	DA	3363	1/1	0.97	0.15	54,54,54,54	0
56	MG	DA	3147	1/1	0.97	0.05	44,44,44,44	0
56	MG	DA	3148	1/1	0.97	0.08	29,29,29,29	0
56	MG	BA	3660	1/1	0.97	0.06	51,51,51,51	0
56	MG	BA	3142	1/1	0.97	0.18	34,34,34,34	0
56	MG	DA	3151	1/1	0.97	0.19	44,44,44,44	0
56	MG	BA	3205	1/1	0.97	0.16	41,41,41,41	0
56	MG	BA	3013	1/1	0.97	0.07	34,34,34,34	0
56	MG	DA	3375	1/1	0.97	0.07	40,40,40,40	0
56	MG	DA	3376	1/1	0.97	0.13	54,54,54,54	0
56	MG	BA	3665	1/1	0.97	0.12	49,49,49,49	0
56	MG	BA	3207	1/1	0.97	0.09	38,38,38,38	0
56	MG	BA	3353	1/1	0.97	0.07	49,49,49,49	0
56	MG	BA	3208	1/1	0.97	0.15	48,48,48,48	0
56	MG	BA	3445	1/1	0.97	0.06	32,32,32,32	0
56	MG	DA	3382	1/1	0.97	0.10	44,44,44,44	0
56	MG	BA	3014	1/1	0.97	0.07	33,33,33,33	0
56	MG	BA	3210	1/1	0.97	0.23	31,31,31,31	0
56	MG	DA	3162	1/1	0.97	0.12	43,43,43,43	0
56	MG	BA	3555	1/1	0.97	0.15	33,33,33,33	0
56	MG	BA	3053	1/1	0.97	0.12	22,22,22,22	0
56	MG	BA	3801	1/1	0.97	0.07	53,53,53,53	0
56	MG	BA	3146	1/1	0.97	0.06	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3391	1/1	0.97	0.05	44,44,44,44	0
56	MG	BA	3803	1/1	0.97	0.05	47,47,47,47	0
56	MG	CA	3021	1/1	0.97	0.05	42,42,42,42	0
56	MG	DA	3394	1/1	0.97	0.09	49,49,49,49	0
56	MG	AA	3009	1/1	0.97	0.10	46,46,46,46	0
56	MG	BA	3805	1/1	0.97	0.05	21,21,21,21	0
56	MG	BA	3216	1/1	0.97	0.05	34,34,34,34	0
56	MG	AA	3227	1/1	0.97	0.15	48,48,48,48	0
56	MG	BA	3151	1/1	0.97	0.07	42,42,42,42	0
56	MG	AA	3053	1/1	0.97	0.24	49,49,49,49	0
56	MG	AA	3160	1/1	0.97	0.14	57,57,57,57	0
56	MG	BA	3222	1/1	0.97	0.11	27,27,27,27	0
56	MG	DA	3180	1/1	0.97	0.10	51,51,51,51	0
56	MG	CA	3030	1/1	0.97	0.06	59,59,59,59	0
56	MG	AA	3193	1/1	0.97	0.08	43,43,43,43	0
56	MG	BA	3458	1/1	0.97	0.13	19,19,19,19	0
56	MG	BA	3816	1/1	0.97	0.06	21,21,21,21	0
56	MG	DA	3637	1/1	0.97	0.06	44,44,44,44	0
56	MG	BA	3817	1/1	0.97	0.10	47,47,47,47	0
56	MG	AA	3077	1/1	0.97	0.12	49,49,49,49	0
56	MG	DA	3641	1/1	0.97	0.06	44,44,44,44	0
56	MG	AA	3132	1/1	0.97	0.05	22,22,22,22	0
56	MG	BA	3821	1/1	0.97	0.08	50,50,50,50	0
56	MG	DA	3189	1/1	0.97	0.19	48,48,48,48	0
56	MG	BA	3687	1/1	0.97	0.05	36,36,36,36	0
56	MG	BA	3226	1/1	0.97	0.09	41,41,41,41	0
56	MG	BA	3161	1/1	0.97	0.21	37,37,37,37	0
56	MG	DA	3193	1/1	0.97	0.32	40,40,40,40	0
56	MG	BA	3572	1/1	0.97	0.10	63,63,63,63	0
56	MG	DA	3004	1/1	0.97	0.11	42,42,42,42	0
56	MG	BA	3162	1/1	0.97	0.15	46,46,46,46	0
56	MG	BA	3165	1/1	0.97	0.16	40,40,40,40	0
56	MG	BA	3296	1/1	0.97	0.12	31,31,31,31	0
56	MG	BA	3297	1/1	0.97	0.31	55,55,55,55	0
56	MG	DA	3656	1/1	0.97	0.16	62,62,62,62	0
56	MG	AF	3001	1/1	0.97	0.14	40,40,40,40	0
56	MG	BA	3299	1/1	0.97	0.09	32,32,32,32	0
56	MG	BA	3835	1/1	0.97	0.14	46,46,46,46	0
56	MG	DA	3018	1/1	0.97	0.12	41,41,41,41	0
56	MG	BA	3836	1/1	0.97	0.22	45,45,45,45	0
56	MG	BA	3837	1/1	0.97	0.09	40,40,40,40	0
56	MG	DA	3021	1/1	0.97	0.14	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3580	1/1	0.97	0.10	42,42,42,42	0
56	MG	DA	3024	1/1	0.97	0.31	40,40,40,40	0
56	MG	BA	3839	1/1	0.97	0.10	38,38,38,38	0
56	MG	BA	3378	1/1	0.97	0.05	34,34,34,34	0
56	MG	AA	3163	1/1	0.97	0.11	37,37,37,37	0
56	MG	AA	3031	1/1	0.97	0.05	44,44,44,44	0
56	MG	BA	3474	1/1	0.97	0.06	61,61,61,61	0
56	MG	DA	3215	1/1	0.97	0.09	37,37,37,37	0
56	MG	BA	3703	1/1	0.97	0.07	48,48,48,48	0
56	MG	DA	3675	1/1	0.97	0.17	44,44,44,44	0
56	MG	BA	3381	1/1	0.97	0.08	43,43,43,43	0
56	MG	DA	3032	1/1	0.97	0.05	40,40,40,40	0
56	MG	AA	3049	1/1	0.97	0.15	52,52,52,52	0
56	MG	BA	3384	1/1	0.97	0.04	30,30,30,30	0
56	MG	BA	3304	1/1	0.97	0.06	39,39,39,39	0
56	MG	BA	3589	1/1	0.97	0.05	17,17,17,17	0
56	MG	BA	3590	1/1	0.97	0.07	32,32,32,32	0
56	MG	BB	3013	1/1	0.97	0.07	42,42,42,42	0
56	MG	DA	3450	1/1	0.97	0.08	36,36,36,36	0
56	MG	BA	3306	1/1	0.97	0.18	31,31,31,31	0
56	MG	BB	3015	1/1	0.97	0.05	51,51,51,51	0
56	MG	DD	301	1/1	0.97	0.09	39,39,39,39	0
56	MG	DA	3042	1/1	0.97	0.05	41,41,41,41	0
56	MG	BB	3016	1/1	0.97	0.12	43,43,43,43	0
56	MG	DD	305	1/1	0.97	0.25	38,38,38,38	0
56	MG	DD	306	1/1	0.97	0.15	44,44,44,44	0
56	MG	DA	3455	1/1	0.97	0.06	27,27,27,27	0
56	MG	BA	3480	1/1	0.97	0.08	56,56,56,56	0
56	MG	BA	3387	1/1	0.97	0.07	65,65,65,65	0
56	MG	BA	3713	1/1	0.97	0.07	54,54,54,54	0
56	MG	BA	3307	1/1	0.97	0.10	37,37,37,37	0
56	MG	BA	3389	1/1	0.97	0.07	37,37,37,37	0
56	MG	DF	302	1/1	0.97	0.06	43,43,43,43	0
56	MG	BB	3023	1/1	0.97	0.08	46,46,46,46	0
56	MG	DF	304	1/1	0.97	0.15	39,39,39,39	0
56	MG	DA	3050	1/1	0.97	0.18	40,40,40,40	0
56	MG	BA	3484	1/1	0.97	0.12	36,36,36,36	0
56	MG	BA	3485	1/1	0.97	0.09	46,46,46,46	0
56	MG	DO	5001	1/1	0.97	0.07	51,51,51,51	0
56	MG	DQ	3001	1/1	0.97	0.06	48,48,48,48	0
56	MG	AA	3070	1/1	0.97	0.19	49,49,49,49	0
56	MG	AA	3137	1/1	0.97	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DQ	3004	1/1	0.97	0.08	51,51,51,51	0
56	MG	BA	3489	1/1	0.97	0.06	44,44,44,44	0
56	MG	BA	3310	1/1	0.97	0.07	57,57,57,57	0
56	MG	AA	3217	1/1	0.97	0.14	55,55,55,55	0
56	MG	DA	3246	1/1	0.97	0.08	39,39,39,39	0
56	MG	AA	3013	1/1	0.97	0.06	51,51,51,51	0
56	MG	DV	3003	1/1	0.97	0.07	52,52,52,52	0
56	MG	DW	3001	1/1	0.97	0.18	43,43,43,43	0
56	MG	DA	3472	1/1	0.97	0.05	33,33,33,33	0
56	MG	BE	303	1/1	0.97	0.15	27,27,27,27	0
56	MG	DY	502	1/1	0.97	0.09	52,52,52,52	0
56	MG	DA	3249	1/1	0.97	0.10	41,41,41,41	0
56	MG	D7	101	1/1	0.97	0.18	39,39,39,39	0
56	MG	BA	3395	1/1	0.97	0.11	44,44,44,44	0
56	MG	DA	3479	1/1	0.97	0.08	50,50,50,50	0
56	MG	BA	3494	1/1	0.97	0.17	57,57,57,57	0
56	MG	DA	3252	1/1	0.97	0.05	29,29,29,29	0
59	ZN	CN	501	1/1	0.97	0.07	92,92,92,92	0
59	ZN	DY	501	1/1	0.97	0.07	106,106,106,106	0
56	MG	BA	3120	1/1	0.97	0.07	32,32,32,32	0
60	K	AX	3001	1/1	0.97	0.08	57,57,57,57	0
56	MG	BA	3497	1/1	0.97	0.14	41,41,41,41	0
56	MG	BA	3573	1/1	0.98	0.04	32,32,32,32	0
56	MG	DA	3011	1/1	0.98	0.07	40,40,40,40	0
56	MG	BA	3735	1/1	0.98	0.13	35,35,35,35	0
56	MG	DA	3013	1/1	0.98	0.07	40,40,40,40	0
56	MG	BA	3498	1/1	0.98	0.07	54,54,54,54	0
56	MG	DA	3140	1/1	0.98	0.10	34,34,34,34	0
56	MG	DA	3016	1/1	0.98	0.04	53,53,53,53	0
56	MG	BA	3827	1/1	0.98	0.12	30,30,30,30	0
56	MG	BA	3425	1/1	0.98	0.09	29,29,29,29	0
56	MG	BA	3426	1/1	0.98	0.04	22,22,22,22	0
56	MG	BA	3830	1/1	0.98	0.10	21,21,21,21	0
56	MG	DA	3146	1/1	0.98	0.10	46,46,46,46	0
56	MG	BA	3189	1/1	0.98	0.08	30,30,30,30	0
56	MG	AA	3117	1/1	0.98	0.07	48,48,48,48	0
56	MG	B3	102	1/1	0.98	0.10	35,35,35,35	0
56	MG	B3	103	1/1	0.98	0.05	45,45,45,45	0
56	MG	DA	3431	1/1	0.98	0.03	25,25,25,25	0
56	MG	BA	3108	1/1	0.98	0.11	24,24,24,24	0
56	MG	BA	3834	1/1	0.98	0.06	35,35,35,35	0
56	MG	BA	3243	1/1	0.98	0.07	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3290	1/1	0.98	0.09	44,44,44,44	0
56	MG	BA	3301	1/1	0.98	0.08	26,26,26,26	0
56	MG	DA	3292	1/1	0.98	0.06	37,37,37,37	0
56	MG	BA	3074	1/1	0.98	0.12	32,32,32,32	0
56	MG	DA	3156	1/1	0.98	0.11	43,43,43,43	0
56	MG	BA	3245	1/1	0.98	0.14	29,29,29,29	0
56	MG	DA	3441	1/1	0.98	0.07	43,43,43,43	0
56	MG	DA	3033	1/1	0.98	0.04	31,31,31,31	0
56	MG	BA	3076	1/1	0.98	0.07	23,23,23,23	0
56	MG	B7	101	1/1	0.98	0.08	33,33,33,33	0
56	MG	BA	3305	1/1	0.98	0.09	33,33,33,33	0
56	MG	CA	3106	1/1	0.98	0.10	50,50,50,50	0
56	MG	BA	3664	1/1	0.98	0.04	43,43,43,43	0
56	MG	B8	102	1/1	0.98	0.07	50,50,50,50	0
56	MG	DA	3165	1/1	0.98	0.09	33,33,33,33	0
56	MG	DA	3304	1/1	0.98	0.04	40,40,40,40	0
56	MG	BA	3368	1/1	0.98	0.05	12,12,12,12	0
56	MG	BA	3050	1/1	0.98	0.06	31,31,31,31	0
56	MG	DA	3307	1/1	0.98	0.07	45,45,45,45	0
56	MG	BA	3080	1/1	0.98	0.04	24,24,24,24	0
56	MG	CA	3112	1/1	0.98	0.05	59,59,59,59	0
56	MG	AA	3056	1/1	0.98	0.10	46,46,46,46	0
56	MG	BA	3440	1/1	0.98	0.09	29,29,29,29	0
56	MG	BA	3147	1/1	0.98	0.10	30,30,30,30	0
56	MG	DA	3173	1/1	0.98	0.05	30,30,30,30	0
56	MG	BA	3148	1/1	0.98	0.07	15,15,15,15	0
56	MG	DA	3175	1/1	0.98	0.08	53,53,53,53	0
56	MG	BA	3443	1/1	0.98	0.03	25,25,25,25	0
56	MG	AA	3138	1/1	0.98	0.07	34,34,34,34	0
56	MG	DA	3622	1/1	0.98	0.04	53,53,53,53	0
56	MG	AX	3005	1/1	0.98	0.04	44,44,44,44	0
56	MG	BA	3054	1/1	0.98	0.09	30,30,30,30	0
56	MG	BA	3009	1/1	0.98	0.05	25,25,25,25	0
56	MG	AA	3035	1/1	0.98	0.06	46,46,46,46	0
56	MG	BB	3017	1/1	0.98	0.04	33,33,33,33	0
56	MG	BA	3037	1/1	0.98	0.20	37,37,37,37	0
56	MG	BA	3088	1/1	0.98	0.14	50,50,50,50	0
56	MG	BA	3157	1/1	0.98	0.11	36,36,36,36	0
56	MG	DA	3473	1/1	0.98	0.05	49,49,49,49	0
56	MG	BA	3121	1/1	0.98	0.20	41,41,41,41	0
56	MG	DA	3475	1/1	0.98	0.05	42,42,42,42	0
56	MG	DA	3476	1/1	0.98	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3017	1/1	0.98	0.06	49,49,49,49	0
56	MG	BA	3383	1/1	0.98	0.05	24,24,24,24	0
56	MG	BA	3159	1/1	0.98	0.12	30,30,30,30	0
56	MG	CA	3131	1/1	0.98	0.06	55,55,55,55	0
56	MG	BA	3160	1/1	0.98	0.09	32,32,32,32	0
56	MG	DA	3640	1/1	0.98	0.07	52,52,52,52	0
56	MG	BA	3122	1/1	0.98	0.20	26,26,26,26	0
56	MG	BA	3607	1/1	0.98	0.07	40,40,40,40	0
56	MG	DA	3334	1/1	0.98	0.06	32,32,32,32	0
56	MG	BD	304	1/1	0.98	0.06	48,48,48,48	0
56	MG	BA	3211	1/1	0.98	0.25	36,36,36,36	0
56	MG	BA	3772	1/1	0.98	0.04	31,31,31,31	0
56	MG	BA	3609	1/1	0.98	0.06	20,20,20,20	0
56	MG	BA	3212	1/1	0.98	0.20	42,42,42,42	0
56	MG	BD	310	1/1	0.98	0.07	31,31,31,31	0
56	MG	BD	311	1/1	0.98	0.09	51,51,51,51	0
56	MG	DA	3492	1/1	0.98	0.07	47,47,47,47	0
56	MG	BA	3691	1/1	0.98	0.04	38,38,38,38	0
56	MG	DA	3494	1/1	0.98	0.11	30,30,30,30	0
56	MG	BE	302	1/1	0.98	0.09	34,34,34,34	0
56	MG	BA	3776	1/1	0.98	0.05	49,49,49,49	0
56	MG	BA	3024	1/1	0.98	0.05	22,22,22,22	0
56	MG	BA	3163	1/1	0.98	0.11	45,45,45,45	0
56	MG	BA	3164	1/1	0.98	0.07	43,43,43,43	0
56	MG	DA	3660	1/1	0.98	0.09	40,40,40,40	0
56	MG	BA	3039	1/1	0.98	0.22	47,47,47,47	0
56	MG	BA	3330	1/1	0.98	0.14	29,29,29,29	0
56	MG	BA	3332	1/1	0.98	0.09	30,30,30,30	0
56	MG	BA	3217	1/1	0.98	0.12	20,20,20,20	0
56	MG	BA	3092	1/1	0.98	0.22	41,41,41,41	0
56	MG	DA	3212	1/1	0.98	0.15	44,44,44,44	0
56	MG	BF	304	1/1	0.98	0.12	32,32,32,32	0
56	MG	BA	3012	1/1	0.98	0.09	26,26,26,26	0
56	MG	DA	3356	1/1	0.98	0.08	20,20,20,20	0
56	MG	DA	3670	1/1	0.98	0.15	38,38,38,38	0
56	MG	BA	3336	1/1	0.98	0.06	35,35,35,35	0
56	MG	BA	3337	1/1	0.98	0.05	35,35,35,35	0
56	MG	BA	3400	1/1	0.98	0.05	25,25,25,25	0
56	MG	BA	3061	1/1	0.98	0.05	40,40,40,40	0
56	MG	CA	3047	1/1	0.98	0.13	35,35,35,35	0
56	MG	BA	3276	1/1	0.98	0.12	41,41,41,41	0
56	MG	BA	3792	1/1	0.98	0.14	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3549	1/1	0.98	0.12	37,37,37,37	0
56	MG	BA	3627	1/1	0.98	0.09	45,45,45,45	0
56	MG	BA	3041	1/1	0.98	0.16	18,18,18,18	0
56	MG	DA	3368	1/1	0.98	0.10	50,50,50,50	0
56	MG	DA	3520	1/1	0.98	0.07	48,48,48,48	0
56	MG	BA	3129	1/1	0.98	0.06	36,36,36,36	0
56	MG	DA	3522	1/1	0.98	0.08	25,25,25,25	0
56	MG	BN	3003	1/1	0.98	0.04	38,38,38,38	0
56	MG	BA	3405	1/1	0.98	0.09	33,33,33,33	0
56	MG	BA	3026	1/1	0.98	0.04	19,19,19,19	0
56	MG	DA	3373	1/1	0.98	0.04	31,31,31,31	0
56	MG	BA	3173	1/1	0.98	0.09	36,36,36,36	0
56	MG	DD	304	1/1	0.98	0.10	31,31,31,31	0
56	MG	DA	3230	1/1	0.98	0.06	33,33,33,33	0
56	MG	BA	3800	1/1	0.98	0.06	39,39,39,39	0
56	MG	BA	3174	1/1	0.98	0.07	34,34,34,34	0
56	MG	BA	3556	1/1	0.98	0.06	45,45,45,45	0
56	MG	DA	3104	1/1	0.98	0.08	46,46,46,46	0
56	MG	BQ	3001	1/1	0.98	0.15	40,40,40,40	0
56	MG	DA	3236	1/1	0.98	0.09	48,48,48,48	0
56	MG	AA	3001	1/1	0.98	0.07	34,34,34,34	0
56	MG	BA	3065	1/1	0.98	0.04	37,37,37,37	0
56	MG	DA	3108	1/1	0.98	0.07	30,30,30,30	0
56	MG	BA	3177	1/1	0.98	0.11	44,44,44,44	0
56	MG	BA	3412	1/1	0.98	0.10	41,41,41,41	0
56	MG	DA	3388	1/1	0.98	0.04	35,35,35,35	0
56	MG	DA	3242	1/1	0.98	0.04	43,43,43,43	0
56	MG	AA	3133	1/1	0.98	0.09	30,30,30,30	0
56	MG	DA	3112	1/1	0.98	0.16	42,42,42,42	0
56	MG	BA	3045	1/1	0.98	0.07	42,42,42,42	0
56	MG	DA	3114	1/1	0.98	0.03	28,28,28,28	0
56	MG	BA	3231	1/1	0.98	0.16	37,37,37,37	0
56	MG	BR	204	1/1	0.98	0.20	42,42,42,42	0
56	MG	BA	3722	1/1	0.98	0.08	50,50,50,50	0
56	MG	AA	3075	1/1	0.98	0.09	33,33,33,33	0
56	MG	DA	3551	1/1	0.98	0.12	55,55,55,55	0
56	MG	AA	3012	1/1	0.98	0.05	33,33,33,33	0
56	MG	BU	205	1/1	0.98	0.20	38,38,38,38	0
56	MG	BA	3814	1/1	0.98	0.11	26,26,26,26	0
56	MG	DA	3255	1/1	0.98	0.06	59,59,59,59	0
56	MG	BU	207	1/1	0.98	0.07	29,29,29,29	0
56	MG	BA	3071	1/1	0.98	0.17	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	D0	101	1/1	0.98	0.07	56,56,56,56	0
56	MG	CA	3077	1/1	0.98	0.04	48,48,48,48	0
56	MG	D3	3001	1/1	0.98	0.06	58,58,58,58	0
56	MG	BA	3183	1/1	0.98	0.06	40,40,40,40	0
56	MG	BA	3104	1/1	0.98	0.07	27,27,27,27	0
56	MG	BV	205	1/1	0.98	0.07	32,32,32,32	0
56	MG	DA	3003	1/1	0.98	0.08	20,20,20,20	0
56	MG	BA	3294	1/1	0.98	0.15	45,45,45,45	0
58	SF4	AD	501	8/8	0.98	0.06	56,62,64,76	0
58	SF4	CD	501	8/8	0.98	0.04	54,64,76,87	0
56	MG	BA	3495	1/1	0.98	0.07	34,34,34,34	0
56	MG	BA	3730	1/1	0.98	0.10	27,27,27,27	0
56	MG	BA	3048	1/1	0.98	0.12	28,28,28,28	0
59	ZN	D9	501	1/1	0.98	0.04	63,63,63,63	0
56	MG	DA	3008	1/1	0.98	0.06	33,33,33,33	0
56	MG	BA	3188	1/1	0.98	0.09	19,19,19,19	0
56	MG	BA	3526	1/1	0.99	0.04	32,32,32,32	0
56	MG	DA	3259	1/1	0.99	0.03	34,34,34,34	0
56	MG	BB	3007	1/1	0.99	0.03	36,36,36,36	0
56	MG	BA	3813	1/1	0.99	0.03	4,4,4,4	0
56	MG	BA	3168	1/1	0.99	0.08	27,27,27,27	0
56	MG	BA	3155	1/1	0.99	0.07	54,54,54,54	0
56	MG	DA	3572	1/1	0.99	0.04	28,28,28,28	0
56	MG	DA	3264	1/1	0.99	0.04	31,31,31,31	0
56	MG	BU	209	1/1	0.99	0.11	27,27,27,27	0
56	MG	DA	3364	1/1	0.99	0.04	38,38,38,38	0
56	MG	DA	3576	1/1	0.99	0.04	37,37,37,37	0
56	MG	BV	201	1/1	0.99	0.14	29,29,29,29	0
56	MG	BV	202	1/1	0.99	0.04	26,26,26,26	0
56	MG	BA	3324	1/1	0.99	0.04	34,34,34,34	0
56	MG	CA	3138	1/1	0.99	0.10	59,59,59,59	0
56	MG	DA	3524	1/1	0.99	0.07	38,38,38,38	0
56	MG	BA	3611	1/1	0.99	0.04	42,42,42,42	0
56	MG	BA	3107	1/1	0.99	0.09	20,20,20,20	0
56	MG	BA	3819	1/1	0.99	0.08	32,32,32,32	0
56	MG	BF	308	1/1	0.99	0.05	36,36,36,36	0
56	MG	BA	3185	1/1	0.99	0.03	32,32,32,32	0
56	MG	DA	3374	1/1	0.99	0.05	37,37,37,37	0
56	MG	AA	3173	1/1	0.99	0.04	47,47,47,47	0
56	MG	BA	3187	1/1	0.99	0.12	36,36,36,36	0
56	MG	BA	3790	1/1	0.99	0.06	32,32,32,32	0
56	MG	BA	3075	1/1	0.99	0.08	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BG	202	1/1	0.99	0.06	46,46,46,46	0
56	MG	BA	3731	1/1	0.99	0.09	23,23,23,23	0
56	MG	BA	3272	1/1	0.99	0.13	11,11,11,11	0
56	MG	DA	3651	1/1	0.99	0.08	47,47,47,47	0
56	MG	BA	3415	1/1	0.99	0.08	29,29,29,29	0
56	MG	BA	3675	1/1	0.99	0.12	37,37,37,37	0
56	MG	BA	3331	1/1	0.99	0.09	32,32,32,32	0
56	MG	BA	3018	1/1	0.99	0.09	34,34,34,34	0
56	MG	BA	3462	1/1	0.99	0.03	11,11,11,11	0
56	MG	BA	3487	1/1	0.99	0.08	25,25,25,25	0
56	MG	BA	3077	1/1	0.99	0.23	34,34,34,34	0
56	MG	BA	3239	1/1	0.99	0.12	31,31,31,31	0
56	MG	AA	3171	1/1	0.99	0.04	48,48,48,48	0
56	MG	BA	3466	1/1	0.99	0.06	28,28,28,28	0
56	MG	BD	309	1/1	0.99	0.15	37,37,37,37	0
56	MG	DA	3444	1/1	0.99	0.05	30,30,30,30	0
56	MG	BA	3069	1/1	0.99	0.08	31,31,31,31	0
56	MG	DA	3015	1/1	0.99	0.09	31,31,31,31	0
56	MG	BA	3091	1/1	0.99	0.13	38,38,38,38	0
56	MG	DA	3017	1/1	0.99	0.08	28,28,28,28	0
56	MG	AM	201	1/1	0.99	0.03	50,50,50,50	0
56	MG	AA	3151	1/1	0.99	0.04	41,41,41,41	0
56	MG	AA	3225	1/1	0.99	0.05	26,26,26,26	0
56	MG	BA	3282	1/1	0.99	0.07	24,24,24,24	0
56	MG	DA	3022	1/1	0.99	0.09	40,40,40,40	0
59	ZN	BY	501	1/1	0.99	0.03	58,58,58,58	0
59	ZN	B4	501	1/1	0.99	0.06	73,73,73,73	0
59	ZN	B6	103	1/1	0.99	0.03	29,29,29,29	0
59	ZN	B9	501	1/1	0.99	0.07	49,49,49,49	0
56	MG	BR	205	1/1	0.99	0.08	29,29,29,29	0
56	MG	DA	3254	1/1	0.99	0.10	21,21,21,21	0
56	MG	BA	3010	1/1	0.99	0.05	29,29,29,29	0
59	ZN	D5	501	1/1	0.99	0.04	53,53,53,53	0
59	ZN	D6	501	1/1	0.99	0.04	73,73,73,73	0
56	MG	DA	3563	1/1	0.99	0.03	42,42,42,42	0
56	MG	BA	3499	1/1	0.99	0.11	33,33,33,33	0
56	MG	BU	203	1/1	0.99	0.04	31,31,31,31	0
59	ZN	AN	501	1/1	1.00	0.02	58,58,58,58	0
56	MG	BA	3003	1/1	1.00	0.05	20,20,20,20	0
56	MG	BA	3078	1/1	1.00	0.04	17,17,17,17	0
59	ZN	B5	104	1/1	1.00	0.02	38,38,38,38	0
56	MG	BA	3265	1/1	1.00	0.12	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3224	1/1	1.00	0.05	33,33,33,33	0
56	MG	DA	3554	1/1	1.00	0.02	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.