



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:48 am BST

PDB ID : 4WOI  
Title : 4,5-linked aminoglycoside antibiotics regulate the bacterial ribosome by targeting dynamic conformational processes within intersubunit bridge B2  
Authors : Pulk, A.; Cate, J.H.D.; Blanchard, S.; Wasserman, M.; Altman, R.; Zhou, Z.; Zinder, J.; Green, K.; Garneau-Tsodikova, S.  
Deposited on : 2014-10-15  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

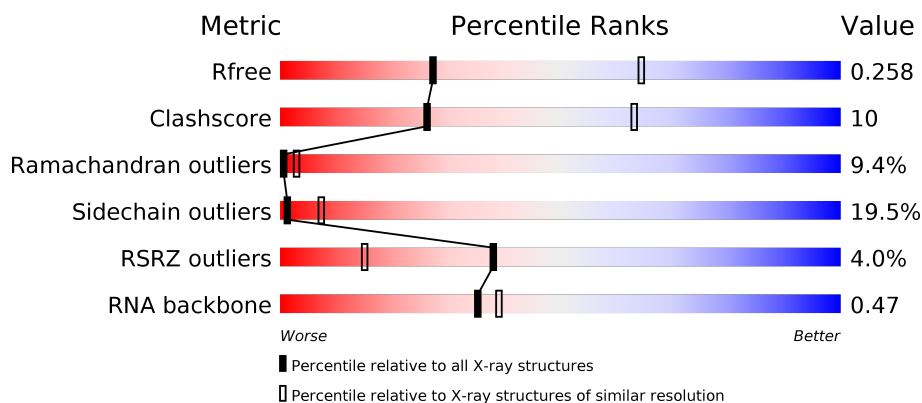
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



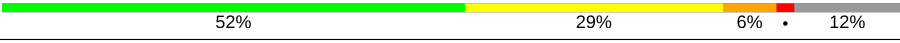

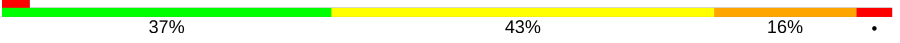
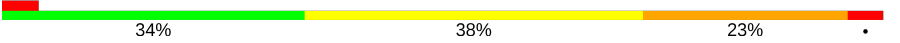


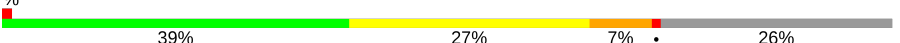
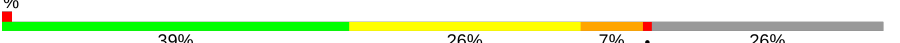
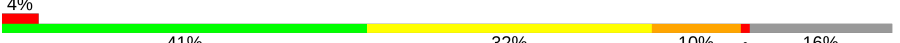




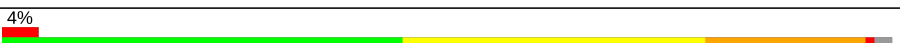
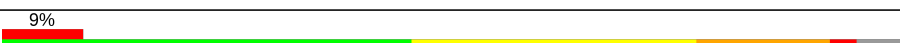

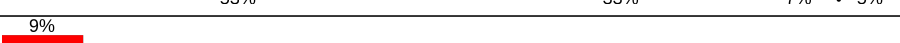
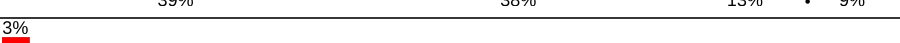
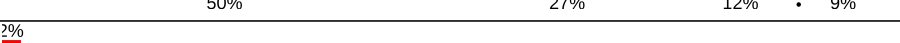

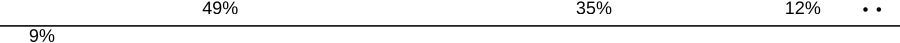
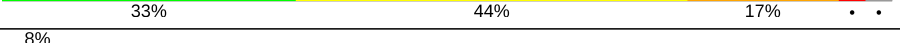

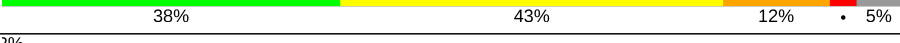

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1542	
1	DA	1542	
2	AB	241	
2	DB	241	

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Mol	Chain	Length	Quality of chain
3	AC	233	
3	DC	233	
4	AD	206	
4	DD	206	
5	AE	167	
5	DE	167	
6	AF	135	
6	DF	135	
7	AG	179	
7	DG	179	
8	AH	130	
8	DH	130	
9	AI	130	
9	DI	130	
10	AJ	103	
10	DJ	103	
11	AK	129	
11	DK	129	
12	AL	124	
12	DL	124	
13	AM	118	
13	DM	118	
14	AN	101	
14	DN	101	
15	AO	89	

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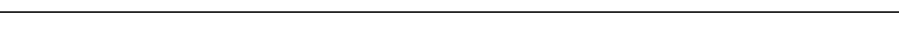

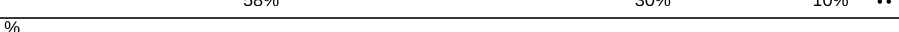

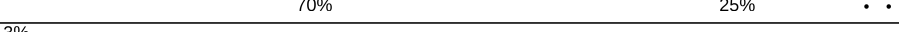






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Mol	Chain	Length	Quality of chain
15	DO	89	
16	AP	82	
16	DP	82	
17	AQ	84	
17	DQ	84	
18	AR	75	
18	DR	75	
19	AS	92	
19	DS	92	
20	AT	87	
20	DT	87	
21	AU	71	
21	DU	71	
22	AV	185	
23	AW	16	
23	DV	16	
24	AX	76	
24	DW	76	
25	BA	2904	
25	CA	2904	
26	BB	120	
26	CB	120	
27	BC	273	
27	CC	273	
28	BD	209	

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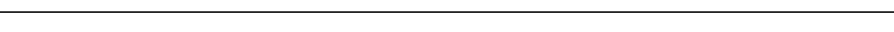

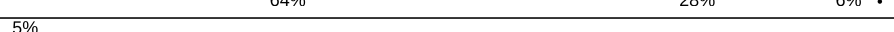

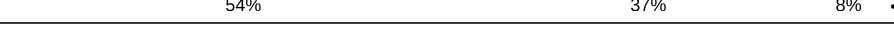








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Mol	Chain	Length	Quality of chain
28	CD	209	
29	BE	201	
29	CE	201	
30	BF	179	
30	CF	179	
31	BG	177	
31	CG	177	
32	BH	149	
32	CH	149	
33	BI	142	
33	CI	142	
34	BJ	142	
34	CJ	142	
35	BK	123	
35	CK	123	
36	BL	144	
36	CL	144	
37	BM	136	
37	CM	136	
38	BN	127	
38	CN	127	
39	BO	117	
39	CO	117	
40	BP	115	
40	CP	115	






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Mol	Chain	Length	Quality of chain
41	BQ	118	
41	CQ	118	
42	BR	103	
42	CR	103	
43	BS	110	
43	CS	110	
44	BT	100	
44	CT	100	
45	BU	104	
45	CU	104	
46	BV	94	
46	CV	94	
47	BW	85	
47	CW	85	
48	BX	78	
48	CX	78	
49	BY	63	
49	CY	63	
50	BZ	59	
50	CZ	59	
51	B0	57	
51	C0	57	
52	B1	55	
52	C1	55	
53	B2	46	

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Mol	Chain	Length	Quality of chain
53	C2	46	
54	B3	65	
54	C3	65	
55	B4	38	
55	C4	38	
56	B5	228	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	1646	-	-	-	X
57	MG	AA	1658	-	-	-	X
57	MG	CA	3013	-	-	-	X
57	MG	CA	3095	-	-	-	X
58	PAR	BA	3005	-	-	X	-
58	PAR	CA	3168	-	-	-	X
58	PAR	CA	3169	-	-	-	X

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 294484 atoms, of which 450 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	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	DA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
2	DB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- 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
			1624	1028	305	288	3			
3	DC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
4	DD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
5	DE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- 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
			817	515	148	148	6			
6	DF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
7	DG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
8	DH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
9	DI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	DJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
11	DK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
12	DL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
13	DM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
14	DN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- 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
			716	440	146	129	1			
15	DO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

- 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
			649	406	128	114	1			
16	DP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
17	DQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			
18	DR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
19	DS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
20	DT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
21	DU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 22 is a protein called Ribosome-recycling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	183	Total	C	N	O	S	0	0	0
			1419	871	260	283	5			

- Molecule 23 is a RNA chain called Messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	15	Total	C	N	O	P	0	0	0
			324	145	61	103	15			
23	DV	16	Total	C	N	O	P	0	0	0
			346	155	66	109	16			

- Molecule 24 is a RNA chain called Phenylalanine specific transfer RNA, tRNA-Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
24	DW	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
25	CA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	119	Total	C	N	O	P	0	0	0
			2549	1135	466	829	119			
26	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			



- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
27	CC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
28	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
29	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
30	CF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
31	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	149	Total	C	N	O	S	0	0	0
			1107	696	197	213	1			
32	CH	149	Total	C	N	O	S	0	0	0
			1107	696	197	213	1			

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
33	CI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
34	CJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
35	CK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
36	CL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
38	CN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BO	116	Total	C	N	O	S	0	0	0
			892	552	178	162				
39	CO	116	Total	C	N	O	S	0	0	0
			892	552	178	162				

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
40	CP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BQ	117	Total	C	N	O	S	0	0	0
			947	604	192	151				
41	CQ	117	Total	C	N	O	S	0	0	0
			947	604	192	151				

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
42	CR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
43	CS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
44	CT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BU	102	Total	C	N	O	0	0	0
			779	492	146	141			
45	CU	102	Total	C	N	O	0	0	0
			779	492	146	141			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
46	CV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BW	76	Total	C	N	O	S	0	0	0
			580	359	117	103	1			
47	CW	75	Total	C	N	O	S	0	0	0
			569	353	113	102	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
48	CX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
49	CY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 50 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
50	CZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
51	C0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	B1	50	Total	C	N	O	0	0	0
			409	263	75	71			
52	C1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	C2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
54	C3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
55	C4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 56 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	B5	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

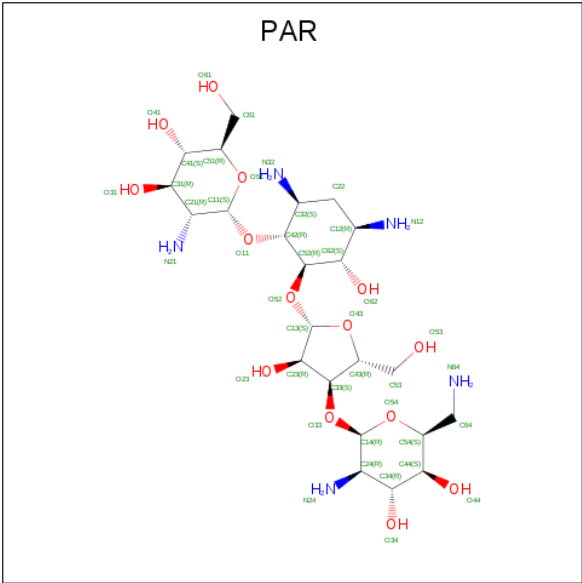
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BB	4	Total	Mg	0	0
			4	4		
57	BO	1	Total	Mg	0	0
			1	1		
57	BA	189	Total	Mg	0	0
			189	189		
57	CA	165	Total	Mg	0	0
			165	165		
57	CB	3	Total	Mg	0	0
			3	3		
57	BL	2	Total	Mg	0	0
			2	2		
57	DA	53	Total	Mg	0	0
			53	53		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CD	1	Total	Mg	0	0
			1	1		
57	AA	71	Total	Mg	0	0
			71	71		
57	BQ	1	Total	Mg	0	0
			1	1		
57	CQ	1	Total	Mg	0	0
			1	1		
57	AN	1	Total	Mg	0	0
			1	1		
57	DN	1	Total	Mg	0	0
			1	1		
57	DD	2	Total	Mg	0	0
			2	2		

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	AA	1	Total	C	H	N	O	0	0
			87	23	45	5	14		
58	BA	1	Total	C	H	N	O	0	0
			87	23	45	5	14		
58	BA	1	Total	C	H	N	O	0	0
			87	23	45	5	14		
58	BA	1	Total	C	H	N	O	0	0
			87	23	45	5	14		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	BA	1	Total C H N O 87 23 45 5 14	0	0
58	BA	1	Total C N O 42 23 5 14	0	0
58	CA	1	Total C N O 42 23 5 14	0	0
58	CA	1	Total C H N O 87 23 45 5 14	0	0
58	CA	1	Total C H N O 87 23 45 5 14	0	0
58	CA	1	Total C N O 42 23 5 14	0	0
58	CA	1	Total C H N O 87 23 45 5 14	0	0
58	DA	1	Total C H N O 87 23 45 5 14	0	0
58	DA	1	Total C H N O 87 23 45 5 14	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	B4	1	Total Zn 1 1	0	0
59	C4	1	Total Zn 1 1	0	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AA	192	Total O 192 192	0	0
60	AE	3	Total O 3 3	0	0
60	AL	1	Total O 1 1	0	0
60	AN	2	Total O 2 2	0	0
60	AT	5	Total O 5 5	0	0
60	BA	626	Total O 626 626	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BB	14	Total 14	O 14	0	0
60	BC	7	Total 7	O 7	0	0
60	BD	2	Total 2	O 2	0	0
60	BE	1	Total 1	O 1	0	0
60	BF	1	Total 1	O 1	0	0
60	BL	8	Total 8	O 8	0	0
60	BN	2	Total 2	O 2	0	0
60	BQ	1	Total 1	O 1	0	0
60	BS	1	Total 1	O 1	0	0
60	BT	3	Total 3	O 3	0	0
60	B3	1	Total 1	O 1	0	0
60	B4	1	Total 1	O 1	0	0
60	CA	608	Total 608	O 608	0	0
60	CB	14	Total 14	O 14	0	0
60	CC	10	Total 10	O 10	0	0
60	CD	5	Total 5	O 5	0	0
60	CE	3	Total 3	O 3	0	0
60	CJ	2	Total 2	O 2	0	0
60	CL	7	Total 7	O 7	0	0
60	CN	2	Total 2	O 2	0	0
60	CT	3	Total 3	O 3	0	0

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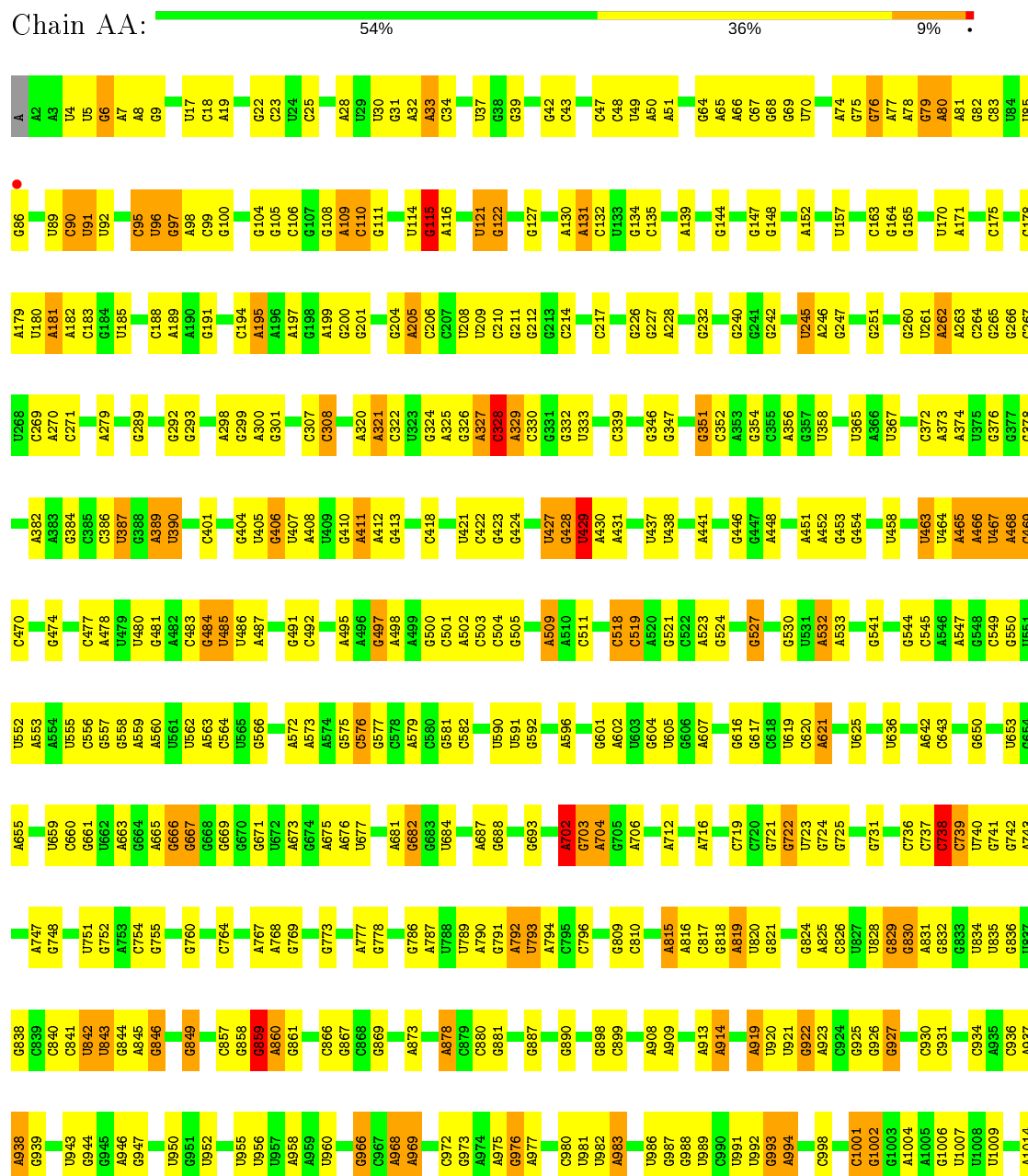
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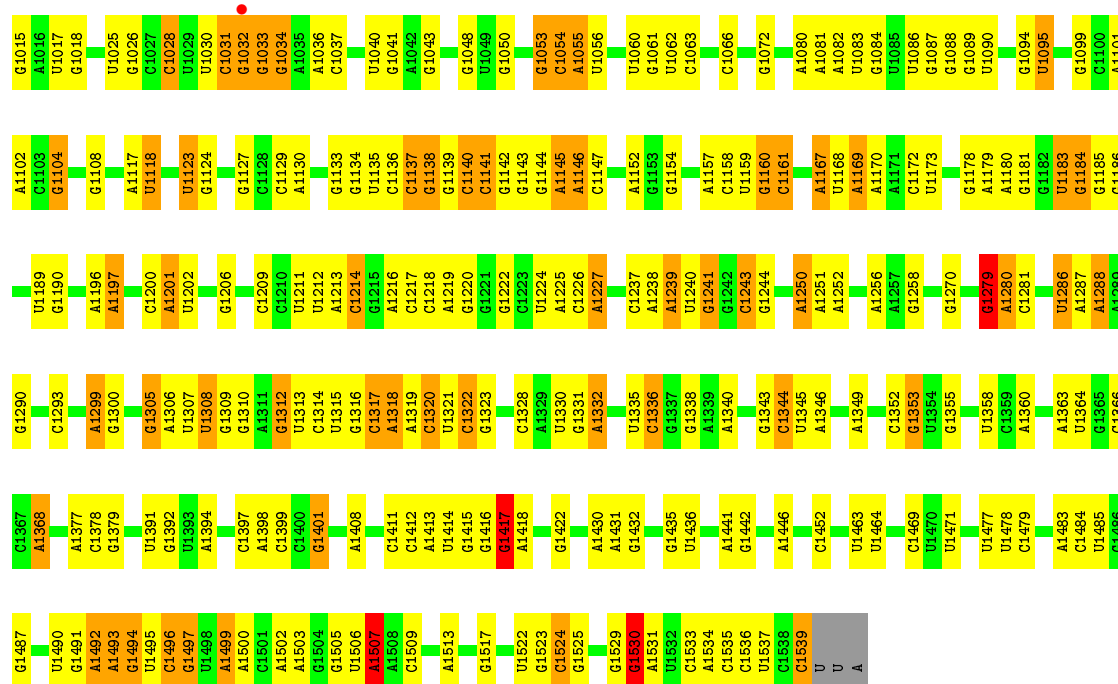
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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60	C3	1	Total 1	O 1	0	0
60	C4	2	Total 2	O 2	0	0
60	DA	184	Total 184	O 184	0	0
60	DD	2	Total 2	O 2	0	0
60	DK	2	Total 2	O 2	0	0
60	DL	2	Total 2	O 2	0	0
60	DN	4	Total 4	O 4	0	0
60	DT	3	Total 3	O 3	0	0
60	DU	1	Total 1	O 1	0	0

### 3 Residue-property plots

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

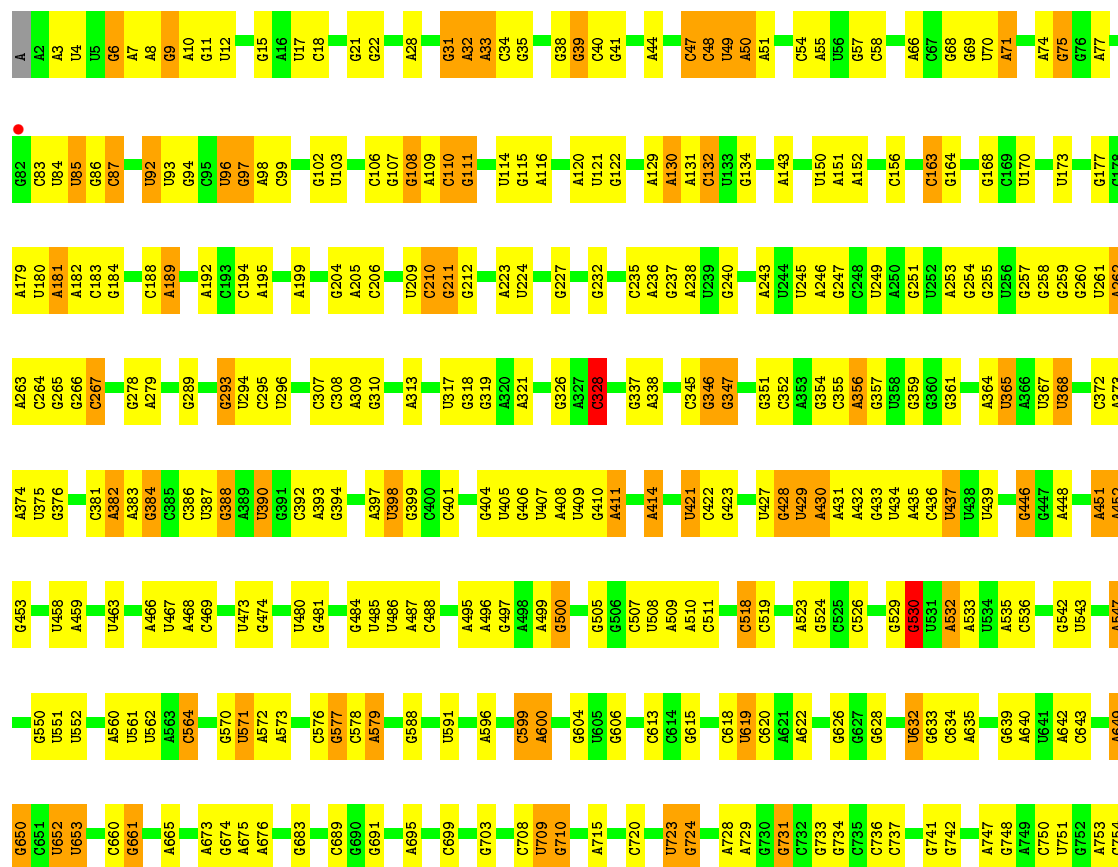
- Molecule 1: 16S ribosomal RNA

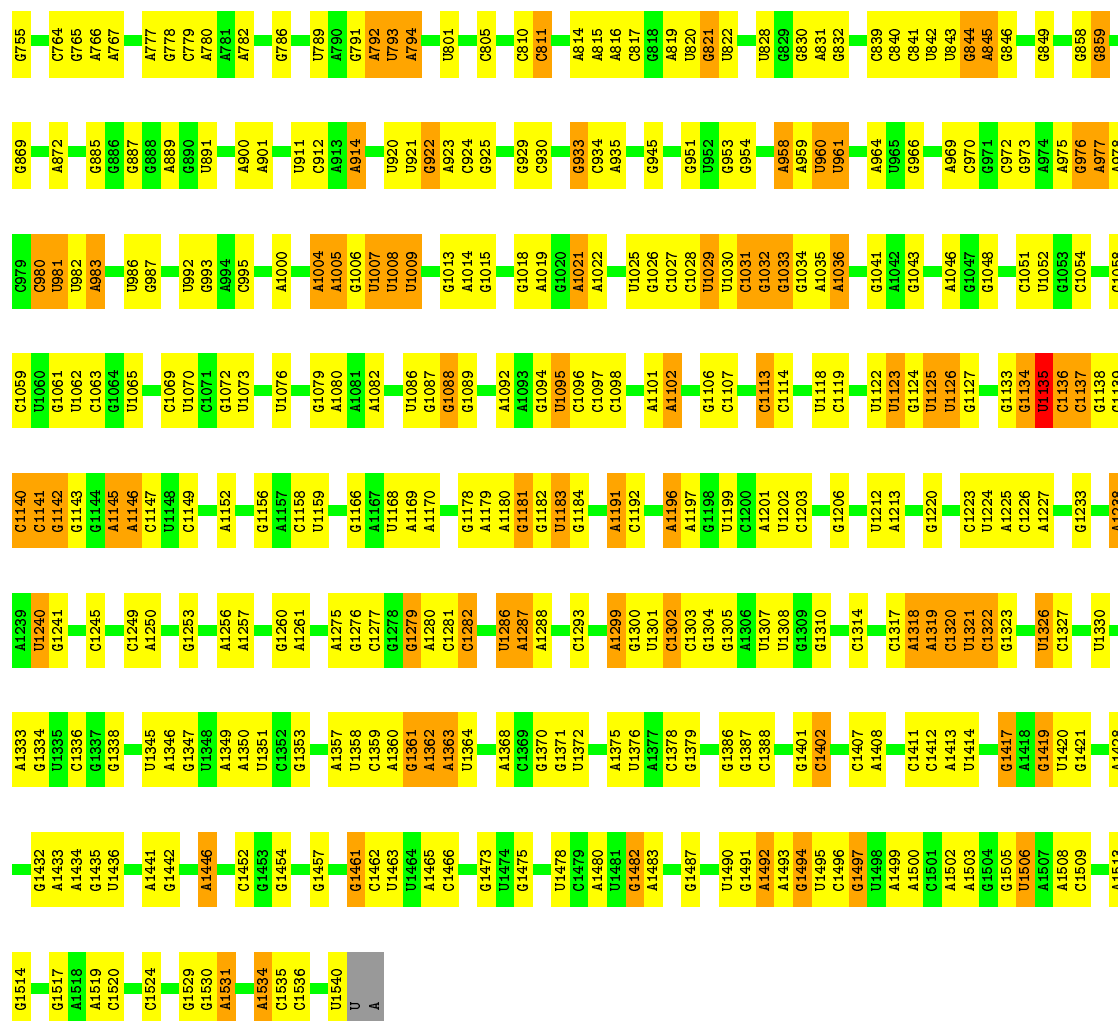




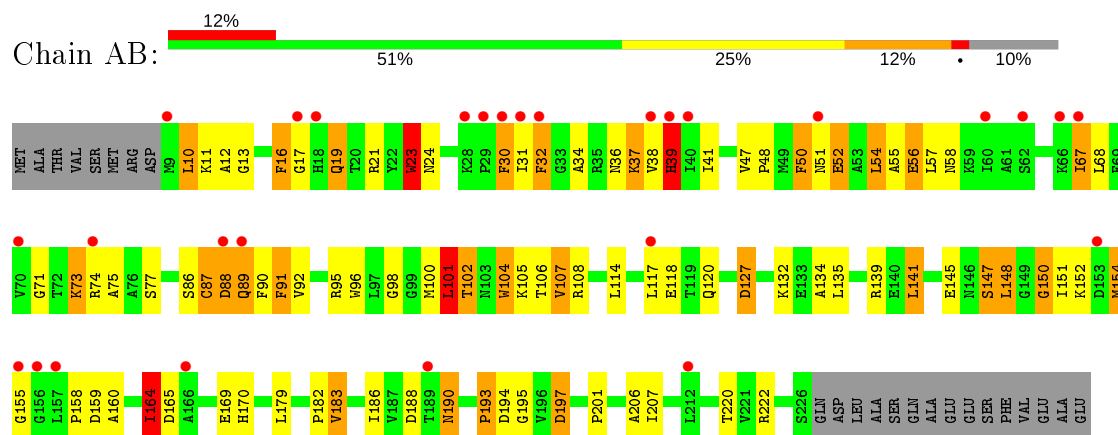
• Molecule 1: 16S ribosomal RNA

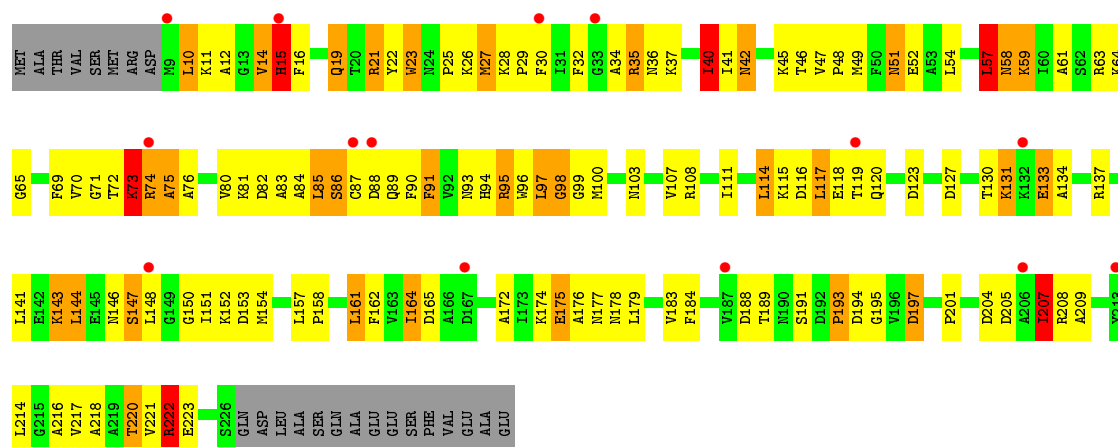
Chain DA: 56% 34% 10%





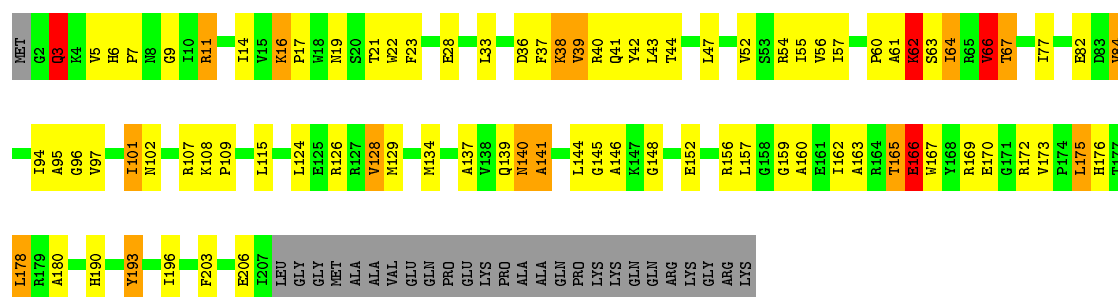
• Molecule 2: 30S ribosomal protein S2





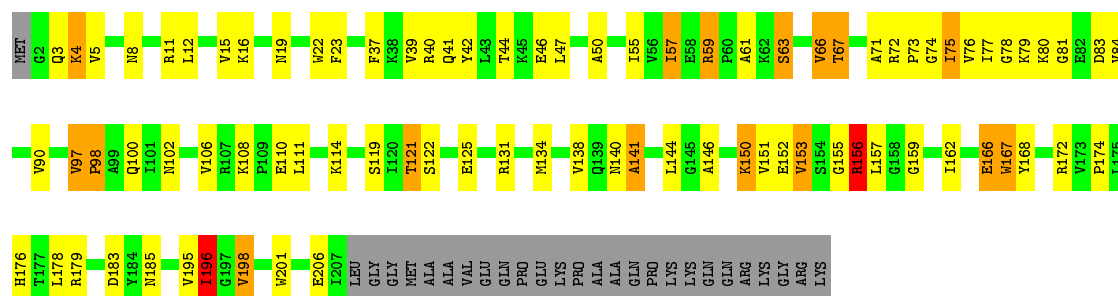
• Molecule 3: 30S ribosomal protein S3

Chain AC: 52% 29% 6% 12%



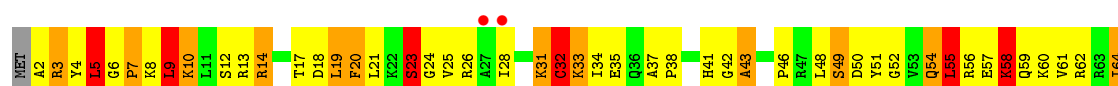
• Molecule 3: 30S ribosomal protein S3

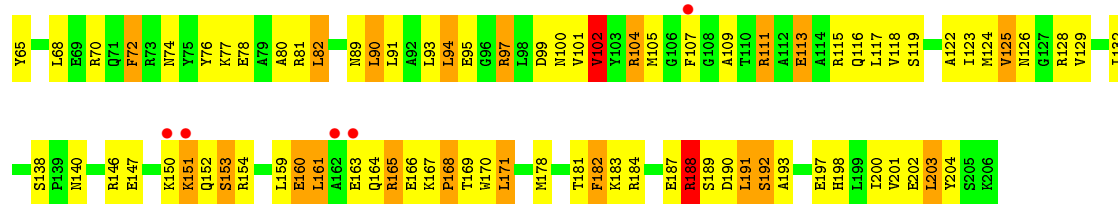
Chain DC: 52% 29% 7% 12%



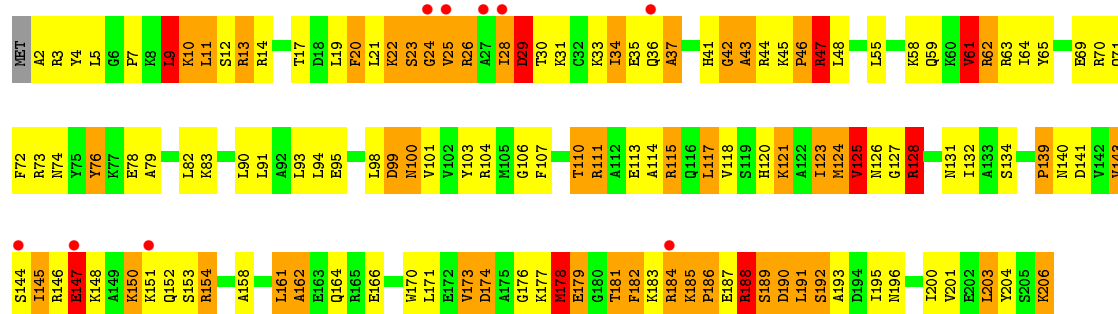
• Molecule 4: 30S ribosomal protein S4

Chain AD: 3% 37% 43% 16%

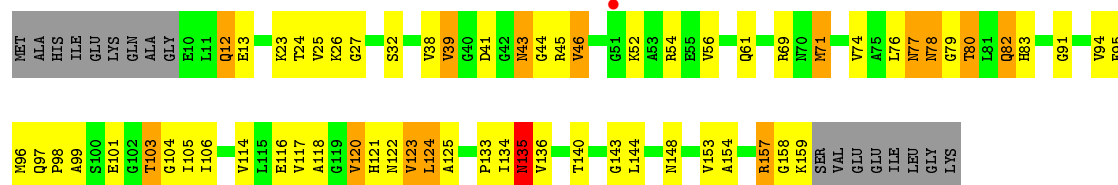




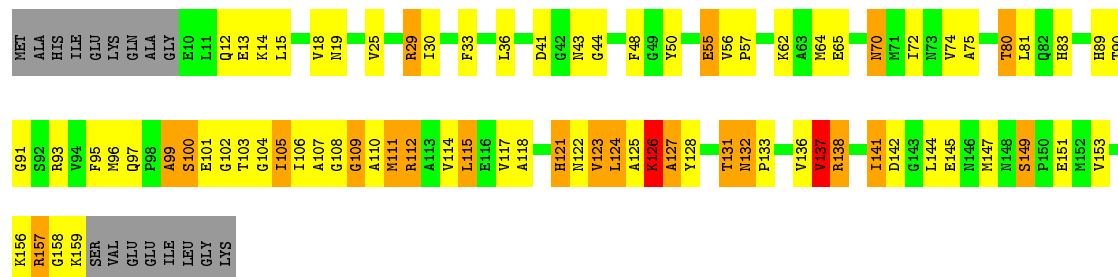
• Molecule 4: 30S ribosomal protein S4



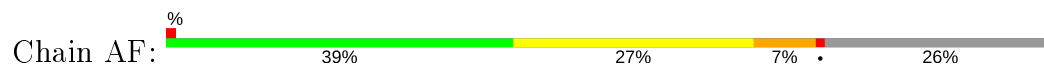
• Molecule 5: 30S ribosomal protein S5

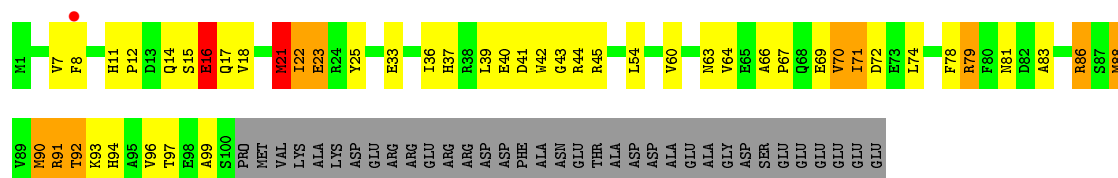


• Molecule 5: 30S ribosomal protein S5

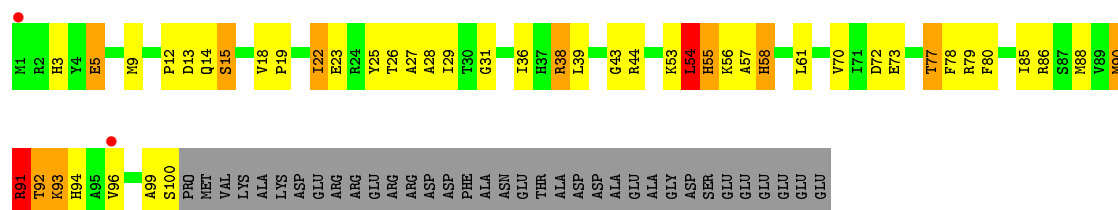
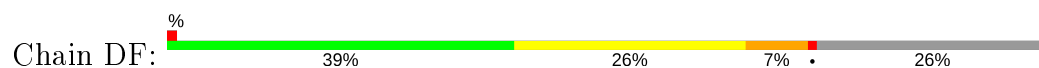


• Molecule 6: 30S ribosomal protein S6

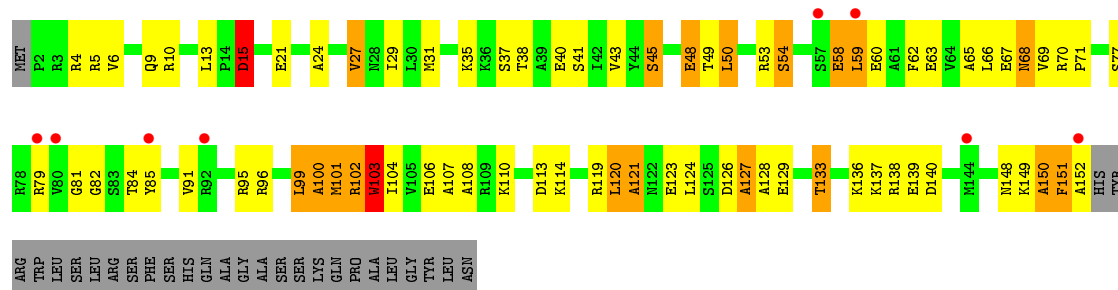




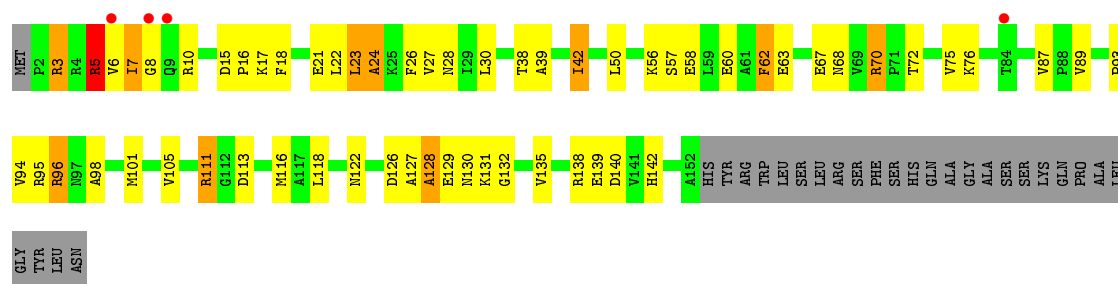
- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7



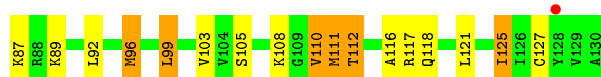
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8



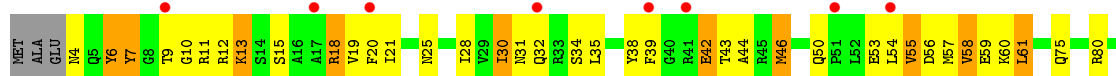




- Molecule 8: 30S ribosomal protein S8



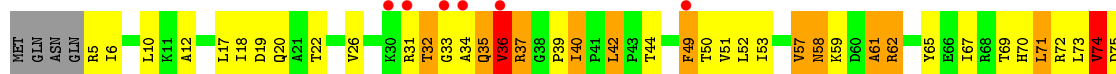
- Molecule 9: 30S ribosomal protein S9



- Molecule 9: 30S ribosomal protein S9

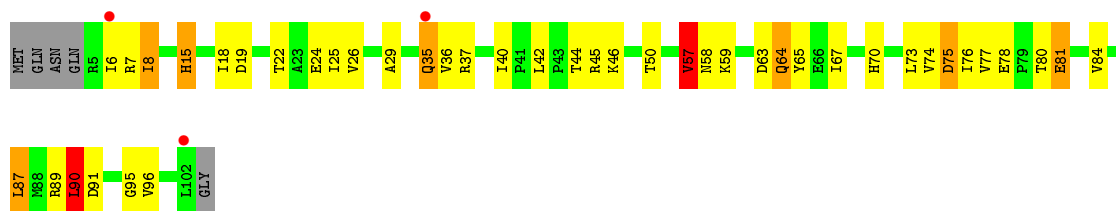


- Molecule 10: 30S ribosomal protein S10

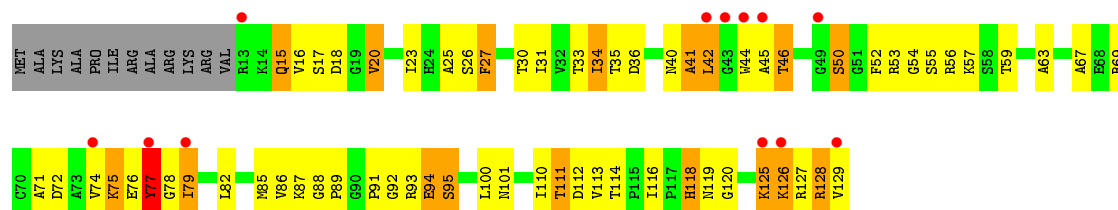
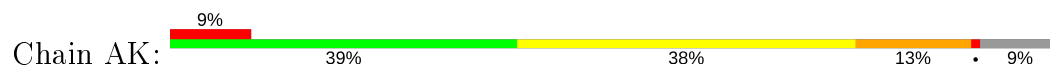


- Molecule 10: 30S ribosomal protein S10

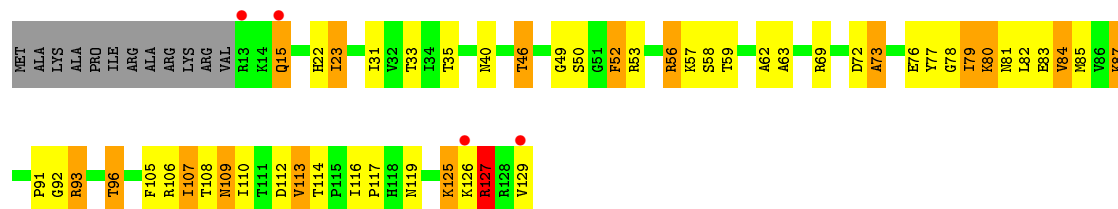




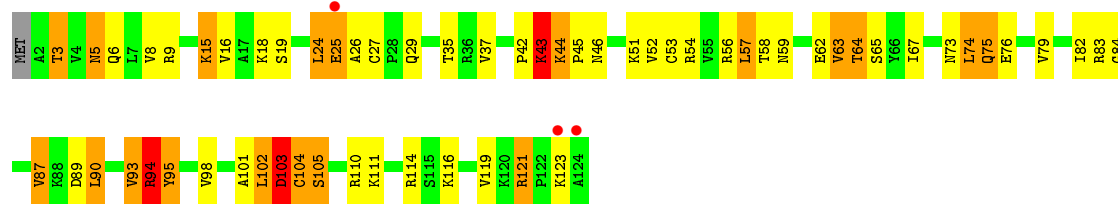
- Molecule 11: 30S ribosomal protein S11



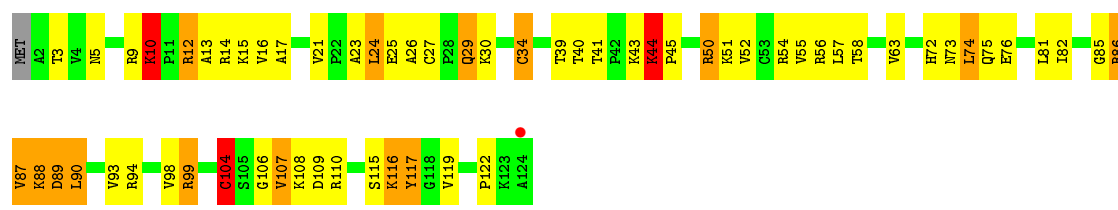
- Molecule 11: 30S ribosomal protein S11



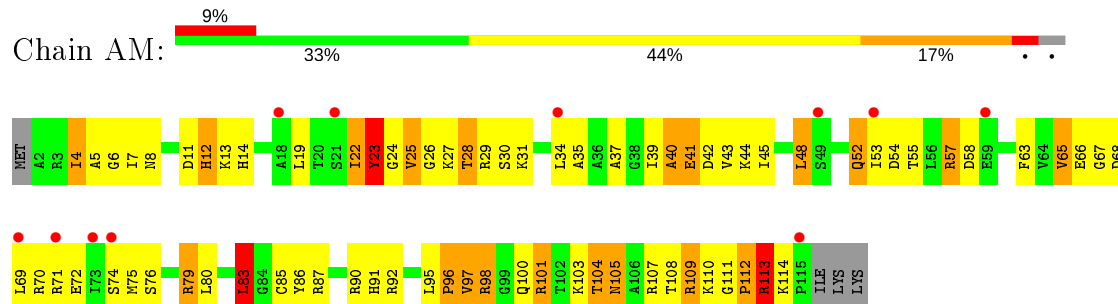
- Molecule 12: 30S ribosomal protein S12



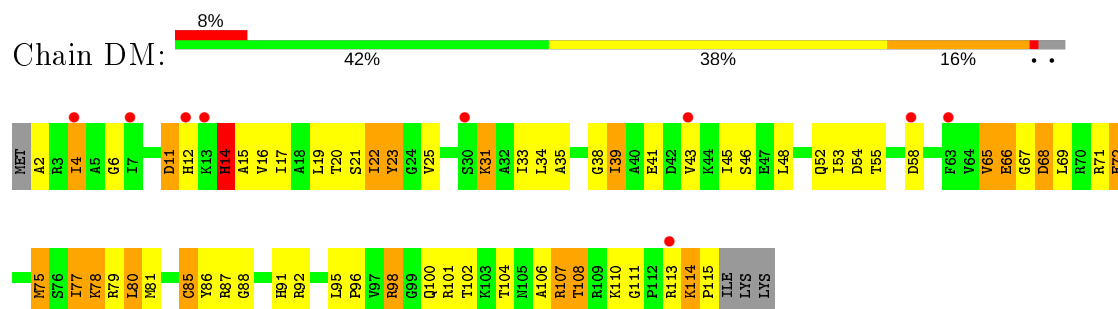
- Molecule 12: 30S ribosomal protein S12



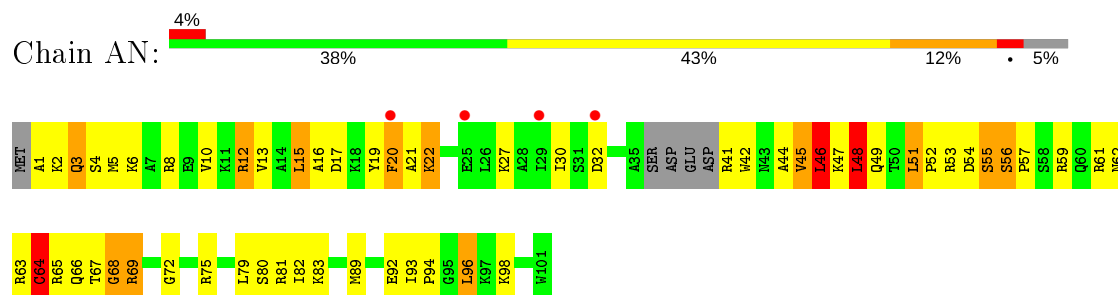
- Molecule 13: 30S ribosomal protein S13



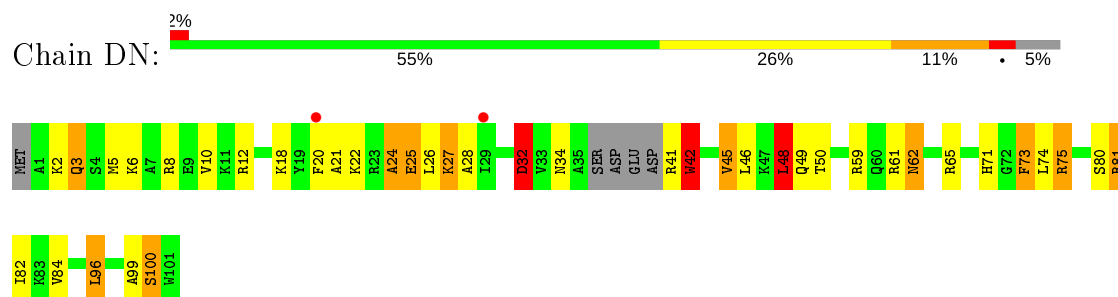
- Molecule 13: 30S ribosomal protein S13



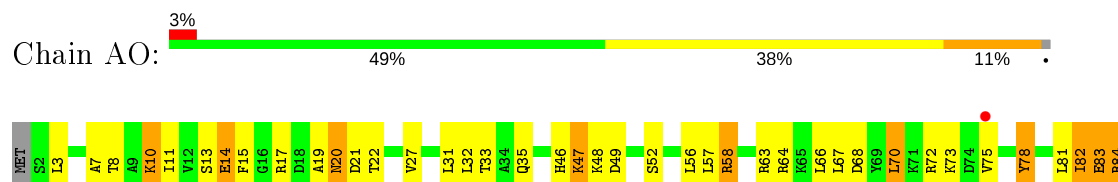
- Molecule 14: 30S ribosomal protein S14

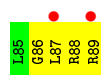


- Molecule 14: 30S ribosomal protein S14

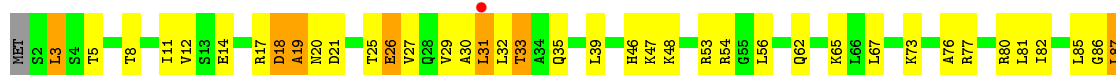


- Molecule 15: 30S ribosomal protein S15

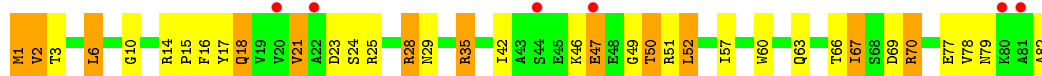




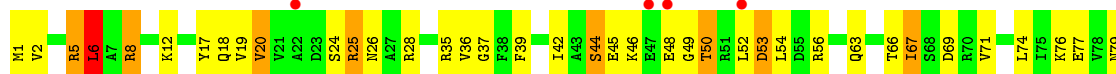
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



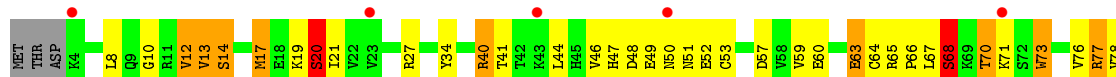
- Molecule 16: 30S ribosomal protein S16



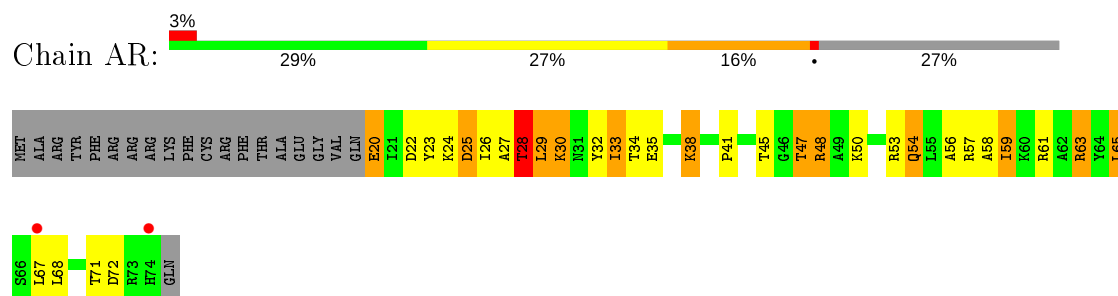
- Molecule 17: 30S ribosomal protein S17



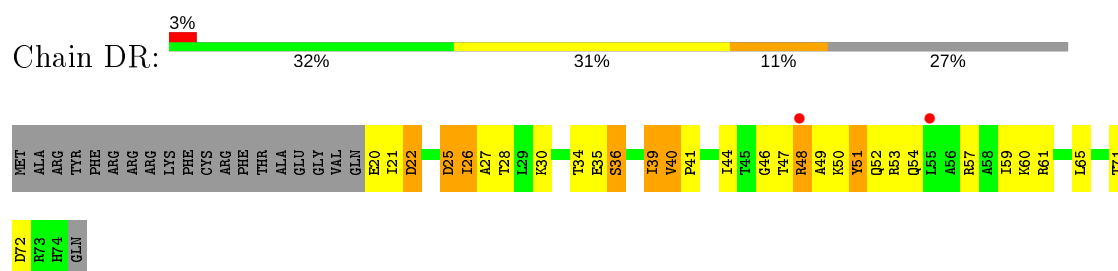
- Molecule 17: 30S ribosomal protein S17



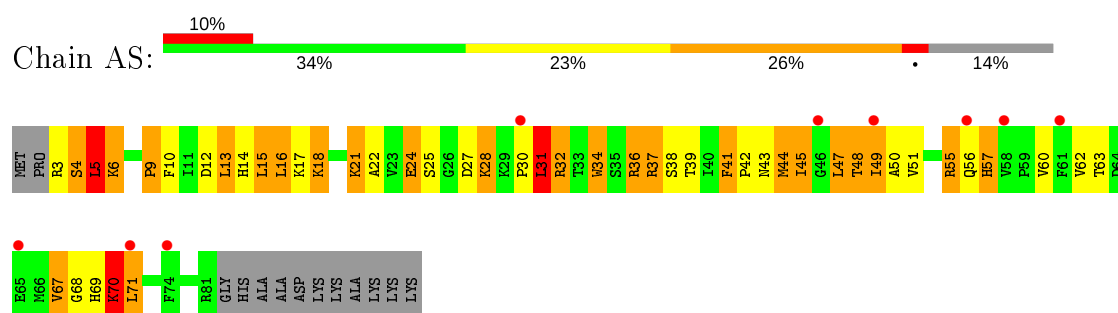
- Molecule 18: 30S ribosomal protein S18



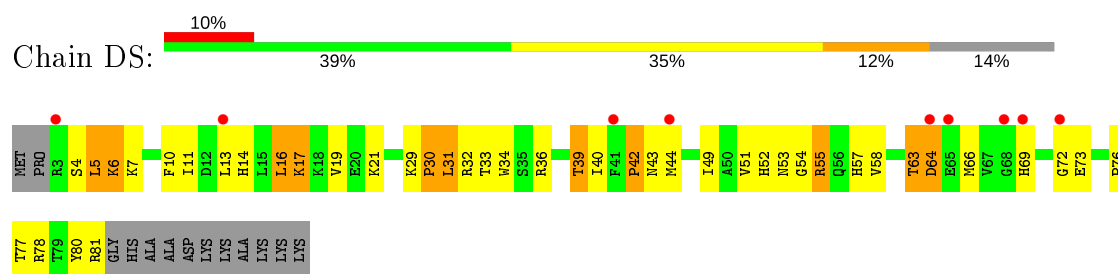
- Molecule 18: 30S ribosomal protein S18



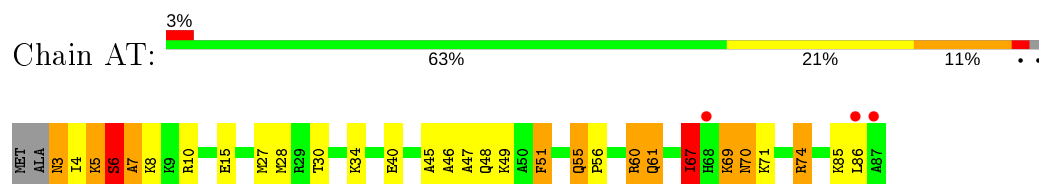
- Molecule 19: 30S ribosomal protein S19



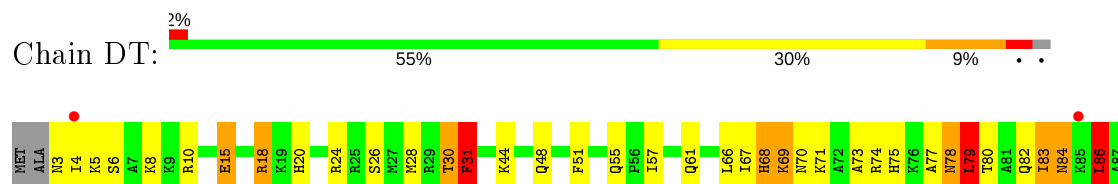
- Molecule 19: 30S ribosomal protein S19



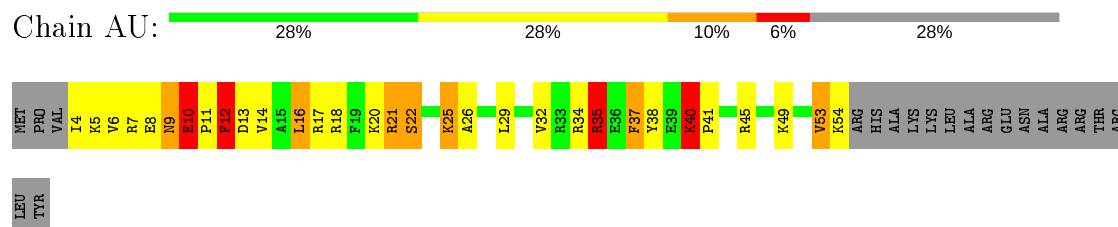
- Molecule 20: 30S ribosomal protein S20



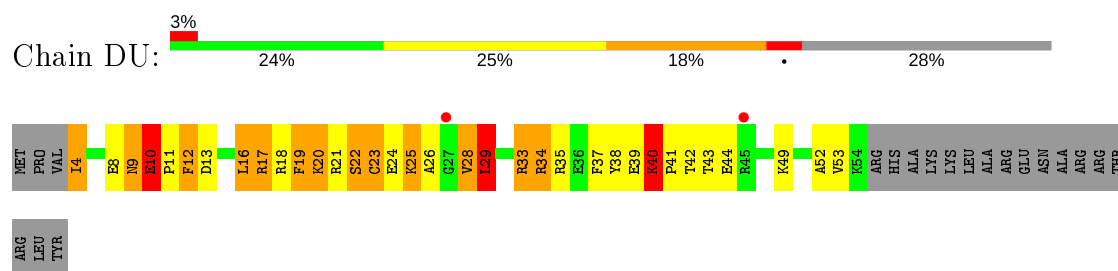
- Molecule 20: 30S ribosomal protein S20



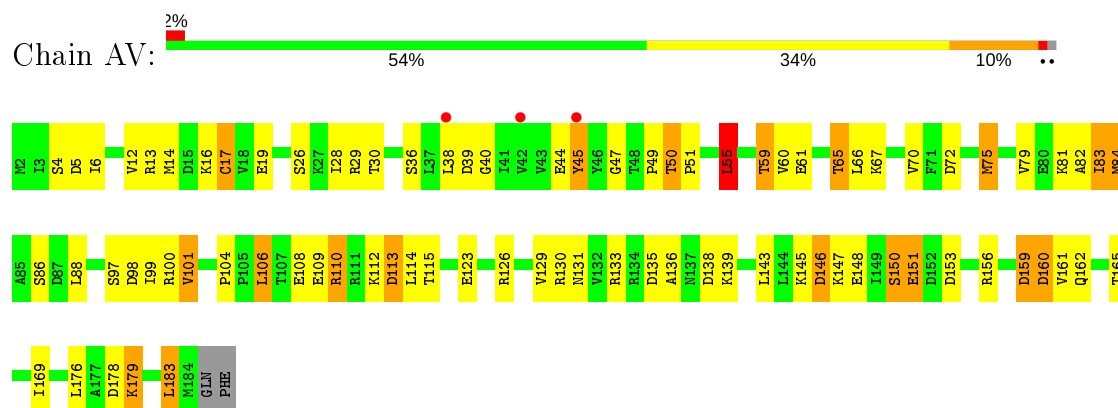
- Molecule 21: 30S ribosomal protein S21



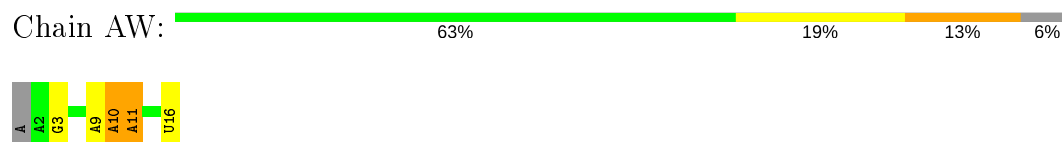
- Molecule 21: 30S ribosomal protein S21



- Molecule 22: Ribosome-recycling factor

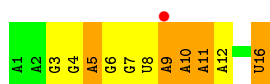


- Molecule 23: Messenger RNA

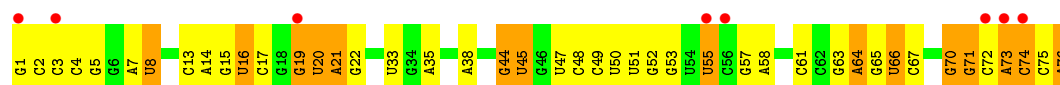
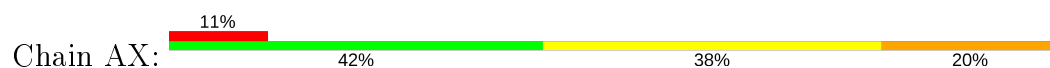


- Molecule 23: Messenger RNA

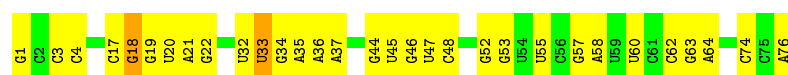




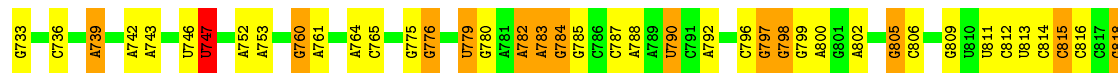
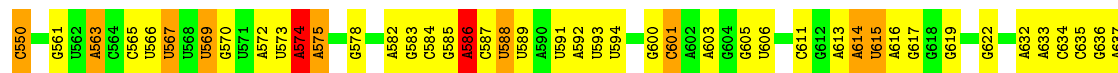
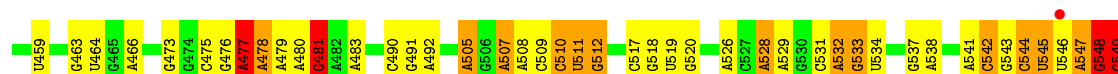
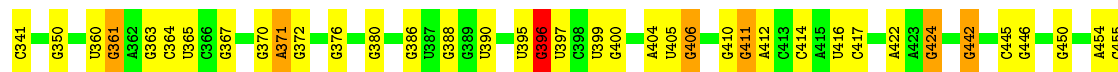
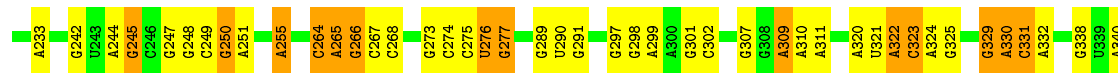
- Molecule 24: Phenylalanine specific transfer RNA, tRNA-Phe



- Molecule 24: Phenylalanine specific transfer RNA, tRNA-Phe



- Molecule 25: 23S ribosomal RNA







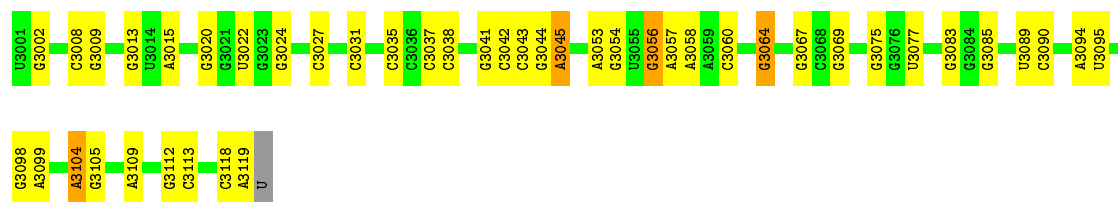


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U847	C848	A849	U850	G858	G859	U860	A861	A866	C867	U868	G869	U870	U871	U872	C873	G874	A877	G881	G882	G883	U884	C885	A	U	C	C	G	A988	G989	A990	G993	C994	C995	A996	G997	C998	C999	A1000	A1001	C1005	C1006	C1007	A1008	A1009	A1010	U1011	C1012	C1013	A1014	G1017	G1022	U1023			

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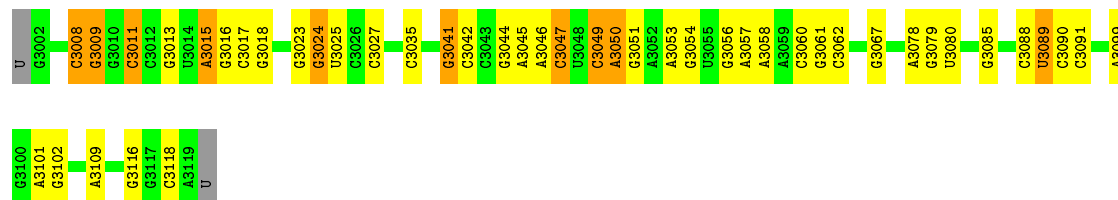
• Molecule 26: 5S ribosomal RNA

Chain BB: 63% 33%



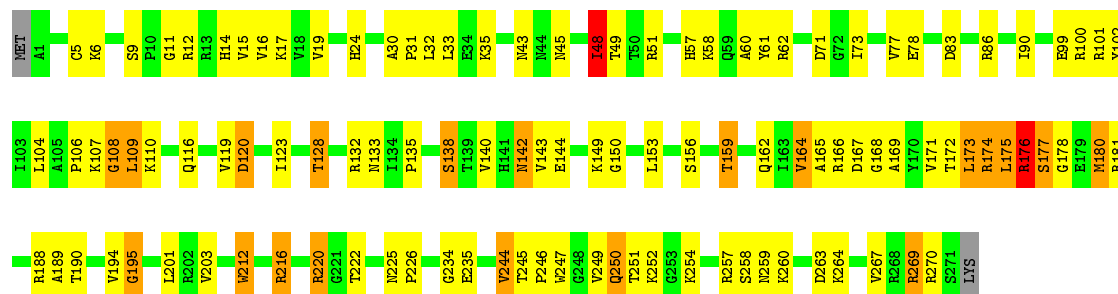
- Molecule 26: 5S ribosomal RNA

Chain CB: 61% 29% 8% .



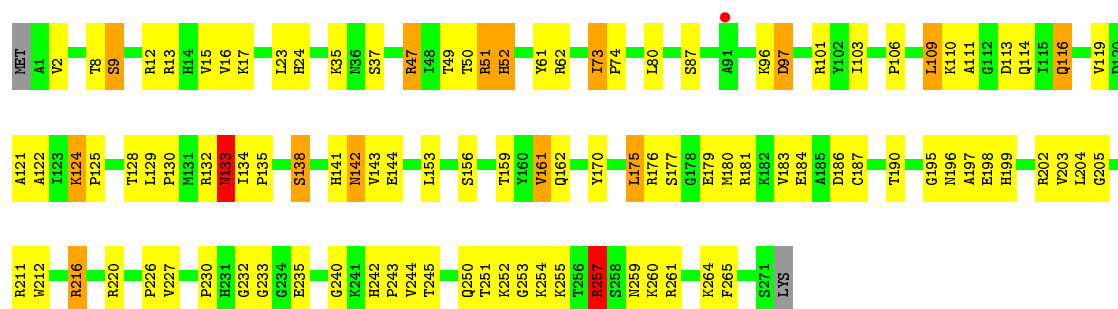
- Molecule 27: 50S ribosomal protein L2

Chain BC: 59% 33% 7% ..



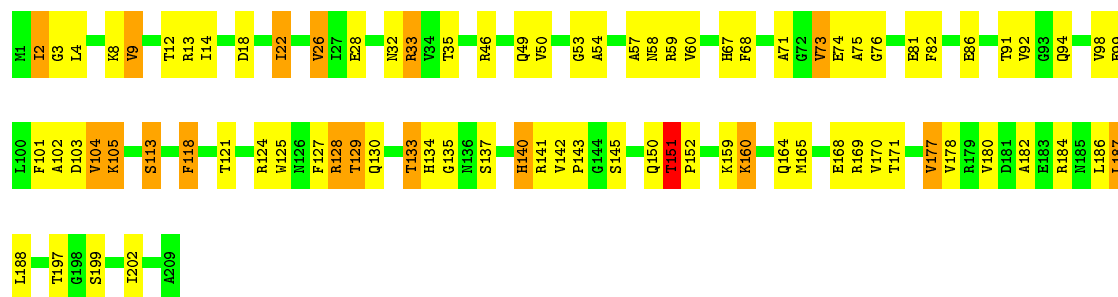
- Molecule 27: 50S ribosomal protein L2

Chain CC: 61% 32% 5% ..

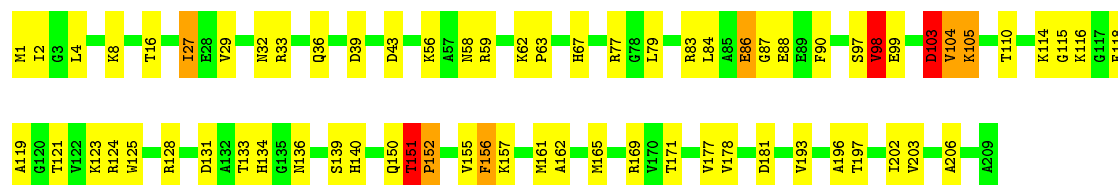


- Molecule 28: 50S ribosomal protein L3

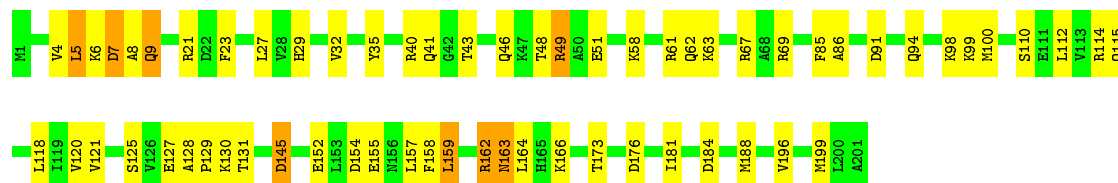
Chain BD: 60% 32% 8%



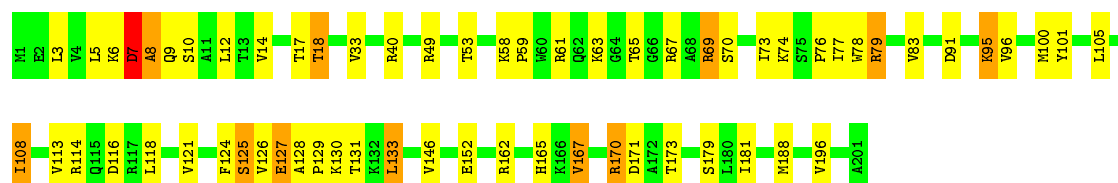
- Molecule 28: 50S ribosomal protein L3



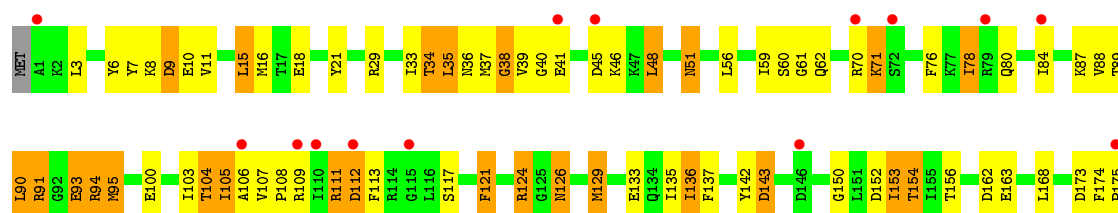
- Molecule 29: 50S ribosomal protein L4



- Molecule 29: 50S ribosomal protein L4

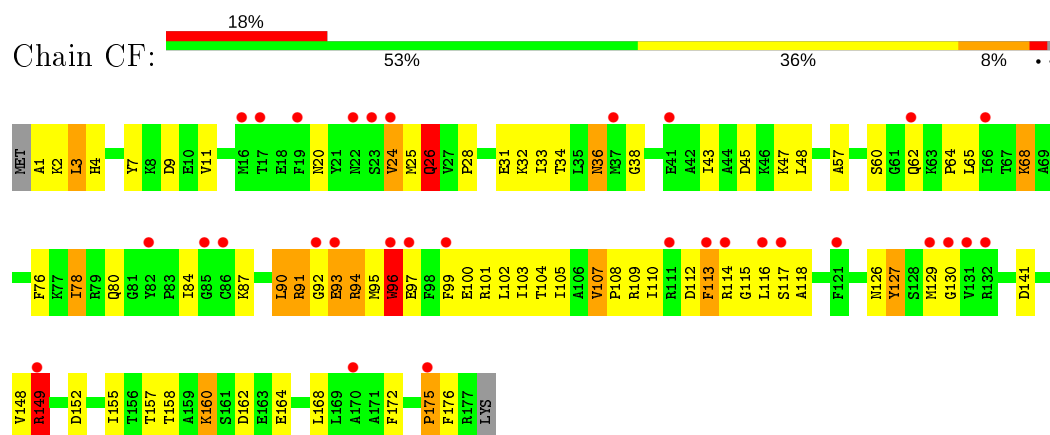


- Molecule 30: 50S ribosomal protein L5

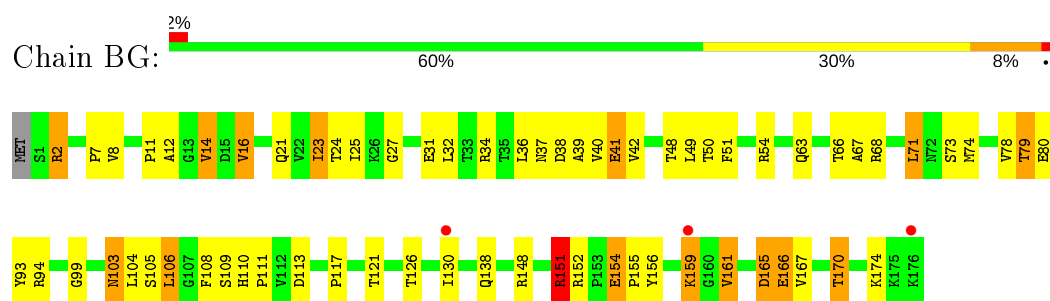




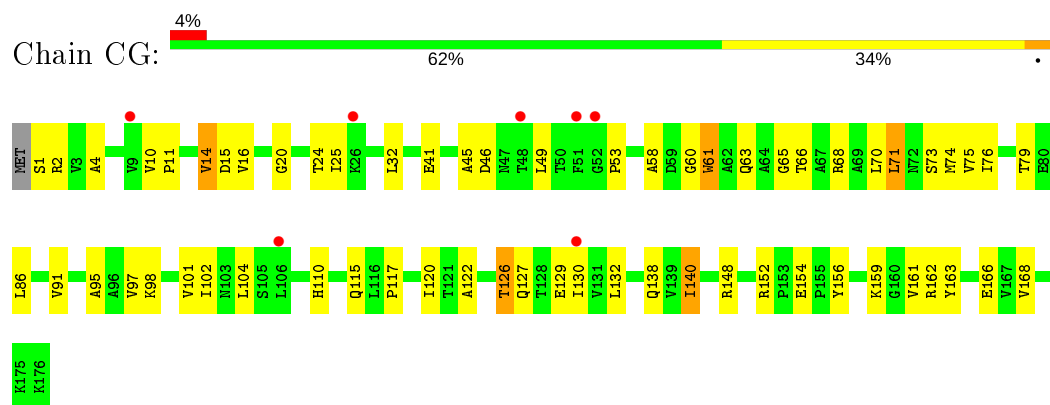
- Molecule 30: 50S ribosomal protein L5



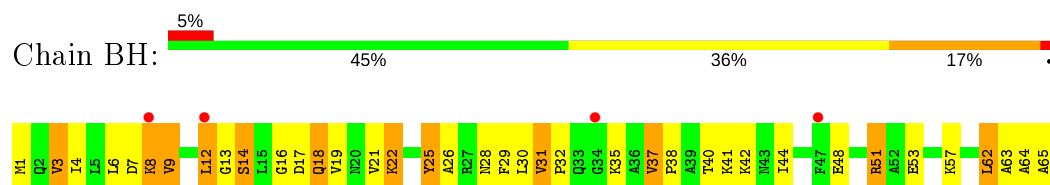
- Molecule 31: 50S ribosomal protein L6

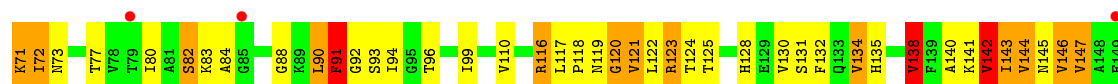


- Molecule 31: 50S ribosomal protein L6

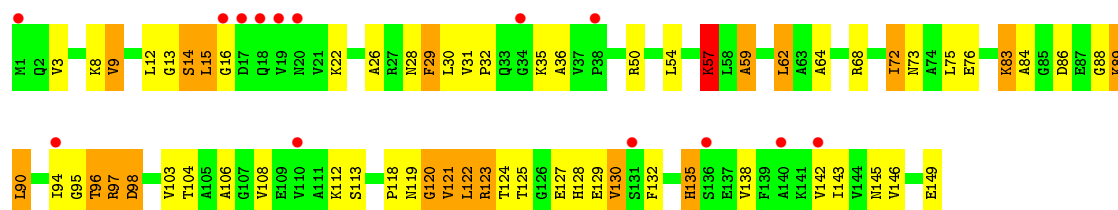


- Molecule 32: 50S ribosomal protein L9

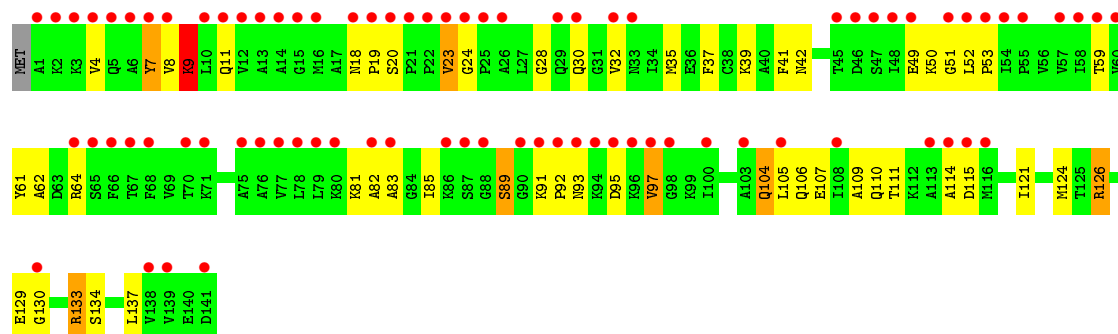




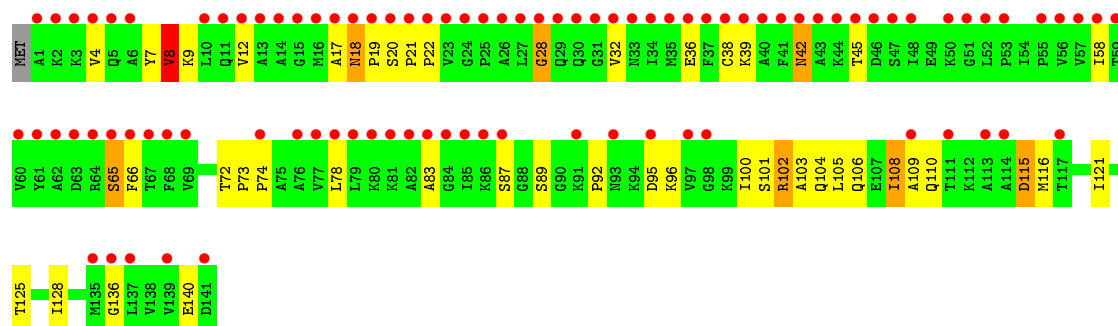
- Molecule 32: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L11

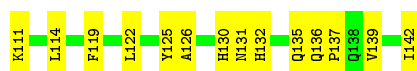


- Molecule 33: 50S ribosomal protein L11



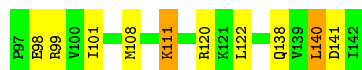
- Molecule 34: 50S ribosomal protein L13





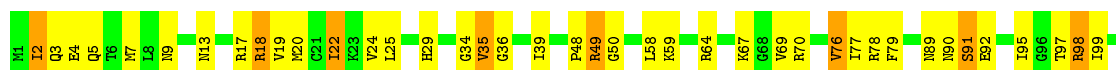
- Molecule 34: 50S ribosomal protein L13

Chain CJ: 68% 26% 6%



- Molecule 35: 50S ribosomal protein L14

Chain BK: 59% 32% 9%



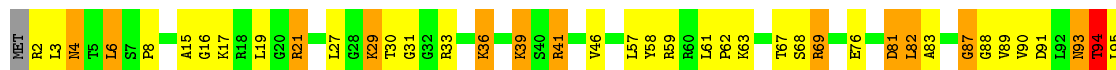
- Molecule 35: 50S ribosomal protein L14

Chain CK: 53% 34% 12%



- Molecule 36: 50S ribosomal protein L15

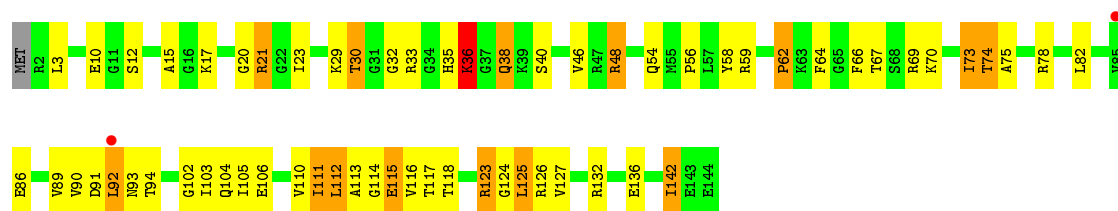
Chain BL: 58% 30% 10%



- Molecule 36: 50S ribosomal protein L15

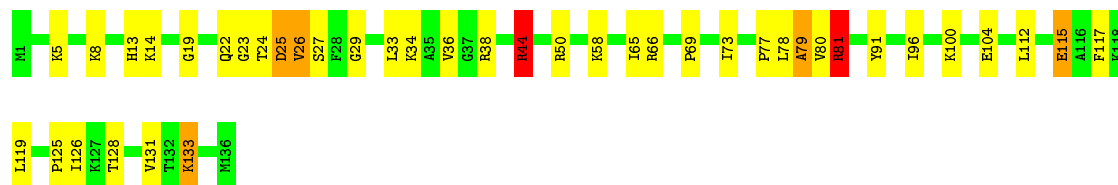
Chain CL: 56% 33% 10%





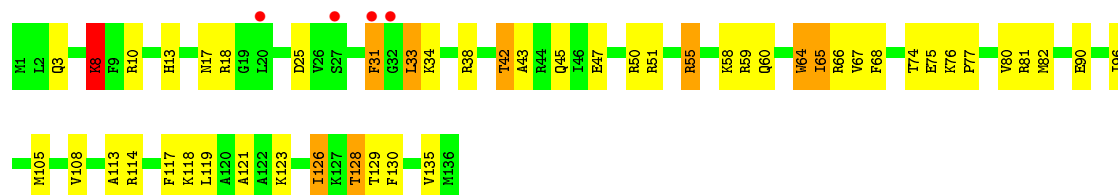
- Molecule 37: 50S ribosomal protein L16

Chain BM: 70% 25% • •



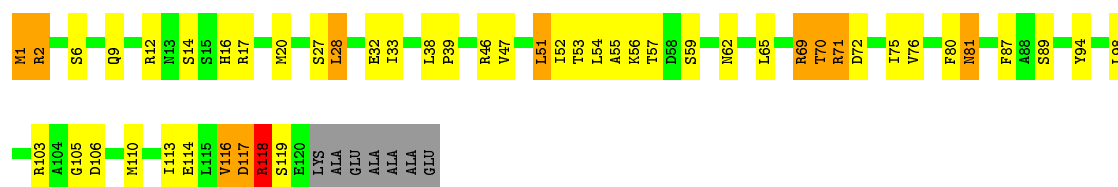
- Molecule 37: 50S ribosomal protein L16

Chain CM: 3% 64% 29% 6% •



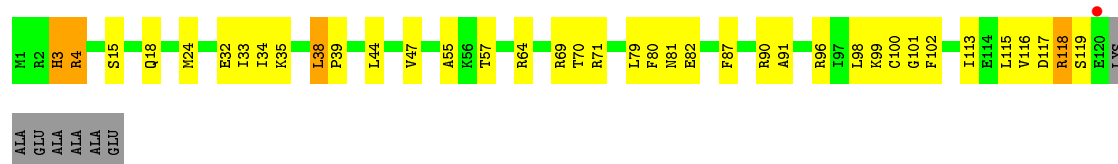
- Molecule 38: 50S ribosomal protein L17

Chain BN: 56% 30% 8% 6% •



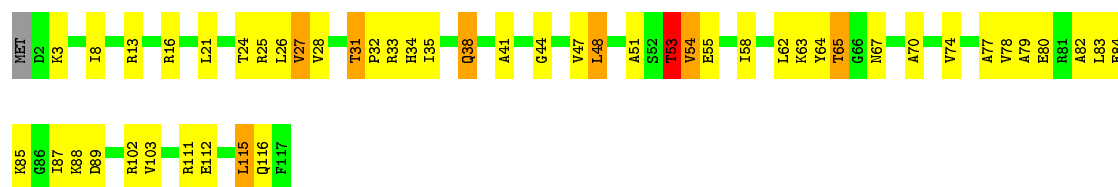
- Molecule 38: 50S ribosomal protein L17

Chain CN: 65% 27% 6% •



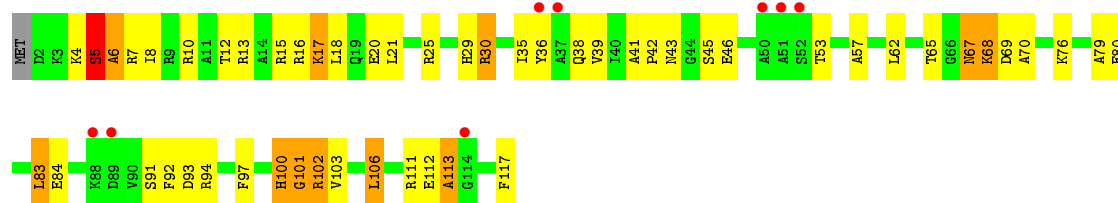
- Molecule 39: 50S ribosomal protein L18

Chain BO:  57% 35% 6% ..



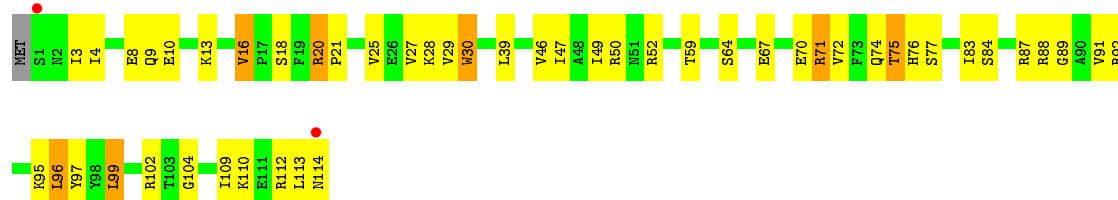
- Molecule 39: 50S ribosomal protein L18

Chain CO:  7% 54% 35% 9% ..



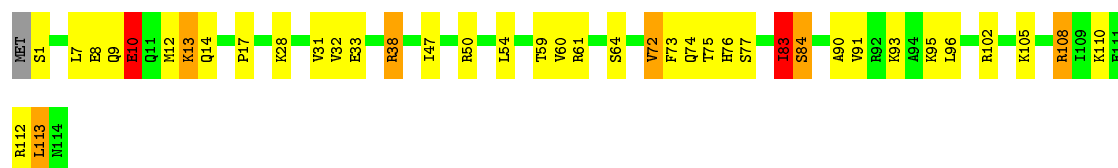
- Molecule 40: 50S ribosomal protein L19

Chain BP:  29% 57% 37% 6% ..



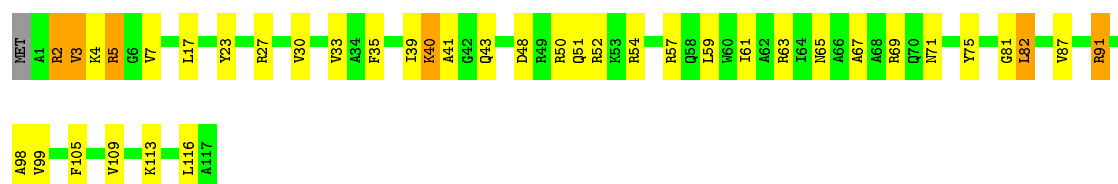
- Molecule 40: 50S ribosomal protein L19

Chain CP:  64% 28% 5% ..

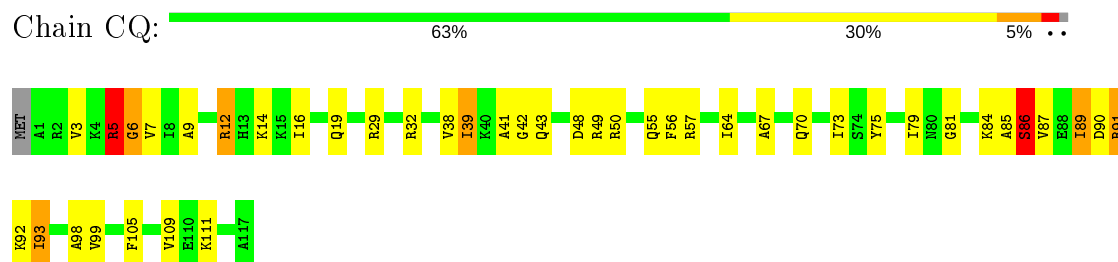


- Molecule 41: 50S ribosomal protein L20

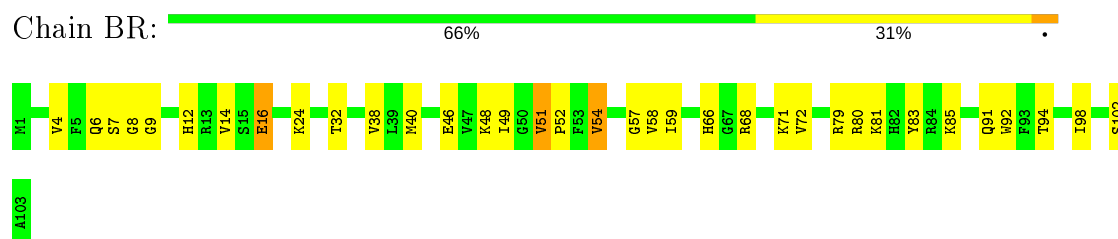
Chain BQ:  66% 28% 5% ..



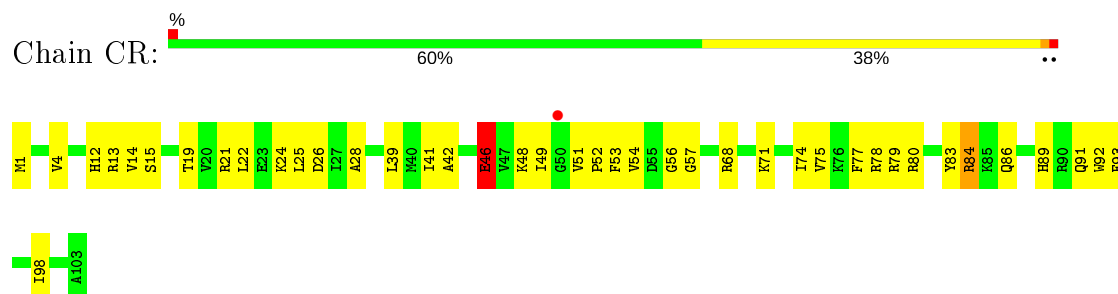
- Molecule 41: 50S ribosomal protein L20



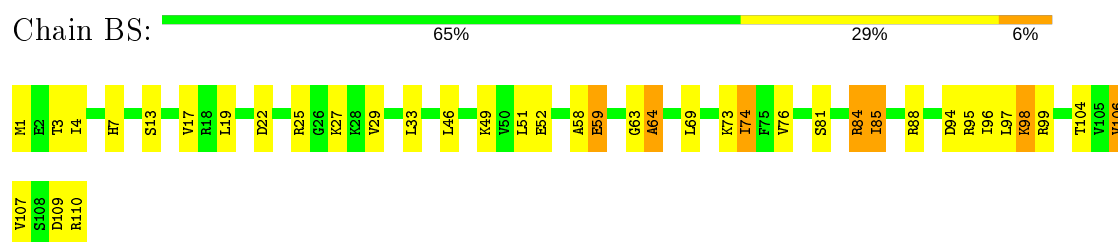
- Molecule 42: 50S ribosomal protein L21



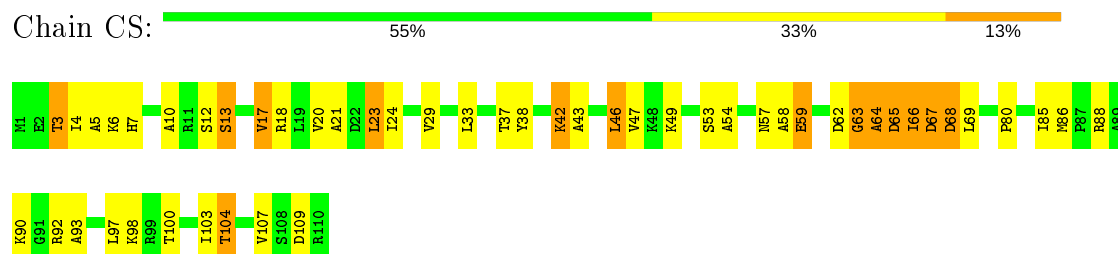
- Molecule 42: 50S ribosomal protein L21



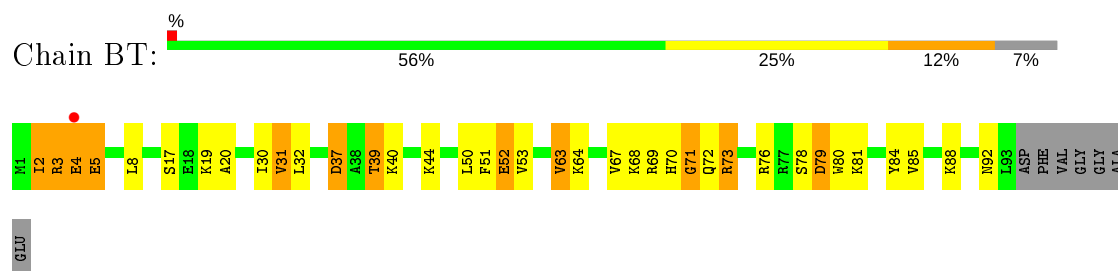
- Molecule 43: 50S ribosomal protein L22



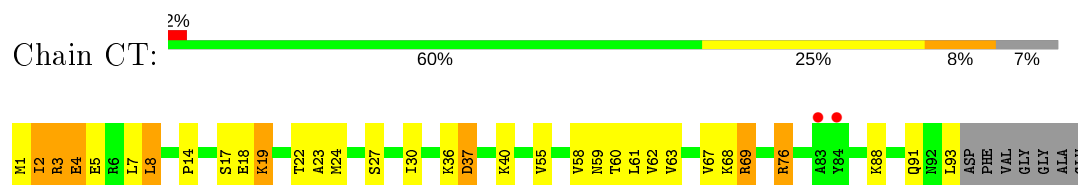
- Molecule 43: 50S ribosomal protein L22



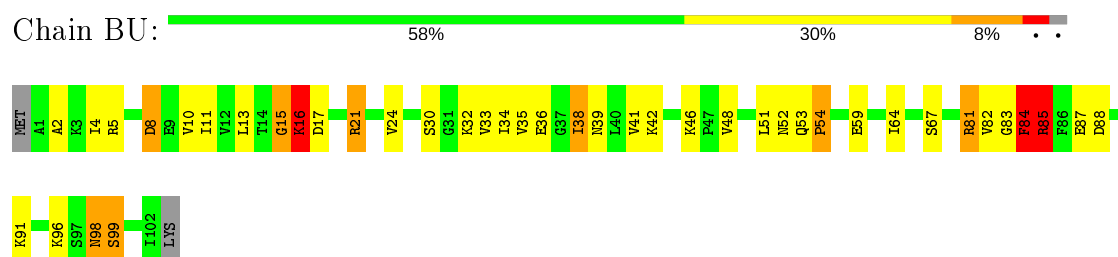
- Molecule 44: 50S ribosomal protein L23



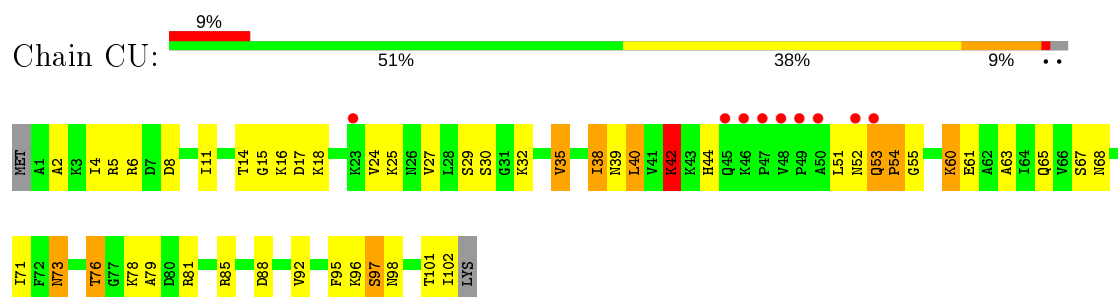
- Molecule 44: 50S ribosomal protein L23



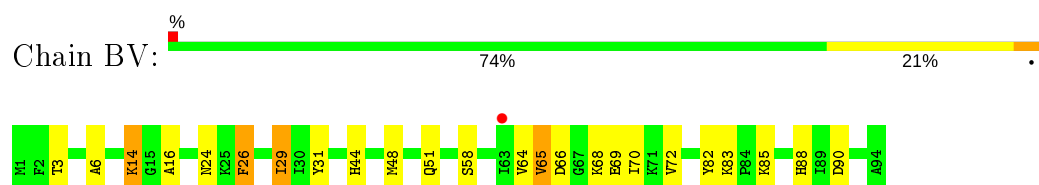
- Molecule 45: 50S ribosomal protein L24



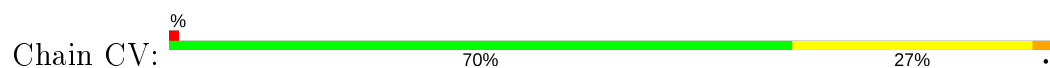
- Molecule 45: 50S ribosomal protein L24



- Molecule 46: 50S ribosomal protein L25



- Molecule 46: 50S ribosomal protein L25





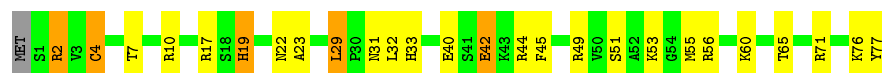
- Molecule 47: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L27



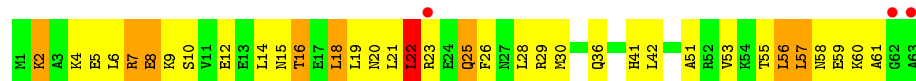
- Molecule 48: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L28




- Molecule 49: 50S ribosomal protein L29

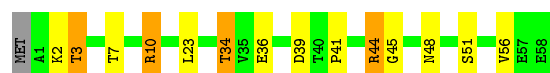


- Molecule 49: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L30

Chain BZ: 



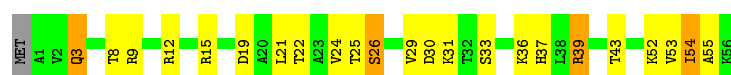
- Molecule 50: 50S ribosomal protein L30

Chain CZ: 



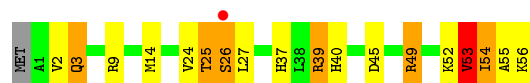
- Molecule 51: 50S ribosomal protein L32

Chain B0: 



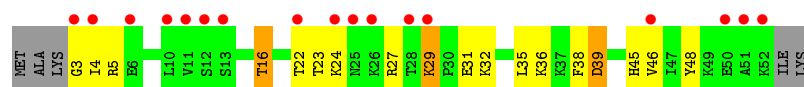
- Molecule 51: 50S ribosomal protein L32

Chain C0: 




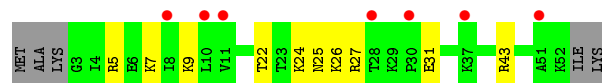
- Molecule 52: 50S ribosomal protein L33

Chain B1: 



- Molecule 52: 50S ribosomal protein L33

Chain C1: 



- Molecule 53: 50S ribosomal protein L34

Chain B2: 



- Molecule 53: 50S ribosomal protein L34

Chain C2:  54% 43% .



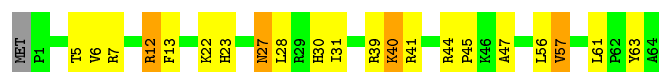
- Molecule 54: 50S ribosomal protein L35

Chain B3:  55% 32% 9% ..



- Molecule 54: 50S ribosomal protein L35

Chain C3:  66% 26% 6% .



- Molecule 55: 50S ribosomal protein L36

Chain B4:  55% 29% 13% .



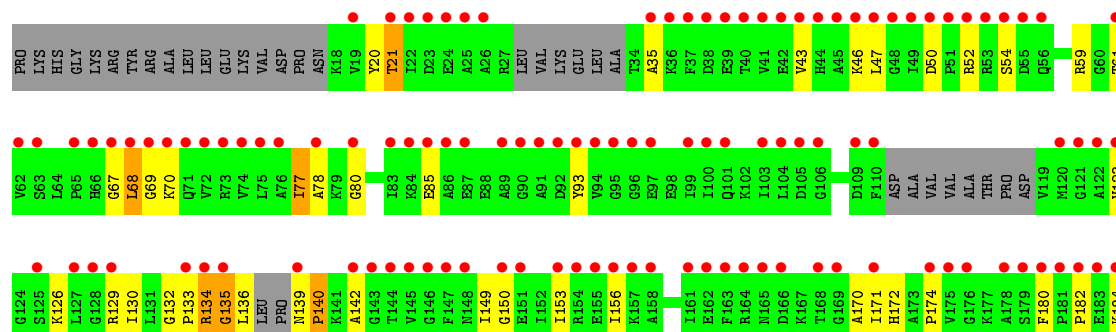
- Molecule 55: 50S ribosomal protein L36

Chain C4:  66% 32% .



- Molecule 56: 50S ribosomal protein L1

Chain B5:  68% 61% 20% 16%



I185	A186	D187	N188	I189	R190	A191	F192	I193	R194	A195	L196	E197	A198	H199	K200	P201	E202	G203	A204	K205	G206	T207	F208	L209	R210	S211	V212	Y213	V214	T215	T216	T217	M218	G219	P220	S221	V222	R223	I224	ASN	PRO	HIS	SER
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.10Å 435.24Å 614.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.00 69.34 – 2.93	Depositor EDS
% Data completeness (in resolution range)	81.1 (70.00-3.00) 76.0 (69.34-2.93)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.174 , 0.253 0.180 , 0.258	Depositor DCC
$R_{free}$ test set	4548 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.9	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 95.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	294484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR

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	0.48	0/36944	0.99	30/57632 (0.1%)
1	DA	0.49	0/36966	1.00	37/57666 (0.1%)
2	AB	0.38	0/1735	0.64	0/2338
2	DB	0.41	0/1735	0.67	1/2338 (0.0%)
3	AC	0.45	0/1651	0.70	0/2225
3	DC	0.42	0/1651	0.66	0/2225
4	AD	0.46	0/1665	0.75	3/2227 (0.1%)
4	DD	0.51	0/1665	0.81	1/2227 (0.0%)
5	AE	0.40	0/1118	0.62	0/1504
5	DE	0.47	0/1118	0.73	0/1504
6	AF	0.42	0/835	0.69	0/1128
6	DF	0.43	0/835	0.71	0/1128
7	AG	2.14	8/1195 (0.7%)	0.81	4/1602 (0.2%)
7	DG	0.38	0/1195	0.57	0/1602
8	AH	0.41	0/989	0.66	0/1326
8	DH	0.45	0/989	0.77	1/1326 (0.1%)
9	AI	0.38	0/1034	0.65	0/1375
9	DI	0.42	0/1034	0.66	0/1375
10	AJ	0.42	0/796	0.69	1/1077 (0.1%)
10	DJ	0.38	0/796	0.64	0/1077
11	AK	0.43	0/893	0.69	0/1205
11	DK	0.43	0/893	0.67	0/1205
12	AL	0.52	0/969	0.77	0/1300
12	DL	0.52	0/969	0.81	1/1300 (0.1%)
13	AM	0.39	0/892	0.74	0/1193
13	DM	0.36	0/892	0.66	0/1193
14	AN	0.44	0/785	0.73	0/1043
14	DN	0.39	0/785	0.67	0/1043
15	AO	0.40	0/724	0.67	0/966
15	DO	0.38	0/724	0.63	0/966
16	AP	0.40	0/659	0.62	0/884
16	DP	0.44	0/659	0.72	1/884 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.40	0/657	0.72	0/881
17	DQ	0.45	0/657	0.69	0/881
18	AR	0.44	0/462	0.63	0/621
18	DR	0.44	0/462	0.71	1/621 (0.2%)
19	AS	0.37	0/652	0.71	0/877
19	DS	0.37	0/652	0.61	0/877
20	AT	0.41	0/671	0.64	0/888
20	DT	0.41	0/671	0.64	0/888
21	AU	0.50	0/430	0.91	1/570 (0.2%)
21	DU	0.58	0/430	0.89	0/570
22	AV	0.43	0/1430	0.63	0/1924
23	AW	0.58	0/363	1.12	0/564
23	DV	0.51	0/388	1.04	0/603
24	AX	0.49	1/1813 (0.1%)	0.95	0/2823
24	DW	0.52	1/1813 (0.1%)	0.95	0/2823
25	BA	0.67	8/69659 (0.0%)	1.20	303/108672 (0.3%)
25	CA	0.52	3/69659 (0.0%)	1.04	112/108672 (0.1%)
26	BB	0.54	0/2850	1.03	7/4444 (0.2%)
26	CB	0.40	0/2828	0.90	2/4410 (0.0%)
27	BC	0.47	0/2121	0.71	0/2852
27	CC	0.42	0/2121	0.68	0/2852
28	BD	0.53	0/1586	0.77	2/2134 (0.1%)
28	CD	0.44	0/1586	0.73	1/2134 (0.0%)
29	BE	0.49	0/1571	0.71	0/2113
29	CE	0.43	0/1571	0.65	0/2113
30	BF	0.40	0/1434	0.65	0/1926
30	CF	0.36	0/1434	0.61	0/1926
31	BG	0.43	0/1343	0.61	0/1816
31	CG	0.35	0/1343	0.56	0/1816
32	BH	0.43	0/1118	0.70	0/1511
32	CH	0.38	0/1118	0.60	1/1511 (0.1%)
33	BI	0.38	0/1046	0.60	0/1410
33	CI	0.33	0/1046	0.55	0/1410
34	BJ	0.53	0/1152	0.67	0/1551
34	CJ	0.43	0/1152	0.62	0/1551
35	BK	0.54	0/947	0.74	0/1268
35	CK	0.47	0/947	0.72	0/1268
36	BL	0.50	0/1054	0.80	0/1403
36	CL	0.45	0/1054	0.70	0/1403
37	BM	0.50	0/1093	0.75	1/1460 (0.1%)
37	CM	0.42	0/1093	0.59	0/1460
38	BN	0.49	0/973	0.69	0/1301
38	CN	0.50	0/973	0.66	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	BO	0.45	0/902	0.65	0/1209
39	CO	0.37	0/902	0.65	0/1209
40	BP	0.49	0/929	0.66	0/1242
40	CP	0.45	0/929	0.65	1/1242 (0.1%)
41	BQ	0.53	0/960	0.74	0/1278
41	CQ	0.49	0/960	0.72	1/1278 (0.1%)
42	BR	0.52	0/829	0.72	0/1107
42	CR	0.49	0/829	0.71	0/1107
43	BS	0.53	0/864	0.70	0/1156
43	CS	0.47	0/864	0.75	0/1156
44	BT	0.48	0/744	0.67	0/994
44	CT	0.40	0/744	0.56	0/994
45	BU	0.51	0/787	0.72	0/1051
45	CU	0.43	0/787	0.64	0/1051
46	BV	0.45	0/766	0.64	0/1025
46	CV	0.34	0/766	0.58	0/1025
47	BW	0.54	0/587	0.73	0/776
47	CW	0.41	0/576	0.65	0/762
48	BX	0.47	0/635	0.71	0/848
48	CX	0.38	0/635	0.64	0/848
49	BY	0.42	0/510	0.69	0/677
49	CY	0.40	0/510	0.72	0/677
50	BZ	0.51	0/453	0.78	0/605
50	CZ	0.41	0/453	0.62	0/605
51	B0	0.54	0/450	0.79	1/599 (0.2%)
51	C0	0.48	0/450	0.73	0/599
52	B1	0.39	0/416	0.61	0/554
52	C1	0.38	0/416	0.62	0/554
53	B2	0.50	0/380	0.74	0/498
53	C2	0.45	0/380	0.66	0/498
54	B3	0.55	0/513	0.78	0/676
54	C3	0.46	0/513	0.71	0/676
55	B4	0.53	0/303	0.77	0/397
55	C4	0.42	0/303	0.60	0/397
56	B5	0.33	0/1145	0.54	0/1556
All	All	0.54	21/316403 (0.0%)	0.99	515/473109 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	1
2	DB	0	1
4	AD	0	1
4	DD	0	1
5	DE	0	2
6	AF	0	1
7	AG	0	1
9	DI	0	1
10	AJ	0	2
11	AK	0	1
12	DL	0	1
14	AN	0	2
17	DQ	0	1
19	AS	0	1
20	AT	0	1
20	DT	0	2
21	AU	0	1
27	BC	0	3
28	BD	0	1
28	CD	0	2
30	BF	0	1
36	BL	0	1
36	CL	0	1
38	BN	0	1
38	CN	0	1
40	CP	0	1
42	CR	0	1
44	BT	0	1
48	CX	0	1
All	All	0	36

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	AG	103	TRP	CE3-CZ3	40.14	2.06	1.38
7	AG	100	ALA	CA-C	39.86	2.56	1.52
7	AG	103	TRP	CZ3-CH2	28.41	1.85	1.40
7	AG	103	TRP	CE2-CZ2	21.77	1.76	1.39
7	AG	103	TRP	CD2-CE2	18.20	1.63	1.41
7	AG	103	TRP	CZ2-CH2	13.78	1.63	1.37
7	AG	103	TRP	CD2-CE3	12.32	1.58	1.40
24	AX	1	G	OP3-P	-10.64	1.48	1.61
24	DW	1	G	OP3-P	-10.17	1.49	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1142	A	N9-C4	-9.04	1.32	1.37
7	AG	100	ALA	CA-CB	8.85	1.71	1.52
25	BA	984	A	N9-C4	-8.83	1.32	1.37
25	CA	984	A	N9-C4	-6.51	1.33	1.37
25	CA	1142	A	N9-C4	-5.95	1.34	1.37
25	BA	974	G	N9-C8	5.65	1.41	1.37
25	CA	752	A	N9-C4	-5.60	1.34	1.37
25	BA	2015	A	N9-C4	-5.46	1.34	1.37
25	BA	528	A	N9-C4	-5.31	1.34	1.37
25	BA	549	G	N9-C4	5.21	1.42	1.38
25	BA	2024	G	P-O5'	-5.10	1.54	1.59
25	BA	528	A	N7-C5	-5.08	1.36	1.39

All (515) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	984	A	C2-N3-C4	-15.53	102.84	110.60
25	BA	1936	A	C2-N3-C4	-12.94	104.13	110.60
28	CD	151	THR	C-N-CD	-11.23	95.90	120.60
25	BA	2623	G	O5'-P-OP1	-10.98	95.82	105.70
25	BA	1936	A	N1-C2-N3	10.97	134.79	129.30
25	CA	984	A	C2-N3-C4	-10.41	105.39	110.60
25	BA	2012	G	O5'-P-OP1	-10.38	96.35	105.70
25	BA	974	G	C5-N7-C8	-10.33	99.14	104.30
25	BA	752	A	C5-N7-C8	-9.96	98.92	103.90
25	BA	549	G	N3-C4-N9	9.84	131.90	126.00
25	BA	984	A	C5-C6-N1	-9.79	112.80	117.70
25	BA	691	C	N1-C2-O2	9.51	124.61	118.90
25	BA	974	G	N3-C4-C5	9.44	133.32	128.60
7	AG	100	ALA	O-C-N	-9.34	107.75	122.70
25	BA	549	G	N3-C4-C5	-9.33	123.94	128.60
25	CA	811	U	O5'-P-OP1	-9.28	97.35	105.70
25	BA	1664	A	O5'-P-OP2	-9.21	97.41	105.70
25	BA	752	A	C4-C5-N7	8.89	115.14	110.70
25	BA	561	G	N1-C6-O6	8.84	125.20	119.90
25	BA	1916	A	N1-C6-N6	8.84	123.90	118.60
25	BA	984	A	N1-C2-N3	8.76	133.68	129.30
25	BA	974	G	N3-C4-N9	-8.65	120.81	126.00
25	CA	542	C	N3-C4-C5	-8.63	118.45	121.90
25	BA	84	A	N1-C6-N6	-8.59	113.44	118.60
7	AG	100	ALA	CB-CA-C	8.51	122.86	110.10
25	CA	2425	A	P-O3'-C3'	8.46	129.85	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	2047	C	O5'-P-OP1	-8.30	98.23	105.70
25	BA	783	A	N1-C6-N6	8.30	123.58	118.60
25	CA	2308	G	C5-C6-O6	-8.27	123.64	128.60
25	BA	549	G	C4-N9-C1'	8.23	137.20	126.50
25	BA	528	A	C2-N3-C4	-8.23	106.49	110.60
25	BA	528	A	N1-C6-N6	8.19	123.51	118.60
25	BA	797	G	O5'-P-OP2	-8.15	98.37	105.70
25	CA	990	A	O5'-P-OP2	-8.11	98.40	105.70
25	BA	2024	G	O5'-P-OP2	-8.10	98.41	105.70
25	BA	2828	G	O5'-P-OP2	-8.08	98.43	105.70
51	B0	19	ASP	CB-CG-OD1	8.07	125.56	118.30
25	BA	1142	A	N1-C6-N6	7.99	123.39	118.60
25	BA	984	A	N3-C4-C5	7.96	132.38	126.80
7	AG	100	ALA	N-CA-CB	-7.95	98.98	110.10
25	BA	1198	U	O5'-P-OP2	-7.89	98.60	105.70
25	CA	2821	A	O5'-P-OP2	-7.87	98.61	105.70
25	CA	740	C	C6-N1-C2	7.79	123.42	120.30
25	CA	846	U	C2-N1-C1'	7.79	127.04	117.70
25	BA	984	A	N3-C4-N9	-7.73	121.22	127.40
25	BA	974	G	C4-C5-C6	-7.72	114.17	118.80
25	BA	752	A	N7-C8-N9	7.71	117.65	113.80
25	BA	2711	A	O5'-P-OP2	-7.70	98.77	105.70
25	BA	1114	C	C6-N1-C2	7.70	123.38	120.30
1	DA	1483	A	O5'-P-OP1	-7.69	98.78	105.70
25	CA	516	C	C6-N1-C2	7.69	123.37	120.30
1	AA	1286	U	C2-N1-C1'	7.63	126.86	117.70
25	BA	974	G	N7-C8-N9	7.63	116.91	113.10
25	BA	2687	U	C5-C6-N1	7.57	126.48	122.70
25	CA	790	U	O5'-P-OP2	-7.57	98.89	105.70
25	CA	752	A	C5-N7-C8	-7.52	100.14	103.90
25	BA	948	C	O5'-P-OP1	7.51	119.72	110.70
25	BA	2417	C	C6-N1-C2	-7.51	117.30	120.30
25	CA	2165	C	C6-N1-C2	-7.50	117.30	120.30
25	BA	2687	U	C6-N1-C2	-7.49	116.50	121.00
25	BA	1379	U	O5'-P-OP2	-7.49	98.96	105.70
25	BA	2044	C	C6-N1-C2	7.49	123.30	120.30
25	BA	1415	U	C2-N1-C1'	7.49	126.68	117.70
25	BA	2024	G	N3-C4-C5	-7.41	124.89	128.60
37	BM	44	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	AA	4	U	C2-N1-C1'	7.39	126.56	117.70
25	CA	962	G	O5'-P-OP2	-7.34	99.09	105.70
25	BA	2250	G	C2-N3-C4	-7.33	108.23	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	CA	2165	C	C2-N1-C1'	7.31	126.84	118.80
25	BA	2326	C	C6-N1-C2	-7.30	117.38	120.30
25	BA	561	G	C5-C6-O6	-7.30	124.22	128.60
25	BA	783	A	C5-N7-C8	-7.26	100.27	103.90
25	BA	752	A	N1-C6-N6	7.24	122.94	118.60
25	BA	1142	A	C5-N7-C8	-7.23	100.28	103.90
25	CA	808	G	N1-C6-O6	7.21	124.23	119.90
25	BA	834	G	N1-C6-O6	7.17	124.20	119.90
25	BA	549	G	C8-N9-C1'	-7.14	117.72	127.00
1	DA	1361	G	C8-N9-C4	-7.13	103.55	106.40
25	BA	542	C	N3-C4-C5	-7.13	119.05	121.90
25	BA	1238	G	O5'-P-OP1	7.12	119.25	110.70
25	BA	1011	G	N3-C4-C5	7.12	132.16	128.60
1	DA	1361	G	N3-C4-C5	-7.11	125.05	128.60
25	CA	984	A	C5-C6-N1	-7.09	114.16	117.70
25	CA	559	G	N1-C6-O6	7.08	124.15	119.90
25	CA	1936	A	C2-N3-C4	-7.03	107.08	110.60
25	BA	1142	A	C2-N3-C4	-7.03	107.09	110.60
21	AU	35	ARG	NE-CZ-NH2	-7.02	116.79	120.30
25	CA	2426	A	O5'-P-OP1	-7.01	99.39	105.70
1	DA	328	C	N1-C2-O2	7.01	123.10	118.90
25	BA	528	A	C5-N7-C8	-6.99	100.40	103.90
25	CA	139	U	C2-N1-C1'	6.99	126.09	117.70
1	DA	1029	U	C2-N1-C1'	6.99	126.09	117.70
25	BA	2250	G	N3-C4-C5	6.96	132.08	128.60
25	BA	691	C	N3-C2-O2	-6.96	117.03	121.90
25	CA	549	G	O4'-C1'-N9	6.95	113.76	108.20
25	CA	1914	C	C2-N1-C1'	6.94	126.44	118.80
25	BA	1434	A	O4'-C1'-N9	6.93	113.75	108.20
25	CA	974	G	C5-N7-C8	-6.93	100.84	104.30
25	BA	2626	C	C6-N1-C2	6.89	123.06	120.30
12	DL	44	LYS	C-N-CD	6.89	142.88	128.40
7	AG	103	TRP	CE3-CZ3-CH2	-6.87	113.64	121.20
1	AA	328	C	N1-C2-O2	6.85	123.01	118.90
25	BA	834	G	C5-C6-O6	-6.83	124.50	128.60
25	BA	60	G	C8-N9-C4	-6.80	103.68	106.40
25	BA	397	U	O5'-P-OP2	-6.80	99.58	105.70
25	BA	2213	U	C2-N1-C1'	6.76	125.81	117.70
25	BA	1913	A	C8-N9-C4	6.75	108.50	105.80
25	BA	752	A	C6-C5-N7	-6.74	127.58	132.30
25	BA	574	A	O5'-P-OP2	6.74	118.79	110.70
25	BA	1378	A	P-O3'-C3'	6.72	127.77	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DA	1495	U	N3-C2-O2	-6.72	117.50	122.20
25	BA	1415	U	N3-C2-O2	-6.71	117.50	122.20
25	BA	1489	C	C6-N1-C2	-6.71	117.62	120.30
25	CA	2590	A	O5'-P-OP2	-6.70	99.67	105.70
25	BA	60	G	P-O3'-C3'	6.70	127.74	119.70
25	CA	2448	A	N1-C6-N6	6.70	122.62	118.60
25	BA	824	U	O5'-P-OP2	-6.67	99.69	105.70
4	DD	203	LEU	CA-CB-CG	6.67	130.64	115.30
25	CA	549	G	C4-N9-C1'	6.67	135.17	126.50
25	BA	2583	G	O5'-P-OP2	-6.66	99.71	105.70
25	BA	2606	C	N1-C2-O2	-6.66	114.91	118.90
1	DA	632	U	C2-N1-C1'	6.66	125.69	117.70
25	BA	1649	G	C8-N9-C4	-6.65	103.74	106.40
25	BA	512	G	O4'-C1'-N9	6.65	113.52	108.20
25	BA	974	G	C4-C5-N7	6.64	113.46	110.80
25	CA	2011	U	C5-C4-O4	6.64	129.88	125.90
25	CA	509	C	C6-N1-C2	-6.62	117.65	120.30
25	BA	1938	A	O5'-P-OP2	6.59	118.61	110.70
25	BA	1784	A	C4-C5-C6	6.58	120.29	117.00
25	CA	2308	G	N1-C6-O6	6.58	123.85	119.90
25	CA	974	G	C4-C5-N7	6.57	113.43	110.80
25	BA	102	U	N1-C2-O2	6.57	127.40	122.80
26	BB	3064	G	N3-C4-N9	-6.55	122.07	126.00
25	BA	1142	A	N3-C4-C5	6.55	131.38	126.80
25	BA	512	G	O5'-P-OP1	-6.55	99.81	105.70
25	BA	2250	G	C5-N7-C8	-6.53	101.04	104.30
25	CA	2060	A	N1-C6-N6	6.51	122.51	118.60
2	DB	117	LEU	CA-CB-CG	6.51	130.27	115.30
1	AA	351	G	C4-C5-N7	6.49	113.40	110.80
25	BA	528	A	C6-C5-N7	-6.46	127.78	132.30
1	AA	429	U	C2-N1-C1'	6.46	125.45	117.70
8	DH	88	ARG	NE-CZ-NH1	6.45	123.52	120.30
25	BA	1133	A	N9-C4-C5	6.43	108.37	105.80
1	AA	859	G	N3-C4-C5	-6.43	125.39	128.60
25	BA	1024	G	C5-C6-O6	-6.42	124.75	128.60
25	CA	275	C	C2-N1-C1'	6.42	125.86	118.80
25	BA	445	C	O5'-P-OP2	-6.42	99.92	105.70
25	BA	60	G	N3-C4-C5	-6.42	125.39	128.60
25	CA	517	C	N3-C2-O2	6.41	126.39	121.90
25	BA	567	U	O5'-P-OP1	6.41	118.39	110.70
25	CA	1802	A	P-O3'-C3'	6.40	127.38	119.70
25	BA	1779	U	C4-C5-C6	6.39	123.54	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	CA	139	U	N3-C2-O2	-6.37	117.74	122.20
25	CA	2311	A	C8-N9-C4	-6.37	103.25	105.80
1	DA	1531	A	N1-C6-N6	6.36	122.42	118.60
25	BA	990	A	O5'-P-OP2	-6.35	99.98	105.70
25	BA	1024	G	N1-C6-O6	6.35	123.71	119.90
25	BA	760	G	O5'-P-OP2	-6.34	100.00	105.70
25	CA	1584	U	C2-N1-C1'	6.33	125.30	117.70
25	CA	2165	C	N1-C2-O2	6.33	122.70	118.90
1	AA	328	C	N3-C2-O2	-6.32	117.48	121.90
25	BA	1022	G	C8-N9-C1'	6.31	135.20	127.00
25	BA	57	C	C6-N1-C2	6.31	122.82	120.30
25	BA	2559	C	C6-N1-C2	6.29	122.81	120.30
25	BA	1916	A	C5-C6-N6	-6.28	118.67	123.70
1	AA	1417	G	C4-C5-N7	6.27	113.31	110.80
25	BA	617	G	C5-C6-O6	6.27	132.36	128.60
25	BA	1064	C	C2-N1-C1'	6.26	125.69	118.80
25	CA	525	U	C5-C4-O4	6.26	129.66	125.90
25	BA	1011	G	N1-C6-O6	6.25	123.65	119.90
1	AA	188	C	C2-N1-C1'	6.24	125.67	118.80
25	BA	2607	G	N3-C4-N9	6.24	129.75	126.00
25	BA	1186	G	N1-C6-O6	6.24	123.64	119.90
25	BA	2437	G	C2-N3-C4	-6.23	108.79	111.90
1	DA	530	G	C4-N9-C1'	6.22	134.59	126.50
25	BA	264	C	N3-C2-O2	-6.22	117.55	121.90
25	BA	2054	A	O5'-P-OP2	-6.21	100.11	105.70
25	CA	974	G	N7-C8-N9	6.21	116.20	113.10
25	CA	2165	C	N3-C2-O2	-6.18	117.58	121.90
25	BA	1022	G	C4-N9-C1'	-6.17	118.48	126.50
25	CA	140	C	C6-N1-C2	-6.17	117.83	120.30
25	BA	473	G	N1-C6-O6	6.16	123.60	119.90
25	BA	2561	U	N1-C2-O2	-6.16	118.49	122.80
1	AA	1417	G	C5-C6-O6	-6.15	124.91	128.60
1	AA	1507	A	N1-C6-N6	6.15	122.29	118.60
1	AA	1320	C	C6-N1-C2	-6.13	117.85	120.30
25	BA	2789	C	N3-C2-O2	-6.12	117.61	121.90
28	BD	124	ARG	NE-CZ-NH1	6.12	123.36	120.30
4	AD	5	LEU	CA-CB-CG	6.12	129.37	115.30
25	BA	1133	A	N1-C6-N6	-6.11	114.93	118.60
25	CA	783	A	C5-N7-C8	-6.11	100.85	103.90
25	BA	783	A	C2-N3-C4	-6.10	107.55	110.60
25	BA	1142	A	C4-C5-N7	6.09	113.75	110.70
25	BA	371	A	C8-N9-C4	6.07	108.23	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DA	754	C	C2-N1-C1'	6.07	125.48	118.80
25	CA	1790	C	O5'-P-OP2	6.06	117.97	110.70
1	AA	1279	G	C8-N9-C4	-6.06	103.98	106.40
25	BA	2689	U	C5-C4-O4	6.05	129.53	125.90
25	BA	1219	U	N3-C4-O4	-6.04	115.17	119.40
1	DA	1361	G	N7-C8-N9	6.03	116.11	113.10
25	BA	1178	C	C6-N1-C2	-6.03	117.89	120.30
25	BA	2448	A	N1-C6-N6	6.03	122.22	118.60
25	BA	2517	C	O4'-C1'-N1	6.03	113.02	108.20
25	BA	209	C	C6-N1-C2	-6.02	117.89	120.30
25	BA	1415	U	N1-C2-O2	6.02	127.01	122.80
25	BA	1064	C	N1-C2-O2	6.01	122.51	118.90
25	BA	828	U	O5'-P-OP2	-6.01	100.29	105.70
25	BA	2211	A	P-O3'-C3'	6.00	126.90	119.70
25	BA	2422	C	P-O3'-C3'	6.00	126.90	119.70
25	BA	2756	U	N3-C2-O2	-6.00	118.00	122.20
26	CB	3089	U	N1-C2-O2	6.00	127.00	122.80
1	DA	1361	G	N3-C4-N9	5.99	129.59	126.00
25	BA	528	A	N7-C8-N9	5.99	116.80	113.80
25	BA	752	A	O4'-C1'-N9	5.97	112.98	108.20
25	BA	2324	U	P-O3'-C3'	5.96	126.85	119.70
26	BB	3083	G	C8-N9-C4	5.95	108.78	106.40
25	CA	1890	A	N1-C6-N6	-5.95	115.03	118.60
25	CA	984	A	N1-C2-N3	5.93	132.27	129.30
25	BA	2044	C	N1-C2-O2	-5.93	115.34	118.90
25	CA	731	C	O5'-P-OP2	-5.93	100.36	105.70
25	BA	747	U	C5-C4-O4	-5.93	122.34	125.90
1	DA	328	C	N3-C2-O2	-5.93	117.75	121.90
25	BA	2275	C	O5'-P-OP2	-5.91	100.38	105.70
28	BD	151	THR	C-N-CD	-5.91	107.61	120.60
1	DA	1482	G	N3-C4-C5	-5.91	125.65	128.60
25	BA	1305	C	O5'-P-OP2	-5.90	100.39	105.70
25	BA	442	G	N1-C6-O6	5.89	123.44	119.90
25	BA	673	C	N1-C2-O2	5.89	122.43	118.90
25	BA	2789	C	N1-C2-O2	5.87	122.42	118.90
25	CA	1938	A	O5'-P-OP2	-5.87	100.42	105.70
25	CA	2817	U	N3-C4-O4	-5.87	115.29	119.40
25	CA	2286	G	C8-N9-C4	-5.86	104.06	106.40
25	BA	676	A	N1-C6-N6	5.86	122.11	118.60
25	BA	102	U	N3-C2-O2	-5.85	118.10	122.20
25	CA	2078	C	O5'-P-OP2	-5.85	100.44	105.70
1	AA	351	G	C5-C6-O6	-5.84	125.09	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	3083	G	N9-C4-C5	-5.83	103.07	105.40
25	CA	549	G	C8-N9-C1'	-5.82	119.43	127.00
25	CA	139	U	N1-C2-O2	5.82	126.87	122.80
1	DA	1361	G	C6-C5-N7	-5.81	126.91	130.40
25	BA	2799	A	N1-C6-N6	5.81	122.09	118.60
25	BA	2751	G	C4-N9-C1'	5.81	134.05	126.50
25	BA	549	G	O4'-C1'-N9	5.80	112.84	108.20
25	CA	456	C	N1-C2-O2	5.80	122.38	118.90
25	CA	512	G	O4'-C1'-N9	5.79	112.83	108.20
25	BA	518	G	C8-N9-C4	5.79	108.71	106.40
25	BA	549	G	N3-C2-N2	5.78	123.95	119.90
25	BA	1308	A	N1-C6-N6	5.78	122.07	118.60
1	DA	328	C	C2-N1-C1'	5.78	125.16	118.80
25	BA	2391	G	N1-C6-O6	-5.78	116.44	119.90
25	BA	2899	A	O5'-P-OP1	5.77	117.62	110.70
25	BA	549	G	C2-N3-C4	5.77	114.78	111.90
1	AA	859	G	N3-C4-N9	5.76	129.45	126.00
25	BA	561	G	C4-C5-N7	5.74	113.10	110.80
1	DA	390	U	O5'-P-OP2	-5.74	100.53	105.70
25	BA	752	A	C5-C6-N6	-5.74	119.11	123.70
1	AA	1286	U	N1-C2-O2	5.73	126.81	122.80
25	CA	808	G	C5-C6-O6	-5.72	125.17	128.60
25	BA	102	U	C2-N1-C1'	5.71	124.55	117.70
25	BA	477	A	C8-N9-C4	-5.71	103.52	105.80
26	BB	3064	G	C4-N9-C1'	-5.71	119.08	126.50
25	BA	84	A	C5-C6-N6	5.70	128.26	123.70
25	BA	752	A	N9-C1'-C2'	5.70	121.41	114.00
25	BA	1328	A	C2-N3-C4	-5.70	107.75	110.60
25	BA	2030	A	N9-C4-C5	5.70	108.08	105.80
25	BA	1609	A	O5'-P-OP2	-5.69	100.58	105.70
25	BA	939	G	N3-C2-N2	-5.68	115.92	119.90
25	BA	601	C	O5'-P-OP2	-5.67	100.60	105.70
25	BA	2609	U	O4'-C1'-N1	5.67	112.73	108.20
25	CA	1896	G	N3-C4-C5	5.65	131.43	128.60
25	BA	140	C	C2-N1-C1'	5.64	125.01	118.80
25	BA	2250	G	N1-C6-O6	5.64	123.28	119.90
25	BA	752	A	C4-N9-C1'	5.64	136.45	126.30
25	BA	783	A	C4-C5-N7	5.63	113.52	110.70
25	CA	740	C	C5-C6-N1	-5.63	118.19	121.00
1	DA	1113	C	C6-N1-C2	-5.63	118.05	120.30
25	BA	1128	G	C4-N9-C1'	-5.62	119.19	126.50
1	AA	859	G	C4-N9-C1'	5.62	133.81	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	776	G	C5-C6-O6	5.62	131.97	128.60
25	CA	1896	G	N3-C4-N9	-5.61	122.63	126.00
26	BB	3064	G	C8-N9-C1'	5.60	134.28	127.00
25	CA	517	C	N1-C2-O2	-5.60	115.54	118.90
1	DA	632	U	N3-C2-O2	-5.60	118.28	122.20
25	BA	2671	G	C4-N9-C1'	-5.60	119.22	126.50
1	AA	1286	U	N3-C2-O2	-5.60	118.28	122.20
25	CA	528	A	C2-N3-C4	-5.60	107.80	110.60
25	BA	1342	A	C8-N9-C4	5.60	108.04	105.80
25	CA	2699	C	C6-N1-C2	-5.60	118.06	120.30
25	BA	586	A	O5'-P-OP1	-5.59	100.67	105.70
1	DA	365	U	C5-C4-O4	5.59	129.26	125.90
25	BA	2627	G	C4-C5-N7	5.59	113.04	110.80
25	BA	2889	C	O5'-P-OP1	-5.59	100.67	105.70
25	CA	276	U	C2-N1-C1'	5.59	124.40	117.70
25	BA	2472	G	N3-C4-C5	5.58	131.39	128.60
25	BA	190	A	P-O3'-C3'	5.58	126.40	119.70
25	BA	2250	G	C4-C5-N7	5.58	113.03	110.80
25	BA	2549	G	P-O3'-C3'	5.58	126.39	119.70
25	BA	1606	C	C6-N1-C2	-5.57	118.07	120.30
25	BA	1622	G	OP1-P-OP2	-5.57	111.25	119.60
25	CA	974	G	C4-N9-C1'	5.57	133.74	126.50
25	BA	2627	G	C5-C6-O6	-5.56	125.26	128.60
1	DA	1279	G	N7-C8-N9	5.56	115.88	113.10
1	AA	115	G	P-O3'-C3'	5.56	126.37	119.70
25	BA	747	U	N3-C2-O2	5.56	126.09	122.20
25	BA	961	C	C6-N1-C2	-5.55	118.08	120.30
25	CA	79	C	C6-N1-C2	-5.55	118.08	120.30
25	CA	808	G	N3-C2-N2	-5.55	116.01	119.90
1	AA	738	C	P-O3'-C3'	5.55	126.36	119.70
25	BA	1567	G	N1-C6-O6	5.55	123.23	119.90
25	BA	2521	C	N1-C2-O2	-5.54	115.58	118.90
25	CA	1934	C	C6-N1-C2	5.54	122.52	120.30
25	BA	400	G	N3-C4-N9	5.54	129.32	126.00
25	BA	1377	G	C8-N9-C4	-5.54	104.19	106.40
25	BA	2766	A	O5'-P-OP2	-5.53	100.72	105.70
1	DA	632	U	N1-C2-O2	5.53	126.67	122.80
1	DA	754	C	C6-N1-C2	-5.53	118.09	120.30
25	BA	2689	U	N3-C4-O4	-5.52	115.53	119.40
25	CA	1968	G	OP2-P-O3'	5.52	117.34	105.20
25	BA	1214	A	O5'-P-OP2	-5.51	100.74	105.70
26	CB	3089	U	N3-C2-O2	-5.51	118.34	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	195	A	C8-N9-C4	-5.51	103.60	105.80
16	DP	6	LEU	CA-CB-CG	5.51	127.96	115.30
25	BA	228	C	N3-C2-O2	-5.50	118.05	121.90
25	BA	2070	A	OP2-P-O3'	5.50	117.30	105.20
25	BA	528	A	C8-N9-C4	-5.50	103.60	105.80
25	CA	2011	U	N3-C2-O2	-5.50	118.35	122.20
1	DA	1495	U	N1-C2-O2	5.50	126.65	122.80
25	BA	1784	A	N1-C6-N6	5.49	121.90	118.60
25	CA	271	G	P-O3'-C3'	5.49	126.29	119.70
25	BA	2044	C	N3-C2-O2	5.49	125.74	121.90
25	BA	687	C	OP1-P-OP2	-5.49	111.37	119.60
25	BA	1115	G	O4'-C1'-N9	5.49	112.59	108.20
25	CA	548	G	OP1-P-O3'	5.48	117.25	105.20
25	BA	1478	G	C4-N9-C1'	-5.48	119.38	126.50
25	CA	1771	C	OP2-P-O3'	5.47	117.23	105.20
25	CA	1343	G	C6-C5-N7	-5.47	127.12	130.40
25	BA	1256	G	OP2-P-O3'	5.46	117.22	105.20
25	CA	752	A	C4-C5-N7	5.46	113.43	110.70
25	BA	1011	G	C8-N9-C4	5.46	108.58	106.40
25	BA	1981	A	N1-C6-N6	5.46	121.88	118.60
25	BA	1994	C	C6-N1-C2	5.46	122.48	120.30
32	CH	62	LEU	CA-CB-CG	5.46	127.85	115.30
25	BA	611	C	C6-N1-C2	-5.46	118.12	120.30
25	BA	140	C	C6-N1-C2	-5.45	118.12	120.30
25	BA	779	U	OP1-P-OP2	5.45	127.78	119.60
1	DA	786	G	N1-C6-O6	-5.45	116.63	119.90
25	BA	195	A	C6-N1-C2	-5.45	115.33	118.60
25	BA	140	C	N1-C2-O2	5.45	122.17	118.90
1	DA	1135	U	C2-N1-C1'	5.45	124.24	117.70
25	BA	673	C	N3-C2-O2	-5.45	118.09	121.90
1	AA	1279	G	N7-C8-N9	5.43	115.82	113.10
25	BA	2601	C	N1-C2-O2	5.43	122.16	118.90
25	BA	980	A	OP2-P-O3'	5.43	117.14	105.20
25	CA	1675	C	C6-N1-C2	-5.42	118.13	120.30
26	BB	3104	A	N1-C6-N6	5.42	121.85	118.60
25	BA	442	G	C5-C6-O6	-5.41	125.35	128.60
25	BA	1131	G	N1-C2-N2	-5.41	111.33	116.20
1	AA	702	A	P-O3'-C3'	5.41	126.19	119.70
1	DA	530	G	C8-N9-C1'	-5.41	119.97	127.00
1	DA	924	C	O5'-P-OP2	-5.41	100.83	105.70
1	AA	621	A	N9-C4-C5	5.40	107.96	105.80
25	BA	2326	C	N3-C2-O2	-5.40	118.12	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	CA	2587	A	N1-C6-N6	5.39	121.83	118.60
25	BA	1259	G	C5-C6-O6	-5.39	125.37	128.60
25	BA	2024	G	N3-C4-N9	5.39	129.23	126.00
25	CA	846	U	C6-N1-C1'	-5.39	113.66	121.20
25	BA	1916	A	N9-C4-C5	-5.38	103.65	105.80
25	CA	559	G	C5-C6-O6	-5.38	125.37	128.60
25	CA	1896	G	C4-N9-C1'	-5.37	119.52	126.50
25	CA	2311	A	P-O3'-C3'	5.37	126.14	119.70
10	AJ	92	LEU	CA-CB-CG	5.36	127.63	115.30
40	CP	113	LEU	CA-CB-CG	5.36	127.63	115.30
1	DA	1031	C	P-O3'-C3'	5.36	126.13	119.70
4	AD	55	LEU	CA-CB-CG	5.36	127.62	115.30
25	BA	396	G	N1-C6-O6	5.36	123.11	119.90
25	BA	548	G	C8-N9-C4	-5.35	104.26	106.40
25	BA	2237	G	N1-C6-O6	-5.35	116.69	119.90
25	BA	648	G	O5'-P-OP2	-5.35	100.89	105.70
25	BA	1779	U	O4'-C1'-N1	5.35	112.48	108.20
1	DA	1146	A	C8-N9-C4	-5.35	103.66	105.80
25	BA	2591	C	OP1-P-O3'	5.34	116.95	105.20
25	CA	516	C	N3-C2-O2	5.34	125.64	121.90
25	BA	1478	G	N3-C4-C5	5.33	131.27	128.60
41	CQ	5	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	DA	85	U	C2-N1-C1'	5.33	124.09	117.70
25	BA	2213	U	C6-N1-C1'	-5.32	113.75	121.20
25	BA	2437	G	N3-C4-C5	5.32	131.26	128.60
25	BA	2878	U	C5-C4-O4	-5.32	122.71	125.90
25	BA	567	U	OP1-P-OP2	-5.32	111.62	119.60
25	BA	818	G	N3-C4-N9	5.32	129.19	126.00
25	BA	739	A	O5'-P-OP2	-5.32	100.91	105.70
25	BA	776	G	C8-N9-C4	-5.32	104.27	106.40
25	BA	400	G	C6-C5-N7	-5.32	127.21	130.40
25	BA	824	U	OP2-P-O3'	5.31	116.89	105.20
1	AA	1530	G	O4'-C1'-N9	5.31	112.45	108.20
25	BA	1757	A	O5'-P-OP2	-5.31	100.92	105.70
1	DA	1279	G	C8-N9-C4	-5.30	104.28	106.40
25	BA	1026	G	N3-C4-C5	-5.30	125.95	128.60
25	BA	1011	G	C4-N9-C1'	-5.30	119.61	126.50
1	AA	328	C	C2-N1-C1'	5.30	124.63	118.80
25	BA	528	A	C4-C5-N7	5.30	113.35	110.70
25	BA	861	A	N1-C6-N6	-5.30	115.42	118.60
25	BA	1238	G	C8-N9-C4	5.30	108.52	106.40
25	BA	2461	A	C8-N9-C4	5.30	107.92	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DA	1417	G	N1-C6-O6	-5.30	116.72	119.90
1	AA	1243	C	C6-N1-C2	-5.30	118.18	120.30
25	BA	1011	G	C5-C6-O6	-5.30	125.42	128.60
25	CA	2899	A	N1-C6-N6	5.29	121.78	118.60
25	BA	1027	A	N7-C8-N9	5.29	116.45	113.80
1	DA	1361	G	N1-C2-N2	-5.29	111.44	116.20
25	BA	1064	C	C6-N1-C2	-5.28	118.19	120.30
25	BA	1677	A	C8-N9-C4	5.28	107.91	105.80
25	BA	2831	G	C5-C6-O6	-5.28	125.43	128.60
1	DA	699	C	C6-N1-C2	5.28	122.41	120.30
25	BA	2472	G	N3-C4-N9	-5.26	122.84	126.00
1	AA	188	C	C6-N1-C2	-5.26	118.19	120.30
25	CA	2828	G	N3-C4-N9	5.25	129.15	126.00
25	BA	2308	G	C4-N9-C1'	-5.25	119.68	126.50
25	BA	2607	G	N3-C4-C5	-5.25	125.98	128.60
25	BA	1993	U	C2-N1-C1'	-5.24	111.41	117.70
25	BA	783	A	C6-C5-N7	-5.24	128.63	132.30
25	CA	275	C	C6-N1-C2	-5.24	118.20	120.30
25	BA	790	U	C5-C4-O4	5.23	129.04	125.90
25	CA	2823	A	N1-C6-N6	5.23	121.74	118.60
25	BA	511	U	OP2-P-O3'	5.23	116.70	105.20
25	CA	1914	C	C6-N1-C1'	-5.23	114.53	120.80
25	BA	1619	G	O5'-P-OP1	-5.22	101.00	105.70
25	BA	331	C	O5'-P-OP1	-5.22	101.00	105.70
25	BA	2606	C	C5-C4-N4	-5.20	116.56	120.20
25	BA	2753	A	O5'-P-OP1	-5.20	101.02	105.70
25	BA	2831	G	N1-C6-O6	5.20	123.02	119.90
25	BA	2053	G	OP2-P-O3'	5.20	116.63	105.20
25	CA	2684	U	C2-N1-C1'	5.19	123.93	117.70
25	CA	752	A	C2-N3-C4	-5.19	108.00	110.60
25	BA	2447	G	N7-C8-N9	-5.19	110.50	113.10
25	BA	2593	U	N3-C4-C5	5.18	117.71	114.60
4	AD	90	LEU	CA-CB-CG	5.18	127.22	115.30
25	BA	1133	A	C5-C6-N6	5.18	127.85	123.70
25	CA	795	C	C6-N1-C2	-5.18	118.23	120.30
25	CA	784	G	P-O3'-C3'	5.18	125.91	119.70
25	BA	2517	C	N3-C4-C5	5.18	123.97	121.90
25	CA	2580	U	OP2-P-O3'	5.18	116.59	105.20
26	BB	3064	G	C6-C5-N7	5.17	133.50	130.40
25	BA	481	G	O4'-C1'-N9	5.17	112.34	108.20
18	DR	51	TYR	CA-CB-CG	5.17	123.22	113.40
25	CA	1137	G	N3-C4-C5	5.17	131.19	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	2324	U	OP2-P-O3'	5.17	116.56	105.20
25	BA	2527	C	O5'-P-OP1	-5.17	101.05	105.70
25	CA	535	G	C4-N9-C1'	-5.16	119.80	126.50
25	BA	729	G	C4-N9-C1'	5.16	133.20	126.50
25	BA	693	A	O5'-P-OP1	5.15	116.88	110.70
25	BA	853	C	N1-C2-O2	-5.15	115.81	118.90
25	BA	1159	U	OP2-P-O3'	5.15	116.53	105.20
25	BA	1779	U	C5-C6-N1	-5.15	120.12	122.70
25	BA	2064	C	C6-N1-C2	5.15	122.36	120.30
25	BA	2751	G	C6-C5-N7	-5.15	127.31	130.40
38	CN	101	GLY	N-CA-C	5.14	125.96	113.10
25	BA	1660	G	N3-C4-N9	-5.14	122.91	126.00
25	CA	2162	G	P-O3'-C3'	5.14	125.87	119.70
25	CA	2642	G	OP2-P-O3'	5.14	116.50	105.20
25	BA	783	A	N7-C8-N9	5.14	116.37	113.80
25	BA	2041	U	C5-C4-O4	-5.14	122.82	125.90
25	BA	2275	C	C6-N1-C2	-5.14	118.25	120.30
25	CA	2590	A	OP2-P-O3'	5.13	116.50	105.20
25	BA	2059	A	C5-C6-N6	-5.13	119.59	123.70
1	DA	1361	G	N3-C2-N2	5.13	123.49	119.90
25	BA	2590	A	O5'-P-OP2	-5.12	101.09	105.70
25	CA	1936	A	N1-C2-N3	5.12	131.86	129.30
25	CA	2308	G	C4-C5-N7	5.12	112.85	110.80
25	CA	1606	C	N1-C2-O2	5.11	121.97	118.90
25	BA	2483	C	N3-C4-N4	5.11	121.58	118.00
25	BA	1128	G	C8-N9-C1'	5.10	133.63	127.00
25	CA	2440	C	N1-C2-O2	5.10	121.96	118.90
25	BA	2671	G	N3-C4-C5	5.10	131.15	128.60
25	BA	1007	C	C6-N1-C2	5.10	122.34	120.30
25	BA	2281	A	C2-N3-C4	-5.10	108.05	110.60
25	BA	2626	C	N3-C4-C5	5.09	123.94	121.90
25	CA	1377	G	C8-N9-C4	-5.08	104.37	106.40
25	BA	1142	A	N3-C4-N9	-5.08	123.33	127.40
25	CA	984	A	N1-C6-N6	5.08	121.65	118.60
25	BA	1414	C	C6-N1-C2	-5.07	118.27	120.30
25	BA	2603	G	C4-C5-N7	5.07	112.83	110.80
25	BA	1420	A	P-O3'-C3'	5.07	125.79	119.70
25	CA	751	A	N1-C6-N6	-5.07	115.56	118.60
25	BA	974	G	O4'-C1'-N9	5.06	112.25	108.20
25	BA	2671	G	N3-C4-N9	-5.06	122.96	126.00
25	CA	1923	U	OP2-P-O3'	5.06	116.34	105.20
25	BA	1167	C	N3-C2-O2	-5.06	118.36	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	CA	2817	U	C5-C4-O4	5.06	128.93	125.90
1	AA	1299	A	P-O3'-C3'	5.06	125.77	119.70
25	CA	1965	C	O5'-P-OP2	-5.06	101.15	105.70
25	BA	181	A	N1-C6-N6	-5.05	115.57	118.60
25	BA	753	A	O5'-P-OP2	-5.05	101.15	105.70
25	BA	1936	A	C5-C6-N1	-5.05	115.17	117.70
25	BA	2545	G	O5'-P-OP2	-5.05	101.16	105.70
1	AA	764	C	C6-N1-C2	-5.04	118.28	120.30
25	BA	2588	G	OP2-P-O3'	5.04	116.29	105.20
1	DA	869	G	N9-C4-C5	-5.04	103.38	105.40
1	AA	1507	A	O5'-P-OP2	-5.03	101.17	105.70
25	BA	2422	C	C6-N1-C2	-5.03	118.29	120.30
25	BA	2627	G	C6-C5-N7	-5.02	127.39	130.40
25	CA	2014	A	OP2-P-O3'	5.02	116.25	105.20
25	BA	1272	A	O5'-P-OP1	-5.02	101.19	105.70
25	CA	1655	A	N1-C6-N6	5.02	121.61	118.60
25	BA	2269	G	N3-C2-N2	5.01	123.41	119.90
25	CA	2619	C	C6-N1-C2	5.01	122.31	120.30
25	BA	20	C	N3-C2-O2	-5.01	118.39	121.90
25	BA	2369	A	N1-C6-N6	5.01	121.61	118.60
25	BA	2597	G	C8-N9-C1'	-5.01	120.48	127.00
25	BA	831	G	C4-C5-N7	5.01	112.80	110.80
25	BA	1695	G	C6-C5-N7	-5.01	127.39	130.40
25	CA	2681	C	C6-N1-C2	5.01	122.30	120.30
25	CA	548	G	C8-N9-C4	-5.00	104.40	106.40
25	BA	645	C	C5-C4-N4	-5.00	116.70	120.20
25	BA	962	G	OP2-P-O3'	5.00	116.20	105.20

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	148	LEU	Peptide
4	AD	18	ASP	Peptide
6	AF	79	ARG	Peptide
7	AG	126	ASP	Peptide
10	AJ	17	LEU	Peptide
10	AJ	91	ASP	Peptide
11	AK	118	HIS	Peptide
14	AN	55	SER	Peptide
14	AN	64	CYS	Peptide
19	AS	4	SER	Peptide

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Mol	Chain	Res	Type	Group
20	AT	67	ILE	Peptide
21	AU	9	ASN	Peptide
27	BC	108	GLY	Peptide
27	BC	11	GLY	Peptide
27	BC	176	ARG	Peptide
28	BD	151	THR	Peptide
30	BF	111	ARG	Peptide
36	BL	102	GLY	Peptide
38	BN	105	GLY	Peptide
44	BT	68	LYS	Peptide
28	CD	1	MET	Peptide
28	CD	151	THR	Peptide
36	CL	112	LEU	Peptide
38	CN	100	CYS	Peptide
40	CP	13	LYS	Peptide
42	CR	1	MET	Peptide
48	CX	31	ASN	Peptide
2	DB	40	ILE	Peptide
4	DD	9	LEU	Peptide
5	DE	110	ALA	Peptide
5	DE	121	HIS	Peptide
9	DI	54	LEU	Peptide
12	DL	23	ALA	Peptide
17	DQ	14	SER	Peptide
20	DT	31	PHE	Peptide
20	DT	68	HIS	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	32995	0	16607	432	1
1	DA	33015	0	16617	426	0
2	AB	1704	0	1732	37	0
2	DB	1704	0	1732	80	0
3	AC	1624	0	1696	45	0
3	DC	1624	0	1696	39	0
4	AD	1643	0	1707	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	DD	1643	0	1707	117	0
5	AE	1105	0	1148	32	0
5	DE	1105	0	1148	53	0
6	AF	817	0	808	20	0
6	DF	817	0	808	22	0
7	AG	1181	0	1238	78	0
7	DG	1181	0	1238	25	0
8	AH	979	0	1031	34	0
8	DH	979	0	1031	49	0
9	AI	1022	0	1070	36	0
9	DI	1022	0	1070	46	0
10	AJ	786	0	828	36	0
10	DJ	786	0	828	16	0
11	AK	877	0	887	46	0
11	DK	877	0	887	35	0
12	AL	955	0	1016	47	0
12	DL	955	0	1016	42	0
13	AM	883	0	941	62	0
13	DM	883	0	941	42	0
14	AN	774	0	827	52	0
14	DN	774	0	827	25	0
15	AO	716	0	739	33	0
15	DO	716	0	739	18	0
16	AP	649	0	666	20	0
16	DP	649	0	666	36	0
17	AQ	648	0	691	17	0
17	DQ	648	0	691	15	0
18	AR	455	0	478	20	0
18	DR	455	0	478	15	0
19	AS	637	0	665	38	0
19	DS	637	0	665	26	0
20	AT	665	0	714	15	0
20	DT	665	0	714	20	0
21	AU	425	0	449	24	0
21	DU	425	0	449	35	0
22	AV	1419	0	1465	45	0
23	AW	324	0	162	4	0
23	DV	346	0	173	15	0
24	AX	1623	0	821	20	0
24	DW	1623	0	821	8	0
25	BA	62195	0	31279	791	0
25	CA	62195	0	31280	774	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	BB	2549	0	1291	25	0
26	CB	2529	0	1281	20	0
27	BC	2082	0	2157	64	0
27	CC	2082	0	2157	61	0
28	BD	1565	0	1616	46	0
28	CD	1565	0	1616	31	0
29	BE	1552	0	1619	39	0
29	CE	1552	0	1619	28	0
30	BF	1410	0	1447	53	0
30	CF	1410	0	1447	49	0
31	BG	1323	0	1374	36	0
31	CG	1323	0	1374	22	0
32	BH	1107	0	1139	90	0
32	CH	1107	0	1138	62	1
33	BI	1032	0	1088	17	0
33	CI	1032	0	1088	17	0
34	BJ	1129	0	1162	24	0
34	CJ	1129	0	1162	27	0
35	BK	938	0	1012	31	0
35	CK	938	0	1012	34	0
36	BL	1045	0	1117	35	0
36	CL	1045	0	1117	39	0
37	BM	1074	0	1157	23	0
37	CM	1074	0	1157	24	0
38	BN	960	0	1000	26	0
38	CN	960	0	1000	25	0
39	BO	892	0	922	24	0
39	CO	892	0	923	32	0
40	BP	917	0	965	30	0
40	CP	917	0	965	31	0
41	BQ	947	0	1022	36	0
41	CQ	947	0	1022	35	0
42	BR	816	0	839	25	0
42	CR	816	0	839	24	0
43	BS	857	0	922	25	0
43	CS	857	0	922	22	0
44	BT	738	0	807	37	0
44	CT	738	0	806	31	0
45	BU	779	0	834	25	0
45	CU	779	0	834	32	0
46	BV	753	0	780	18	0
46	CV	753	0	780	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BW	580	0	594	17	0
47	CW	569	0	581	11	0
48	BX	625	0	655	15	0
48	CX	625	0	655	16	0
49	BY	509	0	543	22	0
49	CY	509	0	543	20	0
50	BZ	449	0	491	6	0
50	CZ	449	0	491	11	0
51	B0	444	0	461	15	0
51	C0	444	0	461	10	0
52	B1	409	0	440	8	0
52	C1	409	0	440	5	0
53	B2	377	0	418	9	0
53	C2	377	0	418	8	0
54	B3	504	0	574	38	0
54	C3	504	0	574	11	0
55	B4	302	0	340	13	0
55	C4	302	0	340	4	0
56	B5	1142	0	865	13	0
57	AA	71	0	0	0	0
57	AN	1	0	0	0	0
57	BA	189	0	0	0	0
57	BB	4	0	0	0	0
57	BL	2	0	0	0	0
57	BO	1	0	0	0	0
57	BQ	1	0	0	0	0
57	CA	165	0	0	0	0
57	CB	3	0	0	0	0
57	CD	1	0	0	0	0
57	CQ	1	0	0	0	0
57	DA	53	0	0	0	0
57	DD	2	0	0	0	0
57	DN	1	0	0	0	0
58	AA	42	45	45	9	0
58	BA	210	180	225	33	0
58	CA	210	135	224	51	0
58	DA	84	90	90	13	0
59	B4	1	0	0	0	0
59	C4	1	0	0	0	0
60	AA	192	0	0	17	0
60	AE	3	0	0	0	0
60	AL	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	AN	2	0	0	1	0
60	AT	5	0	0	0	0
60	B3	1	0	0	0	0
60	B4	1	0	0	0	0
60	BA	626	0	0	92	0
60	BB	14	0	0	3	0
60	BC	7	0	0	0	0
60	BD	2	0	0	1	0
60	BE	1	0	0	0	0
60	BF	1	0	0	0	0
60	BL	8	0	0	4	0
60	BN	2	0	0	0	0
60	BQ	1	0	0	0	0
60	BS	1	0	0	0	0
60	BT	3	0	0	2	0
60	C3	1	0	0	0	0
60	C4	2	0	0	0	0
60	CA	608	0	0	82	0
60	CB	14	0	0	3	0
60	CC	10	0	0	1	0
60	CD	5	0	0	1	0
60	CE	3	0	0	0	0
60	CJ	2	0	0	2	0
60	CL	7	0	0	0	0
60	CN	2	0	0	0	0
60	CT	3	0	0	1	0
60	CU	1	0	0	0	0
60	DA	184	0	0	22	0
60	DD	2	0	0	1	0
60	DK	2	0	0	0	0
60	DL	2	0	0	0	0
60	DN	4	0	0	2	0
60	DT	3	0	0	0	0
60	DU	1	0	0	0	0
All	All	294034	450	196884	4955	1

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 (4955) 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)
7:AG:103:TRP:CE2	7:AG:103:TRP:CZ2	1.76	1.63
7:AG:103:TRP:CH2	7:AG:103:TRP:CZ3	1.85	1.61
7:AG:100:ALA:HA	7:AG:103:TRP:CD2	1.52	1.44
7:AG:103:TRP:CZ3	7:AG:103:TRP:CE3	2.06	1.44
32:BH:124:THR:HG21	32:BH:128:HIS:NE2	1.32	1.44
7:AG:100:ALA:C	7:AG:103:TRP:CZ3	1.99	1.35
7:AG:100:ALA:CA	7:AG:103:TRP:CZ3	2.08	1.35
25:BA:1861:G:O6	58:BA:3005:PAR:C61	1.77	1.33
32:CH:90:LEU:HG	32:CH:123:ARG:CA	1.60	1.32
25:BA:1861:G:O6	58:BA:3005:PAR:H611	1.20	1.27
7:AG:100:ALA:C	7:AG:103:TRP:CH2	2.08	1.27
7:AG:100:ALA:CA	7:AG:103:TRP:CE3	2.19	1.26
7:AG:100:ALA:CA	7:AG:103:TRP:CH2	2.19	1.26
25:CA:1859:U:O4	58:CA:3168:PAR:N12	1.69	1.26
25:BA:139:U:O4	44:BT:2:ILE:HG12	1.33	1.25
25:CA:538:A:C8	58:CA:3169:PAR:N64	2.05	1.24
7:AG:100:ALA:C	7:AG:103:TRP:CE3	2.11	1.23
7:AG:100:ALA:C	7:AG:103:TRP:CZ2	2.13	1.23
25:BA:144:A:O2'	44:BT:3:ARG:NH2	1.73	1.21
25:CA:139:U:C2	44:CT:2:ILE:HD11	1.76	1.20
32:BH:124:THR:CG2	32:BH:128:HIS:CE1	2.23	1.20
7:AG:100:ALA:HA	7:AG:103:TRP:CE3	1.77	1.18
25:CA:508:A:OP1	58:CA:3170:PAR:H641	1.42	1.17
32:CH:94:ILE:H	32:CH:122:LEU:CB	1.56	1.16
7:AG:100:ALA:CA	7:AG:103:TRP:CE2	2.30	1.15
1:DA:1420:U:O4	58:DA:1655:PAR:H222	1.44	1.14
25:BA:1860:G:N7	58:BA:3005:PAR:O41	1.82	1.12
7:AG:100:ALA:C	7:AG:103:TRP:CE2	2.23	1.12
7:AG:100:ALA:CA	7:AG:103:TRP:CD2	2.31	1.12
7:AG:100:ALA:CA	7:AG:103:TRP:CZ2	2.33	1.12
7:AG:101:MET:N	7:AG:103:TRP:CZ3	2.18	1.10
32:BH:124:THR:HG21	32:BH:128:HIS:CE1	1.85	1.10
44:CT:1:MET:HG2	44:CT:2:ILE:HG13	1.11	1.10
7:AG:100:ALA:N	7:AG:103:TRP:CZ3	2.20	1.09
32:CH:90:LEU:CG	32:CH:123:ARG:HA	1.83	1.09
32:BH:124:THR:CG2	32:BH:128:HIS:NE2	2.15	1.08
7:AG:100:ALA:C	7:AG:103:TRP:CD2	2.27	1.08
25:CA:492:A:OP2	58:CA:3170:PAR:N12	1.86	1.07
32:CH:90:LEU:HD23	32:CH:123:ARG:O	1.55	1.07
32:BH:124:THR:HG22	32:BH:128:HIS:CE1	1.84	1.07
25:CA:538:A:N7	58:CA:3169:PAR:N64	2.02	1.07
25:BA:139:U:O4	44:BT:2:ILE:CG1	2.03	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:CT:2:ILE:HG22	44:CT:4:GLU:H	0.90	1.04
25:BA:1861:G:N7	58:BA:3005:PAR:H612	1.73	1.04
25:BA:1861:G:C6	58:BA:3005:PAR:C61	2.41	1.03
1:DA:1480:A:H61	58:DA:1655:PAR:H221	1.20	1.03
25:BA:943:A:OP2	36:BL:39:LYS:NZ	1.92	1.03
25:CA:2673:G:H5'	58:CA:3166:PAR:O53	1.58	1.02
7:AG:100:ALA:CB	7:AG:103:TRP:CZ2	2.41	1.02
44:CT:2:ILE:HG22	44:CT:4:GLU:N	1.73	1.01
44:BT:3:ARG:O	44:BT:5:GLU:N	1.91	1.01
25:CA:139:U:O2	44:CT:2:ILE:HD11	1.59	1.01
25:CA:947:A:HO2'	25:CA:984:A:H2	1.11	0.99
25:BA:144:A:H1'	44:BT:3:ARG:NH1	1.78	0.98
25:BA:144:A:H1'	44:BT:3:ARG:HH12	1.28	0.98
1:DA:547:A:OP1	4:DD:70:ARG:NH1	1.95	0.97
1:AA:1494:G:N7	58:AA:1672:PAR:N32	2.13	0.97
25:BA:192:C:OP1	60:BA:3745:HOH:O	1.82	0.97
58:CA:3169:PAR:H11	58:CA:3169:PAR:O52	1.61	0.97
25:CA:731:C:OP2	60:CA:3689:HOH:O	1.81	0.97
32:CH:121:VAL:HG13	32:CH:122:LEU:H	1.30	0.97
7:AG:100:ALA:HA	7:AG:103:TRP:CE2	1.96	0.96
32:BH:119:ASN:O	32:BH:121:VAL:N	1.98	0.95
25:BA:783:A:OP2	60:BA:3312:HOH:O	1.84	0.94
25:BA:1882:U:O4	58:BA:3005:PAR:O31	1.85	0.94
7:AG:101:MET:N	7:AG:103:TRP:CH2	2.34	0.94
25:BA:510:C:OP1	60:BA:3774:HOH:O	1.86	0.94
1:DA:1420:U:O4	58:DA:1655:PAR:C22	2.15	0.93
25:BA:1257:C:OP1	29:BE:67:ARG:NH2	2.03	0.92
56:B5:136:LEU:O	56:B5:139:ASN:N	2.02	0.92
32:CH:90:LEU:HG	32:CH:123:ARG:HA	0.94	0.92
44:CT:1:MET:HG2	44:CT:2:ILE:CG1	1.98	0.92
21:DU:21:ARG:NH2	23:DV:4:G:N3	2.17	0.92
25:CA:2673:G:C5'	58:CA:3166:PAR:O53	2.18	0.92
36:BL:93:ASN:O	36:BL:95:LEU:N	2.02	0.91
7:AG:100:ALA:O	7:AG:103:TRP:CE2	2.21	0.91
25:CA:2589:A:OP1	60:CA:3312:HOH:O	1.89	0.91
25:BA:1009:A:OP2	60:BA:3784:HOH:O	1.88	0.91
7:AG:100:ALA:HB1	7:AG:103:TRP:CZ2	2.05	0.91
32:CH:90:LEU:CG	32:CH:123:ARG:CA	2.43	0.90
25:CA:550:C:OP2	58:CA:3169:PAR:O62	1.88	0.90
25:BA:1010:A:OP2	60:BA:3784:HOH:O	1.88	0.90
32:CH:122:LEU:O	32:CH:124:THR:N	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:999:U:OP2	60:BA:3359:HOH:O	1.90	0.89
1:AA:1080:A:OP1	5:AE:52:LYS:NZ	2.05	0.88
25:BA:1860:G:O6	58:BA:3005:PAR:H41	1.73	0.88
9:AI:38:TYR:OH	9:AI:75:GLN:OE1	1.92	0.88
13:AM:85:CYS:SG	13:AM:86:TYR:N	2.45	0.88
1:DA:1124:G:O2'	1:DA:1145:A:N6	2.06	0.88
7:AG:100:ALA:O	7:AG:103:TRP:CD2	2.27	0.88
25:CA:139:U:N3	44:CT:2:ILE:HD11	1.88	0.88
39:BO:53:THR:O	39:BO:55:GLU:N	2.07	0.88
32:CH:90:LEU:HG	32:CH:123:ARG:N	1.89	0.88
1:AA:1312:G:N7	19:AS:3:ARG:N	2.22	0.87
19:AS:44:MET:SD	19:AS:45:ILE:N	2.47	0.87
25:BA:733:G:N7	60:BA:3293:HOH:O	2.06	0.87
6:DF:77:THR:O	6:DF:79:ARG:N	2.08	0.87
25:BA:1861:G:C6	58:BA:3005:PAR:H611	2.07	0.86
9:DI:35:LEU:O	9:DI:37:GLN:N	2.07	0.86
25:BA:806:C:OP2	36:BL:41:ARG:NH2	2.08	0.86
25:CA:1265:A:OP2	60:CA:3746:HOH:O	1.93	0.86
25:CA:197:A:OP1	60:CA:3758:HOH:O	1.93	0.86
25:BA:2615:U:OP1	60:BA:3754:HOH:O	1.93	0.86
21:DU:16:LEU:O	21:DU:17:ARG:NH1	2.08	0.86
1:AA:410:G:OP1	4:AD:26:ARG:NH2	2.08	0.86
25:BA:1604:C:OP1	60:BA:3408:HOH:O	1.94	0.86
1:AA:1500:A:OP2	60:AA:1877:HOH:O	1.94	0.86
44:BT:3:ARG:C	44:BT:5:GLU:H	1.77	0.86
32:CH:94:ILE:N	32:CH:122:LEU:CB	2.36	0.86
25:CA:1253:A:N7	60:CA:3331:HOH:O	2.07	0.86
32:BH:94:ILE:HD11	32:BH:121:VAL:HG11	1.55	0.86
5:DE:156:LYS:NZ	5:DE:159:LYS:O	2.09	0.86
1:AA:1308:U:O3'	13:AM:87:ARG:NH2	2.09	0.85
32:BH:124:THR:HG21	32:BH:128:HIS:HE2	1.39	0.85
25:CA:1439:A:OP2	60:CA:3629:HOH:O	1.91	0.85
32:CH:121:VAL:HG21	32:CH:128:HIS:CD2	2.11	0.85
25:CA:1338:G:O2'	44:CT:19:LYS:NZ	2.07	0.85
25:BA:1669:A:OP2	60:BA:3727:HOH:O	1.93	0.85
25:BA:2061:G:OP2	60:BA:3494:HOH:O	1.95	0.85
25:BA:58:G:OP1	44:BT:78:SER:OG	1.94	0.85
25:CA:528:A:OP1	60:CA:3247:HOH:O	1.95	0.85
1:DA:599:C:O2'	8:DH:88:ARG:NH2	2.10	0.85
25:BA:2362:C:OP1	54:B3:39:ARG:NH2	2.09	0.85
25:BA:450:G:O6	60:BA:3244:HOH:O	1.95	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:1013:G:OP2	19:DS:17:LYS:NZ	2.09	0.85
1:DA:958:A:OP1	19:DS:55:ARG:NH2	2.09	0.85
32:CH:121:VAL:HG21	32:CH:128:HIS:CG	2.12	0.85
25:CA:2574:G:OP1	60:CA:3708:HOH:O	1.93	0.85
25:CA:450:G:O6	60:CA:3245:HOH:O	1.95	0.85
25:BA:1861:G:O6	58:BA:3005:PAR:O61	1.94	0.84
30:CF:36:ASN:OD1	30:CF:87:LYS:NZ	2.10	0.84
25:BA:544:C:O2'	25:BA:545:U:OP1	1.94	0.84
6:AF:69:GLU:O	6:AF:71:ILE:N	2.11	0.84
25:BA:322:A:OP2	29:BE:162:ARG:NH2	2.11	0.84
25:CA:243:U:OP2	54:C3:7:ARG:NH1	2.09	0.84
24:DW:18:G:O2'	24:DW:57:G:N2	2.10	0.84
9:AI:53:GLU:O	9:AI:55:VAL:N	2.10	0.84
25:CA:1358:G:N7	60:CA:3400:HOH:O	2.10	0.84
25:CA:1799:G:OP1	27:CC:257:ARG:NH2	2.11	0.84
32:BH:123:ARG:NE	32:BH:123:ARG:H	1.76	0.84
20:DT:79:LEU:O	20:DT:83:ILE:N	2.11	0.83
1:AA:181:A:N6	1:AA:195:A:OP2	2.11	0.83
28:BD:140:HIS:NE2	60:BD:301:HOH:O	2.11	0.83
25:BA:459:U:O2'	44:BT:73:ARG:NH1	2.12	0.83
25:CA:2727:A:OP2	58:CA:3166:PAR:H611	1.79	0.83
13:DM:15:ALA:O	13:DM:17:ILE:N	2.11	0.83
32:BH:1:MET:N	32:BH:21:VAL:O	2.12	0.83
25:BA:1602:U:O4	60:BA:3719:HOH:O	1.95	0.83
25:BA:2742:G:O6	60:BA:3798:HOH:O	1.96	0.82
1:DA:964:A:OP1	60:DA:1833:HOH:O	1.96	0.82
8:DH:111:MET:HE3	8:DH:116:ALA:HA	1.61	0.82
25:BA:2707:U:O2	38:BN:71:ARG:NH1	2.11	0.82
25:CA:733:G:N7	60:CA:3297:HOH:O	2.11	0.82
25:BA:1861:G:C5	58:BA:3005:PAR:H612	2.14	0.82
25:CA:539:G:N7	58:CA:3169:PAR:N64	2.27	0.82
25:CA:784:G:OP2	60:CA:3312:HOH:O	1.97	0.82
25:CA:84:A:OP1	45:CU:5:ARG:NH2	2.12	0.82
25:CA:517:C:OP2	51:C0:9:ARG:NH2	2.13	0.82
27:CC:142:ASN:ND2	27:CC:142:ASN:O	2.13	0.82
4:DD:41:HIS:O	4:DD:43:ALA:N	2.12	0.82
25:BA:587:C:OP2	36:BL:21:ARG:NH1	2.14	0.81
5:DE:99:ALA:O	5:DE:122:ASN:ND2	2.13	0.81
25:BA:1921:G:N7	58:BA:3001:PAR:N12	2.29	0.81
25:CA:139:U:O2	44:CT:2:ILE:CD1	2.27	0.81
1:AA:1118:U:O4'	9:AI:106:ARG:NH2	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:CA:508:A:OP1	58:CA:3170:PAR:C64	2.28	0.81
43:BS:25:ARG:NH1	43:BS:74:ILE:O	2.13	0.81
25:CA:2589:A:OP2	60:CA:3314:HOH:O	1.97	0.81
25:CA:1669:A:OP2	60:CA:3721:HOH:O	1.98	0.81
25:CA:1859:U:C4	58:CA:3168:PAR:N12	2.43	0.81
7:DG:127:ALA:O	7:DG:129:GLU:N	2.14	0.81
1:DA:375:U:O2'	16:DP:5:ARG:NH2	2.13	0.81
11:DK:49:GLY:O	11:DK:69:ARG:NH2	2.14	0.81
11:DK:127:ARG:O	21:DU:34:ARG:NH1	2.14	0.80
25:CA:1923:U:O4	58:CA:3167:PAR:N32	2.14	0.80
25:BA:686:U:OP2	60:BA:3721:HOH:O	1.99	0.80
25:CA:2498:C:OP2	60:CA:3680:HOH:O	1.97	0.80
25:CA:1824:G:O6	60:CA:3655:HOH:O	2.00	0.80
25:BA:2299:U:OP1	30:BF:70:ARG:NH1	2.14	0.80
25:CA:1010:A:OP2	60:CA:3778:HOH:O	1.97	0.80
25:CA:691:C:OP1	27:CC:216:ARG:NH2	2.14	0.80
1:DA:1505:G:OP2	60:DA:1872:HOH:O	2.00	0.80
1:AA:980:C:OP2	60:AA:1861:HOH:O	1.99	0.80
25:BA:1604:C:OP2	60:BA:3410:HOH:O	1.98	0.80
25:CA:1995:U:OP1	28:CD:128:ARG:NH1	2.14	0.80
25:BA:1827:U:OP2	27:BC:220:ARG:NH1	2.16	0.79
25:CA:2795:C:O2	25:CA:2802:G:N2	2.15	0.79
1:AA:429:U:OP1	4:AD:13:ARG:NH1	2.16	0.79
25:BA:690:G:O3'	27:BC:216:ARG:NH2	2.14	0.79
24:AX:19:G:O2'	24:AX:20:U:OP1	2.00	0.79
32:BH:71:LYS:O	32:BH:73:ASN:N	2.16	0.79
25:BA:1670:C:OP1	60:BA:3435:HOH:O	1.99	0.79
27:CC:259:ASN:O	27:CC:261:ARG:N	2.16	0.79
28:CD:140:HIS:NE2	60:CD:404:HOH:O	2.14	0.79
25:BA:1860:G:O6	58:BA:3005:PAR:C41	2.31	0.79
32:BH:124:THR:HG21	32:BH:128:HIS:CD2	2.18	0.79
25:BA:2720:U:OP1	40:BP:52:ARG:NH2	2.15	0.79
25:BA:572:A:OP2	42:BR:80:ARG:NH2	2.15	0.79
1:DA:1323:G:O2'	1:DA:1362:A:N3	2.16	0.79
3:DC:19:ASN:O	3:DC:40:ARG:NH2	2.15	0.79
25:CA:1393:A:N1	44:CT:19:LYS:NZ	2.31	0.79
49:CY:56:LEU:O	49:CY:58:ASN:N	2.16	0.79
25:BA:2407:A:OP1	60:BA:3568:HOH:O	2.00	0.78
1:DA:536:C:OP1	60:DA:1770:HOH:O	2.00	0.78
1:AA:972:C:OP1	10:AJ:59:LYS:NZ	2.11	0.78
25:CA:1395:A:OP2	60:CA:3408:HOH:O	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:58:GLU:O	7:AG:60:GLU:N	2.16	0.78
55:B4:11:CYS:SG	55:B4:33:HIS:ND1	2.55	0.78
25:BA:600:G:H1'	29:BE:100:MET:HE1	1.65	0.78
25:CA:761:A:OP1	60:CA:3689:HOH:O	2.01	0.78
4:DD:124:MET:SD	4:DD:127:GLY:N	2.56	0.78
1:AA:1054:C:OP2	60:AA:1845:HOH:O	2.02	0.78
1:AA:1408:A:N1	58:AA:1672:PAR:O61	2.16	0.78
25:BA:578:G:OP2	60:BA:3271:HOH:O	2.01	0.78
1:AA:1270:G:HO2'	1:AA:1313:U:HO2'	1.25	0.78
25:BA:2579:C:OP1	60:BA:3544:HOH:O	2.00	0.78
32:BH:62:LEU:O	32:BH:64:ALA:N	2.17	0.77
32:CH:90:LEU:CD2	32:CH:123:ARG:C	2.53	0.77
32:CH:88:GLY:O	32:CH:123:ARG:O	2.01	0.77
4:AD:100:ASN:OD1	4:AD:111:ARG:NH2	2.18	0.77
44:CT:1:MET:HE3	44:CT:2:ILE:HD12	1.64	0.77
4:AD:19:LEU:O	4:AD:21:LEU:N	2.16	0.77
5:AE:25:VAL:O	5:AE:27:GLY:N	2.17	0.77
25:BA:947:A:HO2'	25:BA:984:A:H2	1.32	0.77
25:BA:509:C:O3'	60:BA:3775:HOH:O	2.01	0.77
43:CS:66:ILE:O	43:CS:68:ASP:N	2.17	0.77
25:BA:2589:A:OP1	60:BA:3312:HOH:O	2.01	0.77
25:CA:1670:C:OP2	60:CA:3721:HOH:O	2.01	0.77
25:BA:511:U:OP2	60:BA:3774:HOH:O	2.03	0.77
25:BA:2445:G:OP1	29:BE:69:ARG:NH2	2.18	0.77
1:DA:751:U:OP1	15:DO:17:ARG:NH2	2.18	0.77
1:AA:1147:C:HO2'	9:AI:7:TYR:HH	1.33	0.77
13:AM:54:ASP:O	13:AM:57:ARG:NH1	2.17	0.77
13:DM:77:ILE:O	13:DM:79:ARG:N	2.18	0.77
25:BA:2243:U:OP1	60:BA:3745:HOH:O	2.02	0.76
2:DB:221:VAL:O	2:DB:223:GLU:N	2.18	0.76
1:DA:1048:G:OP2	60:DA:1883:HOH:O	2.03	0.76
25:BA:2683:C:OP1	40:BP:50:ARG:NH2	2.18	0.76
44:CT:1:MET:CE	44:CT:2:ILE:HD12	2.14	0.76
25:BA:2017:U:OP2	60:BA:3273:HOH:O	2.04	0.76
25:BA:2594:C:N4	60:BA:3795:HOH:O	2.17	0.76
32:CH:90:LEU:CD2	32:CH:123:ARG:O	2.32	0.76
25:CA:491:G:O6	43:CS:49:LYS:NZ	2.18	0.76
32:BH:82:SER:OG	32:BH:83:LYS:N	2.16	0.76
20:DT:3:ASN:O	20:DT:5:LYS:N	2.18	0.76
1:AA:1095:U:OP2	60:AA:1851:HOH:O	2.03	0.76
25:BA:1420:A:O2'	25:BA:1421:G:O5'	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:739:A:N1	60:BA:3300:HOH:O	2.18	0.76
44:BT:69:ARG:NH2	60:BT:201:HOH:O	2.19	0.76
1:DA:1181:G:O2'	1:DA:1182:G:N7	2.18	0.76
1:AA:1147:C:O2	9:AI:18:ARG:NH1	2.17	0.76
1:AA:451:A:OP2	16:AP:70:ARG:NH2	2.19	0.76
26:BB:3031:C:O2	26:BB:3053:A:N6	2.17	0.76
31:BG:103:ASN:ND2	31:BG:113:ASP:OD1	2.19	0.76
25:CA:250:G:OP2	54:C3:12:ARG:NH1	2.19	0.76
4:DD:185:LYS:O	4:DD:187:GLU:N	2.19	0.76
25:BA:2758:A:O4'	60:BA:3821:HOH:O	2.04	0.75
25:CA:730:A:OP2	60:CA:3689:HOH:O	2.04	0.75
1:DA:980:C:O2'	14:DN:59:ARG:NH1	2.19	0.75
9:AI:25:ASN:O	9:AI:60:LYS:N	2.20	0.75
18:AR:28:THR:O	18:AR:30:LYS:N	2.20	0.75
25:BA:2017:U:OP1	60:BA:3269:HOH:O	2.03	0.75
25:BA:1861:G:C5	58:BA:3005:PAR:C61	2.69	0.75
25:BA:787:C:OP1	60:BA:3760:HOH:O	2.05	0.75
32:CH:90:LEU:CG	32:CH:123:ARG:N	2.48	0.75
25:BA:948:C:O2	25:BA:984:A:O2'	2.04	0.75
25:CA:1986:C:OP1	60:CA:3428:HOH:O	2.04	0.75
13:AM:24:GLY:O	13:AM:29:ARG:NH1	2.20	0.75
14:AN:64:CYS:O	14:AN:83:LYS:NZ	2.19	0.75
25:BA:2615:U:OP1	60:BA:3753:HOH:O	2.04	0.75
36:CL:74:THR:OG1	36:CL:75:ALA:N	2.19	0.75
12:AL:24:LEU:O	12:AL:26:ALA:N	2.18	0.75
47:BW:9:ARG:O	47:BW:12:ARG:NH2	2.19	0.75
25:BA:1064:C:N4	25:BA:1070:A:OP1	2.19	0.75
25:BA:945:A:OP2	60:BA:3347:HOH:O	2.04	0.75
25:CA:474:G:O6	60:CA:3212:HOH:O	2.04	0.75
15:DO:46:HIS:O	15:DO:48:LYS:N	2.19	0.75
1:DA:1500:A:OP2	60:DA:1873:HOH:O	2.04	0.75
32:BH:40:THR:O	32:BH:42:LYS:N	2.21	0.74
14:DN:32:ASP:O	14:DN:34:ASN:ND2	2.19	0.74
25:BA:1417:C:HO2'	25:BA:1587:G:HO2'	1.30	0.74
1:DA:1421:G:O6	58:DA:1655:PAR:N32	2.21	0.74
4:DD:170:TRP:NE1	4:DD:184:ARG:O	2.21	0.74
4:DD:70:ARG:O	4:DD:74:ASN:ND2	2.20	0.74
13:AM:65:VAL:O	13:AM:67:GLY:N	2.20	0.74
28:BD:101:PHE:O	28:BD:103:ASP:N	2.21	0.74
25:CA:324:A:N6	25:CA:338:G:O2'	2.19	0.74
30:CF:100:GLU:O	30:CF:102:LEU:N	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:CA:877:A:O2'	25:CA:900:A:N6	2.20	0.74
1:AA:386:C:H2'	1:AA:387:U:H5'	1.69	0.74
25:CA:1603:A:OP1	60:CA:3407:HOH:O	2.05	0.74
25:CA:2094:A:OP1	32:CH:22:LYS:NZ	2.17	0.74
16:DP:79:ASN:ND2	16:DP:82:ALA:O	2.21	0.74
1:AA:553:A:O2'	12:AL:26:ALA:O	2.06	0.73
2:AB:89:GLN:OE1	2:AB:90:PHE:N	2.21	0.73
15:AO:13:SER:O	15:AO:15:PHE:N	2.20	0.73
32:BH:62:LEU:O	32:BH:65:ALA:N	2.21	0.73
49:BY:51:ALA:O	49:BY:55:THR:OG1	2.04	0.73
25:CA:1722:A:OP2	25:CA:1737:G:N2	2.20	0.73
14:DN:3:GLN:NE2	60:DN:303:HOH:O	2.20	0.73
25:CA:996:A:OP2	41:CQ:92:LYS:NZ	2.21	0.73
25:BA:512:G:N7	60:BA:3774:HOH:O	2.21	0.73
60:BA:3292:HOH:O	29:BE:98:LYS:NZ	2.20	0.73
25:BA:585:G:N7	41:BQ:5:ARG:NH1	2.36	0.73
25:CA:1857:G:N2	25:CA:1884:G:O2'	2.21	0.73
25:CA:761:A:N7	60:CA:3297:HOH:O	2.20	0.73
25:BA:2573:C:OP1	60:BA:3717:HOH:O	2.05	0.73
25:BA:1799:G:O6	27:BC:176:ARG:NH1	2.21	0.73
25:BA:2611:C:OP2	60:BA:3544:HOH:O	2.06	0.73
36:BL:81:ASP:O	36:BL:83:ALA:N	2.20	0.73
34:CJ:111:LYS:NZ	60:CJ:202:HOH:O	2.21	0.73
49:CY:2:LYS:O	49:CY:5:GLU:N	2.21	0.73
7:AG:100:ALA:CB	7:AG:103:TRP:CH2	2.69	0.73
25:BA:2080:A:OP1	48:BX:19:HIS:ND1	2.21	0.73
32:CH:124:THR:HG23	32:CH:128:HIS:NE2	2.04	0.73
7:AG:100:ALA:CA	7:AG:100:ALA:C	2.56	0.73
16:AP:23:ASP:O	16:AP:25:ARG:N	2.22	0.73
25:BA:1269:A:OP2	60:BA:3384:HOH:O	2.05	0.73
25:BA:2588:G:OP1	60:BA:3315:HOH:O	2.06	0.73
1:AA:1499:A:OP2	60:AA:1877:HOH:O	2.06	0.73
38:BN:117:ASP:O	38:BN:119:SER:N	2.22	0.73
25:CA:1268:A:OP1	60:CA:3377:HOH:O	2.06	0.73
32:CH:90:LEU:CD1	32:CH:123:ARG:H	2.01	0.73
58:AA:1672:PAR:H612	25:BA:1913:A:N1	2.03	0.73
25:CA:1952:A:OP1	35:CK:44:LYS:NZ	2.21	0.73
32:CH:95:GLY:O	32:CH:97:ARG:N	2.22	0.73
33:CI:17:ALA:O	33:CI:18:ASN:ND2	2.21	0.73
56:B5:134:ARG:O	56:B5:135:GLY:O	2.06	0.73
25:BA:2657:A:O2'	31:BG:159:LYS:NZ	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:137:U:O2'	25:BA:138:U:OP1	2.07	0.72
25:BA:194:G:OP2	60:BA:3765:HOH:O	2.06	0.72
25:BA:2484:G:OP1	37:BM:44:ARG:NH2	2.22	0.72
58:CA:3169:PAR:C11	58:CA:3169:PAR:O52	2.35	0.72
2:AB:154:MET:SD	2:AB:155:GLY:N	2.61	0.72
25:BA:826:U:OP1	60:BA:3703:HOH:O	2.07	0.72
26:BB:3057:A:OP2	60:BB:3301:HOH:O	2.07	0.72
9:AI:57:MET:O	9:AI:59:GLU:N	2.22	0.72
45:BU:85:ARG:NH1	45:BU:99:SER:O	2.22	0.72
25:CA:1845:G:OP1	27:CC:255:LYS:NZ	2.16	0.72
58:CA:3166:PAR:N21	58:CA:3166:PAR:H531	2.03	0.72
17:AQ:19:LYS:NZ	17:AQ:49:GLU:OE2	2.20	0.72
13:AM:104:THR:OG1	13:AM:105:ASN:N	2.23	0.72
25:CA:1009:A:OP2	60:CA:3778:HOH:O	2.07	0.72
25:CA:1921:G:O6	58:CA:3167:PAR:N12	2.23	0.72
25:BA:250:G:OP2	54:B3:12:ARG:NH1	2.23	0.72
17:DQ:49:GLU:O	17:DQ:51:ASN:N	2.23	0.72
25:CA:774:G:OP1	27:CC:47:ARG:NH1	2.23	0.72
32:CH:120:GLY:O	32:CH:121:VAL:C	2.28	0.72
44:CT:69:ARG:NH2	60:CT:201:HOH:O	2.22	0.72
2:DB:58:ASN:ND2	2:DB:223:GLU:OE2	2.22	0.72
25:CA:1604:C:OP1	60:CA:3404:HOH:O	2.05	0.72
25:CA:2387:U:O2'	47:CW:39:ARG:NH1	2.23	0.72
1:DA:689:C:OP1	11:DK:46:THR:OG1	2.06	0.72
25:BA:1861:G:N7	58:BA:3005:PAR:C61	2.52	0.71
28:CD:86:GLU:O	28:CD:88:GLU:N	2.23	0.71
21:DU:26:ALA:HB3	23:DV:5:A:H5''	1.71	0.71
1:AA:939:G:O3'	7:AG:102:ARG:NH2	2.24	0.71
22:AV:112:LYS:O	22:AV:114:LEU:N	2.23	0.71
25:CA:2483:C:O2	37:CM:123:LYS:NZ	2.23	0.71
44:CT:1:MET:CG	44:CT:2:ILE:HG13	2.06	0.71
2:AB:86:SER:O	2:AB:88:ASP:N	2.22	0.71
40:CP:105:LYS:O	40:CP:108:ARG:NH2	2.22	0.71
6:DF:91:ARG:O	6:DF:92:THR:OG1	2.09	0.71
1:AA:1309:G:OP1	13:AM:87:ARG:NH1	2.23	0.71
25:BA:2243:U:OP1	60:BA:3748:HOH:O	2.09	0.71
25:BA:2313:C:O4'	30:BF:36:ASN:ND2	2.23	0.71
25:CA:1061:U:OP1	33:CI:9:LYS:NZ	2.16	0.71
25:CA:192:C:OP1	60:CA:3738:HOH:O	2.08	0.71
25:CA:2406:A:O5'	36:CL:69:ARG:NH2	2.23	0.71
3:DC:114:LYS:NZ	3:DC:183:ASP:OD2	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1371:G:N7	60:BA:3402:HOH:O	2.22	0.71
26:BB:3008:C:O3'	39:BO:25:ARG:NH1	2.24	0.71
1:AA:110:C:O2'	16:AP:25:ARG:O	2.07	0.71
54:B3:30:HIS:O	54:B3:32:LEU:N	2.24	0.71
25:CA:1922:G:O6	58:CA:3167:PAR:H221	1.91	0.71
25:CA:2056:G:OP2	60:CA:3487:HOH:O	2.07	0.71
25:CA:2285:C:OP2	52:C1:5:ARG:NH2	2.23	0.71
4:DD:146:ARG:O	4:DD:150:LYS:NZ	2.18	0.71
9:DI:86:ALA:O	9:DI:88:MET:N	2.24	0.71
1:AA:544:G:OP1	4:AD:59:GLN:NE2	2.22	0.71
9:AI:57:MET:SD	9:AI:58:VAL:N	2.64	0.71
25:CA:2115:G:O2'	25:CA:2166:U:O2	2.07	0.71
45:CU:15:GLY:O	45:CU:17:ASP:N	2.24	0.71
1:DA:259:G:OP2	60:DA:1724:HOH:O	2.08	0.71
1:DA:518:C:OP2	1:DA:530:G:O2'	2.07	0.71
19:DS:76:PRO:O	19:DS:78:ARG:N	2.24	0.71
1:AA:1224:U:O2'	1:AA:1322:C:OP1	2.09	0.70
25:BA:144:A:O2'	44:BT:3:ARG:CZ	2.38	0.70
2:DB:207:ILE:O	2:DB:209:ALA:N	2.23	0.70
18:DR:25:ASP:O	18:DR:27:ALA:N	2.24	0.70
2:AB:67:ILE:O	2:AB:89:GLN:NE2	2.24	0.70
4:AD:58:LYS:HZ3	4:AD:203:LEU:CB	2.04	0.70
27:CC:196:ASN:O	27:CC:198:GLU:N	2.23	0.70
1:DA:1095:U:OP2	60:DA:1847:HOH:O	2.09	0.70
25:BA:1440:U:O4	60:BA:3636:HOH:O	2.10	0.70
1:AA:702:A:N6	25:BA:1847:A:OP1	2.23	0.70
58:BA:3005:PAR:H21	58:BA:3005:PAR:O53	1.90	0.70
1:DA:978:A:OP1	1:DA:1362:A:N6	2.24	0.70
5:AE:41:ASP:OD1	5:AE:43:ASN:N	2.25	0.70
10:AJ:5:ARG:N	10:AJ:76:ILE:O	2.25	0.70
25:BA:1268:A:OP1	60:BA:3381:HOH:O	2.08	0.70
25:CA:273:G:N2	25:CA:365:U:O2	2.24	0.70
25:BA:1827:U:O2'	25:BA:1970:A:N3	2.24	0.70
45:BU:85:ARG:NH2	45:BU:87:GLU:OE2	2.23	0.70
4:AD:10:LYS:O	4:AD:14:ARG:N	2.25	0.70
11:AK:46:THR:O	11:AK:50:SER:OG	2.10	0.70
2:DB:21:ARG:O	2:DB:23:TRP:N	2.25	0.70
3:AC:40:ARG:O	3:AC:44:THR:OG1	2.09	0.70
11:AK:125:LYS:HA	21:AU:35:ARG:HE	1.55	0.70
25:BA:1817:G:OP1	27:BC:86:ARG:NH2	2.25	0.70
32:BH:90:LEU:O	32:BH:92:GLY:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:CA:675:A:OP1	29:CE:58:LYS:NZ	2.24	0.70
33:CI:108:ILE:O	33:CI:110:GLN:N	2.25	0.70
1:AA:405:U:OP2	4:AD:3:ARG:NH2	2.25	0.70
1:AA:558:G:OP1	60:AA:1728:HOH:O	2.09	0.70
41:CQ:39:ILE:HD11	42:CR:77:PHE:CG	2.26	0.70
48:CX:51:SER:OG	48:CX:52:ALA:N	2.20	0.70
5:DE:41:ASP:OD1	5:DE:43:ASN:N	2.25	0.70
25:BA:818:G:OP2	60:BA:3583:HOH:O	2.09	0.69
32:BH:117:LEU:HD11	32:BH:121:VAL:HG23	1.71	0.69
25:CA:993:G:OP1	41:CQ:49:ARG:NH2	2.24	0.69
25:CA:1001:A:OP2	60:CA:3734:HOH:O	2.08	0.69
25:CA:1921:G:N7	58:CA:3167:PAR:N12	2.40	0.69
11:AK:75:LYS:NZ	11:AK:79:ILE:O	2.25	0.69
25:BA:1014:A:OP2	60:BA:3607:HOH:O	2.10	0.69
25:BA:1901:A:OP2	27:BC:252:LYS:NZ	2.24	0.69
25:CA:1359:A:OP1	60:CA:3615:HOH:O	2.10	0.69
25:CA:2375:G:N2	25:CA:2378:A:OP2	2.22	0.69
20:DT:26:SER:O	20:DT:30:THR:OG1	2.10	0.69
1:AA:8:A:N6	4:AD:202:GLU:O	2.25	0.69
26:CB:3009:G:OP1	39:CO:25:ARG:NH1	2.26	0.69
25:BA:2057:G:OP2	60:BA:3488:HOH:O	2.10	0.69
25:CA:422:A:OP2	60:CA:3559:HOH:O	2.10	0.69
12:AL:101:ALA:O	12:AL:103:ASP:N	2.25	0.69
1:AA:980:C:O3'	14:AN:12:ARG:NH2	2.26	0.69
1:DA:1480:A:N6	58:DA:1655:PAR:H221	2.01	0.69
25:CA:2732:G:O6	58:CA:3166:PAR:H641	1.93	0.69
25:CA:605:G:O6	60:CA:3292:HOH:O	2.10	0.69
25:CA:2418:A:O3'	54:C3:40:LYS:NZ	2.26	0.69
32:CH:121:VAL:HG13	32:CH:122:LEU:N	2.04	0.69
39:CO:5:SER:OG	39:CO:6:ALA:N	2.22	0.69
2:DB:83:ALA:O	2:DB:89:GLN:NE2	2.26	0.69
1:AA:79:G:O2'	1:AA:80:A:O5'	2.09	0.69
1:AA:1239:A:O2'	7:AG:114:LYS:O	2.08	0.69
26:BB:3045:A:OP1	30:BF:91:ARG:NE	2.26	0.69
30:CF:105:ILE:O	30:CF:109:ARG:NH2	2.26	0.69
1:AA:1366:C:O2'	10:AJ:62:ARG:NH2	2.26	0.69
25:BA:616:A:OP2	60:BA:3291:HOH:O	2.11	0.69
32:BH:122:LEU:CB	32:BH:123:ARG:HA	2.22	0.69
26:CB:3060:C:N4	60:CB:3304:HOH:O	2.25	0.69
1:DA:811:C:O2'	1:DA:901:A:N1	2.26	0.69
9:AI:30:ILE:O	9:AI:32:GLN:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1378:A:O2'	60:BA:3758:HOH:O	2.10	0.69
26:BB:3043:C:O3'	30:BF:94:ARG:NH2	2.26	0.69
8:DH:39:VAL:O	8:DH:41:LYS:N	2.26	0.69
1:AA:1197:A:OP2	60:AA:1847:HOH:O	2.09	0.68
5:AE:77:ASN:O	5:AE:79:GLY:N	2.26	0.68
44:BT:4:GLU:HG2	49:BY:18:LEU:HD11	1.75	0.68
4:DD:150:LYS:O	4:DD:152:GLN:NE2	2.25	0.68
25:BA:1359:A:OP1	60:BA:3620:HOH:O	2.11	0.68
33:BI:42:ASN:OD1	33:BI:50:LYS:NZ	2.26	0.68
38:BN:114:GLU:OE2	38:BN:118:ARG:NH2	2.25	0.68
11:DK:56:ARG:O	11:DK:58:SER:N	2.26	0.68
25:BA:370:G:O2'	25:BA:424:G:OP1	2.10	0.68
1:AA:1241:G:O3'	60:AA:1865:HOH:O	2.10	0.68
2:AB:106:THR:O	2:AB:108:ARG:N	2.26	0.68
3:AC:3:GLN:OE1	3:AC:3:GLN:N	2.26	0.68
45:BU:32:LYS:NZ	45:BU:64:ILE:O	2.26	0.68
25:CA:447:A:OP2	60:CA:3210:HOH:O	2.12	0.68
26:CB:3045:A:O4'	30:CF:91:ARG:NH2	2.26	0.68
26:CB:3057:A:OP2	60:CB:3303:HOH:O	2.09	0.68
58:CA:3169:PAR:H11	58:CA:3169:PAR:C13	2.23	0.68
25:CA:881:G:N2	25:CA:895:U:O2	2.25	0.68
20:DT:78:ASN:O	20:DT:80:THR:N	2.27	0.68
4:AD:170:TRP:O	4:AD:183:LYS:N	2.26	0.68
8:AH:15:ARG:NH1	8:AH:75:ILE:O	2.25	0.68
25:CA:1423:G:N7	60:CA:3628:HOH:O	2.24	0.68
39:CO:5:SER:O	39:CO:7:ARG:N	2.27	0.68
1:AA:1222:G:O6	60:AA:1861:HOH:O	2.09	0.68
7:AG:48:GLU:OE1	7:AG:49:THR:N	2.27	0.68
21:AU:17:ARG:NH2	21:AU:22:SER:OG	2.27	0.68
25:BA:1342:A:OP2	60:BA:3719:HOH:O	2.11	0.68
25:BA:1603:A:OP1	60:BA:3410:HOH:O	2.10	0.68
25:BA:139:U:C4	44:BT:2:ILE:HG12	2.24	0.68
40:CP:8:GLU:O	40:CP:10:GLU:N	2.27	0.68
1:DA:1304:G:OP2	60:DA:1857:HOH:O	2.11	0.68
5:AE:101:GLU:OE1	5:AE:122:ASN:ND2	2.26	0.68
7:AG:127:ALA:O	7:AG:129:GLU:N	2.26	0.68
25:CA:2458:G:O2'	25:CA:2460:U:O4	2.08	0.68
25:CA:77:G:OP1	49:CY:52:ARG:NH2	2.27	0.68
1:DA:1199:U:OP1	60:DA:1833:HOH:O	2.11	0.68
1:AA:878:A:O5'	8:AH:80:ARG:NH2	2.27	0.68
1:DA:267:C:N4	60:DA:1723:HOH:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:101:ASN:ND2	21:AU:13:ASP:OD1	2.26	0.68
25:BA:197:A:OP1	60:BA:3764:HOH:O	2.11	0.68
25:BA:831:G:OP1	60:BL:302:HOH:O	2.11	0.68
25:CA:411:G:OP1	60:CA:3561:HOH:O	2.12	0.68
25:CA:398:C:OP1	48:CX:31:ASN:ND2	2.27	0.68
9:DI:89:GLU:O	9:DI:91:ASP:N	2.27	0.68
2:AB:193:PRO:O	2:AB:195:GLY:N	2.27	0.67
1:DA:741:G:OP1	15:DO:35:GLN:NE2	2.27	0.67
25:BA:2056:G:OP2	60:BA:3491:HOH:O	2.12	0.67
25:BA:2339:C:O3'	26:BB:3041:G:N2	2.28	0.67
25:CA:2615:U:OP1	60:CA:3747:HOH:O	2.12	0.67
25:CA:492:A:P	58:CA:3170:PAR:H122	2.16	0.67
21:DU:37:PHE:O	21:DU:40:LYS:NZ	2.23	0.67
1:AA:427:U:O2'	1:AA:541:G:OP1	2.12	0.67
44:BT:63:VAL:HG21	44:BT:80:TRP:CE2	2.29	0.67
13:AM:111:GLY:O	13:AM:113:ARG:N	2.28	0.67
25:CA:2588:G:OP1	60:CA:3314:HOH:O	2.13	0.67
25:CA:635:C:OP2	36:CL:126:ARG:NH2	2.27	0.67
29:BE:145:ASP:OD1	29:BE:184:ASP:N	2.27	0.67
25:CA:2133:G:O2'	25:CA:2158:A:N6	2.28	0.67
25:CA:2743:U:O2'	31:CG:152:ARG:NH2	2.28	0.67
25:BA:1358:G:N7	60:BA:3402:HOH:O	2.26	0.67
32:BH:116:ARG:NH1	32:BH:131:SER:OG	2.28	0.67
1:DA:652:U:O2'	1:DA:653:U:OP2	2.13	0.67
5:AE:157:ARG:O	5:AE:159:LYS:N	2.27	0.67
52:B1:3:GLY:O	52:B1:5:ARG:N	2.28	0.67
25:BA:1378:A:O2'	60:BA:3756:HOH:O	2.11	0.67
34:BJ:31:GLU:OE2	34:BJ:35:ARG:NH1	2.28	0.67
1:AA:1108:G:O6	60:AA:1853:HOH:O	2.11	0.67
3:AC:40:ARG:NH1	3:AC:55:ILE:O	2.28	0.67
30:BF:60:SER:OG	30:BF:61:GLY:N	2.27	0.67
25:BA:2683:C:O2	35:BK:70:ARG:NH2	2.27	0.67
27:BC:166:ARG:O	27:BC:168:GLY:N	2.28	0.66
1:DA:951:G:HO2'	1:DA:970:C:HO2'	1.39	0.66
4:DD:95:GLU:OE2	4:DD:100:ASN:ND2	2.28	0.66
11:AK:88:GLY:O	11:AK:93:ARG:NH1	2.28	0.66
12:AL:79:VAL:O	12:AL:103:ASP:HB2	1.95	0.66
25:BA:2585:U:O2'	25:BA:2586:U:OP2	2.13	0.66
25:BA:636:G:N2	36:BL:76:GLU:OE2	2.29	0.66
25:CA:2406:A:OP2	60:CA:3560:HOH:O	2.12	0.66
25:CA:512:G:N7	60:CA:3769:HOH:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:66:LEU:O	7:AG:68:ASN:N	2.27	0.66
12:AL:93:VAL:HG22	12:AL:94:ARG:N	2.10	0.66
25:BA:686:U:OP1	53:B2:11:LYS:NZ	2.28	0.66
25:CA:372:G:O2'	25:CA:400:G:O6	2.08	0.66
25:BA:2268:A:OP1	60:BA:3512:HOH:O	2.13	0.66
25:BA:811:U:OP1	60:BA:3337:HOH:O	2.12	0.66
25:CA:999:U:OP2	60:CA:3355:HOH:O	2.13	0.66
1:DA:510:A:OP2	60:DA:1760:HOH:O	2.12	0.66
2:DB:193:PRO:O	2:DB:195:GLY:N	2.28	0.66
14:AN:27:LYS:HA	14:AN:30:ILE:HG12	1.77	0.66
25:BA:1077:A:OP1	33:BI:93:ASN:ND2	2.29	0.66
25:BA:526:A:OP1	60:BA:3246:HOH:O	2.13	0.66
25:BA:784:G:OP1	60:BA:3317:HOH:O	2.13	0.66
1:AA:157:U:O2	1:AA:165:G:N1	2.27	0.66
9:AI:130:ARG:NH1	24:AX:35:A:OP2	2.28	0.66
25:BA:2589:A:OP1	60:BA:3313:HOH:O	2.14	0.66
25:CA:2756:U:OP2	55:C4:19:ARG:NE	2.28	0.66
1:AA:1123:U:O2'	10:AJ:37:ARG:NH2	2.29	0.66
25:CA:2066:C:OP1	60:CA:3503:HOH:O	2.13	0.66
36:CL:132:ARG:NH1	36:CL:136:GLU:OE2	2.29	0.66
7:DG:23:LEU:O	7:DG:27:VAL:N	2.29	0.66
1:DA:107:G:N7	20:DT:10:ARG:NH2	2.41	0.66
25:BA:1998:A:OP2	28:BD:141:ARG:NH2	2.29	0.66
36:CL:123:ARG:O	36:CL:125:LEU:N	2.27	0.66
1:DA:375:U:O3'	16:DP:5:ARG:NH1	2.29	0.66
13:AM:26:GLY:O	13:AM:28:THR:N	2.29	0.66
25:BA:2574:G:OP1	60:BA:3716:HOH:O	2.14	0.66
49:BY:36:GLN:N	49:BY:36:GLN:OE1	2.29	0.66
49:BY:8:GLU:O	49:BY:60:LYS:NZ	2.28	0.66
25:BA:1358:G:O6	60:BA:3405:HOH:O	2.12	0.66
25:BA:2448:A:N1	60:BA:3263:HOH:O	2.28	0.66
25:CA:2819:G:OP1	60:CA:3801:HOH:O	2.13	0.66
9:DI:59:GLU:O	9:DI:61:LEU:N	2.28	0.66
1:AA:1507:A:OP2	11:AK:128:ARG:NH1	2.29	0.65
25:CA:675:A:N3	25:CA:2443:C:O2'	2.28	0.65
32:CH:121:VAL:CG2	32:CH:128:HIS:CD2	2.79	0.65
1:DA:1386:G:N7	60:DA:1861:HOH:O	2.28	0.65
7:DG:22:LEU:O	7:DG:24:ALA:N	2.28	0.65
21:DU:17:ARG:HA	21:DU:17:ARG:CZ	2.26	0.65
1:AA:869:G:N7	60:AA:1818:HOH:O	2.30	0.65
1:AA:1055:A:HO2'	3:AC:193:TYR:HH	1.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:19:ASN:OD1	3:AC:54:ARG:NH1	2.28	0.65
25:CA:2684:U:OP2	40:CP:50:ARG:NH1	2.28	0.65
28:CD:97:SER:O	28:CD:99:GLU:N	2.29	0.65
1:AA:69:G:O6	1:AA:98:A:N6	2.29	0.65
1:AA:22:G:O2'	1:AA:913:A:N1	2.21	0.65
28:BD:121:THR:HB	28:BD:127:PHE:CD2	2.31	0.65
29:BE:21:ARG:N	29:BE:110:SER:OG	2.29	0.65
32:BH:124:THR:HG22	32:BH:125:THR:H	1.62	0.65
25:CA:2061:G:OP2	60:CA:3490:HOH:O	2.13	0.65
1:DA:1032:G:N2	1:DA:1033:G:O4'	2.30	0.65
1:AA:842:U:H3'	1:AA:843:U:H4'	1.78	0.65
2:AB:19:GLN:NE2	2:AB:188:ASP:OD2	2.29	0.65
13:AM:6:GLY:O	13:AM:8:ASN:N	2.30	0.65
1:AA:1307:U:O5'	13:AM:98:ARG:NH2	2.29	0.65
6:AF:21:MET:O	6:AF:23:GLU:N	2.29	0.65
25:BA:2006:C:OP1	60:BA:3381:HOH:O	2.14	0.65
25:BA:2061:G:OP2	60:BA:3493:HOH:O	2.13	0.65
25:BA:2757:A:N1	31:BG:66:THR:HG21	2.12	0.65
25:BA:730:A:OP2	60:BA:3698:HOH:O	2.13	0.65
5:DE:149:SER:O	5:DE:153:VAL:N	2.27	0.65
1:AA:509:A:OP2	60:AA:1758:HOH:O	2.14	0.65
12:AL:87:VAL:HG23	12:AL:93:VAL:HG21	1.77	0.65
1:DA:780:A:OP2	60:DA:1804:HOH:O	2.15	0.65
8:AH:66:PHE:O	8:AH:68:GLY:N	2.30	0.65
25:CA:538:A:H8	58:CA:3169:PAR:N64	1.92	0.65
1:DA:376:G:OP1	16:DP:5:ARG:NH1	2.29	0.65
1:AA:404:G:O2'	1:AA:498:A:N1	2.29	0.65
41:BQ:51:GLN:O	41:BQ:54:ARG:N	2.29	0.65
26:CB:3058:A:OP2	60:CB:3303:HOH:O	2.14	0.65
25:CA:824:U:O4	25:CA:825:A:N6	2.30	0.65
32:CH:90:LEU:HD23	32:CH:123:ARG:C	2.17	0.65
11:DK:79:ILE:O	11:DK:81:ASN:N	2.30	0.65
11:AK:76:GLU:O	11:AK:78:GLY:N	2.30	0.65
56:B5:67:GLY:O	56:B5:69:GLY:N	2.29	0.65
4:AD:78:GLU:OE2	4:AD:81:ARG:NH1	2.29	0.64
27:BC:71:ASP:OD1	27:BC:188:ARG:NH1	2.29	0.64
35:BK:104:THR:OG1	35:BK:106:GLU:OE1	2.13	0.64
25:CA:2134:A:N6	25:CA:2157:G:O2'	2.30	0.64
25:CA:251:A:OP1	36:CL:58:TYR:OH	2.14	0.64
25:BA:1263:U:O2'	51:B0:3:GLN:OE1	2.14	0.64
25:BA:1860:G:C5	58:BA:3005:PAR:O41	2.36	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2614:A:OP2	60:BA:3487:HOH:O	2.14	0.64
7:AG:104:ILE:O	7:AG:107:ALA:N	2.30	0.64
58:BA:3002:PAR:H532	58:BA:3002:PAR:HN61	1.62	0.64
42:CR:24:LYS:NZ	42:CR:26:ASP:OD1	2.30	0.64
4:DD:178:MET:SD	4:DD:179:GLU:N	2.71	0.64
8:DH:70:ALA:O	8:DH:72:VAL:N	2.30	0.64
12:DL:25:GLU:O	12:DL:27:CYS:N	2.30	0.64
16:DP:76:LYS:O	16:DP:79:ASN:N	2.31	0.64
7:AG:107:ALA:HB1	7:AG:133:THR:HG21	1.79	0.64
55:B4:11:CYS:SG	55:B4:33:HIS:CE1	2.91	0.64
25:BA:2310:C:O2'	30:BF:70:ARG:NH2	2.31	0.64
30:CF:164:GLU:N	30:CF:164:GLU:OE1	2.30	0.64
2:DB:99:GLY:O	2:DB:103:ASN:N	2.30	0.64
1:AA:1134:G:N2	1:AA:1140:C:N3	2.44	0.64
25:BA:2211:A:O2'	25:BA:2212:A:OP1	2.15	0.64
25:BA:2269:G:OP1	60:BA:3513:HOH:O	2.14	0.64
25:CA:810:U:OP1	36:CL:29:LYS:NZ	2.30	0.64
25:CA:818:G:OP2	60:CA:3576:HOH:O	2.14	0.64
35:CK:34:GLY:O	35:CK:36:GLY:N	2.31	0.64
25:CA:2876:G:OP1	40:CP:1:SER:N	2.31	0.64
4:DD:70:ARG:NH1	60:DD:402:HOH:O	2.19	0.64
25:BA:965:C:OP2	60:BA:3342:HOH:O	2.15	0.64
25:CA:1013:C:OP2	60:CA:3602:HOH:O	2.15	0.64
25:CA:139:U:O2'	44:CT:1:MET:SD	2.47	0.64
1:AA:1033:G:H2'	1:AA:1034:G:H5'	1.79	0.64
5:DE:157:ARG:O	5:DE:159:LYS:N	2.31	0.64
18:DR:71:THR:OG1	18:DR:72:ASP:N	2.30	0.64
25:BA:1187:G:N2	25:BA:1188:U:O4	2.27	0.64
25:CA:1094:U:O2'	25:CA:1096:A:N7	2.18	0.64
39:CO:80:GLU:O	39:CO:83:LEU:N	2.30	0.64
21:DU:40:LYS:O	21:DU:44:GLU:N	2.31	0.64
9:AI:130:ARG:NH2	24:AX:33:U:OP2	2.30	0.64
25:BA:1779:U:H5	25:BA:1784:A:N7	1.96	0.64
32:BH:123:ARG:HE	32:BH:123:ARG:H	1.45	0.64
47:BW:28:SER:OG	47:BW:29:VAL:N	2.31	0.64
25:CA:2248:C:OP2	60:CA:3505:HOH:O	2.15	0.64
25:CA:570:G:OP1	60:CA:3771:HOH:O	2.16	0.64
1:DA:376:G:H5''	16:DP:5:ARG:NE	2.13	0.64
1:DA:933:G:OP2	7:DG:5:ARG:NH2	2.30	0.64
25:CA:560:C:OP1	60:CA:3251:HOH:O	2.15	0.63
1:AA:1178:G:N2	1:AA:1181:G:OP2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2060:A:O2'	25:BA:2061:G:OP2	2.16	0.63
31:CG:41:GLU:N	31:CG:41:GLU:OE1	2.32	0.63
1:DA:1358:U:O5'	14:DN:75:ARG:NH2	2.31	0.63
1:AA:688:G:O2'	1:AA:704:A:N1	2.25	0.63
25:CA:1722:A:N6	25:CA:1737:G:O2'	2.31	0.63
2:DB:177:ASN:ND2	2:DB:195:GLY:O	2.32	0.63
1:DA:1358:U:OP2	14:DN:75:ARG:CZ	2.47	0.63
25:BA:1654:A:O2'	28:BD:118:PHE:O	2.17	0.63
27:BC:83:ASP:OD2	27:BC:86:ARG:NH1	2.32	0.63
18:AR:29:LEU:O	18:AR:32:TYR:N	2.31	0.63
26:BB:3058:A:OP2	60:BB:3301:HOH:O	2.15	0.63
11:DK:93:ARG:NH2	11:DK:112:ASP:OD2	2.27	0.63
1:AA:1494:G:C8	58:AA:1672:PAR:N32	2.66	0.63
7:AG:133:THR:O	7:AG:136:LYS:NZ	2.31	0.63
12:AL:57:LEU:O	12:AL:59:ASN:N	2.32	0.63
25:BA:2163:A:OP1	25:BA:2170:A:O2'	2.15	0.63
41:BQ:48:ASP:HA	41:BQ:51:GLN:HB2	1.81	0.63
1:DA:1310:G:OP2	13:DM:87:ARG:NH2	2.30	0.63
4:DD:178:MET:HE1	4:DD:179:GLU:HA	1.81	0.63
25:CA:2249:U:O4	60:CA:3506:HOH:O	2.15	0.63
58:CA:3169:PAR:O23	34:CJ:2:LYS:NZ	2.23	0.63
4:AD:58:LYS:HD3	4:AD:203:LEU:HD22	1.80	0.63
25:BA:1992:G:N2	25:BA:1996:C:O2'	2.32	0.63
25:CA:811:U:H2'	36:CL:21:ARG:HA	1.81	0.63
16:AP:79:ASN:ND2	16:AP:82:ALA:O	2.31	0.62
17:AQ:50:ASN:ND2	17:AQ:50:ASN:O	2.32	0.62
25:CA:537:G:OP2	58:CA:3169:PAR:O61	2.15	0.62
4:DD:189:SER:OG	4:DD:190:ASP:N	2.31	0.62
6:DF:25:TYR:O	6:DF:28:ALA:N	2.32	0.62
25:BA:833:A:H2'	25:BA:834:G:C8	2.34	0.62
32:BH:90:LEU:HD21	32:BH:124:THR:H	1.63	0.62
25:CA:226:A:O2'	25:CA:229:C:N4	2.29	0.62
25:CA:861:A:N3	26:CB:3079:G:O2'	2.29	0.62
32:CH:90:LEU:CD2	32:CH:123:ARG:CA	2.77	0.62
7:AG:100:ALA:CB	7:AG:103:TRP:CE2	2.82	0.62
14:AN:32:ASP:O	14:AN:41:ARG:NH2	2.32	0.62
25:BA:2502:G:H5''	25:BA:2503:A:H5''	1.81	0.62
32:BH:91:PHE:O	1:DA:357:G:O2'	2.14	0.62
42:BR:7:SER:O	42:BR:9:GLY:N	2.29	0.62
25:CA:1210:G:H4'	25:CA:1211:C:H5''	1.80	0.62
26:CB:3008:C:OP1	39:CO:29:HIS:NE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:DT:15:GLU:OE2	20:DT:18:ARG:NH1	2.32	0.62
4:AD:58:LYS:HZ3	4:AD:203:LEU:HB2	1.64	0.62
25:BA:1952:A:C6	35:BK:22:ILE:HG12	2.34	0.62
58:BA:3003:PAR:O44	58:BA:3003:PAR:N24	2.30	0.62
25:CA:728:G:O3'	27:CC:12:ARG:NH2	2.32	0.62
1:DA:626:G:OP1	16:DP:35:ARG:NH2	2.33	0.62
25:CA:1064:C:O2'	25:CA:1075:C:O2	2.13	0.62
25:CA:2673:G:H5'	58:CA:3166:PAR:HO53	1.64	0.62
21:DU:33:ARG:NH2	23:DV:6:G:OP1	2.33	0.62
1:AA:430:A:H4'	4:AD:7:PRO:HB3	1.82	0.62
16:AP:18:GLN:OE1	16:AP:35:ARG:NH1	2.33	0.62
36:BL:29:LYS:O	36:BL:31:GLY:N	2.33	0.62
25:CA:1014:A:OP2	60:CA:3602:HOH:O	2.16	0.62
14:DN:24:ALA:O	14:DN:26:LEU:N	2.33	0.62
16:DP:6:LEU:HA	16:DP:19:VAL:HA	1.82	0.62
5:AE:80:THR:OG1	5:AE:98:PRO:O	2.17	0.62
25:CA:1173:U:H2'	25:CA:1174:U:H4'	1.81	0.62
25:CA:1360:G:OP2	60:CA:3614:HOH:O	2.15	0.62
25:CA:509:C:O2'	25:CA:510:C:OP1	2.17	0.62
17:DQ:17:MET:HG2	17:DQ:20:SER:HB2	1.79	0.62
1:AA:590:U:OP1	8:AH:31:LYS:N	2.33	0.62
25:CA:1255:U:O2'	60:CA:3274:HOH:O	2.16	0.62
25:CA:2639:A:O3'	34:CJ:96:ARG:NH2	2.33	0.62
17:AQ:4:LYS:NZ	17:AQ:5:ILE:O	2.28	0.62
25:BA:2355:G:O3'	47:BW:22:LYS:NZ	2.32	0.62
25:BA:2314:A:OP1	30:BF:87:LYS:NZ	2.33	0.62
25:CA:2550:G:OP1	60:CA:3721:HOH:O	2.16	0.62
1:DA:1419:G:O6	58:DA:1655:PAR:N12	2.31	0.62
20:DT:73:ALA:O	20:DT:77:ALA:N	2.32	0.62
14:AN:64:CYS:SG	14:AN:83:LYS:CE	2.88	0.61
36:BL:36:LYS:NZ	60:BL:302:HOH:O	2.11	0.61
25:CA:2674:G:OP2	58:CA:3166:PAR:N21	2.26	0.61
27:CC:132:ARG:NH1	27:CC:186:ASP:OD1	2.33	0.61
38:CN:69:ARG:O	38:CN:71:ARG:N	2.33	0.61
46:CV:34:LYS:N	46:CV:35:GLU:OE2	2.33	0.61
1:DA:1320:C:N3	19:DS:36:ARG:NH1	2.48	0.61
6:AF:70:VAL:O	6:AF:74:LEU:N	2.33	0.61
1:AA:503:C:OP1	12:AL:116:LYS:NZ	2.33	0.61
25:CA:2615:U:OP1	60:CA:3748:HOH:O	2.16	0.61
20:AT:70:ASN:N	20:AT:70:ASN:OD1	2.33	0.61
25:BA:2840:C:H5''	38:BN:53:THR:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BT:3:ARG:C	44:BT:5:GLU:N	2.47	0.61
32:CH:90:LEU:HD11	32:CH:123:ARG:H	1.65	0.61
1:DA:397:A:O2'	1:DA:399:G:OP2	2.18	0.61
1:DA:600:A:P	8:DH:88:ARG:HD2	2.41	0.61
1:AA:878:A:P	8:AH:80:ARG:NH2	2.73	0.61
25:BA:2751:G:OP2	31:BG:2:ARG:NH2	2.34	0.61
25:CA:2872:A:H2'	25:CA:2873:A:H5'	1.83	0.61
25:CA:537:G:OP2	58:CA:3169:PAR:C61	2.48	0.61
25:BA:1072:C:O2	25:BA:1093:G:N1	2.33	0.61
25:BA:819:A:C4	25:BA:1189:A:C2	2.88	0.61
32:BH:88:GLY:HA2	32:BH:125:THR:OG1	2.01	0.61
25:CA:2091:C:H4'	48:CX:55:MET:HE1	1.82	0.61
2:DB:93:ASN:O	2:DB:94:HIS:ND1	2.32	0.61
4:DD:191:LEU:O	4:DD:192:SER:OG	2.10	0.61
1:AA:1288:A:N3	1:AA:1352:C:O2'	2.28	0.61
25:BA:1446:C:N4	60:BA:3642:HOH:O	2.32	0.61
25:BA:2230:G:H1'	48:BX:31:ASN:HB3	1.81	0.61
25:BA:592:A:HO2'	54:B3:63:TYR:HH	1.48	0.61
22:AV:59:THR:OG1	22:AV:60:VAL:N	2.30	0.61
31:BG:21:GLN:NE2	31:BG:40:VAL:O	2.34	0.61
45:BU:35:VAL:HB	45:BU:38:ILE:CG1	2.31	0.61
1:AA:790:A:OP1	24:AX:38:A:O2'	2.15	0.61
25:BA:1119:U:OP1	46:BV:83:LYS:NZ	2.30	0.61
60:BA:3821:HOH:O	31:BG:63:GLN:NE2	2.26	0.61
25:CA:1268:A:OP2	60:CA:3380:HOH:O	2.16	0.61
25:CA:1376:C:OP2	60:CA:3392:HOH:O	2.16	0.61
29:CE:128:ALA:O	29:CE:130:LYS:N	2.33	0.61
32:CH:124:THR:HG23	32:CH:124:THR:O	2.01	0.61
25:BA:1600:C:OP1	44:BT:81:LYS:NZ	2.34	0.61
32:BH:117:LEU:HD22	32:BH:119:ASN:O	2.01	0.61
1:AA:504:C:OP2	60:AA:1768:HOH:O	2.16	0.61
10:AJ:37:ARG:NH1	10:AJ:37:ARG:O	2.34	0.61
16:AP:50:THR:OG1	16:AP:50:THR:O	2.18	0.61
21:AU:20:LYS:O	21:AU:22:SER:N	2.34	0.61
36:BL:99:ASN:ND2	60:BL:307:HOH:O	2.27	0.61
25:BA:1340:U:OP1	44:BT:19:LYS:NZ	2.34	0.61
25:CA:1754:A:N1	25:CA:2716:C:O2'	2.29	0.61
44:CT:2:ILE:O	44:CT:3:ARG:HB2	2.01	0.61
1:AA:1225:A:H2'	1:AA:1226:C:C5	2.36	0.60
14:AN:64:CYS:SG	14:AN:83:LYS:NZ	2.74	0.60
25:CA:1440:U:O4	60:CA:3631:HOH:O	2.12	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:CA:669:G:O2'	25:CA:670:A:OP1	2.18	0.60
25:CA:2262:U:OP1	47:CW:39:ARG:NH1	2.32	0.60
7:DG:24:ALA:O	7:DG:27:VAL:N	2.33	0.60
12:DL:34:CYS:HA	12:DL:55:VAL:HA	1.83	0.60
20:DT:68:HIS:CG	20:DT:69:LYS:HB2	2.36	0.60
25:BA:790:U:OP2	60:BA:3762:HOH:O	2.15	0.60
25:CA:669:G:HO2'	25:CA:670:A:P	2.24	0.60
31:CG:1:SER:OG	31:CG:2:ARG:N	2.34	0.60
35:CK:92:GLU:OE2	35:CK:111:LYS:NZ	2.32	0.60
25:BA:1174:U:O2'	25:BA:1176:U:O2	2.19	0.60
25:BA:998:C:OP2	41:BQ:57:ARG:NH2	2.35	0.60
1:AA:835:U:OP1	18:AR:53:ARG:NH1	2.32	0.60
6:AF:91:ARG:O	6:AF:92:THR:OG1	2.19	0.60
25:BA:784:G:OP2	60:BA:3313:HOH:O	2.15	0.60
26:CB:3011:C:O2'	26:CB:3015:A:N6	2.33	0.60
36:CL:78:ARG:HB2	36:CL:113:ALA:HB2	1.83	0.60
4:DD:34:ILE:O	4:DD:36:GLN:N	2.34	0.60
29:CE:170:ARG:NH1	29:CE:179:SER:OG	2.32	0.60
45:CU:95:PHE:CE1	45:CU:102:ILE:HD13	2.36	0.60
3:DC:73:PRO:O	3:DC:75:ILE:N	2.34	0.60
1:DA:35:G:O2'	12:DL:115:SER:O	2.18	0.60
1:DA:1307:U:OP2	13:DM:98:ARG:NH1	2.34	0.60
1:DA:473:U:OP1	16:DP:76:LYS:NZ	2.33	0.60
20:DT:70:ASN:O	20:DT:74:ARG:N	2.33	0.60
1:AA:135:C:N4	16:AP:1:MET:SD	2.74	0.60
19:AS:13:LEU:O	19:AS:16:LEU:N	2.30	0.60
19:AS:32:ARG:HA	19:AS:50:ALA:HB3	1.83	0.60
25:BA:1066:U:N3	25:BA:1069:A:OP2	2.34	0.60
25:BA:1097:U:O2'	33:BI:7:TYR:O	2.18	0.60
25:BA:2162:G:OP2	25:BA:2164:C:N4	2.35	0.60
29:BE:162:ARG:HE	29:BE:162:ARG:N	2.00	0.60
39:BO:53:THR:OG1	39:BO:54:VAL:N	2.34	0.60
25:CA:1026:G:OP1	60:CA:3705:HOH:O	2.16	0.60
25:CA:322:A:OP1	29:CE:162:ARG:NH2	2.35	0.60
9:DI:49:ARG:O	9:DI:52:LEU:N	2.33	0.60
4:AD:165:ARG:O	4:AD:167:LYS:N	2.34	0.60
25:BA:1266:G:O2'	25:BA:2012:G:O6	2.16	0.60
25:BA:790:U:OP2	60:BA:3760:HOH:O	2.16	0.60
25:CA:15:G:OP2	60:CA:3550:HOH:O	2.16	0.60
16:DP:24:SER:O	16:DP:26:ASN:N	2.35	0.60
1:AA:1422:G:O2'	35:BK:49:ARG:NH2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:101:LEU:O	2:AB:104:TRP:N	2.34	0.60
30:BF:51:ASN:N	30:BF:51:ASN:OD1	2.34	0.60
35:BK:34:GLY:O	35:BK:36:GLY:N	2.35	0.60
25:CA:2119:A:O2'	25:CA:2120:G:O5'	2.18	0.60
1:DA:977:A:OP1	14:DN:61:ARG:NH2	2.35	0.60
2:DB:100:MET:HA	2:DB:107:VAL:HG21	1.83	0.60
8:DH:102:ALA:HB3	8:DH:113:ASP:HB3	1.84	0.60
21:DU:29:LEU:O	21:DU:33:ARG:N	2.34	0.60
4:AD:57:GLU:O	4:AD:59:GLN:N	2.29	0.60
54:B3:31:ILE:HD11	54:B3:35:LYS:CE	2.32	0.60
1:DA:976:G:OP2	1:DA:1358:U:O2'	2.20	0.60
1:DA:319:G:N7	60:DA:1732:HOH:O	2.32	0.60
5:AE:133:PRO:O	5:AE:135:ASN:N	2.33	0.60
25:BA:2236:U:H2'	25:BA:2237:G:O4'	2.02	0.60
44:BT:69:ARG:O	44:BT:71:GLY:N	2.34	0.60
25:CA:2099:U:O2'	25:CA:2190:G:O6	2.20	0.60
1:DA:260:G:N2	1:DA:265:G:N7	2.50	0.60
14:DN:48:LEU:O	14:DN:50:THR:N	2.34	0.60
1:AA:675:A:O2'	11:AK:116:ILE:O	2.20	0.59
14:AN:3:GLN:NE2	60:AN:301:HOH:O	2.35	0.59
25:BA:1199:U:O2'	41:BQ:2:ARG:NH2	2.34	0.59
25:CA:537:G:OP2	58:CA:3169:PAR:H612	2.01	0.59
39:CO:67:ASN:ND2	39:CO:69:ASP:OD1	2.35	0.59
1:DA:401:C:N4	60:DA:1773:HOH:O	2.25	0.59
7:AG:49:THR:O	7:AG:53:ARG:N	2.33	0.59
44:BT:4:GLU:O	44:BT:8:LEU:HD12	2.02	0.59
2:DB:183:VAL:N	2:DB:197:ASP:OD1	2.34	0.59
25:CA:1097:U:N3	33:CI:7:TYR:O	2.36	0.59
25:CA:1450:G:N2	25:CA:1452:G:O6	2.35	0.59
25:CA:85:G:OP2	45:CU:6:ARG:NH2	2.35	0.59
2:DB:73:LYS:O	2:DB:75:ALA:N	2.35	0.59
1:AA:1147:C:O2'	9:AI:7:TYR:OH	2.08	0.59
1:AA:204:G:H3'	1:AA:205:A:H5''	1.85	0.59
13:AM:11:ASP:O	13:AM:13:LYS:N	2.35	0.59
25:BA:2345:G:H4'	25:BA:2346:A:C5'	2.33	0.59
25:BA:2743:U:O2'	31:BG:152:ARG:NH1	2.36	0.59
45:BU:2:ALA:O	45:BU:5:ARG:NH2	2.36	0.59
25:CA:1181:U:H2'	25:CA:1182:G:C8	2.37	0.59
25:CA:2006:C:OP1	60:CA:3377:HOH:O	2.15	0.59
25:CA:455:C:N3	25:CA:472:A:H2'	2.18	0.59
25:CA:997:G:OP1	41:CQ:91:ARG:HG2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:DR:48:ARG:O	18:DR:50:LYS:N	2.36	0.59
4:AD:150:LYS:O	4:AD:152:GLN:N	2.35	0.59
13:AM:98:ARG:NE	13:AM:100:GLN:OE1	2.35	0.59
25:BA:1026:G:OP1	60:BA:3714:HOH:O	2.17	0.59
58:AA:1672:PAR:C61	25:BA:1913:A:H61	2.16	0.59
35:BK:78:ARG:NH1	40:BP:70:GLU:OE2	2.36	0.59
25:CA:2321:U:H3'	25:CA:2322:A:H5''	1.84	0.59
1:AA:858:G:O6	60:AA:1816:HOH:O	2.16	0.59
25:BA:606:U:OP2	29:BE:99:LYS:NZ	2.34	0.59
25:CA:2243:U:OP1	60:CA:3740:HOH:O	2.16	0.59
9:DI:123:ARG:HB2	9:DI:123:ARG:NH1	2.17	0.59
25:CA:2728:U:OP1	58:CA:3166:PAR:N12	2.30	0.59
4:DD:111:ARG:HA	4:DD:114:ALA:HB3	1.85	0.59
20:DT:44:LYS:NZ	20:DT:86:LEU:O	2.35	0.59
14:AN:67:THR:OG1	14:AN:68:GLY:N	2.34	0.59
44:BT:69:ARG:NH2	60:BT:202:HOH:O	2.35	0.59
25:CA:539:G:OP2	58:CA:3169:PAR:H34	2.03	0.59
25:CA:576:U:OP1	60:CA:3665:HOH:O	2.17	0.59
25:CA:1006:C:O2'	34:CJ:108:MET:O	2.19	0.59
4:DD:146:ARG:O	4:DD:148:LYS:N	2.35	0.59
5:AE:76:LEU:O	5:AE:82:GLN:NE2	2.36	0.59
30:BF:126:ASN:HB3	30:BF:156:THR:HA	1.85	0.59
25:CA:2445:G:OP1	29:CE:69:ARG:NH2	2.36	0.59
22:AV:45:TYR:OH	22:AV:51:PRO:O	2.19	0.59
32:BH:14:SER:OG	32:BH:17:ASP:OD2	2.19	0.59
50:BZ:3:THR:OG1	50:BZ:3:THR:O	2.21	0.59
25:CA:1723:G:O6	25:CA:1737:G:O2'	2.21	0.59
25:CA:996:A:C2	25:CA:997:G:C8	2.91	0.59
1:AA:1530:G:O2'	1:AA:1531:A:OP2	2.17	0.58
1:AA:509:A:OP2	60:AA:1757:HOH:O	2.17	0.58
23:AW:10:A:O2'	23:AW:11:A:OP2	2.19	0.58
25:BA:139:U:C4	44:BT:2:ILE:CG1	2.85	0.58
32:BH:124:THR:HG22	32:BH:128:HIS:HE1	1.57	0.58
25:CA:684:G:OP1	53:C2:16:HIS:ND1	2.36	0.58
25:CA:1105:U:H2'	25:CA:1106:G:C8	2.38	0.58
1:DA:1349:A:O3'	9:DI:123:ARG:NH1	2.36	0.58
16:DP:5:ARG:NE	16:DP:6:LEU:O	2.36	0.58
1:AA:386:C:C2'	1:AA:387:U:H5'	2.32	0.58
25:BA:517:C:OP2	51:B0:9:ARG:NH2	2.36	0.58
25:CA:2119:A:N6	25:CA:2167:U:O2'	2.36	0.58
1:DA:430:A:OP1	4:DD:9:LEU:HD23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DD:23:SER:O	4:DD:25:VAL:N	2.36	0.58
25:CA:2364:C:OP1	47:CW:53:ARG:NH1	2.36	0.58
25:CA:5:A:H2'	25:CA:6:A:C8	2.39	0.58
1:DA:1226:C:O2'	13:DM:102:THR:O	2.15	0.58
54:B3:15:LYS:NZ	54:B3:64:ALA:OXT	2.33	0.58
1:DA:116:A:N1	1:DA:313:A:O2'	2.31	0.58
22:AV:123:GLU:OE1	22:AV:126:ARG:NH1	2.36	0.58
25:BA:537:G:OP2	58:BA:3003:PAR:O62	2.16	0.58
25:CA:2657:A:O3'	31:CG:159:LYS:NZ	2.36	0.58
26:CB:3041:G:O6	30:CF:68:LYS:NZ	2.37	0.58
21:AU:10:GLU:HB3	21:AU:11:PRO:HD3	1.86	0.58
42:BR:14:VAL:HG11	42:BR:98:ILE:HG21	1.85	0.58
43:BS:109:ASP:OD1	43:BS:110:ARG:N	2.37	0.58
25:CA:265:A:N1	25:CA:427:U:O2'	2.30	0.58
25:CA:2757:A:N1	31:CG:66:THR:HG21	2.18	0.58
25:CA:1153:C:OP1	41:CQ:91:ARG:NH1	2.31	0.58
2:DB:144:LEU:O	2:DB:148:LEU:N	2.36	0.58
1:DA:1534:A:N6	23:DV:3:G:N7	2.51	0.58
23:DV:8:U:H3'	23:DV:9:A:C5'	2.34	0.58
1:AA:791:G:N2	1:AA:1497:G:O3'	2.36	0.58
12:AL:24:LEU:HB2	12:AL:59:ASN:HD22	1.68	0.58
25:BA:684:G:OP1	53:B2:16:HIS:ND1	2.36	0.58
25:BA:731:C:OP2	60:BA:3697:HOH:O	2.17	0.58
43:BS:17:VAL:HG12	43:BS:76:VAL:HG21	1.86	0.58
25:CA:45:G:H5''	25:CA:46:G:H5'	1.85	0.58
30:CF:112:ASP:O	30:CF:114:ARG:N	2.36	0.58
4:AD:9:LEU:HD13	4:AD:10:LYS:N	2.19	0.58
29:CE:17:THR:O	29:CE:18:THR:OG1	2.16	0.58
1:AA:208:U:O2	1:AA:212:G:N2	2.37	0.58
25:BA:116:C:O2'	25:BA:126:A:N3	2.35	0.58
25:BA:1509:A:O2'	25:BA:1510:G:OP2	2.16	0.58
32:BH:90:LEU:CD1	32:BH:123:ARG:HB3	2.33	0.58
49:BY:16:THR:O	49:BY:20:ASN:N	2.36	0.58
30:BF:90:LEU:HD13	30:BF:95:MET:HB2	1.86	0.58
25:BA:2657:A:O3'	31:BG:159:LYS:NZ	2.37	0.58
32:CH:121:VAL:HG22	32:CH:122:LEU:N	2.19	0.58
7:DG:113:ASP:OD2	7:DG:122:ASN:ND2	2.37	0.58
9:AI:25:ASN:O	9:AI:61:LEU:N	2.36	0.57
32:BH:4:ILE:N	32:BH:37:VAL:O	2.36	0.57
49:BY:25:GLN:O	49:BY:29:ARG:N	2.31	0.57
25:CA:1693:U:O2'	27:CC:13:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:429:U:OP1	4:DD:9:LEU:HD13	2.04	0.57
4:DD:26:ARG:NH2	4:DD:28:ILE:O	2.36	0.57
9:DI:18:ARG:HD3	9:DI:66:THR:CG2	2.34	0.57
25:CA:1466:U:HO2'	25:CA:1546:G:HO2'	1.51	0.57
25:CA:2502:G:H5''	25:CA:2503:A:H5''	1.86	0.57
1:DA:1182:G:C4'	1:DA:1183:U:H5'	2.34	0.57
14:DN:20:PHE:O	14:DN:22:LYS:N	2.36	0.57
25:CA:714:U:OP2	15:DO:89:ARG:NH2	2.36	0.57
1:AA:1491:G:C8	58:AA:1672:PAR:O31	2.57	0.57
25:BA:743:A:O2'	25:BA:1659:G:OP1	2.19	0.57
25:BA:798:G:O6	60:BA:3323:HOH:O	2.17	0.57
39:BO:62:LEU:CD2	39:BO:70:ALA:HA	2.35	0.57
25:CA:402:A:H2'	25:CA:403:U:H5'	1.86	0.57
32:CH:90:LEU:CD1	32:CH:123:ARG:N	2.67	0.57
41:CQ:9:ALA:O	41:CQ:12:ARG:N	2.36	0.57
3:DC:63:SER:HA	3:DC:97:VAL:HG13	1.86	0.57
8:DH:77:ARG:NE	8:DH:79:SER:O	2.37	0.57
1:AA:1129:C:O2	1:AA:1130:A:N6	2.38	0.57
8:DH:34:VAL:O	8:DH:37:ALA:N	2.38	0.57
1:DA:376:G:H5''	16:DP:5:ARG:HD3	1.85	0.57
27:BC:175:LEU:O	27:BC:178:GLY:N	2.36	0.57
37:CM:58:LYS:O	37:CM:60:GLN:N	2.37	0.57
1:DA:86:G:O2'	1:DA:87:C:O5'	2.21	0.57
1:DA:885:G:O2'	1:DA:914:A:N1	2.25	0.57
4:DD:58:LYS:NZ	4:DD:69:GLU:OE1	2.38	0.57
1:AA:1015:G:OP1	19:AS:14:HIS:NE2	2.37	0.57
14:AN:20:PHE:O	14:AN:22:LYS:NZ	2.38	0.57
25:BA:2298:A:C2	25:BA:2321:U:C2	2.92	0.57
25:BA:1922:G:O6	58:BA:3001:PAR:H221	2.05	0.57
32:BH:91:PHE:HB3	1:DA:368:U:N3	2.19	0.57
25:BA:144:A:C1'	44:BT:3:ARG:HH12	2.10	0.57
60:CA:3261:HOH:O	36:CL:36:LYS:NZ	2.28	0.57
2:DB:82:ASP:OD1	2:DB:82:ASP:N	2.38	0.57
23:DV:10:A:O2'	23:DV:11:A:OP2	2.19	0.57
3:AC:39:VAL:O	3:AC:43:LEU:N	2.38	0.57
25:CA:2579:C:OP1	60:CA:3538:HOH:O	2.17	0.57
25:CA:2821:A:OP2	38:CN:3:HIS:NE2	2.37	0.57
35:CK:71:ARG:NH1	35:CK:106:GLU:OE2	2.36	0.57
1:DA:376:G:H5''	16:DP:5:ARG:CD	2.35	0.57
1:AA:1160:G:O2'	1:AA:1161:C:O5'	2.19	0.57
11:AK:125:LYS:HD2	11:AK:126:LYS:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:CA:1826:G:O2'	25:CA:1971:U:OP2	2.23	0.57
25:CA:2128:G:N2	25:CA:2161:C:O2	2.38	0.57
30:CF:3:LEU:O	30:CF:7:TYR:N	2.38	0.57
60:CA:3333:HOH:O	36:CL:29:LYS:NZ	2.37	0.57
47:CW:52:GLY:O	47:CW:54:ASP:N	2.38	0.57
1:DA:1125:U:O2	1:DA:1126:U:O2'	2.13	0.57
4:AD:5:LEU:HG	4:AD:6:GLY:H	1.70	0.57
19:AS:48:THR:OG1	19:AS:49:ILE:N	2.37	0.57
25:BA:947:A:O2'	25:BA:984:A:H2	1.88	0.57
35:BK:2:ILE:HD11	35:BK:39:ILE:HG21	1.87	0.57
41:BQ:39:ILE:O	41:BQ:43:GLN:HG3	2.04	0.57
54:C3:57:VAL:O	54:C3:61:LEU:N	2.37	0.57
28:CD:27:ILE:HD11	28:CD:203:VAL:HG21	1.86	0.57
35:CK:71:ARG:O	35:CK:73:ASP:N	2.38	0.57
35:CK:76:VAL:HG12	40:CP:72:VAL:HG23	1.87	0.57
18:DR:20:GLU:O	18:DR:22:ASP:N	2.38	0.57
1:AA:1493:A:OP2	58:AA:1672:PAR:O41	2.16	0.57
17:AQ:81:LYS:O	17:AQ:83:VAL:N	2.37	0.57
1:DA:1062:U:H2'	1:DA:1063:C:C6	2.40	0.57
1:DA:108:G:H5'	1:DA:109:A:H5''	1.86	0.57
4:DD:13:ARG:NH2	4:DD:37:ALA:O	2.37	0.57
4:DD:61:VAL:O	4:DD:64:ILE:N	2.37	0.57
1:AA:1305:G:HO2'	1:AA:1306:A:H8	1.52	0.56
11:AK:112:ASP:OD1	21:AU:25:LYS:NZ	2.27	0.56
18:AR:28:THR:OG1	18:AR:29:LEU:N	2.34	0.56
25:BA:1860:G:C6	58:BA:3005:PAR:O41	2.54	0.56
41:CQ:39:ILE:HD11	42:CR:77:PHE:CD2	2.40	0.56
1:DA:1345:U:O5'	9:DI:122:ARG:NH2	2.38	0.56
18:DR:40:VAL:HG22	18:DR:41:PRO:HD2	1.87	0.56
13:AM:107:ARG:HH21	13:AM:112:PRO:HA	1.69	0.56
25:CA:1799:G:N2	25:CA:1819:A:OP2	2.33	0.56
45:CU:65:GLN:O	45:CU:68:ASN:N	2.38	0.56
1:DA:1156:G:O2'	1:DA:1180:A:N1	2.35	0.56
25:BA:2345:G:H4'	25:BA:2346:A:H5''	1.87	0.56
25:CA:2171:A:O2'	25:CA:2173:A:OP1	2.24	0.56
48:CX:4:CYS:O	48:CX:8:GLY:N	2.37	0.56
1:DA:1286:U:O2'	1:DA:1287:A:OP1	2.17	0.56
1:DA:405:U:O4	4:DD:2:ALA:N	2.38	0.56
1:AA:1081:A:H5'	5:AE:23:LYS:HD3	1.88	0.56
1:AA:693:G:OP1	11:AK:127:ARG:NH2	2.38	0.56
7:AG:100:ALA:N	7:AG:103:TRP:CE3	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:100:ALA:HB1	7:AG:103:TRP:CE2	2.41	0.56
11:AK:25:ALA:N	11:AK:87:LYS:O	2.30	0.56
35:BK:7:MET:SD	35:BK:20:MET:HB2	2.45	0.56
37:BM:77:PRO:O	37:BM:80:VAL:HG12	2.05	0.56
48:BX:71:ARG:NH1	48:BX:77:TYR:OH	2.39	0.56
25:CA:1047:G:HO2'	25:CA:1110:G:H1	1.51	0.56
25:CA:9:G:O2'	25:CA:2800:A:N6	2.38	0.56
25:CA:630:G:H3'	25:CA:631:A:H5''	1.87	0.56
3:DC:156:ARG:NH1	3:DC:159:GLY:O	2.37	0.56
12:AL:44:LYS:HB3	12:AL:45:PRO:HD3	1.88	0.56
25:BA:2681:C:OP1	28:BD:8:LYS:NZ	2.36	0.56
25:BA:27:G:O2'	25:BA:28:A:OP2	2.22	0.56
25:BA:395:U:O2'	25:BA:396:G:N7	2.27	0.56
25:BA:446:G:OP1	41:BQ:2:ARG:HG3	2.06	0.56
35:CK:107:LEU:O	35:CK:109:SER:N	2.39	0.56
39:CO:67:ASN:O	39:CO:69:ASP:N	2.35	0.56
40:CP:17:PRO:HD2	40:CP:83:ILE:HG12	1.88	0.56
1:DA:227:G:O2'	16:DP:63:GLN:OE1	2.21	0.56
1:DA:257:G:O6	60:DA:1718:HOH:O	2.18	0.56
1:DA:618:C:H3'	1:DA:619:U:H5''	1.88	0.56
19:DS:10:PHE:O	19:DS:39:THR:OG1	2.24	0.56
25:BA:2014:A:H2'	25:BA:2015:A:C8	2.41	0.56
30:BF:143:ASP:OD1	30:BF:143:ASP:N	2.38	0.56
25:CA:555:G:H22	58:CA:3169:PAR:H642	1.70	0.56
41:CQ:89:ILE:CD1	41:CQ:93:ILE:HB	2.36	0.56
48:CX:66:VAL:O	48:CX:69:GLU:N	2.37	0.56
1:DA:1225:A:H2'	1:DA:1226:C:C5	2.40	0.56
2:DB:63:ARG:O	2:DB:65:GLY:N	2.39	0.56
8:DH:90:ASP:OD2	8:DH:90:ASP:N	2.38	0.56
22:AV:150:SER:O	22:AV:153:ASP:N	2.39	0.56
25:BA:1136:G:HO2'	25:BA:2038:G:HO2'	1.51	0.56
38:BN:59:SER:OG	38:BN:62:ASN:OD1	2.24	0.56
25:CA:948:C:O2	25:CA:984:A:O2'	2.22	0.56
25:CA:2681:C:OP1	28:CD:8:LYS:NZ	2.38	0.56
37:CM:118:LYS:NZ	37:CM:128:THR:O	2.38	0.56
2:DB:69:PHE:CZ	2:DB:84:ALA:HB1	2.41	0.56
1:AA:121:U:O2'	1:AA:122:G:OP1	2.18	0.56
8:AH:14:ILE:HD11	8:AH:75:ILE:HG12	1.88	0.56
1:AA:527:G:O6	12:AL:46:ASN:ND2	2.39	0.56
1:AA:667:G:O2'	15:AO:49:ASP:OD1	2.17	0.56
28:BD:128:ARG:HA	28:BD:128:ARG:HE	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BY:2:LYS:HE3	49:BY:6:LEU:HD22	1.87	0.56
25:CA:31:C:O3'	25:CA:1238:G:H5''	2.06	0.56
25:CA:381:G:OP1	48:CX:17:ARG:NH2	2.39	0.56
32:CH:90:LEU:HD21	32:CH:123:ARG:C	2.26	0.56
50:CZ:8:GLN:HB2	50:CZ:28:LEU:HD23	1.88	0.56
1:AA:1179:A:H2'	1:AA:1180:A:O4'	2.05	0.56
4:AD:76:TYR:O	4:AD:80:ALA:N	2.39	0.56
24:AX:44:G:H4'	24:AX:45:U:OP1	2.06	0.56
25:BA:192:C:O2'	25:BA:802:A:N3	2.37	0.56
40:BP:91:VAL:HG12	40:BP:92:ARG:N	2.21	0.56
1:DA:980:C:H5''	1:DA:981:U:C5	2.40	0.56
1:AA:523:A:N6	12:AL:87:VAL:HG12	2.21	0.56
25:BA:636:G:OP2	36:BL:109:LYS:NZ	2.19	0.56
25:CA:2230:G:H1'	48:CX:31:ASN:CB	2.36	0.56
1:DA:1307:U:OP1	13:DM:100:GLN:NE2	2.39	0.56
8:DH:88:ARG:NH2	8:DH:122:GLY:O	2.39	0.56
11:DK:125:LYS:O	21:DU:34:ARG:NH2	2.38	0.56
1:AA:114:U:C2'	1:AA:115:G:H5'	2.36	0.56
4:AD:100:ASN:O	4:AD:102:VAL:N	2.34	0.56
13:AM:107:ARG:HD2	13:AM:110:LYS:HZ2	1.71	0.56
25:CA:1509:A:O2'	25:CA:1510:G:OP2	2.20	0.56
25:CA:1590:A:H2'	25:CA:1591:A:C8	2.41	0.56
25:CA:739:A:H1'	25:CA:740:C:H5	1.70	0.56
25:CA:885:C:O3'	13:DM:92:ARG:NH2	2.39	0.56
30:CF:33:ILE:H	30:CF:95:MET:HE1	1.70	0.56
36:CL:102:GLY:O	36:CL:104:GLN:N	2.38	0.56
39:CO:111:ARG:O	39:CO:113:ALA:N	2.39	0.56
1:AA:1412:C:H2'	1:AA:1413:A:C8	2.41	0.55
11:AK:17:SER:HA	11:AK:79:ILE:N	2.21	0.55
25:BA:1178:C:H2'	25:BA:1179:G:C8	2.41	0.55
25:BA:1313:U:OP1	44:BT:69:ARG:NH2	2.39	0.55
25:BA:1952:A:C6	35:BK:22:ILE:HD11	2.41	0.55
25:BA:1930:G:O2'	25:BA:1968:G:O6	2.17	0.55
25:BA:2418:A:OP1	54:B3:44:ARG:NH1	2.39	0.55
28:BD:125:TRP:CD2	28:BD:160:LYS:HG2	2.41	0.55
32:BH:25:TYR:CE1	32:BH:30:LEU:HD13	2.41	0.55
25:CA:2884:U:O4'	51:C0:49:ARG:NH2	2.39	0.55
25:CA:1779:U:H5	25:CA:1784:A:N7	2.03	0.55
2:DB:96:TRP:O	2:DB:98:GLY:N	2.39	0.55
4:DD:145:ILE:HG22	4:DD:178:MET:SD	2.46	0.55
22:AV:135:ASP:O	22:AV:138:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BH:125:THR:HG23	32:BH:146:VAL:CG1	2.37	0.55
37:CM:105:MET:HE1	37:CM:113:ALA:HA	1.88	0.55
8:DH:88:ARG:O	8:DH:90:ASP:N	2.39	0.55
1:AA:1250:A:N1	1:AA:1353:G:N2	2.52	0.55
25:BA:1859:U:O4	58:BA:3005:PAR:H31	2.06	0.55
28:BD:32:ASN:HB3	28:BD:50:VAL:HG21	1.87	0.55
31:BG:34:ARG:HH11	31:BG:74:MET:HE1	1.72	0.55
36:CL:110:VAL:HG22	36:CL:127:VAL:HA	1.88	0.55
45:CU:97:SER:OG	45:CU:98:ASN:N	2.39	0.55
12:DL:44:LYS:HB2	12:DL:45:PRO:HD3	1.88	0.55
15:DO:87:LEU:HD12	15:DO:88:ARG:H	1.71	0.55
1:AA:1279:G:O2'	1:AA:1281:C:OP2	2.23	0.55
25:BA:1327:A:H2'	25:BA:1328:A:O4'	2.06	0.55
25:BA:2325:G:C6	25:BA:2326:C:N4	2.74	0.55
25:BA:2547:A:H2'	25:BA:2548:U:C6	2.41	0.55
58:BA:3003:PAR:H51	58:BA:3003:PAR:H322	1.72	0.55
25:BA:761:A:OP1	60:BA:3697:HOH:O	2.18	0.55
25:CA:1055:G:N2	25:CA:1104:C:N3	2.50	0.55
25:CA:1265:A:OP2	60:CA:3747:HOH:O	2.17	0.55
25:CA:1838:C:H4'	25:CA:1839:G:C8	2.42	0.55
2:AB:73:LYS:O	2:AB:75:ALA:N	2.40	0.55
4:AD:97:ARG:NH1	4:AD:99:ASP:OD2	2.39	0.55
7:AG:69:VAL:O	7:AG:138:ARG:NH2	2.35	0.55
25:BA:2728:U:O2'	25:BA:2729:G:P	2.65	0.55
27:BC:16:VAL:N	27:BC:203:VAL:HG12	2.22	0.55
38:BN:81:ASN:OD1	38:BN:81:ASN:N	2.39	0.55
49:BY:2:LYS:CE	49:BY:6:LEU:HD22	2.36	0.55
25:CA:1252:G:C2	41:CQ:32:ARG:HG3	2.41	0.55
44:CT:8:LEU:HD22	49:CY:21:LEU:HB3	1.88	0.55
1:DA:1359:C:H5	14:DN:75:ARG:NH2	2.05	0.55
1:DA:150:U:H2'	1:DA:151:A:H8	1.72	0.55
5:DE:90:THR:OG1	5:DE:91:GLY:N	2.37	0.55
23:DV:4:G:C2'	23:DV:5:A:H5'	2.36	0.55
1:AA:736:C:H2'	1:AA:737:C:C6	2.41	0.55
25:BA:1309:G:H4'	53:B2:7:PRO:HB2	1.87	0.55
25:BA:1794:A:H2'	25:BA:1795:C:C6	2.42	0.55
25:BA:1860:G:O6	58:BA:3005:PAR:O41	2.24	0.55
32:BH:90:LEU:N	32:BH:90:LEU:HD12	2.21	0.55
25:CA:630:G:H3'	25:CA:631:A:C5'	2.37	0.55
30:CF:38:GLY:O	30:CF:149:ARG:NH1	2.39	0.55
32:CH:90:LEU:HG	32:CH:123:ARG:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:DU:18:ARG:HA	21:DU:21:ARG:HB3	1.88	0.55
15:AO:82:ILE:O	15:AO:86:GLY:N	2.37	0.55
17:AQ:28:PHE:HB3	17:AQ:39:LYS:HA	1.88	0.55
25:BA:274:C:O2	25:BA:363:G:N2	2.34	0.55
31:BG:165:ASP:OD1	31:BG:165:ASP:N	2.34	0.55
48:BX:31:ASN:HB2	48:BX:33:HIS:HE1	1.71	0.55
25:CA:2640:G:OP1	34:CJ:96:ARG:NH1	2.39	0.55
1:DA:1508:A:H2'	1:DA:1509:C:O4'	2.07	0.55
1:AA:1123:U:O3'	10:AJ:37:ARG:NH1	2.40	0.55
13:AM:87:ARG:O	13:AM:91:HIS:N	2.34	0.55
20:AT:45:ALA:O	20:AT:48:GLN:NE2	2.40	0.55
24:AX:14:A:H2'	24:AX:15:G:O4'	2.07	0.55
54:B3:31:ILE:HD13	54:B3:34:LYS:HZ2	1.72	0.55
25:BA:370:G:OP2	60:BA:3564:HOH:O	2.18	0.55
25:CA:1313:U:H2'	25:CA:1610:A:C2	2.42	0.55
25:CA:555:G:N2	58:CA:3169:PAR:N64	2.54	0.55
25:CA:1799:G:O2'	27:CC:179:GLU:OE2	2.12	0.55
35:CK:53:LYS:N	35:CK:56:ASP:OD2	2.39	0.55
25:CA:2377:A:H1'	39:CO:92:PHE:HZ	1.72	0.55
50:CZ:48:ASN:O	50:CZ:51:SER:OG	2.25	0.55
5:AE:104:GLY:HA3	5:AE:122:ASN:HB2	1.89	0.55
25:BA:2305:U:C2	30:BF:150:GLY:HA3	2.41	0.55
30:CF:91:ARG:O	30:CF:93:GLU:N	2.39	0.55
39:CO:18:LEU:HA	39:CO:21:LEU:HB2	1.89	0.55
25:CA:1251:C:OP2	41:CQ:5:ARG:NH2	2.40	0.55
1:AA:1505:G:OP2	60:AA:1878:HOH:O	2.18	0.55
1:AA:518:C:H2'	1:AA:530:G:C8	2.42	0.55
8:AH:110:VAL:O	8:AH:111:MET:CB	2.54	0.55
10:AJ:53:ILE:HG12	10:AJ:61:ALA:HB1	1.88	0.55
25:BA:2543:G:H2'	25:BA:2544:G:C8	2.41	0.55
1:AA:1124:G:O2'	1:AA:1145:A:N6	2.40	0.54
1:AA:429:U:H5	1:AA:431:A:N7	2.04	0.54
7:AG:45:SER:OG	7:AG:45:SER:O	2.24	0.54
25:BA:1071:G:OP2	25:BA:1088:A:O2'	2.25	0.54
25:BA:477:A:O2'	25:BA:478:A:OP1	2.21	0.54
25:BA:83:A:OP1	45:BU:91:LYS:NZ	2.39	0.54
25:CA:1993:U:H4'	28:CD:133:THR:CG2	2.36	0.54
34:CJ:19:ASP:O	34:CJ:23:LYS:NZ	2.22	0.54
1:DA:1319:A:O2'	1:DA:1323:G:N7	2.30	0.54
8:DH:111:MET:CE	8:DH:116:ALA:HA	2.34	0.54
8:DH:27:MET:HB3	8:DH:28:PRO:HD2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:DM:11:ASP:HA	13:DM:45:ILE:HG12	1.89	0.54
9:AI:50:GLN:HB3	9:AI:103:PHE:HZ	1.72	0.54
14:AN:15:LEU:O	14:AN:17:ASP:N	2.40	0.54
54:B3:44:ARG:HB3	54:B3:45:PRO:HD3	1.89	0.54
40:BP:74:GLN:O	40:BP:76:HIS:N	2.40	0.54
25:CA:2714:G:OP2	60:CA:3544:HOH:O	2.18	0.54
1:DA:660:C:H2'	1:DA:661:G:O4'	2.07	0.54
4:AD:32:CYS:SG	4:AD:33:LYS:N	2.79	0.54
56:B5:136:LEU:CB	56:B5:139:ASN:CB	2.86	0.54
25:BA:1853:A:N1	25:BA:2087:G:H1'	2.22	0.54
25:BA:1669:A:H5''	25:BA:2550:G:OP1	2.07	0.54
32:BH:135:HIS:O	32:BH:135:HIS:ND1	2.40	0.54
25:CA:1044:C:O2'	25:CA:1111:A:N1	2.39	0.54
6:DF:92:THR:HG22	6:DF:93:LYS:N	2.21	0.54
4:AD:76:TYR:CZ	4:AD:204:TYR:HB3	2.43	0.54
1:AA:1124:G:O5'	10:AJ:37:ARG:NE	2.40	0.54
25:BA:1274:A:N3	25:BA:1297:C:H1'	2.23	0.54
25:BA:544:C:H3'	25:BA:545:U:C6	2.42	0.54
34:BJ:80:HIS:O	34:BJ:82:GLY:N	2.40	0.54
25:CA:1671:U:OP2	60:CA:3432:HOH:O	2.18	0.54
32:CH:90:LEU:CG	32:CH:123:ARG:H	2.16	0.54
41:CQ:75:TYR:CZ	41:CQ:79:ILE:CD1	2.91	0.54
41:CQ:39:ILE:HD11	42:CR:77:PHE:CD1	2.42	0.54
1:AA:1317:C:O2'	1:AA:1318:A:OP1	2.26	0.54
51:B0:24:VAL:O	51:B0:26:SER:N	2.36	0.54
27:BC:140:VAL:HG21	27:BC:189:ALA:HB1	1.90	0.54
25:BA:1063:G:N2	33:BI:89:SER:OG	2.41	0.54
25:CA:526:A:O2'	25:CA:2043:C:O2	2.23	0.54
32:CH:90:LEU:HD11	32:CH:123:ARG:N	2.21	0.54
33:CI:102:ARG:O	33:CI:106:GLN:NE2	2.40	0.54
34:CJ:111:LYS:NZ	60:CJ:201:HOH:O	2.39	0.54
4:DD:189:SER:O	4:DD:191:LEU:N	2.40	0.54
1:AA:663:A:O3'	18:AR:53:ARG:NH2	2.39	0.54
25:BA:1059:G:N2	33:BI:130:GLY:O	2.40	0.54
25:BA:1668:A:H4'	25:BA:1669:A:O5'	2.08	0.54
25:BA:2590:A:H2'	25:BA:2591:C:C6	2.42	0.54
32:BH:117:LEU:CD2	32:BH:119:ASN:O	2.55	0.54
32:CH:72:ILE:HD11	32:CH:132:PHE:CD2	2.42	0.54
46:CV:35:GLU:N	46:CV:35:GLU:OE2	2.41	0.54
49:CY:13:GLU:O	49:CY:17:GLU:N	2.36	0.54
15:DO:19:ALA:O	15:DO:21:ASP:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:101:LEU:H	2:AB:101:LEU:HD22	1.73	0.54
25:BA:307:G:N2	25:BA:309:A:H3'	2.22	0.54
25:BA:446:G:OP2	41:BQ:2:ARG:NE	2.35	0.54
25:CA:2418:A:O2'	25:CA:2419:U:OP1	2.22	0.54
1:DA:1277:C:HO2'	1:DA:1279:G:H8	1.54	0.54
10:DJ:7:ARG:NE	10:DJ:75:ASP:OD1	2.37	0.54
1:AA:68:G:C5	1:AA:69:G:H1'	2.43	0.54
7:AG:148:ASN:O	7:AG:150:ALA:N	2.40	0.54
28:BD:13:ARG:NH2	40:BP:74:GLN:OE1	2.37	0.54
25:CA:1782:U:H1'	25:CA:2609:U:H5'	1.89	0.54
2:DB:57:LEU:HD12	2:DB:58:ASN:H	1.72	0.54
4:DD:29:ASP:O	4:DD:31:LYS:N	2.38	0.54
5:DE:107:ALA:CB	5:DE:125:ALA:HB3	2.38	0.54
16:DP:5:ARG:CZ	16:DP:6:LEU:HB2	2.37	0.54
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.43	0.54
1:AA:378:G:C2	1:AA:386:C:O2	2.61	0.54
1:AA:719:C:O4'	18:AR:38:LYS:NZ	2.41	0.54
25:BA:2390:U:O5'	54:B3:34:LYS:HE2	2.07	0.54
25:BA:301:G:OP2	45:BU:81:ARG:NH1	2.41	0.54
25:CA:2346:A:H3'	25:CA:2347:C:H5''	1.89	0.54
25:CA:2673:G:H5''	58:CA:3166:PAR:O53	2.01	0.54
30:CF:72:SER:OG	30:CF:80:GLN:N	2.40	0.54
1:AA:90:C:O2'	1:AA:91:U:OP2	2.21	0.54
25:BA:2420:C:OP1	54:B3:33:THR:HG23	2.08	0.54
25:BA:221:A:N1	25:BA:265:A:O2'	2.41	0.54
32:BH:91:PHE:CE2	1:DA:55:A:C4	2.96	0.54
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.42	0.53
1:AA:131:A:H2'	1:AA:132:C:C6	2.43	0.53
3:AC:165:THR:HG22	3:AC:166:GLU:N	2.22	0.53
25:BA:2527:C:H5''	55:B4:31:PRO:HB3	1.89	0.53
25:CA:1153:C:OP2	60:CA:3358:HOH:O	2.18	0.53
25:CA:1269:A:N1	25:CA:2011:U:H5	2.07	0.53
25:CA:2683:C:OP1	40:CP:50:ARG:NH2	2.40	0.53
25:CA:139:U:H3	44:CT:2:ILE:HD11	1.72	0.53
1:DA:606:G:N2	1:DA:632:U:OP1	2.39	0.53
2:DB:188:ASP:HB2	2:DB:204:ASP:CG	2.29	0.53
2:AB:10:LEU:O	2:AB:12:ALA:N	2.40	0.53
22:AV:29:ARG:NH2	22:AV:88:LEU:O	2.41	0.53
25:BA:1378:A:O3'	60:BA:3756:HOH:O	2.19	0.53
25:BA:2514:U:H2'	25:BA:2515:C:C6	2.44	0.53
25:BA:324:A:N6	25:BA:338:G:O2'	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BH:122:LEU:CB	32:BH:123:ARG:CA	2.86	0.53
25:BA:1952:A:N6	35:BK:22:ILE:HD11	2.23	0.53
49:CY:24:GLU:O	49:CY:26:PHE:N	2.41	0.53
1:DA:58:C:O2'	1:DA:388:G:N7	2.34	0.53
8:DH:101:ILE:HG22	8:DH:129:VAL:HG23	1.89	0.53
1:AA:1124:G:O5'	10:AJ:37:ARG:CZ	2.56	0.53
15:AO:46:HIS:O	15:AO:48:LYS:N	2.34	0.53
20:AT:5:LYS:O	20:AT:7:ALA:N	2.41	0.53
25:BA:1475:G:O2'	25:BA:1514:G:O6	2.17	0.53
26:BB:3013:G:H1	26:BB:3069:G:HO2'	1.55	0.53
32:BH:122:LEU:HA	32:BH:124:THR:N	2.23	0.53
32:CH:122:LEU:O	32:CH:124:THR:HG22	2.09	0.53
4:DD:107:PHE:CE2	4:DD:145:ILE:HD12	2.44	0.53
13:DM:22:ILE:HD11	13:DM:65:VAL:HB	1.90	0.53
14:AN:64:CYS:O	14:AN:64:CYS:SG	2.67	0.53
18:AR:56:ALA:HA	18:AR:59:ILE:HG22	1.89	0.53
56:B5:134:ARG:O	56:B5:135:GLY:C	2.47	0.53
56:B5:136:LEU:CA	56:B5:139:ASN:CB	2.85	0.53
31:BG:109:SER:OG	31:BG:110:HIS:N	2.42	0.53
31:BG:148:ARG:HA	31:BG:161:VAL:CG2	2.38	0.53
25:BA:1952:A:C5	35:BK:22:ILE:HG12	2.43	0.53
39:BO:34:HIS:ND1	39:BO:53:THR:OG1	2.41	0.53
34:CJ:75:TYR:HB3	34:CJ:84:ILE:HD11	1.91	0.53
41:CQ:16:ILE:O	41:CQ:19:GLN:N	2.42	0.53
2:DB:146:ASN:O	2:DB:146:ASN:ND2	2.41	0.53
6:DF:5:GLU:OE2	6:DF:38:ARG:NH2	2.41	0.53
1:DA:1350:A:P	9:DI:123:ARG:NH1	2.81	0.53
1:AA:339:C:OP2	35:BK:98:ARG:NH1	2.39	0.53
1:AA:390:U:O3'	16:AP:28:ARG:NH1	2.38	0.53
1:AA:509:A:OP1	4:AD:49:SER:OG	2.23	0.53
25:BA:137:U:O2'	25:BA:139:U:H2'	2.09	0.53
25:BA:614:A:O2'	25:BA:615:U:OP2	2.23	0.53
25:BA:2376:A:N3	39:BO:111:ARG:NH1	2.57	0.53
25:CA:954:G:O2'	25:CA:2274:A:N1	2.26	0.53
25:CA:2392:A:OP2	25:CA:2422:C:N4	2.42	0.53
30:CF:3:LEU:HD13	30:CF:172:PHE:CE2	2.44	0.53
1:DA:375:U:O3'	16:DP:5:ARG:CZ	2.56	0.53
16:AP:1:MET:HG2	16:AP:2:VAL:N	2.24	0.53
54:B3:31:ILE:HD13	54:B3:34:LYS:NZ	2.23	0.53
25:BA:2298:A:N1	25:BA:2321:U:N3	2.56	0.53
32:BH:68:ARG:NH2	32:BH:134:VAL:HG23	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BT:2:ILE:HG22	44:BT:3:ARG:N	2.22	0.53
25:CA:691:C:P	27:CC:216:ARG:NH2	2.82	0.53
1:DA:507:C:OP2	60:DA:1758:HOH:O	2.18	0.53
1:DA:789:U:O2'	1:DA:791:G:N7	2.31	0.53
4:AD:41:HIS:O	4:AD:43:ALA:N	2.42	0.53
10:AJ:12:ALA:HB3	10:AJ:18:ILE:HG23	1.89	0.53
25:BA:1253:A:OP2	60:BA:3283:HOH:O	2.19	0.53
25:BA:2776:A:H4'	25:BA:2777:G:H5''	1.90	0.53
50:BZ:41:PRO:O	50:BZ:45:GLY:N	2.41	0.53
29:CE:8:ALA:O	29:CE:10:SER:N	2.42	0.53
40:CP:33:GLU:HB2	40:CP:38:ARG:NH1	2.23	0.53
13:AM:45:ILE:HD12	13:AM:48:LEU:HD11	1.91	0.53
13:AM:68:ASP:O	30:BF:109:ARG:NH1	2.42	0.53
11:AK:126:LYS:N	21:AU:35:ARG:NE	2.56	0.53
22:AV:178:ASP:OD1	22:AV:179:LYS:N	2.42	0.53
54:B3:31:ILE:CD1	54:B3:34:LYS:HB3	2.39	0.53
25:BA:1080:A:O2'	33:BI:126:ARG:O	2.26	0.53
25:BA:783:A:H2'	25:BA:784:G:H4'	1.90	0.53
29:BE:131:THR:OG1	29:BE:162:ARG:NH1	2.41	0.53
32:BH:123:ARG:CD	32:BH:123:ARG:H	2.17	0.53
35:BK:9:ASN:OD1	35:BK:18:ARG:NH1	2.41	0.53
37:BM:66:ARG:NH1	37:BM:104:GLU:OE2	2.42	0.53
44:BT:79:ASP:OD2	44:BT:79:ASP:N	2.41	0.53
41:CQ:81:GLY:O	41:CQ:84:LYS:N	2.42	0.53
3:DC:155:GLY:O	3:DC:157:LEU:N	2.42	0.53
6:DF:70:VAL:O	6:DF:73:GLU:N	2.41	0.53
1:AA:411:A:OP1	4:AD:31:LYS:NZ	2.34	0.53
25:BA:1022:G:O6	34:BJ:68:LYS:HE3	2.08	0.53
25:BA:2094:A:OP1	32:BH:22:LYS:NZ	2.31	0.53
27:BC:120:ASP:OD1	27:BC:120:ASP:N	2.40	0.53
25:CA:2285:C:P	52:C1:5:ARG:HH22	2.32	0.53
9:DI:26:GLY:N	9:DI:59:GLU:O	2.42	0.53
11:DK:50:SER:OG	11:DK:69:ARG:NH1	2.41	0.53
2:AB:23:TRP:HA	2:AB:190:ASN:HA	1.90	0.53
53:B2:1:MET:H3	53:B2:1:MET:HE3	1.73	0.53
25:BA:600:G:H1'	29:BE:100:MET:CE	2.39	0.53
50:BZ:48:ASN:O	50:BZ:51:SER:OG	2.27	0.53
1:DA:1359:C:C5	14:DN:75:ARG:NH2	2.77	0.53
1:DA:376:G:P	16:DP:5:ARG:NH1	2.82	0.53
3:DC:57:ILE:HA	3:DC:66:VAL:HA	1.91	0.53
6:DF:27:ALA:O	6:DF:31:GLY:N	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:132:C:OP1	20:DT:69:LYS:NZ	2.42	0.53
20:DT:70:ASN:O	20:DT:73:ALA:N	2.42	0.53
1:AA:791:G:C5	1:AA:792:A:N7	2.77	0.52
4:AD:118:VAL:HA	4:AD:123:ILE:HD13	1.90	0.52
9:AI:13:LYS:O	9:AI:15:SER:N	2.40	0.52
15:AO:81:LEU:HA	15:AO:84:ARG:HB2	1.90	0.52
36:BL:58:TYR:O	54:B3:12:ARG:NE	2.42	0.52
27:BC:57:HIS:CD2	27:BC:58:LYS:N	2.78	0.52
34:BJ:78:THR:OG1	34:BJ:80:HIS:HB2	2.10	0.52
44:BT:51:PHE:O	44:BT:53:VAL:N	2.41	0.52
48:BX:4:CYS:SG	48:BX:7:THR:HG22	2.49	0.52
25:CA:1668:A:O2'	25:CA:1674:G:N7	2.31	0.52
25:CA:2392:A:OP2	54:C3:30:HIS:NE2	2.42	0.52
25:CA:2898:U:H2'	25:CA:2899:A:H8	1.73	0.52
13:DM:46:SER:O	13:DM:48:LEU:N	2.39	0.52
4:AD:117:LEU:HG	4:AD:123:ILE:HD11	1.91	0.52
12:AL:43:LYS:HB2	12:AL:89:ASP:HA	1.91	0.52
39:BO:87:ILE:O	39:BO:89:ASP:N	2.42	0.52
25:CA:1379:U:OP1	25:CA:1379:U:C6	2.62	0.52
25:CA:1905:C:O2'	25:CA:1906:G:OP2	2.20	0.52
25:CA:348:A:H2'	25:CA:349:U:O4'	2.09	0.52
25:CA:630:G:C3'	25:CA:631:A:H5''	2.39	0.52
25:CA:77:G:H5''	49:CY:2:LYS:HD3	1.90	0.52
25:CA:86:G:O6	25:CA:96:C:N4	2.40	0.52
44:CT:19:LYS:HA	44:CT:22:THR:HG22	1.91	0.52
1:DA:255:G:OP1	17:DQ:71:LYS:NZ	2.40	0.52
1:DA:434:U:H2'	1:DA:435:A:C8	2.44	0.52
4:DD:45:LYS:O	4:DD:47:ARG:NE	2.41	0.52
1:DA:192:A:N3	20:DT:55:GLN:NE2	2.54	0.52
17:AQ:48:ASP:CB	17:AQ:75:LEU:HD23	2.39	0.52
25:BA:197:A:N6	25:BA:2430:A:H2'	2.25	0.52
26:BB:3075:G:H1'	46:BV:29:ILE:HG12	1.90	0.52
47:BW:37:ARG:HA	47:BW:56:THR:HG22	1.90	0.52
25:CA:690:G:O3'	27:CC:216:ARG:NH2	2.42	0.52
27:CC:220:ARG:NH2	60:CC:307:HOH:O	2.42	0.52
41:CQ:42:GLY:HA3	42:CR:75:VAL:HG11	1.91	0.52
14:DN:5:MET:SD	14:DN:8:ARG:NH2	2.78	0.52
54:B3:31:ILE:HD11	54:B3:35:LYS:HE2	1.91	0.52
25:BA:2590:A:H2'	25:BA:2591:C:H6	1.75	0.52
25:BA:544:C:HO2'	25:BA:545:U:P	2.25	0.52
45:BU:35:VAL:HB	45:BU:38:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:C2:13:ASN:O	53:C2:17:GLY:N	2.38	0.52
31:CG:71:LEU:O	31:CG:74:MET:N	2.42	0.52
25:CA:1190:G:H5'	36:CL:32:GLY:HA2	1.90	0.52
25:CA:1614:A:N1	43:CS:93:ALA:HB2	2.25	0.52
1:DA:960:U:H4'	1:DA:961:U:C5'	2.40	0.52
3:AC:6:HIS:O	3:AC:9:GLY:N	2.42	0.52
40:BP:89:GLY:O	40:BP:112:ARG:NH1	2.42	0.52
25:CA:2094:A:C2	25:CA:2196:C:C2	2.97	0.52
25:CA:2267:A:H5''	25:CA:2268:A:H5'	1.91	0.52
25:CA:2345:G:H4'	25:CA:2346:A:H5''	1.91	0.52
58:CA:3168:PAR:O62	58:CA:3168:PAR:H13	2.08	0.52
27:CC:114:GLN:O	27:CC:124:LYS:NZ	2.24	0.52
30:CF:91:ARG:HA	30:CF:95:MET:SD	2.50	0.52
1:DA:6:G:O2'	1:DA:7:A:O5'	2.27	0.52
16:DP:6:LEU:HD12	16:DP:71:VAL:HG12	1.92	0.52
1:AA:958:A:C8	19:AS:55:ARG:NH2	2.77	0.52
25:BA:1837:C:O2'	25:BA:1927:A:N3	2.34	0.52
25:BA:2405:G:O2'	25:BA:2406:A:OP1	2.22	0.52
32:BH:94:ILE:HD11	32:BH:121:VAL:CG1	2.33	0.52
37:BM:112:LEU:O	37:BM:115:GLU:N	2.42	0.52
41:BQ:65:ASN:OD1	41:BQ:69:ARG:NE	2.42	0.52
25:CA:1447:C:O2'	25:CA:1544:A:N3	2.39	0.52
25:CA:2816:G:O3'	38:CN:99:LYS:NZ	2.35	0.52
25:CA:520:G:H2'	25:CA:521:U:H6	1.75	0.52
4:DD:65:TYR:CD1	4:DD:65:TYR:N	2.78	0.52
12:DL:107:VAL:HG12	12:DL:108:LYS:H	1.74	0.52
1:AA:1435:G:H2'	1:AA:1436:U:C6	2.44	0.52
1:AA:655:A:C2	1:AA:754:C:N4	2.78	0.52
1:AA:829:G:C2'	1:AA:830:G:H5'	2.40	0.52
7:AG:95:ARG:O	7:AG:99:LEU:N	2.42	0.52
17:AQ:28:PHE:CB	17:AQ:39:LYS:HA	2.40	0.52
25:BA:481:G:C4	25:BA:507:A:C2	2.97	0.52
25:CA:1912:A:N1	1:DA:1407:C:O2'	2.34	0.52
25:CA:2675:A:H62	58:CA:3166:PAR:HN62	1.58	0.52
31:CG:120:ILE:HD12	31:CG:140:ILE:CG2	2.39	0.52
1:DA:179:A:H2'	1:DA:180:U:O4'	2.10	0.52
2:DB:218:ALA:HA	2:DB:221:VAL:HG12	1.92	0.52
8:DH:101:ILE:CG1	8:DH:112:THR:HB	2.40	0.52
10:AJ:42:LEU:HB3	10:AJ:71:LEU:CD1	2.40	0.52
11:AK:36:ASP:OD1	11:AK:40:ASN:N	2.40	0.52
26:BB:3043:C:C4'	30:BF:62:GLN:HE21	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BC:165:ALA:HB3	27:BC:172:THR:HB	1.92	0.52
30:BF:76:PHE:HB2	30:BF:78:ILE:HG12	1.90	0.52
25:CA:2579:C:OP1	60:CA:3539:HOH:O	2.19	0.52
44:CT:24:MET:SD	44:CT:30:ILE:HD13	2.50	0.52
1:DA:337:G:H2'	1:DA:338:A:C8	2.45	0.52
9:DI:90:TYR:HD1	9:DI:91:ASP:H	1.56	0.52
12:DL:87:VAL:HG13	12:DL:93:VAL:HG13	1.91	0.52
16:DP:49:GLY:O	16:DP:50:THR:OG1	2.24	0.52
21:DU:33:ARG:CG	21:DU:34:ARG:N	2.72	0.52
1:AA:702:A:O2'	1:AA:703:G:OP1	2.17	0.52
32:BH:90:LEU:HD11	32:BH:123:ARG:HB3	1.92	0.52
48:BX:17:ARG:CZ	48:BX:23:ALA:HB2	2.40	0.52
25:CA:1096:A:O2'	25:CA:1097:U:O4'	2.24	0.52
25:CA:2405:G:OP1	36:CL:70:LYS:NZ	2.43	0.52
2:DB:23:TRP:CE3	2:DB:25:PRO:HA	2.45	0.52
5:DE:104:GLY:CA	5:DE:122:ASN:HA	2.40	0.52
19:DS:31:LEU:HD12	19:DS:32:ARG:N	2.24	0.52
21:DU:24:GLU:OE2	21:DU:25:LYS:N	2.43	0.52
1:AA:428:G:H4'	4:AD:9:LEU:CD2	2.39	0.52
2:AB:21:ARG:HG2	2:AB:37:LYS:HD2	1.92	0.52
3:AC:7:PRO:O	3:AC:11:ARG:HD3	2.10	0.52
7:AG:107:ALA:HA	7:AG:110:LYS:HG2	1.92	0.52
7:AG:66:LEU:HD11	7:AG:71:PRO:HD2	1.92	0.52
11:AK:88:GLY:H	11:AK:114:THR:HG22	1.74	0.52
11:AK:50:SER:O	11:AK:69:ARG:NH1	2.43	0.52
25:BA:307:G:N2	25:BA:310:A:C8	2.78	0.52
37:BM:44:ARG:HG3	37:BM:44:ARG:HH21	1.74	0.52
25:BA:2230:G:C1'	48:BX:31:ASN:HB3	2.40	0.52
25:CA:2872:A:C2'	25:CA:2873:A:H5'	2.40	0.52
25:CA:448:U:O4'	29:CE:79:ARG:NH2	2.43	0.52
47:CW:24:PHE:N	47:CW:27:GLU:OE1	2.40	0.52
1:DA:889:A:H5'	1:DA:891:U:H1'	1.92	0.52
4:DD:26:ARG:NH1	4:DD:29:ASP:O	2.42	0.52
8:DH:13:ARG:NH1	8:DH:27:MET:HB2	2.25	0.52
1:DA:720:C:H1'	18:DR:39:ILE:HD11	1.91	0.52
19:DS:51:VAL:O	19:DS:58:VAL:N	2.42	0.52
24:DW:32:U:H3'	24:DW:33:U:H5''	1.92	0.52
13:AM:72:GLU:HA	13:AM:75:MET:HG2	1.90	0.51
25:BA:1203:U:O2'	36:BL:4:ASN:OD1	2.16	0.51
44:BT:30:ILE:CG1	44:BT:85:VAL:HG13	2.40	0.51
25:CA:2774:C:H2'	25:CA:2775:G:O4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:CC:251:THR:HG22	27:CC:252:LYS:N	2.25	0.51
35:CK:2:ILE:HD11	35:CK:39:ILE:HD13	1.92	0.51
36:CL:29:LYS:O	36:CL:30:THR:HB	2.10	0.51
1:DA:1411:C:O3'	12:DL:54:ARG:NH2	2.43	0.51
3:DC:168:TYR:OH	5:DE:55:GLU:OE2	2.28	0.51
1:DA:845:A:O3'	18:DR:48:ARG:NH2	2.43	0.51
21:DU:26:ALA:HA	21:DU:29:LEU:HB3	1.92	0.51
21:DU:26:ALA:HB3	23:DV:5:A:C5'	2.39	0.51
1:AA:299:G:C6	1:AA:300:A:C6	2.99	0.51
10:AJ:57:VAL:HG12	10:AJ:58:ASN:H	1.76	0.51
1:AA:37:U:C5'	12:AL:121:ARG:HH12	2.23	0.51
13:AM:76:SER:OG	30:BF:111:ARG:NH1	2.43	0.51
11:AK:125:LYS:CA	21:AU:35:ARG:HE	2.22	0.51
25:BA:1799:G:OP2	27:BC:269:ARG:NH2	2.43	0.51
25:BA:1952:A:C6	35:BK:22:ILE:CG1	2.93	0.51
25:BA:569:U:H5'	25:BA:569:U:H6	1.74	0.51
25:CA:1802:A:H2'	25:CA:1803:A:C8	2.45	0.51
25:CA:2848:G:O2'	25:CA:2867:G:N2	2.37	0.51
25:CA:450:G:OP1	25:CA:1248:G:N1	2.43	0.51
25:CA:476:G:H4'	25:CA:502:A:N1	2.25	0.51
25:CA:2563:U:H5''	35:CK:27:GLY:H	1.75	0.51
1:DA:976:G:N2	1:DA:1363:A:C4	2.78	0.51
10:DJ:50:THR:HG22	10:DJ:64:GLN:OE1	2.10	0.51
1:AA:1216:A:H2'	1:AA:1217:C:H6	1.76	0.51
25:BA:1026:G:H2'	25:BA:1027:A:H8	1.76	0.51
25:BA:2306:C:N4	30:BF:38:GLY:O	2.42	0.51
28:BD:133:THR:CG2	28:BD:134:HIS:N	2.73	0.51
38:CN:70:THR:OG1	38:CN:71:ARG:N	2.44	0.51
2:DB:99:GLY:N	2:DB:175:GLU:OE2	2.41	0.51
3:DC:79:LYS:O	3:DC:81:GLY:N	2.43	0.51
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.46	0.51
2:AB:50:PHE:O	2:AB:54:LEU:N	2.43	0.51
21:AU:40:LYS:N	21:AU:41:PRO:CD	2.74	0.51
22:AV:79:VAL:O	22:AV:82:ALA:N	2.43	0.51
25:BA:1265:A:C8	25:BA:1267:U:C2	2.98	0.51
28:BD:104:VAL:CG2	28:BD:177:VAL:HG11	2.41	0.51
28:BD:125:TRP:CE3	28:BD:160:LYS:HG2	2.45	0.51
36:BL:94:THR:HG22	36:BL:95:LEU:N	2.25	0.51
35:BK:76:VAL:HB	40:BP:72:VAL:CG2	2.40	0.51
44:BT:37:ASP:OD1	44:BT:37:ASP:N	2.39	0.51
58:CA:3170:PAR:H322	58:CA:3170:PAR:H51	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:CD:125:TRP:CZ3	28:CD:161:MET:N	2.78	0.51
1:AA:430:A:OP1	4:AD:9:LEU:HG	2.10	0.51
19:AS:24:GLU:OE1	19:AS:25:SER:N	2.44	0.51
25:BA:45:G:H5'	25:BA:46:G:OP1	2.10	0.51
28:BD:133:THR:O	28:BD:135:GLY:N	2.44	0.51
34:BJ:32:LEU:HD22	34:BJ:122:LEU:HD12	1.92	0.51
37:BM:23:GLY:O	37:BM:25:ASP:N	2.38	0.51
25:CA:2291:U:O2'	25:CA:2374:C:O2'	2.12	0.51
32:CH:98:ASP:N	32:CH:98:ASP:OD2	2.43	0.51
1:DA:1408:A:N1	58:DA:1654:PAR:O61	2.42	0.51
1:DA:407:U:OP1	4:DD:3:ARG:NH2	2.41	0.51
1:DA:409:U:H2'	1:DA:410:G:O4'	2.10	0.51
2:DB:14:VAL:O	2:DB:15:HIS:ND1	2.43	0.51
6:DF:3:HIS:H	6:DF:92:THR:HG23	1.76	0.51
3:AC:16:LYS:HG3	3:AC:17:PRO:HD2	1.93	0.51
5:AE:99:ALA:HB3	5:AE:123:VAL:HA	1.91	0.51
1:AA:684:U:O2'	11:AK:40:ASN:OD1	2.20	0.51
11:AK:54:GLY:O	11:AK:56:ARG:N	2.43	0.51
16:AP:1:MET:HG2	16:AP:2:VAL:HG22	1.92	0.51
16:AP:67:ILE:HD12	16:AP:67:ILE:N	2.25	0.51
22:AV:146:ASP:O	22:AV:148:GLU:N	2.43	0.51
25:BA:1882:U:H3	58:BA:3005:PAR:H41	1.76	0.51
25:BA:657:U:H2'	25:BA:658:U:C6	2.45	0.51
25:CA:545:U:C6	25:CA:547:A:H4'	2.45	0.51
25:CA:1805:A:N3	27:CC:49:THR:CG2	2.74	0.51
29:CE:5:LEU:O	29:CE:7:ASP:N	2.44	0.51
1:DA:831:A:P	2:DB:21:ARG:HH12	2.34	0.51
12:DL:86:ARG:HA	12:DL:94:ARG:HA	1.92	0.51
23:DV:11:A:N6	23:DV:12:A:C2	2.79	0.51
13:AM:54:ASP:OD1	13:AM:55:THR:N	2.44	0.51
17:AQ:51:ASN:N	17:AQ:51:ASN:OD1	2.42	0.51
11:AK:127:ARG:CB	21:AU:35:ARG:HH22	2.24	0.51
25:BA:686:U:H2'	25:BA:788:A:N1	2.25	0.51
27:BC:156:SER:O	27:BC:159:THR:HB	2.11	0.51
28:BD:33:ARG:NH1	28:BD:53:GLY:O	2.41	0.51
31:BG:51:PHE:CE1	31:BG:68:ARG:HA	2.46	0.51
37:BM:34:LYS:HB2	37:BM:131:VAL:CG2	2.40	0.51
37:BM:26:VAL:CG1	37:BM:133:LYS:HA	2.41	0.51
4:DD:173:VAL:HG12	4:DD:174:ASP:H	1.75	0.51
4:DD:95:GLU:OE2	4:DD:104:ARG:NH1	2.42	0.51
1:DA:1240:U:OP2	7:DG:116:MET:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:DI:119:ARG:NH1	9:DI:123:ARG:HD3	2.26	0.51
12:DL:107:VAL:HG23	12:DL:117:TYR:HB3	1.92	0.51
19:DS:63:THR:HG22	19:DS:66:MET:SD	2.51	0.51
13:DM:86:TYR:H	19:DS:73:GLU:HB2	1.76	0.51
1:AA:324:G:N2	1:AA:326:G:H3'	2.25	0.51
1:AA:467:U:H3'	1:AA:468:A:H5''	1.92	0.51
13:AM:72:GLU:HA	13:AM:75:MET:CG	2.40	0.51
19:AS:39:THR:HA	19:AS:70:LYS:HA	1.92	0.51
24:AX:63:G:N3	52:B1:27:ARG:NH1	2.59	0.51
25:BA:157:C:H42	25:BA:169:G:H1	1.58	0.51
25:BA:19:A:H2'	25:BA:20:C:C6	2.45	0.51
25:CA:1794:A:H2'	25:CA:1795:C:C6	2.46	0.51
25:CA:1847:A:O2'	25:CA:1848:A:O5'	2.28	0.51
25:CA:2162:G:H4'	25:CA:2163:A:OP1	2.10	0.51
25:CA:572:A:H3'	25:CA:573:U:O4'	2.11	0.51
39:CO:103:VAL:O	39:CO:106:LEU:N	2.43	0.51
2:DB:35:ARG:O	2:DB:37:LYS:N	2.39	0.51
5:DE:74:VAL:HG23	5:DE:75:ALA:N	2.26	0.51
19:AS:18:LYS:C	19:AS:18:LYS:HE2	2.30	0.51
25:BA:84:A:H62	25:BA:101:A:H2	1.59	0.51
25:BA:215:G:O3'	25:BA:216:A:H4'	2.10	0.51
28:BD:142:VAL:HB	28:BD:143:PRO:HD2	1.93	0.51
28:BD:57:ALA:O	28:BD:59:ARG:N	2.42	0.51
33:BI:104:GLN:HG2	33:BI:105:LEU:N	2.25	0.51
25:CA:544:C:C4	25:CA:545:U:C5	2.98	0.51
31:CG:154:GLU:OE2	31:CG:156:TYR:N	2.44	0.51
49:CY:17:GLU:HB3	49:CY:53:VAL:HG11	1.93	0.51
4:DD:127:GLY:O	4:DD:128:ARG:HB2	2.11	0.51
4:DD:170:TRP:CZ2	4:DD:182:PHE:CE2	2.99	0.51
5:DE:44:GLY:CA	5:DE:74:VAL:HG21	2.40	0.51
9:DI:46:MET:SD	9:DI:49:ARG:N	2.83	0.51
1:AA:1014:A:H4'	19:AS:14:HIS:CE1	2.46	0.51
4:AD:5:LEU:CG	4:AD:6:GLY:H	2.24	0.51
5:AE:46:VAL:HG13	5:AE:118:ALA:HB2	1.91	0.51
8:AH:112:THR:O	8:AH:116:ALA:N	2.40	0.51
13:AM:22:ILE:HG13	13:AM:25:VAL:CG2	2.41	0.51
22:AV:162:GLN:NE2	25:BA:1942:C:H4'	2.26	0.51
25:BA:2091:C:H4'	48:BX:55:MET:CE	2.41	0.51
25:BA:2365:G:H4'	47:BW:58:PHE:CE1	2.46	0.51
25:BA:2731:G:N7	58:BA:3002:PAR:H34	2.26	0.51
25:BA:533:G:H5'	41:BQ:23:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:601:C:O2'	25:BA:605:G:OP1	2.26	0.51
25:BA:714:U:O2'	25:BA:716:A:N7	2.36	0.51
25:BA:78:U:H2'	25:BA:79:C:C6	2.46	0.51
25:BA:297:G:O3'	45:BU:84:PHE:CG	2.64	0.51
25:CA:2800:A:C2	25:CA:2895:G:H1'	2.46	0.51
27:CC:106:PRO:HD2	27:CC:109:LEU:HD21	1.93	0.51
27:CC:8:THR:HG23	27:CC:12:ARG:HD2	1.93	0.51
32:CH:124:THR:HG23	32:CH:128:HIS:CE1	2.46	0.51
34:CJ:93:ILE:HD12	34:CJ:94:ALA:N	2.26	0.51
39:CO:92:PHE:N	39:CO:92:PHE:CD1	2.78	0.51
1:DA:238:A:OP1	17:DQ:40:ARG:NH1	2.42	0.51
7:DG:38:THR:HG23	7:DG:39:ALA:N	2.26	0.51
16:DP:5:ARG:NH2	16:DP:6:LEU:HB2	2.25	0.51
17:DQ:52:GLU:N	17:DQ:52:GLU:OE1	2.44	0.51
55:B4:27:CYS:SG	55:B4:33:HIS:ND1	2.84	0.50
25:BA:646:U:H5'	25:BA:647:G:H5''	1.93	0.50
32:BH:9:VAL:O	32:BH:13:GLY:N	2.41	0.50
25:CA:1936:A:H2	25:CA:1943:U:H3	1.58	0.50
58:CA:3168:PAR:H11	58:CA:3168:PAR:O52	2.10	0.50
27:CC:196:ASN:HB3	27:CC:199:HIS:HB2	1.93	0.50
32:CH:125:THR:OG1	32:CH:146:VAL:O	2.25	0.50
37:CM:117:PHE:O	37:CM:121:ALA:N	2.38	0.50
1:AA:378:G:N2	1:AA:386:C:O2	2.45	0.50
3:AC:63:SER:OG	3:AC:64:ILE:N	2.44	0.50
1:AA:428:G:H5'	4:AD:9:LEU:HD21	1.94	0.50
13:AM:87:ARG:NH1	13:AM:97:VAL:HG21	2.26	0.50
25:BA:2279:G:N7	47:BW:12:ARG:NH1	2.59	0.50
32:BH:120:GLY:O	32:BH:122:LEU:N	2.44	0.50
34:BJ:45:THR:HG22	41:BQ:63:ARG:HH21	1.77	0.50
25:CA:1023:U:OP2	60:CA:3705:HOH:O	2.19	0.50
25:CA:2702:G:C6	25:CA:2703:C:C4	2.99	0.50
1:DA:1122:U:H2'	1:DA:1123:U:H5'	1.93	0.50
1:DA:577:G:C8	1:DA:816:A:C6	2.99	0.50
1:DA:736:C:H2'	1:DA:737:C:C6	2.46	0.50
7:DG:56:LYS:NZ	7:DG:60:GLU:OE1	2.34	0.50
1:AA:643:C:OP1	8:AH:31:LYS:NZ	2.44	0.50
8:AH:29:SER:HB3	8:AH:57:PRO:HB2	1.94	0.50
13:AM:95:LEU:HB3	13:AM:96:PRO:CD	2.41	0.50
21:AU:53:VAL:HG13	21:AU:54:LYS:H	1.77	0.50
54:B3:16:THR:O	54:B3:19:GLY:N	2.43	0.50
25:BA:1379:U:P	60:BA:3756:HOH:O	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1778:U:H2'	25:BA:1784:A:N6	2.26	0.50
25:BA:2633:G:N2	25:BA:2785:C:O2	2.39	0.50
25:BA:600:G:N3	29:BE:100:MET:HE1	2.27	0.50
25:BA:2685:G:OP1	35:BK:78:ARG:NH2	2.43	0.50
42:BR:16:GLU:HA	42:BR:98:ILE:CD1	2.41	0.50
25:CA:1171:G:N2	25:CA:1178:C:N3	2.46	0.50
25:CA:2207:C:N3	25:CA:2218:G:C2	2.79	0.50
25:CA:2822:G:H2'	25:CA:2823:A:H5''	1.92	0.50
25:CA:458:G:O2'	25:CA:469:G:O6	2.25	0.50
27:CC:144:GLU:HB3	27:CC:187:CYS:HB2	1.94	0.50
35:CK:61:VAL:HG21	35:CK:112:PHE:HE1	1.76	0.50
37:CM:47:GLU:OE2	37:CM:51:ARG:NH2	2.43	0.50
1:DA:66:A:H4'	1:DA:173:U:C5	2.46	0.50
1:DA:791:G:C6	1:DA:792:A:N7	2.80	0.50
1:DA:839:C:H2'	1:DA:840:C:O4'	2.11	0.50
4:DD:61:VAL:O	4:DD:63:ARG:N	2.44	0.50
13:DM:23:TYR:CG	13:DM:69:LEU:HD21	2.47	0.50
20:DT:67:ILE:HD12	20:DT:68:HIS:H	1.75	0.50
18:AR:20:GLU:N	18:AR:22:ASP:O	2.44	0.50
19:AS:18:LYS:HZ2	19:AS:31:LEU:HD13	1.76	0.50
19:AS:67:VAL:HG12	19:AS:68:GLY:N	2.27	0.50
39:BO:31:THR:HG22	39:BO:34:HIS:H	1.77	0.50
40:BP:91:VAL:HG12	40:BP:92:ARG:H	1.77	0.50
48:BX:31:ASN:HB2	48:BX:33:HIS:CE1	2.46	0.50
25:CA:1266:G:O2'	25:CA:2012:G:O6	2.26	0.50
25:CA:2297:A:C2	25:CA:2298:A:C8	3.00	0.50
25:CA:892:A:H2'	25:CA:892:A:N3	2.27	0.50
32:CH:121:VAL:HG23	32:CH:128:HIS:CE1	2.46	0.50
35:CK:76:VAL:CG1	40:CP:72:VAL:HG23	2.42	0.50
1:DA:346:G:O2'	1:DA:347:G:OP1	2.26	0.50
1:DA:437:U:O2'	4:DD:120:HIS:ND1	2.34	0.50
2:DB:216:ALA:O	2:DB:220:THR:OG1	2.29	0.50
8:DH:87:LYS:NZ	8:DH:93:PRO:HD3	2.26	0.50
1:DA:1358:U:P	14:DN:75:ARG:NH2	2.85	0.50
16:DP:8:ARG:H	16:DP:28:ARG:HD3	1.76	0.50
16:DP:67:ILE:HG22	16:DP:71:VAL:CG2	2.42	0.50
3:AC:156:ARG:HA	3:AC:163:ALA:HA	1.93	0.50
7:AG:49:THR:HG21	7:AG:121:ALA:HB1	1.93	0.50
14:AN:56:SER:CB	14:AN:57:PRO:CD	2.89	0.50
56:B5:20:TYR:O	56:B5:21:THR:OG1	2.17	0.50
25:BA:1074:G:H2'	25:BA:1075:C:H5'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1786:A:H1'	25:BA:1938:A:N6	2.27	0.50
25:BA:2088:A:C5	25:BA:2089:C:C5	2.99	0.50
25:BA:2504:U:OP2	60:BA:3676:HOH:O	2.20	0.50
25:BA:671:C:H6	25:BA:671:C:H5'	1.77	0.50
25:BA:861:A:C2	25:BA:917:A:C4	2.98	0.50
36:BL:39:LYS:NZ	60:BL:305:HOH:O	2.44	0.50
42:BR:38:VAL:HG13	42:BR:54:VAL:HG13	1.93	0.50
43:BS:95:ARG:HD3	43:BS:96:ILE:O	2.11	0.50
25:CA:1693:U:H4'	25:CA:1694:C:OP2	2.12	0.50
1:AA:722:G:H3'	21:AU:45:ARG:NH2	2.26	0.50
1:AA:950:U:OP2	13:AM:101:ARG:NH1	2.45	0.50
12:AL:87:VAL:H	12:AL:93:VAL:HG11	1.77	0.50
25:BA:422:A:OP2	60:BA:3564:HOH:O	2.20	0.50
25:BA:2304:G:O2'	30:BF:129:MET:O	2.29	0.50
32:BH:96:THR:HA	32:BH:99:ILE:CG2	2.41	0.50
25:CA:1667:G:O2'	25:CA:1991:U:O4	2.19	0.50
25:CA:1992:G:N2	25:CA:1996:C:O2'	2.44	0.50
25:CA:547:A:N7	25:CA:548:G:N2	2.58	0.50
28:CD:119:ALA:HB3	28:CD:165:MET:HE3	1.93	0.50
30:CF:90:LEU:HD12	30:CF:90:LEU:N	2.27	0.50
25:CA:927:A:O2'	50:CZ:38:GLU:OE2	2.29	0.50
8:DH:31:LYS:O	8:DH:33:LYS:N	2.43	0.50
1:AA:815:A:O2'	1:AA:816:A:OP1	2.24	0.50
4:AD:23:SER:O	4:AD:25:VAL:N	2.44	0.50
7:AG:107:ALA:CB	7:AG:133:THR:HG21	2.41	0.50
10:AJ:35:GLN:HE21	10:AJ:80:THR:HG22	1.76	0.50
1:AA:706:A:H4'	11:AK:31:ILE:HD11	1.93	0.50
25:BA:1399:C:H2'	25:BA:1400:U:C6	2.47	0.50
25:BA:2502:G:C5'	25:BA:2503:A:H5''	2.41	0.50
25:BA:1789:A:P	27:BC:220:ARG:HE	2.35	0.50
28:BD:184:ARG:NH2	40:BP:10:GLU:OE1	2.44	0.50
31:BG:148:ARG:NH1	31:BG:166:GLU:OE2	2.45	0.50
25:CA:811:U:C2	25:CA:1251:C:C5	3.00	0.50
29:CE:108:ILE:HD13	29:CE:181:ILE:HG13	1.93	0.50
1:DA:1072:G:OP1	5:DE:62:LYS:NZ	2.44	0.50
4:DD:120:HIS:O	4:DD:121:LYS:HB2	2.12	0.50
4:DD:145:ILE:HD13	4:DD:150:LYS:HE2	1.92	0.50
1:AA:1124:G:O2'	1:AA:1127:G:O6	2.30	0.50
1:AA:1496:C:H5''	1:AA:1497:G:OP2	2.11	0.50
1:AA:642:A:N3	8:AH:105:SER:HB3	2.27	0.50
14:AN:64:CYS:HB2	14:AN:80:SER:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AV:126:ARG:HG2	22:AV:169:ILE:HG13	1.94	0.50
54:B3:31:ILE:O	54:B3:33:THR:N	2.45	0.50
32:BH:146:VAL:HG13	32:BH:147:VAL:H	1.77	0.50
25:CA:2026:U:H2'	25:CA:2027:G:O4'	2.11	0.50
25:CA:2771:C:H2'	25:CA:2772:C:C6	2.47	0.50
30:CF:115:GLY:HA2	30:CF:175:PRO:HB2	1.94	0.50
38:CN:79:LEU:O	38:CN:81:ASN:N	2.42	0.50
43:CS:29:VAL:HG21	43:CS:107:VAL:HG21	1.93	0.50
43:CS:23:LEU:HD12	43:CS:24:ILE:HG23	1.94	0.50
49:CY:5:GLU:O	49:CY:7:ARG:N	2.41	0.50
1:DA:640:A:O3'	8:DH:108:LYS:NZ	2.44	0.50
4:DD:99:ASP:HB2	4:DD:115:ARG:CZ	2.41	0.50
1:AA:825:A:O2'	8:AH:13:ARG:NH1	2.45	0.50
1:AA:860:A:H2'	1:AA:861:G:O4'	2.12	0.50
4:AD:9:LEU:CD1	4:AD:10:LYS:N	2.75	0.50
10:AJ:19:ASP:OD1	10:AJ:72:ARG:NH1	2.45	0.50
12:AL:93:VAL:HG22	12:AL:95:TYR:H	1.76	0.50
25:BA:1060:U:N1	25:BA:1062:G:H5'	2.26	0.50
25:BA:1861:G:C6	58:BA:3005:PAR:O61	2.53	0.50
27:BC:143:VAL:HB	27:BC:153:LEU:HB2	1.94	0.50
29:BE:162:ARG:NE	29:BE:163:ASN:H	2.10	0.50
43:BS:63:GLY:O	43:BS:64:ALA:HB3	2.12	0.50
25:CA:1026:G:H1'	25:CA:1134:A:C2	2.47	0.50
25:CA:2813:A:H2'	25:CA:2814:A:O4'	2.12	0.50
25:CA:959:A:N3	25:CA:2457:U:O2'	2.45	0.50
30:CF:1:ALA:HA	30:CF:96:TRP:HB2	1.94	0.50
35:CK:88:ASN:O	35:CK:90:ASN:N	2.44	0.50
24:DW:55:U:O2'	24:DW:57:G:N7	2.33	0.50
1:AA:147:G:H2'	1:AA:148:G:C8	2.47	0.49
4:AD:151:LYS:HB3	4:AD:178:MET:HE3	1.94	0.49
14:AN:5:MET:SD	14:AN:8:ARG:NH2	2.85	0.49
16:AP:10:GLY:HA3	16:AP:15:PRO:HA	1.94	0.49
25:BA:1820:U:H4'	25:BA:1821:A:OP2	2.12	0.49
25:BA:2315:G:O2'	30:BF:124:ARG:NE	2.44	0.49
32:BH:146:VAL:HG22	32:BH:147:VAL:N	2.27	0.49
25:CA:139:U:N3	44:CT:2:ILE:CD1	2.68	0.49
25:CA:1940:U:C2	25:CA:1965:C:OP2	2.65	0.49
25:CA:2615:U:C2	51:C0:3:GLN:HA	2.47	0.49
25:CA:2728:U:O2'	25:CA:2729:G:P	2.70	0.49
40:CP:12:MET:HB2	40:CP:76:HIS:CD2	2.47	0.49
1:DA:675:A:O2'	11:DK:116:ILE:O	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:DU:33:ARG:HG2	21:DU:34:ARG:N	2.27	0.49
1:AA:1186:G:O3'	9:AI:115:LYS:NZ	2.45	0.49
1:AA:809:G:H2'	1:AA:810:C:O5'	2.12	0.49
1:AA:993:G:O2'	1:AA:994:A:N7	2.44	0.49
13:AM:109:ARG:NH1	13:AM:109:ARG:HB2	2.27	0.49
14:AN:96:LEU:C	14:AN:96:LEU:HD12	2.33	0.49
24:AX:73:A:O2'	24:AX:74:C:OP1	2.20	0.49
25:BA:2356:U:O3'	47:BW:18:ARG:HD3	2.12	0.49
34:BJ:19:ASP:O	34:BJ:23:LYS:NZ	2.41	0.49
34:BJ:30:THR:HG22	34:BJ:31:GLU:N	2.27	0.49
43:BS:25:ARG:HH12	43:BS:74:ILE:H	1.60	0.49
47:BW:38:GLN:OE1	47:BW:42:LYS:N	2.45	0.49
25:CA:1102:C:H2'	25:CA:1103:A:C8	2.47	0.49
27:CC:73:ILE:O	27:CC:116:GLN:NE2	2.45	0.49
29:CE:146:VAL:HG13	29:CE:167:VAL:HG23	1.94	0.49
2:DB:164:ILE:HG23	2:DB:165:ASP:N	2.27	0.49
4:DD:76:TYR:O	4:DD:79:ALA:N	2.45	0.49
9:DI:75:GLN:O	9:DI:78:ALA:N	2.45	0.49
16:DP:6:LEU:HB3	16:DP:17:TYR:HB3	1.95	0.49
20:DT:83:ILE:HG22	20:DT:84:ASN:N	2.27	0.49
4:AD:140:ASN:N	4:AD:182:PHE:CZ	2.80	0.49
30:BF:133:GLU:HG2	30:BF:136:ILE:HD11	1.93	0.49
25:CA:910:A:H2'	25:CA:911:A:C8	2.47	0.49
27:CC:97:ASP:N	27:CC:97:ASP:OD1	2.44	0.49
25:CA:534:U:O2'	41:CQ:48:ASP:OD2	2.20	0.49
8:DH:87:LYS:NZ	8:DH:125:ILE:HG21	2.27	0.49
9:DI:18:ARG:HD3	9:DI:66:THR:HG23	1.95	0.49
3:AC:19:ASN:O	3:AC:40:ARG:NH2	2.46	0.49
25:BA:815:C:OP1	42:BR:85:LYS:NZ	2.46	0.49
32:BH:145:ASN:CG	32:BH:146:VAL:N	2.65	0.49
30:CF:130:GLY:HA2	30:CF:152:ASP:HA	1.93	0.49
45:CU:5:ARG:O	45:CU:24:VAL:HG21	2.12	0.49
1:DA:11:G:C5	1:DA:12:U:C5	3.01	0.49
1:DA:496:A:H2'	1:DA:497:G:C8	2.48	0.49
1:DA:731:G:H5'	1:DA:766:A:H4'	1.94	0.49
1:AA:79:G:H2'	1:AA:80:A:C8	2.47	0.49
2:AB:164:ILE:HG23	2:AB:165:ASP:H	1.76	0.49
4:AD:65:TYR:CD2	4:AD:94:LEU:HD22	2.48	0.49
11:AK:35:THR:OG1	11:AK:40:ASN:N	2.46	0.49
13:AM:72:GLU:OE1	30:BF:109:ARG:NH1	2.43	0.49
25:BA:1343:G:C6	25:BA:1344:U:O4	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1450:G:C6	25:BA:1451:C:N4	2.80	0.49
25:BA:2142:A:H2'	25:BA:2143:C:C5	2.47	0.49
30:BF:100:GLU:O	30:BF:104:THR:OG1	2.30	0.49
32:BH:53:GLU:O	32:BH:57:LYS:N	2.45	0.49
29:BE:23:PHE:CE1	36:BL:2:ARG:NH2	2.80	0.49
42:BR:51:VAL:HB	42:BR:52:PRO:CD	2.42	0.49
25:CA:2096:C:H2'	25:CA:2097:A:C8	2.48	0.49
25:CA:374:A:N6	25:CA:400:G:O2'	2.44	0.49
25:CA:669:G:O2'	25:CA:670:A:P	2.69	0.49
25:CA:674:G:H1'	29:CE:69:ARG:CD	2.42	0.49
25:CA:728:G:H1'	27:CC:12:ARG:NH2	2.28	0.49
30:CF:24:VAL:O	30:CF:26:GLN:N	2.44	0.49
37:CM:129:THR:OG1	37:CM:130:PHE:N	2.44	0.49
41:CQ:39:ILE:O	41:CQ:43:GLN:HG2	2.13	0.49
47:CW:29:VAL:CG2	47:CW:33:SER:HB2	2.43	0.49
1:DA:184:G:N2	1:DA:194:C:C2	2.81	0.49
3:DC:134:MET:O	3:DC:138:VAL:N	2.44	0.49
4:DD:124:MET:CG	4:DD:143:VAL:HA	2.42	0.49
4:DD:177:LYS:O	4:DD:178:MET:HB3	2.11	0.49
4:DD:7:PRO:HB3	4:DD:9:LEU:HD21	1.95	0.49
9:DI:23:PRO:HA	9:DI:61:LEU:CB	2.42	0.49
8:AH:110:VAL:O	8:AH:111:MET:HB3	2.11	0.49
1:AA:127:G:O2'	17:AQ:6:ARG:NH1	2.46	0.49
54:B3:31:ILE:HG13	54:B3:35:LYS:HE3	1.95	0.49
25:BA:1320:C:N3	25:BA:1331:G:O6	2.44	0.49
25:BA:2323:G:C2'	25:BA:2324:U:H5''	2.43	0.49
32:BH:91:PHE:HB3	1:DA:368:U:C4	2.48	0.49
34:BJ:98:GLU:CD	34:BJ:126:ALA:HB2	2.31	0.49
25:CA:2461:A:H1'	25:CA:2492:U:C2	2.48	0.49
25:CA:26:G:C6	25:CA:27:G:N1	2.81	0.49
26:CB:3101:A:H2'	26:CB:3102:G:O4'	2.12	0.49
32:BH:91:PHE:HB3	1:DA:368:U:C2	2.48	0.49
1:DA:428:G:H4'	4:DD:9:LEU:HD22	1.93	0.49
9:DI:47:VAL:O	9:DI:50:GLN:NE2	2.44	0.49
9:DI:6:TYR:OH	9:DI:87:LEU:N	2.45	0.49
1:AA:1216:A:H2'	1:AA:1217:C:C6	2.48	0.49
1:AA:1344:C:OP1	9:AI:124:ARG:NH2	2.45	0.49
1:AA:663:A:N1	1:AA:743:A:C2	2.80	0.49
8:AH:78:VAL:HG12	8:AH:127:CYS:HA	1.93	0.49
20:AT:6:SER:O	20:AT:8:LYS:N	2.45	0.49
22:AV:14:MET:O	22:AV:17:CYS:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:B3:35:LYS:O	54:B3:40:LYS:NZ	2.39	0.49
25:BA:675:A:N3	25:BA:2443:C:O2'	2.43	0.49
29:BE:129:PRO:CB	29:BE:159:LEU:HD11	2.43	0.49
36:BL:62:PRO:HG2	54:B3:24:LYS:CG	2.42	0.49
38:BN:55:ALA:HA	38:BN:80:PHE:CE1	2.48	0.49
25:CA:1847:A:HO2'	25:CA:1848:A:P	2.35	0.49
25:CA:2242:G:N7	60:CA:3498:HOH:O	2.35	0.49
25:CA:612:G:C6	25:CA:614:A:C2	3.00	0.49
50:CZ:39:ASP:OD2	50:CZ:44:ARG:NH1	2.45	0.49
1:DA:21:G:H2'	1:DA:22:G:C8	2.48	0.49
2:DB:143:LYS:O	2:DB:146:ASN:N	2.43	0.49
2:DB:70:VAL:N	2:DB:162:PHE:O	2.39	0.49
21:DU:37:PHE:O	21:DU:39:GLU:N	2.39	0.49
4:AD:203:LEU:HD23	4:AD:204:TYR:N	2.28	0.49
14:AN:45:VAL:O	14:AN:47:LYS:N	2.45	0.49
19:AS:51:VAL:HG22	19:AS:71:LEU:HD13	1.94	0.49
25:BA:1124:G:H2'	25:BA:1125:G:H5'	1.95	0.49
25:BA:475:C:O2'	25:BA:505:A:N3	2.31	0.49
25:BA:819:A:OP2	25:BA:1187:G:N2	2.39	0.49
26:BB:3060:C:N4	60:BB:3302:HOH:O	2.45	0.49
27:BC:175:LEU:O	27:BC:177:SER:N	2.46	0.49
27:BC:251:THR:HG22	27:BC:252:LYS:N	2.28	0.49
25:CA:959:A:N6	37:CM:82:MET:HE3	2.28	0.49
28:CD:133:THR:OG1	28:CD:134:HIS:N	2.44	0.49
1:DA:110:C:N4	1:DA:111:G:C6	2.81	0.49
1:DA:307:C:C5	1:DA:308:C:C5	3.01	0.49
1:DA:421:U:H4'	1:DA:422:C:OP2	2.13	0.49
9:DI:54:LEU:O	9:DI:55:VAL:HG22	2.12	0.49
1:AA:386:C:H2'	1:AA:387:U:C5'	2.39	0.49
24:AX:20:U:H3'	24:AX:21:A:C5'	2.43	0.49
25:BA:2210:U:H4'	25:BA:2211:A:H5'	1.95	0.49
25:BA:2291:U:H2'	25:BA:2292:U:C6	2.48	0.49
25:BA:492:A:OP2	58:BA:3004:PAR:N12	2.44	0.49
29:BE:127:GLU:N	29:BE:127:GLU:OE1	2.41	0.49
39:BO:79:ALA:HA	39:BO:115:LEU:CD1	2.42	0.49
27:CC:8:THR:O	27:CC:9:SER:HB3	2.13	0.49
36:CL:36:LYS:O	36:CL:40:SER:OG	2.28	0.49
37:CM:42:THR:OG1	37:CM:43:ALA:N	2.45	0.49
1:DA:708:C:O2'	1:DA:709:U:H5'	2.12	0.49
7:DG:67:GLU:HA	7:DG:70:ARG:HE	1.76	0.49
1:AA:1089:G:N2	1:AA:1090:U:H1'	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:530:G:H2'	1:AA:530:G:N3	2.27	0.49
2:AB:141:LEU:HD23	2:AB:145:GLU:HG3	1.95	0.49
7:AG:102:ARG:HG3	7:AG:103:TRP:CE3	2.48	0.49
13:AM:87:ARG:NH2	13:AM:97:VAL:HG11	2.27	0.49
19:AS:18:LYS:HD2	19:AS:31:LEU:HD11	1.95	0.49
25:BA:136:G:H2'	25:BA:137:U:C6	2.48	0.49
25:BA:320:A:H4'	25:BA:322:A:N7	2.27	0.49
25:BA:1952:A:N1	35:BK:22:ILE:HD11	2.27	0.49
51:C0:24:VAL:O	51:C0:26:SER:N	2.41	0.49
25:CA:1456:G:C5	25:CA:1457:U:C5	3.01	0.49
25:CA:2038:G:H2'	25:CA:2039:U:O4'	2.12	0.49
27:CC:8:THR:O	27:CC:12:ARG:NH1	2.45	0.49
1:DA:1122:U:H2'	1:DA:1123:U:C5'	2.42	0.49
1:DA:458:U:H2'	1:DA:459:A:C8	2.48	0.49
3:DC:41:GLN:N	3:DC:41:GLN:OE1	2.39	0.49
5:DE:106:ILE:HD11	5:DE:124:LEU:HD22	1.95	0.49
13:DM:95:LEU:HB2	13:DM:96:PRO:HD2	1.95	0.49
1:AA:881:G:OP2	12:AL:6:GLN:NE2	2.43	0.48
4:AD:125:VAL:HG13	4:AD:126:ASN:H	1.78	0.48
9:AI:83:ILE:O	9:AI:86:ALA:N	2.46	0.48
10:AJ:53:ILE:CG1	10:AJ:61:ALA:HB1	2.43	0.48
13:AM:48:LEU:HD13	13:AM:53:ILE:HD11	1.95	0.48
53:B2:1:MET:N	53:B2:1:MET:HE3	2.27	0.48
25:BA:2737:G:H2'	25:BA:2738:A:C8	2.48	0.48
35:BK:121:GLU:OE2	40:BP:64:SER:OG	2.26	0.48
25:CA:2112:G:N3	25:CA:2112:G:H2'	2.28	0.48
25:CA:642:U:O2'	25:CA:644:A:N7	2.27	0.48
30:CF:95:MET:O	30:CF:97:GLU:N	2.46	0.48
43:CS:12:SER:OG	43:CS:13:SER:N	2.45	0.48
1:DA:1330:U:H4'	13:DM:23:TYR:CE1	2.48	0.48
1:DA:1347:G:H8	9:DI:109:ARG:HB3	1.78	0.48
1:DA:1490:U:OP2	58:DA:1654:PAR:N64	2.46	0.48
1:DA:929:G:C5	1:DA:930:C:C5	3.01	0.48
3:DC:131:ARG:NH2	3:DC:166:GLU:OE2	2.46	0.48
4:AD:5:LEU:HD12	4:AD:6:GLY:N	2.28	0.48
4:AD:59:GLN:HA	4:AD:62:ARG:HG2	1.93	0.48
25:BA:1093:G:HO2'	25:BA:1099:G:H1	1.62	0.48
25:BA:2839:G:OP1	38:BN:46:ARG:HG2	2.13	0.48
27:BC:244:VAL:HG22	27:BC:245:THR:O	2.13	0.48
37:BM:50:ARG:HD3	37:BM:65:ILE:HD11	1.94	0.48
38:BN:12:ARG:NH2	38:BN:20:MET:HE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:BR:66:HIS:CG	42:BR:94:THR:HG22	2.48	0.48
25:CA:1063:G:O6	25:CA:1075:C:N4	2.41	0.48
25:CA:942:G:O2'	25:CA:1189:A:N3	2.45	0.48
25:CA:1747:U:H2'	25:CA:1748:C:C6	2.48	0.48
25:CA:281:C:H2'	25:CA:282:A:C8	2.48	0.48
30:CF:43:ILE:HG12	30:CF:78:ILE:HD11	1.94	0.48
34:CJ:62:VAL:HG11	34:CJ:101:ILE:HD11	1.94	0.48
35:CK:76:VAL:CG1	40:CP:72:VAL:CG2	2.91	0.48
43:CS:42:LYS:O	43:CS:46:LEU:HD12	2.13	0.48
45:CU:60:LYS:HG3	45:CU:61:GLU:N	2.28	0.48
1:DA:1191:A:H2'	1:DA:1192:C:C6	2.48	0.48
1:DA:188:C:N4	1:DA:189:A:N1	2.62	0.48
1:DA:382:A:C2	1:DA:383:A:C4	3.01	0.48
5:DE:136:VAL:C	5:DE:138:ARG:H	2.17	0.48
8:DH:10:MET:SD	8:DH:36:ILE:HD11	2.53	0.48
1:DA:1249:C:H4'	9:DI:75:GLN:HE22	1.79	0.48
9:DI:89:GLU:HG3	9:DI:90:TYR:CG	2.48	0.48
1:AA:264:C:N4	1:AA:265:G:C6	2.81	0.48
5:AE:69:ARG:O	5:AE:71:MET:N	2.39	0.48
7:AG:21:GLU:O	7:AG:24:ALA:N	2.45	0.48
7:AG:27:VAL:HG21	7:AG:40:GLU:HB3	1.94	0.48
7:AG:49:THR:HG23	7:AG:50:LEU:N	2.27	0.48
12:AL:87:VAL:HG23	12:AL:93:VAL:HG11	1.95	0.48
12:AL:8:VAL:HG23	17:AQ:31:HIS:CD2	2.48	0.48
19:AS:31:LEU:O	19:AS:50:ALA:N	2.44	0.48
1:AA:263:A:OP2	20:AT:74:ARG:NH2	2.47	0.48
32:BH:99:ILE:CD1	32:BH:130:VAL:HG21	2.43	0.48
34:BJ:136:GLN:N	34:BJ:137:PRO:HD3	2.29	0.48
36:BL:68:SER:O	36:BL:69:ARG:CB	2.61	0.48
38:BN:9:GLN:O	38:BN:17:ARG:NH2	2.45	0.48
46:BV:26:PHE:CD1	46:BV:26:PHE:C	2.86	0.48
25:CA:1478:G:H1	25:CA:1513:U:H3	1.61	0.48
27:CC:119:VAL:O	27:CC:133:ASN:ND2	2.45	0.48
31:CG:163:TYR:HB2	31:CG:166:GLU:HB2	1.95	0.48
42:CR:68:ARG:HD3	42:CR:92:TRP:CE2	2.48	0.48
43:CS:54:ALA:HA	43:CS:57:ASN:HB2	1.95	0.48
1:DA:1182:G:H4'	1:DA:1183:U:H5'	1.94	0.48
1:DA:1238:A:C2	1:DA:1303:C:H4'	2.48	0.48
1:DA:28:A:OP1	4:DD:73:ARG:NH1	2.45	0.48
5:DE:114:VAL:O	5:DE:118:ALA:N	2.38	0.48
1:DA:1318:A:H4'	19:DS:10:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1200:C:H4'	1:AA:1201:A:H5''	1.96	0.48
2:AB:114:LEU:O	2:AB:118:GLU:N	2.45	0.48
12:AL:35:THR:N	12:AL:54:ARG:O	2.46	0.48
25:BA:1192:G:OP2	36:BL:17:LYS:NZ	2.46	0.48
25:BA:1794:A:H1'	25:BA:1900:A:C2	2.48	0.48
25:BA:2009:A:N6	60:BA:3376:HOH:O	2.46	0.48
28:BD:99:GLU:HG2	28:BD:182:ALA:HB2	1.96	0.48
38:BN:12:ARG:CZ	38:BN:20:MET:HE1	2.43	0.48
47:BW:35:ILE:HG21	47:BW:78:ILE:HG21	1.95	0.48
50:BZ:39:ASP:OD1	50:BZ:44:ARG:NE	2.45	0.48
25:CA:2376:A:H2'	25:CA:2377:A:O4'	2.13	0.48
25:CA:2854:G:N2	25:CA:2864:G:C4	2.82	0.48
2:DB:57:LEU:CD1	2:DB:58:ASN:H	2.26	0.48
4:DD:9:LEU:HG	4:DD:10:LYS:N	2.28	0.48
1:AA:1343:G:N2	1:AA:1349:A:O2'	2.46	0.48
1:AA:1536:C:H2'	1:AA:1537:U:C6	2.49	0.48
1:AA:922:G:H4'	5:AE:25:VAL:HA	1.95	0.48
7:AG:4:ARG:HG3	7:AG:5:ARG:H	1.79	0.48
11:AK:20:VAL:HG13	11:AK:35:THR:HG23	1.94	0.48
11:AK:40:ASN:O	11:AK:41:ALA:CB	2.62	0.48
25:BA:1566:A:C6	27:BC:212:TRP:CZ3	3.02	0.48
25:BA:566:U:H2'	25:BA:567:U:O4'	2.14	0.48
25:BA:634:C:H2'	25:BA:635:C:C6	2.48	0.48
25:BA:1568:G:H4'	27:BC:58:LYS:HG2	1.93	0.48
27:BC:78:GLU:OE1	27:BC:100:ARG:NH1	2.46	0.48
31:BG:41:GLU:OE1	31:BG:54:ARG:NE	2.47	0.48
39:BO:64:TYR:O	39:BO:67:ASN:ND2	2.47	0.48
25:CA:796:C:H2'	25:CA:797:G:C8	2.48	0.48
25:CA:833:A:H2'	25:CA:834:G:C8	2.49	0.48
27:CC:143:VAL:HG21	27:CC:161:VAL:HG21	1.95	0.48
32:CH:64:ALA:O	32:CH:68:ARG:NH2	2.47	0.48
39:CO:30:ARG:HE	39:CO:102:ARG:HE	1.61	0.48
1:DA:376:G:C5'	16:DP:5:ARG:NE	2.76	0.48
14:DN:80:SER:O	14:DN:82:ILE:N	2.45	0.48
1:AA:1144:G:N1	1:AA:1145:A:N1	2.61	0.48
4:AD:91:LEU:HD12	4:AD:197:GLU:HG3	1.96	0.48
8:AH:32:LEU:O	8:AH:35:ALA:N	2.46	0.48
1:AA:981:U:P	14:AN:12:ARG:HH22	2.36	0.48
21:AU:6:VAL:HG21	21:AU:17:ARG:HD3	1.96	0.48
24:AX:53:G:H1	24:AX:58:A:H2'	1.79	0.48
53:B2:43:THR:HG23	53:B2:44:VAL:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:B4:27:CYS:SG	55:B4:30:GLU:OE2	2.71	0.48
25:BA:2115:G:N2	25:BA:2119:A:N7	2.62	0.48
25:BA:2499:C:OP2	60:BA:3689:HOH:O	2.19	0.48
26:BB:3037:C:C4	26:BB:3038:C:C4	3.02	0.48
26:BB:3094:A:C6	26:BB:3095:U:C4	3.02	0.48
39:BO:31:THR:O	39:BO:102:ARG:NH1	2.41	0.48
40:BP:91:VAL:HG11	40:BP:96:LEU:CD2	2.44	0.48
25:CA:2214:C:H2'	25:CA:2215:C:O4'	2.13	0.48
25:CA:463:G:N2	25:CA:466:A:OP2	2.39	0.48
25:CA:657:U:H2'	25:CA:658:U:C6	2.47	0.48
30:CF:100:GLU:O	30:CF:103:ILE:N	2.39	0.48
31:CG:115:GLN:OE1	31:CG:115:GLN:N	2.47	0.48
35:CK:88:ASN:OD1	35:CK:91:SER:N	2.46	0.48
25:CA:2230:G:H1'	48:CX:31:ASN:HB3	1.93	0.48
25:CA:988:A:P	50:CZ:11:SER:HB3	2.53	0.48
4:DD:178:MET:C	4:DD:178:MET:SD	2.92	0.48
1:AA:1330:U:C4	1:AA:1331:G:C6	3.01	0.48
1:AA:204:G:H3'	1:AA:205:A:C5'	2.43	0.48
2:AB:101:LEU:HD23	2:AB:102:THR:N	2.28	0.48
4:AD:13:ARG:NH2	4:AD:37:ALA:O	2.42	0.48
8:AH:54:ASP:CG	8:AH:55:THR:H	2.17	0.48
12:AL:63:VAL:HG12	12:AL:64:THR:H	1.78	0.48
25:BA:466:A:N3	25:BA:683:U:H1'	2.29	0.48
25:BA:813:U:H2'	25:BA:814:C:C6	2.49	0.48
43:BS:73:LYS:HB2	43:BS:106:VAL:CG1	2.44	0.48
25:CA:1068:G:H2'	25:CA:1068:G:N3	2.28	0.48
25:CA:634:C:H2'	25:CA:635:C:C6	2.49	0.48
25:CA:708:G:N2	25:CA:724:U:H1'	2.29	0.48
1:DA:1119:C:OP2	9:DI:11:ARG:NH2	2.46	0.48
1:DA:1166:G:N1	1:DA:1169:A:OP2	2.46	0.48
1:DA:925:G:H1'	1:DA:1502:A:C4	2.49	0.48
1:DA:386:C:N4	1:DA:387:U:O4	2.47	0.48
1:DA:858:G:N7	60:DA:1815:HOH:O	2.35	0.48
4:DD:58:LYS:HA	4:DD:200:ILE:HD11	1.96	0.48
6:DF:3:HIS:HB2	6:DF:92:THR:HG23	1.95	0.48
7:DG:101:MET:O	7:DG:105:VAL:HG12	2.13	0.48
12:DL:12:ARG:HG2	12:DL:13:ALA:N	2.29	0.48
1:AA:1310:G:OP1	13:AM:79:ARG:NE	2.46	0.48
2:AB:47:VAL:HG23	2:AB:48:PRO:HD3	1.95	0.48
4:AD:55:LEU:HA	4:AD:58:LYS:HD2	1.96	0.48
21:AU:17:ARG:HE	21:AU:20:LYS:CE	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AV:98:ASP:O	22:AV:100:ARG:N	2.47	0.48
24:AX:70:G:H2'	24:AX:71:G:H5'	1.96	0.48
25:BA:2420:C:P	54:B3:33:THR:HG23	2.54	0.48
25:BA:1001:A:OP2	60:BA:3741:HOH:O	2.20	0.48
25:BA:1059:G:C5'	25:BA:1060:U:H2'	2.43	0.48
25:BA:1154:G:OP2	41:BQ:57:ARG:NH1	2.47	0.48
25:BA:2307:G:N2	25:BA:2311:A:H2'	2.29	0.48
25:BA:2607:G:H2'	25:BA:2608:G:O4'	2.13	0.48
25:BA:2800:A:C2	25:BA:2895:G:H1'	2.49	0.48
25:BA:324:A:H2'	25:BA:325:G:O4'	2.14	0.48
25:BA:519:U:O3'	43:BS:25:ARG:NH2	2.47	0.48
30:BF:37:MET:O	30:BF:39:VAL:N	2.47	0.48
29:BE:32:VAL:HG11	36:BL:6:LEU:HD13	1.96	0.48
25:CA:2755:C:O2'	25:CA:2756:U:H2'	2.14	0.48
37:CM:58:LYS:C	37:CM:60:GLN:H	2.17	0.48
49:CY:21:LEU:HA	49:CY:25:GLN:HB3	1.96	0.48
1:DA:1182:G:C3'	1:DA:1183:U:H5'	2.43	0.48
3:DC:172:ARG:CD	3:DC:174:PRO:HG3	2.43	0.48
4:DD:145:ILE:HD13	4:DD:150:LYS:CE	2.43	0.48
4:DD:99:ASP:HB2	4:DD:115:ARG:NH1	2.28	0.48
8:DH:10:MET:HA	8:DH:13:ARG:HE	1.79	0.48
13:DM:20:THR:C	13:DM:22:ILE:H	2.17	0.48
17:DQ:77:ARG:HG3	17:DQ:78:VAL:H	1.78	0.48
1:AA:815:A:N7	1:AA:1509:C:O2'	2.40	0.48
1:AA:976:G:OP2	1:AA:1358:U:O2'	2.31	0.48
2:AB:67:ILE:N	2:AB:89:GLN:HG3	2.29	0.48
5:AE:96:MET:HB3	5:AE:125:ALA:HB2	1.94	0.48
13:AM:12:HIS:N	13:AM:45:ILE:HG13	2.27	0.48
15:AO:89:ARG:HH22	25:BA:716:A:P	2.37	0.48
22:AV:44:GLU:OE2	22:AV:45:TYR:N	2.47	0.48
25:BA:975:A:H2	25:BA:1156:A:HO2'	1.61	0.48
25:BA:2121:G:N3	56:B5:170:ALA:N	2.61	0.48
25:BA:360:U:C4	25:BA:361:G:C6	3.01	0.48
25:BA:533:G:H5'	41:BQ:23:TYR:CD1	2.48	0.48
28:BD:104:VAL:HG23	28:BD:177:VAL:HG11	1.96	0.48
40:BP:59:THR:HG23	40:BP:72:VAL:HG12	1.96	0.48
42:BR:24:LYS:HA	42:BR:94:THR:HG23	1.95	0.48
25:CA:1378:A:O2'	25:CA:1380:G:N7	2.46	0.48
25:CA:1808:A:H3'	25:CA:1809:A:C8	2.49	0.48
25:CA:2409:G:C6	25:CA:2410:G:C5	3.02	0.48
25:CA:555:G:N2	58:CA:3169:PAR:H642	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:CU:73:ASN:HA	45:CU:95:PHE:CE2	2.49	0.48
48:CX:67:LEU:HA	48:CX:70:LEU:HG	1.96	0.48
1:DA:1013:G:OP1	19:DS:21:LYS:NZ	2.47	0.48
4:DD:58:LYS:HA	4:DD:200:ILE:CD1	2.44	0.48
1:AA:1494:G:OP2	58:AA:1672:PAR:N32	2.46	0.48
1:AA:390:U:O2'	16:AP:28:ARG:NH1	2.43	0.48
10:AJ:18:ILE:O	10:AJ:22:THR:N	2.45	0.48
51:B0:52:LYS:CE	51:B0:55:ALA:HA	2.44	0.48
54:B3:30:HIS:ND1	54:B3:31:ILE:HG23	2.28	0.48
25:BA:2070:A:H2'	25:BA:2071:A:O4'	2.14	0.48
25:BA:2571:U:O2'	28:BD:151:THR:OG1	2.31	0.48
30:BF:136:ILE:N	30:BF:136:ILE:HD13	2.28	0.48
32:BH:80:ILE:CD1	32:BH:82:SER:HB3	2.44	0.48
34:BJ:81:ILE:HG13	34:BJ:82:GLY:N	2.29	0.48
43:BS:85:ILE:H	43:BS:85:ILE:HD12	1.79	0.48
44:BT:20:ALA:HA	44:BT:31:VAL:HG21	1.96	0.48
51:C0:39:ARG:HB3	51:C0:40:HIS:HD2	1.79	0.48
25:CA:2377:A:H1'	39:CO:92:PHE:CZ	2.49	0.48
27:CC:16:VAL:HB	27:CC:203:VAL:HG22	1.96	0.48
28:CD:62:LYS:N	28:CD:63:PRO:CD	2.77	0.48
29:CE:113:VAL:HG12	29:CE:118:LEU:HD23	1.95	0.48
4:DD:65:TYR:HD1	4:DD:65:TYR:N	2.10	0.48
5:DE:109:GLY:HA2	5:DE:112:ARG:HG2	1.95	0.48
12:DL:88:LYS:O	12:DL:89:ASP:HB2	2.14	0.48
17:DQ:12:VAL:HG12	17:DQ:13:VAL:N	2.29	0.48
18:DR:52:GLN:C	18:DR:54:GLN:H	2.17	0.48
1:AA:1087:G:N2	1:AA:1099:G:H1'	2.29	0.47
1:AA:114:U:H2'	1:AA:115:G:H5'	1.96	0.47
12:AL:93:VAL:CG2	12:AL:94:ARG:N	2.76	0.47
14:AN:56:SER:HB3	14:AN:57:PRO:CD	2.43	0.47
25:BA:1432:G:H2'	25:BA:1433:A:C8	2.49	0.47
25:BA:1840:G:C6	25:BA:1841:U:C4	3.02	0.47
25:BA:2323:G:H2'	25:BA:2324:U:C5'	2.44	0.47
25:BA:2517:C:C6	25:BA:2542:A:N7	2.82	0.47
25:BA:974:G:N3	25:BA:974:G:H2'	2.28	0.47
42:BR:16:GLU:CA	42:BR:98:ILE:HD11	2.43	0.47
45:BU:15:GLY:O	45:BU:17:ASP:N	2.47	0.47
25:CA:2284:A:H3'	52:C1:5:ARG:NH2	2.29	0.47
25:CA:2391:G:O2'	25:CA:2424:C:N4	2.40	0.47
25:CA:616:A:H4'	29:CE:101:TYR:CE2	2.49	0.47
25:CA:84:A:N3	25:CA:85:G:H1'	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CH:130:VAL:HG22	32:CH:132:PHE:CE1	2.49	0.47
37:CM:33:LEU:HD21	37:CM:128:THR:HB	1.96	0.47
40:CP:90:ALA:HB2	40:CP:112:ARG:HA	1.95	0.47
1:DA:258:G:N7	60:DA:1721:HOH:O	2.36	0.47
1:DA:499:A:C6	1:DA:547:A:C8	3.01	0.47
4:DD:9:LEU:CG	4:DD:10:LYS:H	2.26	0.47
4:DD:65:TYR:CE2	4:DD:94:LEU:HB3	2.49	0.47
8:DH:10:MET:HE1	8:DH:36:ILE:HG12	1.95	0.47
8:DH:31:LYS:HA	8:DH:34:VAL:HG12	1.95	0.47
11:DK:125:LYS:O	21:DU:34:ARG:NE	2.44	0.47
1:DA:564:C:H5'	17:DQ:34:TYR:HE1	1.78	0.47
3:AC:39:VAL:HG23	3:AC:40:ARG:H	1.78	0.47
7:AG:35:LYS:O	7:AG:37:SER:N	2.44	0.47
14:AN:12:ARG:NE	14:AN:54:ASP:OD1	2.47	0.47
21:AU:17:ARG:HB2	21:AU:20:LYS:HG2	1.95	0.47
24:AX:55:U:H1'	24:AX:57:G:N7	2.29	0.47
25:BA:102:U:H2'	25:BA:102:U:O2	2.14	0.47
25:BA:1433:A:N1	25:BA:1434:A:C6	2.83	0.47
27:BC:142:ASN:ND2	27:BC:142:ASN:O	2.40	0.47
32:BH:82:SER:OG	32:BH:146:VAL:HG21	2.14	0.47
25:CA:1267:U:H2'	25:CA:1268:A:H5'	1.96	0.47
25:CA:1386:C:H2'	25:CA:1387:A:C8	2.49	0.47
31:CG:102:ILE:HG22	31:CG:104:LEU:CD1	2.44	0.47
38:CN:33:ILE:HG13	38:CN:118:ARG:CZ	2.44	0.47
1:DA:1152:A:H4'	10:DJ:15:HIS:CD2	2.49	0.47
1:DA:1360:A:H62	1:DA:1361:G:H21	1.61	0.47
1:DA:40:C:H2'	1:DA:41:G:C8	2.49	0.47
2:DB:131:LYS:HA	2:DB:134:ALA:HB3	1.96	0.47
15:DO:82:ILE:O	15:DO:86:GLY:N	2.47	0.47
1:AA:205:A:OP1	1:AA:205:A:H4'	2.13	0.47
7:AG:35:LYS:NZ	7:AG:38:THR:HG23	2.28	0.47
51:B0:12:ARG:HG3	51:B0:15:ARG:NH1	2.28	0.47
38:CN:98:LEU:HD11	51:C0:53:VAL:HG11	1.96	0.47
25:CA:118:A:C8	25:CA:119:A:C8	3.03	0.47
25:CA:1792:G:P	27:CC:204:LEU:HD12	2.55	0.47
25:CA:244:A:C2	25:CA:255:A:C4	3.02	0.47
25:CA:2727:A:O2'	35:CK:70:ARG:NH2	2.47	0.47
45:CU:40:LEU:HA	45:CU:61:GLU:HA	1.96	0.47
25:CA:2331:G:H4'	47:CW:41:THR:H	1.79	0.47
1:DA:328:C:O2	1:DA:328:C:H2'	2.14	0.47
1:DA:564:C:H5'	17:DQ:34:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:791:G:C5	1:DA:792:A:N7	2.82	0.47
2:DB:221:VAL:HG13	2:DB:222:ARG:N	2.28	0.47
5:DE:133:PRO:HA	5:DE:136:VAL:HG12	1.95	0.47
1:AA:1183:U:H3'	1:AA:1184:G:H5''	1.97	0.47
1:AA:386:C:C3'	1:AA:387:U:H5'	2.45	0.47
1:AA:937:A:H2'	1:AA:938:A:H5'	1.96	0.47
3:AC:108:LYS:N	3:AC:109:PRO:CD	2.77	0.47
13:AM:101:ARG:CD	13:AM:104:THR:HG23	2.44	0.47
25:BA:2756:U:OP2	55:B4:19:ARG:NE	2.47	0.47
25:BA:2798:U:H4'	25:BA:2799:A:H5'	1.96	0.47
25:BA:388:G:N7	25:BA:390:U:H2'	2.29	0.47
25:BA:533:G:C6	25:BA:534:U:C4	3.01	0.47
27:BC:43:ASN:HB3	27:BC:49:THR:HG21	1.97	0.47
32:BH:144:VAL:HG22	32:BH:145:ASN:H	1.80	0.47
42:BR:4:VAL:HA	42:BR:12:HIS:O	2.14	0.47
48:BX:32:LEU:HA	48:BX:51:SER:HA	1.95	0.47
25:CA:1475:G:O2'	25:CA:1514:G:O6	2.28	0.47
25:CA:1921:G:C6	58:CA:3167:PAR:N12	2.81	0.47
27:CC:251:THR:CG2	27:CC:252:LYS:N	2.77	0.47
1:DA:1492:A:H5'	12:DL:44:LYS:HA	1.96	0.47
1:DA:346:G:HO2'	1:DA:347:G:P	2.37	0.47
6:DF:13:ASP:C	6:DF:15:SER:H	2.17	0.47
6:DF:43:GLY:HA2	6:DF:58:HIS:CE1	2.49	0.47
1:DA:951:G:OP2	13:DM:101:ARG:NH2	2.45	0.47
1:AA:109:A:H2'	1:AA:326:G:N2	2.29	0.47
1:AA:532:A:N6	1:AA:1206:G:O2'	2.46	0.47
1:AA:790:A:C6	1:AA:791:G:C6	3.03	0.47
1:AA:824:G:H1'	8:AH:2:SER:CB	2.44	0.47
12:AL:54:ARG:HD2	12:AL:64:THR:HB	1.95	0.47
13:AM:12:HIS:N	13:AM:45:ILE:CG1	2.77	0.47
25:BA:1132:U:H3'	25:BA:1133:A:H5''	1.96	0.47
25:BA:1563:U:H2'	25:BA:1564:C:C6	2.48	0.47
25:BA:2024:G:C4	25:BA:2040:G:N2	2.82	0.47
25:BA:674:G:OP2	29:BE:49:ARG:NH1	2.47	0.47
25:BA:687:C:H2'	25:BA:688:U:O4'	2.15	0.47
31:BG:148:ARG:HA	31:BG:161:VAL:HG22	1.95	0.47
35:BK:59:LYS:NZ	35:BK:92:GLU:OE2	2.46	0.47
51:C0:24:VAL:O	51:C0:25:THR:HG22	2.15	0.47
25:CA:2091:C:H4'	48:CX:55:MET:CE	2.44	0.47
25:CA:2551:C:OP2	60:CA:3720:HOH:O	2.20	0.47
25:CA:2676:C:OP1	35:CK:31:ARG:NH2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:CD:151:THR:HG22	28:CD:152:PRO:HD2	1.95	0.47
35:CK:61:VAL:HG23	35:CK:87:LEU:HD13	1.95	0.47
41:CQ:86:SER:HB3	42:CR:52:PRO:HD3	1.97	0.47
1:DA:32:A:C2	1:DA:33:A:C4	3.03	0.47
2:DB:69:PHE:CE2	2:DB:84:ALA:HB1	2.49	0.47
4:DD:147:GLU:HA	4:DD:150:LYS:HD3	1.96	0.47
4:DD:42:GLY:O	4:DD:44:ARG:N	2.47	0.47
4:DD:45:LYS:O	4:DD:47:ARG:N	2.46	0.47
8:DH:101:ILE:HG12	8:DH:112:THR:HB	1.97	0.47
15:DO:85:LEU:CD1	15:DO:87:LEU:HD23	2.45	0.47
19:DS:11:ILE:HD13	19:DS:16:LEU:HD12	1.96	0.47
1:AA:1430:A:C2	1:AA:1471:U:C2	3.03	0.47
1:AA:1418:A:C2	1:AA:1483:A:C2	3.03	0.47
2:AB:91:PHE:O	2:AB:150:GLY:HA2	2.14	0.47
6:AF:16:GLU:OE1	4:DD:193:ALA:N	2.47	0.47
6:AF:66:ALA:HB1	6:AF:67:PRO:HD2	1.97	0.47
7:AG:9:GLN:HG2	7:AG:10:ARG:N	2.30	0.47
10:AJ:36:VAL:HG22	10:AJ:76:ILE:HA	1.96	0.47
13:AM:87:ARG:HE	13:AM:91:HIS:CE1	2.32	0.47
1:AA:981:U:H4'	14:AN:61:ARG:HD3	1.96	0.47
24:AX:65:G:C2	24:AX:66:U:H1'	2.50	0.47
25:BA:2063:C:C5	25:BA:2064:C:C5	3.03	0.47
25:BA:2129:C:H42	25:BA:2159:G:H22	1.62	0.47
25:BA:2324:U:H4'	25:BA:2325:G:OP2	2.13	0.47
25:BA:690:G:C3'	27:BC:216:ARG:HH22	2.28	0.47
37:BM:81:ARG:NH1	37:BM:81:ARG:HA	2.30	0.47
41:BQ:30:VAL:HG12	41:BQ:33:VAL:H	1.79	0.47
25:CA:2854:G:H2'	25:CA:2855:C:C6	2.50	0.47
32:CH:120:GLY:O	32:CH:121:VAL:O	2.33	0.47
35:CK:16:ALA:HB2	35:CK:43:ILE:HD13	1.96	0.47
25:CA:910:A:C4	37:CM:13:HIS:CE1	3.02	0.47
25:CA:85:G:OP1	45:CU:5:ARG:HG2	2.15	0.47
1:DA:978:A:P	1:DA:1362:A:N6	2.88	0.47
4:DD:139:PRO:O	4:DD:141:ASP:N	2.48	0.47
24:DW:63:G:H2'	24:DW:64:A:O4'	2.14	0.47
1:AA:982:U:H4'	1:AA:983:A:H5'	1.96	0.47
24:AX:76:A:N6	25:BA:2422:C:O5'	2.48	0.47
25:BA:247:G:C8	25:BA:249:C:C6	3.02	0.47
26:BB:3037:C:C5	26:BB:3038:C:C5	3.03	0.47
28:BD:188:LEU:N	28:BD:188:LEU:HD23	2.30	0.47
29:BE:128:ALA:HB1	29:BE:129:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BL:57:LEU:HD22	54:B3:53:ASP:HB3	1.96	0.47
37:BM:44:ARG:CG	37:BM:44:ARG:HH21	2.28	0.47
25:BA:446:G:P	41:BQ:2:ARG:HE	2.38	0.47
25:CA:1365:A:OP1	48:CX:27:ARG:NH2	2.43	0.47
27:CC:110:LYS:HG2	27:CC:111:ALA:H	1.80	0.47
1:DA:1435:G:H2'	1:DA:1436:U:C6	2.50	0.47
32:BH:91:PHE:CZ	1:DA:55:A:C8	3.03	0.47
1:DA:977:A:HO2'	1:DA:981:U:H3	1.63	0.47
10:DJ:35:GLN:HG2	10:DJ:77:VAL:CG1	2.44	0.47
12:DL:43:LYS:HG2	12:DL:44:LYS:HD3	1.97	0.47
16:DP:5:ARG:NH1	16:DP:6:LEU:HD13	2.30	0.47
1:AA:1033:G:H2'	1:AA:1034:G:C5'	2.45	0.47
1:AA:716:A:N3	11:AK:120:GLY:HA2	2.29	0.47
3:AC:77:ILE:HA	3:AC:84:VAL:HG13	1.97	0.47
1:AA:966:G:O2'	9:AI:129:LYS:O	2.32	0.47
19:AS:21:LYS:NZ	19:AS:21:LYS:O	2.36	0.47
19:AS:5:LEU:HD22	19:AS:9:PRO:HA	1.96	0.47
22:AV:133:ARG:HE	25:BA:1942:C:H1'	1.79	0.47
25:BA:1050:A:C2	25:BA:2751:G:C4	3.02	0.47
25:BA:1607:C:N4	25:BA:1622:G:N7	2.62	0.47
39:BO:27:VAL:HG13	39:BO:38:GLN:O	2.15	0.47
40:BP:96:LEU:HD13	40:BP:99:LEU:HD22	1.97	0.47
47:BW:28:SER:O	47:BW:63:GLY:O	2.33	0.47
25:CA:2345:G:N3	25:CA:2381:A:H2'	2.30	0.47
25:CA:2377:A:HO2'	39:CO:92:PHE:HZ	1.59	0.47
25:CA:518:G:H4'	43:CS:18:ARG:CZ	2.44	0.47
32:CH:31:VAL:HB	32:CH:32:PRO:HD3	1.97	0.47
25:CA:2271:G:H5'	47:CW:18:ARG:HE	1.79	0.47
2:DB:144:LEU:HA	2:DB:147:SER:OG	2.14	0.47
4:DD:124:MET:HG3	4:DD:125:VAL:N	2.30	0.47
8:DH:112:THR:O	8:DH:116:ALA:N	2.47	0.47
8:DH:34:VAL:HG13	8:DH:35:ALA:N	2.30	0.47
11:DK:82:LEU:HD22	11:DK:105:PHE:CD1	2.50	0.47
1:AA:1189:U:OP1	14:AN:98:LYS:NZ	2.48	0.47
1:AA:1209:C:O2'	1:AA:1214:C:N4	2.48	0.47
4:AD:104:ARG:CZ	4:AD:170:TRP:CH2	2.98	0.47
5:AE:122:ASN:N	5:AE:122:ASN:OD1	2.48	0.47
8:AH:38:ASN:HA	8:AH:49:PHE:CE2	2.50	0.47
9:AI:7:TYR:HB2	9:AI:20:PHE:HA	1.97	0.47
10:AJ:78:GLU:O	10:AJ:80:THR:N	2.48	0.47
15:AO:75:VAL:HA	15:AO:78:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AV:112:LYS:HA	22:AV:115:THR:HG22	1.96	0.47
51:B0:52:LYS:HE2	51:B0:55:ALA:CA	2.45	0.47
25:BA:118:A:C8	25:BA:119:A:C8	3.02	0.47
25:BA:1414:C:C4	25:BA:1415:U:H5	2.32	0.47
25:BA:1606:C:H4'	25:BA:1607:C:H5''	1.96	0.47
25:BA:289:G:H2'	25:BA:290:U:O4'	2.14	0.47
25:BA:725:G:C6	25:BA:726:G:N1	2.83	0.47
27:BC:135:PRO:O	27:BC:138:SER:HB2	2.15	0.47
39:BO:41:ALA:HB2	39:BO:48:LEU:HD11	1.95	0.47
49:BY:41:HIS:CE1	49:BY:42:LEU:CD1	2.98	0.47
25:CA:2522:U:H2'	25:CA:2523:G:C5'	2.45	0.47
25:CA:2519:U:C6	25:CA:2542:A:N6	2.82	0.47
30:CF:1:ALA:HB1	30:CF:4:HIS:HB3	1.96	0.47
42:CR:42:ALA:HA	42:CR:46:GLU:HA	1.97	0.47
43:CS:17:VAL:HG21	43:CS:103:ILE:CG2	2.45	0.47
1:DA:983:A:N3	1:DA:983:A:C2'	2.77	0.47
4:DD:154:ARG:O	4:DD:158:ALA:N	2.47	0.47
11:DK:72:ASP:O	11:DK:73:ALA:CB	2.63	0.47
4:AD:104:ARG:NH2	4:AD:168:PRO:HA	2.30	0.47
5:AE:133:PRO:HA	5:AE:136:VAL:HG22	1.96	0.47
12:AL:65:SER:HB2	12:AL:82:ILE:HD11	1.96	0.47
18:AR:71:THR:OG1	18:AR:72:ASP:N	2.47	0.47
25:BA:2365:G:H4'	47:BW:58:PHE:CZ	2.50	0.47
25:BA:476:G:N1	25:BA:479:A:OP2	2.48	0.47
27:BC:48:ILE:HD13	27:BC:48:ILE:O	2.15	0.47
42:BR:68:ARG:HD3	42:BR:92:TRP:CE2	2.50	0.47
25:CA:1434:A:H2'	25:CA:1435:G:C8	2.50	0.47
25:CA:1647:U:P	25:CA:1647:U:H3'	2.55	0.47
25:CA:743:A:O2'	25:CA:1659:G:OP1	2.28	0.47
25:CA:2681:C:OP2	28:CD:114:LYS:NZ	2.40	0.47
25:CA:2685:G:OP1	35:CK:78:ARG:NH2	2.47	0.47
29:CE:125:SER:OG	29:CE:126:VAL:N	2.46	0.47
36:CL:132:ARG:HD2	36:CL:142:ILE:CD1	2.44	0.47
1:DA:1009:U:C2	1:DA:1021:A:N1	2.83	0.47
1:DA:1493:A:OP1	58:DA:1654:PAR:N32	2.48	0.47
1:DA:830:G:O2'	2:DB:21:ARG:NH2	2.47	0.47
1:DA:986:U:H2'	1:DA:987:G:O4'	2.14	0.47
2:DB:10:LEU:O	2:DB:12:ALA:N	2.43	0.47
3:DC:42:TYR:CZ	3:DC:46:GLU:HG3	2.50	0.47
3:DC:22:TRP:O	3:DC:59:ARG:NH1	2.47	0.47
12:DL:116:LYS:O	12:DL:117:TYR:CG	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:DM:66:GLU:O	13:DM:68:ASP:N	2.48	0.47
7:AG:99:LEU:C	7:AG:103:TRP:CE3	2.88	0.47
1:AA:1048:G:H5''	14:AN:2:LYS:HZ3	1.79	0.47
19:AS:44:MET:CG	19:AS:45:ILE:H	2.28	0.47
20:AT:28:MET:HE2	20:AT:61:GLN:HG2	1.96	0.47
52:B1:22:THR:OG1	52:B1:23:THR:N	2.44	0.47
54:B3:31:ILE:HD11	54:B3:35:LYS:HE3	1.96	0.47
25:BA:1009:A:OP2	34:BJ:39:LYS:NZ	2.37	0.47
25:BA:1670:C:OP2	60:BA:3727:HOH:O	2.20	0.47
25:BA:864:G:C6	25:BA:865:C:N4	2.83	0.47
27:BC:14:HIS:O	27:BC:203:VAL:HG11	2.14	0.47
30:BF:7:TYR:O	30:BF:11:VAL:HB	2.15	0.47
33:BI:23:VAL:HG13	33:BI:24:GLY:H	1.80	0.47
37:BM:44:ARG:HG3	37:BM:44:ARG:NH2	2.29	0.47
37:BM:73:ILE:HG21	37:BM:91:TYR:CZ	2.50	0.47
42:BR:66:HIS:CD2	42:BR:94:THR:HG22	2.50	0.47
26:BB:3077:U:P	46:BV:14:LYS:HZ3	2.38	0.47
25:CA:103:A:H2'	25:CA:104:A:O4'	2.15	0.47
25:CA:2570:G:C5	25:CA:2571:U:C5	3.03	0.47
30:CF:107:VAL:N	30:CF:108:PRO:CD	2.78	0.47
30:CF:116:LEU:O	30:CF:118:ALA:N	2.47	0.47
38:CN:115:LEU:H	38:CN:115:LEU:HD12	1.80	0.47
41:CQ:73:ILE:HG21	41:CQ:109:VAL:HG13	1.97	0.47
43:CS:109:ASP:N	43:CS:109:ASP:OD1	2.43	0.47
2:DB:57:LEU:O	2:DB:59:LYS:N	2.48	0.47
8:DH:88:ARG:HG2	8:DH:89:LYS:N	2.30	0.47
16:DP:19:VAL:HG23	16:DP:36:VAL:HG23	1.96	0.47
3:AC:28:GLU:OE1	3:AC:28:GLU:N	2.46	0.46
1:AA:1082:A:OP1	5:AE:23:LYS:NZ	2.48	0.46
55:B4:25:VAL:HB	55:B4:35:GLN:HB2	1.97	0.46
25:BA:1426:G:H1'	25:BA:1572:A:N6	2.30	0.46
25:BA:1918:A:N3	25:BA:1919:A:N6	2.61	0.46
25:BA:2531:A:OP1	31:BG:174:LYS:NZ	2.38	0.46
25:BA:672:C:C2	25:BA:809:G:N2	2.83	0.46
32:BH:91:PHE:HA	1:DA:55:A:N6	2.30	0.46
45:BU:4:ILE:HD11	45:BU:10:VAL:HG11	1.97	0.46
47:BW:21:VAL:HG11	47:BW:24:PHE:CD1	2.50	0.46
25:CA:2617:U:H2'	25:CA:2618:G:O4'	2.14	0.46
25:CA:2685:G:H2'	25:CA:2686:G:H8	1.79	0.46
25:CA:275:C:C5	25:CA:276:U:H1'	2.50	0.46
32:CH:86:ASP:O	32:CH:89:LYS:NZ	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:CK:61:VAL:HG11	35:CK:112:PHE:CE1	2.49	0.46
39:CO:69:ASP:OD1	39:CO:70:ALA:N	2.44	0.46
48:CX:37:PHE:CE2	48:CX:58:ILE:HG21	2.49	0.46
1:DA:652:U:O2'	1:DA:653:U:P	2.73	0.46
1:DA:953:G:H2'	1:DA:954:G:O4'	2.14	0.46
3:DC:195:VAL:HG12	3:DC:196:ILE:N	2.30	0.46
4:DD:124:MET:HA	4:DD:128:ARG:O	2.16	0.46
10:DJ:81:GLU:HA	10:DJ:84:VAL:HG22	1.96	0.46
12:DL:40:THR:HG22	12:DL:41:THR:N	2.30	0.46
15:DO:39:LEU:HD11	15:DO:56:LEU:HD13	1.96	0.46
21:DU:37:PHE:HB3	21:DU:41:PRO:HD2	1.96	0.46
1:AA:1320:C:H5	1:AA:1321:U:C4	2.33	0.46
1:AA:1478:U:H2'	1:AA:1479:C:C6	2.50	0.46
1:AA:920:U:H2'	1:AA:921:U:C6	2.50	0.46
4:AD:105:MET:HE2	4:AD:107:PHE:HE1	1.80	0.46
14:AN:19:TYR:OH	14:AN:55:SER:C	2.53	0.46
25:BA:586:A:C2	25:BA:1254:A:C2	3.04	0.46
25:BA:142:A:H2'	25:BA:143:C:C6	2.50	0.46
25:BA:2120:G:N2	25:BA:2178:C:O2	2.48	0.46
25:BA:2686:G:H2'	25:BA:2687:U:O4'	2.15	0.46
25:BA:833:A:H2'	25:BA:834:G:H8	1.78	0.46
25:BA:934:U:H2'	25:BA:935:C:C6	2.50	0.46
43:BS:63:GLY:O	43:BS:64:ALA:CB	2.63	0.46
49:BY:9:LYS:O	49:BY:12:GLU:N	2.48	0.46
25:CA:126:A:C6	25:CA:127:A:N1	2.83	0.46
25:CA:871:U:H2'	25:CA:872:U:C6	2.50	0.46
27:CC:175:LEU:O	27:CC:177:SER:N	2.48	0.46
41:CQ:98:ALA:HB2	41:CQ:105:PHE:CD1	2.50	0.46
1:DA:38:G:N2	1:DA:397:A:C4	2.83	0.46
1:DA:68:G:C6	1:DA:69:G:H1'	2.50	0.46
1:DA:922:G:H2'	1:DA:923:A:C8	2.50	0.46
2:DB:32:PHE:HB2	2:DB:42:ASN:HB2	1.97	0.46
4:DD:125:VAL:HG22	4:DD:126:ASN:N	2.30	0.46
4:DD:124:MET:SD	4:DD:127:GLY:CA	3.03	0.46
8:DH:106:THR:HG22	8:DH:109:GLY:O	2.15	0.46
8:DH:40:LEU:O	8:DH:45:PHE:N	2.38	0.46
9:DI:25:ASN:O	9:DI:27:LYS:N	2.48	0.46
1:AA:1179:A:H5''	9:AI:104:VAL:HG22	1.96	0.46
1:AA:406:G:C2	1:AA:407:U:C6	3.04	0.46
1:AA:677:U:O2	1:AA:777:A:O2'	2.29	0.46
1:AA:842:U:C3'	1:AA:843:U:H4'	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:140:ASN:O	3:AC:141:ALA:CB	2.64	0.46
4:AD:138:SER:O	4:AD:182:PHE:CZ	2.69	0.46
4:AD:181:THR:O	4:AD:182:PHE:HB3	2.15	0.46
12:AL:94:ARG:NH1	12:AL:95:TYR:CG	2.83	0.46
15:AO:81:LEU:HD12	15:AO:82:ILE:N	2.31	0.46
25:BA:1091:G:O2'	25:BA:1092:C:OP2	2.31	0.46
25:BA:1124:G:C2'	25:BA:1125:G:H5'	2.45	0.46
25:BA:1880:U:O4	58:BA:3005:PAR:H62	2.15	0.46
25:BA:1952:A:C6	35:BK:22:ILE:CD1	2.98	0.46
25:BA:207:A:H2'	25:BA:208:C:O4'	2.15	0.46
25:BA:197:A:H62	25:BA:2430:A:H2'	1.80	0.46
25:BA:2580:U:OP1	28:BD:137:SER:OG	2.27	0.46
25:BA:329:G:H4'	25:BA:330:A:OP2	2.15	0.46
25:BA:528:A:C2	25:BA:2043:C:H4'	2.50	0.46
25:BA:832:U:H2'	25:BA:833:A:C8	2.51	0.46
27:BC:140:VAL:CG2	27:BC:189:ALA:HB1	2.45	0.46
27:BC:174:ARG:HB2	27:BC:180:MET:HG3	1.96	0.46
28:BD:180:VAL:HG22	28:BD:187:LEU:HD23	1.98	0.46
35:BK:2:ILE:HD12	35:BK:3:GLN:N	2.31	0.46
41:BQ:87:VAL:CB	42:BR:49:ILE:HG21	2.45	0.46
45:BU:82:VAL:HG12	45:BU:83:GLY:N	2.31	0.46
49:BY:25:GLN:O	49:BY:28:LEU:N	2.48	0.46
25:CA:1188:U:C2'	25:CA:1189:A:H5'	2.45	0.46
25:CA:874:G:N2	25:CA:904:G:C4	2.84	0.46
25:CA:1252:G:N2	41:CQ:32:ARG:HG3	2.31	0.46
43:CS:6:LYS:HD3	43:CS:104:THR:HB	1.98	0.46
1:DA:1358:U:OP2	14:DN:75:ARG:NH2	2.49	0.46
1:DA:57:G:C6	1:DA:58:C:N3	2.83	0.46
1:DA:1191:A:OP1	3:DC:4:LYS:HE3	2.15	0.46
4:DD:110:THR:CG2	4:DD:113:GLU:H	2.28	0.46
5:DE:104:GLY:HA3	5:DE:122:ASN:HA	1.96	0.46
1:AA:1251:A:H2'	1:AA:1252:A:O4'	2.15	0.46
1:AA:560:A:H5'	1:AA:566:G:N2	2.30	0.46
10:AJ:18:ILE:HD12	10:AJ:19:ASP:N	2.30	0.46
14:AN:1:ALA:O	14:AN:2:LYS:HB3	2.16	0.46
15:AO:75:VAL:HA	15:AO:78:TYR:OH	2.16	0.46
25:BA:1020:A:C2	25:BA:1141:U:C2	3.04	0.46
25:BA:1272:A:C2	25:BA:1618:A:C2	3.04	0.46
25:BA:2323:G:H2'	25:BA:2324:U:H5''	1.97	0.46
25:BA:2698:U:H2'	25:BA:2699:C:C6	2.51	0.46
25:BA:547:A:N7	25:BA:548:G:N3	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:866:A:C8	25:BA:914:G:C2	3.04	0.46
27:BC:99:GLU:OE1	27:BC:101:ARG:NH2	2.42	0.46
40:BP:21:PRO:HA	40:BP:46:VAL:CG2	2.46	0.46
25:CA:1468:U:H2'	25:CA:1522:A:N6	2.30	0.46
25:CA:2591:C:H2'	25:CA:2592:G:C8	2.50	0.46
25:CA:2727:A:P	58:CA:3166:PAR:H611	2.55	0.46
58:CA:3169:PAR:H13	58:CA:3169:PAR:O62	2.15	0.46
25:CA:454:A:H4'	25:CA:455:C:OP2	2.15	0.46
25:CA:877:A:HO2'	25:CA:900:A:N6	2.14	0.46
25:CA:995:C:O2	34:CJ:3:THR:HB	2.15	0.46
32:CH:121:VAL:CG1	32:CH:122:LEU:N	2.73	0.46
44:CT:67:VAL:HG23	44:CT:76:ARG:HB3	1.98	0.46
1:DA:68:G:C5	1:DA:69:G:H1'	2.50	0.46
3:DC:106:VAL:C	3:DC:108:LYS:H	2.19	0.46
4:DD:124:MET:CG	4:DD:125:VAL:N	2.78	0.46
4:DD:161:LEU:O	4:DD:162:ALA:HB2	2.16	0.46
8:DH:71:VAL:HG13	8:DH:72:VAL:N	2.30	0.46
16:DP:74:LEU:O	16:DP:77:GLU:N	2.48	0.46
17:DQ:68:SER:OG	17:DQ:68:SER:O	2.28	0.46
1:AA:604:G:H2'	1:AA:605:U:O4'	2.15	0.46
1:AA:983:A:C2'	1:AA:983:A:N3	2.78	0.46
1:AA:1321:U:O2	19:AS:36:ARG:NH2	2.49	0.46
19:AS:5:LEU:HD21	19:AS:10:PHE:CD2	2.50	0.46
25:BA:2078:C:H2'	25:BA:2079:U:O4'	2.16	0.46
25:BA:588:U:H2'	25:BA:589:U:C6	2.50	0.46
25:BA:691:C:O2'	25:BA:692:C:H5'	2.15	0.46
29:BE:162:ARG:HG2	29:BE:163:ASN:N	2.31	0.46
30:BF:126:ASN:N	30:BF:126:ASN:OD1	2.48	0.46
30:BF:153:ILE:O	30:BF:154:THR:CB	2.64	0.46
42:BR:49:ILE:HG12	42:BR:51:VAL:O	2.15	0.46
47:BW:49:VAL:HG21	47:BW:78:ILE:O	2.16	0.46
25:CA:2271:G:O6	60:CA:3510:HOH:O	2.20	0.46
25:CA:2689:U:OP2	25:CA:2719:G:N2	2.37	0.46
25:CA:639:U:H2'	25:CA:640:C:C6	2.50	0.46
30:CF:107:VAL:HG12	30:CF:108:PRO:HD3	1.97	0.46
33:CI:101:SER:O	33:CI:103:ALA:N	2.43	0.46
37:CM:17:ASN:O	37:CM:38:ARG:NH1	2.48	0.46
25:CA:2875:C:OP1	38:CN:4:ARG:NH2	2.48	0.46
43:CS:7:HIS:HB3	43:CS:103:ILE:CG1	2.45	0.46
1:DA:1224:U:O2'	1:DA:1322:C:OP1	2.30	0.46
8:DH:41:LYS:HB3	8:DH:46:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:1492:A:P	12:DL:44:LYS:HZ2	2.39	0.46
13:DM:80:LEU:HD12	13:DM:81:MET:H	1.80	0.46
19:DS:31:LEU:HD11	19:DS:49:ILE:HB	1.97	0.46
1:AA:1477:U:H2'	1:AA:1478:U:C6	2.51	0.46
10:AJ:49:PHE:CD1	10:AJ:49:PHE:N	2.84	0.46
11:AK:69:ARG:HD3	25:BA:2146:C:N3	2.31	0.46
11:AK:94:GLU:OE1	11:AK:95:SER:N	2.48	0.46
14:AN:64:CYS:O	14:AN:66:GLN:N	2.38	0.46
15:AO:19:ALA:O	15:AO:21:ASP:N	2.47	0.46
18:AR:34:THR:OG1	18:AR:35:GLU:N	2.48	0.46
53:B2:9:VAL:HG23	53:B2:12:ARG:NH1	2.30	0.46
25:BA:1057:A:N6	25:BA:1087:G:OP2	2.47	0.46
25:BA:1420:A:HO2'	25:BA:1421:G:C5'	2.26	0.46
25:BA:1838:C:H4'	25:BA:1839:G:C8	2.51	0.46
25:BA:963:U:O4'	25:BA:2250:G:N2	2.49	0.46
25:BA:2848:G:H1'	25:BA:2867:G:N2	2.30	0.46
25:BA:858:G:N3	25:BA:2268:A:H2'	2.31	0.46
31:BG:155:PRO:O	31:BG:170:THR:HA	2.15	0.46
32:BH:84:ALA:HA	32:BH:90:LEU:HA	1.98	0.46
38:BN:1:MET:O	38:BN:2:ARG:CB	2.63	0.46
25:BA:998:C:OP1	41:BQ:91:ARG:NH2	2.48	0.46
42:BR:4:VAL:CG1	42:BR:40:MET:HB3	2.45	0.46
25:CA:1434:A:H2'	25:CA:1435:G:H8	1.80	0.46
25:CA:1799:G:N1	25:CA:1819:A:OP2	2.49	0.46
25:CA:528:A:C2	25:CA:2042:A:H2'	2.50	0.46
25:CA:2773:C:OP1	28:CD:171:THR:OG1	2.34	0.46
32:CH:26:ALA:O	32:CH:28:ASN:N	2.42	0.46
47:CW:41:THR:O	47:CW:41:THR:CG2	2.63	0.46
1:DA:960:U:C5	1:DA:1225:A:C8	3.04	0.46
1:DA:1524:C:OP2	11:DK:125:LYS:NZ	2.43	0.46
1:DA:390:U:H4'	16:DP:28:ARG:NH1	2.31	0.46
1:DA:673:A:H2'	1:DA:674:G:C8	2.51	0.46
2:DB:161:LEU:O	2:DB:184:PHE:N	2.44	0.46
2:DB:69:PHE:HB3	2:DB:162:PHE:HB3	1.97	0.46
13:DM:75:MET:HA	13:DM:78:LYS:HB3	1.97	0.46
1:AA:333:U:OP1	20:AT:3:ASN:ND2	2.47	0.46
1:AA:33:A:H2'	1:AA:34:C:C6	2.50	0.46
1:AA:751:U:C4	1:AA:752:G:C6	3.03	0.46
1:AA:96:U:HO2'	1:AA:97:G:P	2.39	0.46
6:AF:78:PHE:N	6:AF:78:PHE:CD1	2.84	0.46
1:AA:939:G:C4'	7:AG:102:ARG:HH22	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AH:78:VAL:HG22	8:AH:79:SER:N	2.30	0.46
52:B1:35:LEU:O	52:B1:48:TYR:N	2.39	0.46
25:BA:811:U:C2	25:BA:1251:C:C5	3.04	0.46
25:BA:1570:A:H2'	25:BA:1571:A:C8	2.51	0.46
25:BA:2303:G:H4'	30:BF:121:PHE:H	1.81	0.46
25:BA:483:A:OP2	58:BA:3004:PAR:O41	2.27	0.46
27:BC:15:VAL:HG12	27:BC:16:VAL:N	2.29	0.46
27:BC:251:THR:HG22	27:BC:252:LYS:H	1.80	0.46
32:BH:132:PHE:HE2	32:BH:142:VAL:HG21	1.80	0.46
32:BH:90:LEU:HD21	32:BH:124:THR:O	2.15	0.46
33:BI:52:LEU:HB3	33:BI:53:PRO:CD	2.46	0.46
41:BQ:35:PHE:CZ	41:BQ:39:ILE:HD11	2.50	0.46
42:BR:91:GLN:HG3	42:BR:92:TRP:N	2.29	0.46
43:BS:3:THR:HG21	43:BS:58:ALA:N	2.31	0.46
25:CA:1113:U:H2'	25:CA:1114:C:C6	2.51	0.46
25:CA:1340:U:H4'	25:CA:1341:G:OP2	2.16	0.46
38:CN:117:ASP:O	38:CN:118:ARG:CB	2.63	0.46
39:CO:92:PHE:CE1	39:CO:117:PHE:HB2	2.50	0.46
48:CX:32:LEU:HA	48:CX:51:SER:HA	1.98	0.46
1:DA:1387:G:H2'	1:DA:1388:C:C6	2.50	0.46
1:DA:591:U:OP1	8:DH:31:LYS:NZ	2.45	0.46
1:DA:986:U:C2	1:DA:1220:G:N2	2.84	0.46
1:AA:1219:A:OP1	14:AN:53:ARG:NH1	2.45	0.46
1:AA:742:G:OP1	15:AO:58:ARG:NH1	2.49	0.46
3:AC:66:VAL:HG13	3:AC:67:THR:H	1.81	0.46
5:AE:104:GLY:HA3	5:AE:122:ASN:CB	2.46	0.46
7:AG:91:VAL:HG11	7:AG:96:ARG:HG3	1.98	0.46
13:AM:72:GLU:HB3	13:AM:75:MET:SD	2.55	0.46
14:AN:51:LEU:HB2	14:AN:52:PRO:HD2	1.96	0.46
18:AR:65:LEU:HD23	18:AR:65:LEU:N	2.31	0.46
25:BA:1425:G:N2	25:BA:1573:G:N7	2.64	0.46
25:BA:1690:A:H2'	25:BA:1691:C:O4'	2.16	0.46
25:BA:250:G:C6	25:BA:251:A:C6	3.04	0.46
25:BA:671:C:C6	25:BA:671:C:H5'	2.51	0.46
26:BB:3024:G:N7	26:BB:3056:G:H2'	2.30	0.46
31:BG:7:PRO:HB3	31:BG:50:THR:HG22	1.97	0.46
36:BL:95:LEU:O	36:BL:100:ILE:HG22	2.16	0.46
25:CA:1207:C:C2	25:CA:1208:C:C5	3.03	0.46
25:CA:1682:G:C2	25:CA:1757:A:H1'	2.51	0.46
25:CA:1916:A:H2'	25:CA:1917:U:O4'	2.15	0.46
25:CA:2619:C:H1'	28:CD:155:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:CC:24:HIS:N	27:CC:80:LEU:O	2.43	0.46
28:CD:136:ASN:HD21	28:CD:139:SER:C	2.20	0.46
43:CS:63:GLY:O	43:CS:64:ALA:CB	2.64	0.46
1:DA:1118:U:P	9:DI:106:ARG:HE	2.39	0.46
1:DA:1102:A:O2'	2:DB:97:LEU:O	2.34	0.46
1:DA:8:A:C6	4:DD:206:LYS:HG2	2.50	0.46
12:DL:110:ARG:HE	12:DL:117:TYR:HD2	1.62	0.46
13:DM:107:ARG:O	13:DM:111:GLY:N	2.47	0.46
1:AA:262:A:N6	1:AA:263:A:N6	2.63	0.46
4:AD:55:LEU:HA	4:AD:58:LYS:CD	2.45	0.46
7:AG:62:PHE:O	7:AG:65:ALA:N	2.47	0.46
13:AM:101:ARG:HD2	13:AM:104:THR:HG23	1.96	0.46
14:AN:46:LEU:HD12	14:AN:46:LEU:O	2.16	0.46
14:AN:64:CYS:CB	14:AN:83:LYS:HZ1	2.29	0.46
15:AO:64:ARG:NH2	15:AO:68:ASP:OD2	2.49	0.46
20:AT:6:SER:OG	20:AT:7:ALA:N	2.49	0.46
22:AV:45:TYR:OH	22:AV:50:THR:O	2.31	0.46
24:AX:51:U:H1'	24:AX:64:A:N1	2.30	0.46
25:BA:1306:C:H5''	25:BA:1306:C:H6	1.81	0.46
25:BA:1456:G:C6	25:BA:1457:U:C4	3.04	0.46
25:BA:1682:G:H2'	25:BA:1683:U:C6	2.50	0.46
25:BA:404:A:C8	25:BA:406:G:C6	3.04	0.46
25:BA:662:G:O3'	36:BL:16:GLY:HA2	2.15	0.46
29:BE:29:HIS:CE1	36:BL:8:PRO:HB3	2.50	0.46
34:BJ:65:THR:O	34:BJ:68:LYS:HD3	2.16	0.46
41:BQ:87:VAL:HB	42:BR:49:ILE:HG21	1.96	0.46
25:CA:1385:A:H1'	25:CA:1386:C:C6	2.51	0.46
25:CA:137:U:C5	25:CA:140:C:H1'	2.51	0.46
25:CA:165:A:N3	48:CX:43:LYS:NZ	2.62	0.46
30:CF:126:ASN:OD1	30:CF:157:THR:N	2.43	0.46
31:CG:122:ALA:HB2	31:CG:132:LEU:HB3	1.98	0.46
32:CH:124:THR:CG2	32:CH:128:HIS:CE1	2.99	0.46
35:CK:108:ARG:HA	35:CK:116:ILE:HD11	1.98	0.46
36:CL:20:GLY:O	36:CL:21:ARG:NE	2.49	0.46
1:DA:109:A:C6	1:DA:326:G:C6	3.04	0.46
1:DA:1276:G:N3	1:DA:1282:C:O2'	2.47	0.46
1:DA:181:A:N1	1:DA:195:A:C8	2.84	0.46
1:DA:57:G:H2'	1:DA:58:C:O4'	2.16	0.46
1:DA:900:A:H2'	1:DA:901:A:C8	2.51	0.46
2:DB:144:LEU:H	2:DB:144:LEU:CD2	2.29	0.46
4:DD:25:VAL:HG13	4:DD:26:ARG:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:DE:95:PHE:HE2	5:DE:97:GLN:HG2	1.80	0.46
12:DL:44:LYS:HD2	12:DL:44:LYS:N	2.31	0.46
13:DM:114:LYS:HG3	13:DM:115:PRO:HD2	1.98	0.46
1:AA:1160:G:HO2'	1:AA:1161:C:C5'	2.28	0.46
1:AA:68:G:C6	1:AA:69:G:H1'	2.51	0.46
1:AA:666:G:C2	1:AA:741:G:C4	3.04	0.46
2:AB:183:VAL:HG21	2:AB:197:ASP:N	2.30	0.46
4:AD:124:MET:HA	4:AD:129:VAL:HA	1.98	0.46
4:AD:70:ARG:O	4:AD:74:ASN:ND2	2.39	0.46
6:AF:21:MET:HB3	6:AF:25:TYR:HE1	1.81	0.46
11:AK:71:ALA:HA	11:AK:74:VAL:HG22	1.97	0.46
13:AM:29:ARG:NH1	13:AM:29:ARG:HB2	2.31	0.46
20:AT:69:LYS:NZ	20:AT:69:LYS:O	2.42	0.46
25:BA:2419:U:O3'	54:B3:33:THR:HG23	2.16	0.46
25:BA:70:G:H5''	25:BA:112:U:O2	2.16	0.46
25:BA:1153:C:OP1	41:BQ:91:ARG:NH1	2.48	0.46
30:BF:15:LEU:HA	30:BF:18:GLU:HB3	1.98	0.46
46:BV:70:ILE:HG22	46:BV:72:VAL:HG13	1.97	0.46
25:CA:1509:A:N3	25:CA:1510:G:C8	2.84	0.46
25:CA:1672:A:C2	25:CA:2582:G:H5'	2.50	0.46
25:CA:1687:G:H2'	25:CA:1688:U:C6	2.51	0.46
58:CA:3166:PAR:H11	58:CA:3166:PAR:O52	2.15	0.46
25:CA:333:G:H5''	25:CA:334:C:OP2	2.16	0.46
25:CA:811:U:OP2	36:CL:29:LYS:N	2.46	0.46
25:CA:88:G:C6	25:CA:89:A:N7	2.84	0.46
33:CI:28:GLY:HA2	33:CI:32:VAL:HG21	1.97	0.46
45:CU:53:GLN:N	45:CU:54:PRO:HD3	2.31	0.46
1:DA:831:A:OP1	2:DB:21:ARG:NH1	2.48	0.46
5:DE:56:VAL:N	5:DE:57:PRO:HD2	2.31	0.46
5:DE:44:GLY:HA2	5:DE:74:VAL:HG21	1.98	0.46
6:DF:12:PRO:HG3	6:DF:57:ALA:HA	1.97	0.46
13:DM:31:LYS:O	13:DM:33:ILE:N	2.47	0.46
15:DO:11:ILE:HD11	15:DO:31:LEU:HB3	1.96	0.46
1:AA:502:A:H2'	1:AA:503:C:O4'	2.16	0.45
1:AA:880:C:OP1	12:AL:9:ARG:NH2	2.49	0.45
4:AD:14:ARG:HD3	4:AD:56:ARG:NH2	2.31	0.45
4:AD:58:LYS:HB2	4:AD:200:ILE:HG23	1.99	0.45
4:AD:58:LYS:CD	4:AD:203:LEU:HD22	2.46	0.45
5:AE:44:GLY:HA2	5:AE:74:VAL:HG23	1.98	0.45
6:AF:15:SER:O	6:AF:17:GLN:N	2.49	0.45
6:AF:8:PHE:CE2	6:AF:60:VAL:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:151:PHE:CD1	7:AG:152:ALA:N	2.84	0.45
8:AH:78:VAL:HG12	8:AH:127:CYS:CA	2.46	0.45
13:AM:31:LYS:HZ3	13:AM:35:ALA:HB2	1.81	0.45
14:AN:20:PHE:C	14:AN:22:LYS:H	2.20	0.45
24:AX:50:U:H1'	24:AX:65:G:N2	2.31	0.45
25:BA:1120:G:C6	25:BA:1121:C:C4	3.04	0.45
25:BA:1569:A:H2'	25:BA:1570:A:C8	2.52	0.45
25:BA:1850:G:C5	25:BA:1851:U:C5	3.05	0.45
25:BA:1936:A:H2	25:BA:1943:U:N3	2.14	0.45
25:BA:2651:C:H2'	25:BA:2652:C:C6	2.51	0.45
25:BA:2796:U:H3	25:BA:2799:A:H61	1.63	0.45
25:BA:475:C:C4	25:BA:481:G:O6	2.69	0.45
25:BA:541:A:H2'	25:BA:542:C:O4'	2.16	0.45
25:BA:927:A:H2'	25:BA:928:A:C8	2.51	0.45
29:BE:41:GLN:HB3	29:BE:43:THR:HG23	1.98	0.45
39:BO:35:ILE:O	39:BO:53:THR:HG23	2.16	0.45
45:BU:15:GLY:CA	45:BU:16:LYS:HZ2	2.30	0.45
46:BV:29:ILE:HD12	46:BV:90:ASP:HA	1.98	0.45
25:CA:2151:U:H2'	25:CA:2152:G:C8	2.51	0.45
33:CI:115:ASP:N	33:CI:115:ASP:OD1	2.42	0.45
35:CK:118:LEU:O	35:CK:119:ALA:HB3	2.15	0.45
36:CL:125:LEU:N	36:CL:125:LEU:HD13	2.31	0.45
39:CO:67:ASN:C	39:CO:69:ASP:H	2.19	0.45
46:CV:80:HIS:CG	46:CV:83:LYS:O	2.68	0.45
1:DA:15:G:O2'	5:DE:29:ARG:NH1	2.49	0.45
1:DA:258:G:C2	1:DA:259:G:H1'	2.51	0.45
1:DA:383:A:C5	1:DA:384:G:H1'	2.51	0.45
3:DC:22:TRP:HB3	3:DC:59:ARG:HD2	1.98	0.45
6:DF:29:ILE:HG21	6:DF:36:ILE:CG2	2.46	0.45
8:DH:88:ARG:HB2	8:DH:88:ARG:HH11	1.80	0.45
11:DK:105:PHE:C	11:DK:107:ILE:H	2.20	0.45
4:AD:95:GLU:OE1	4:AD:100:ASN:ND2	2.45	0.45
6:AF:21:MET:CB	6:AF:25:TYR:HE1	2.30	0.45
13:AM:40:ALA:O	13:AM:42:ASP:N	2.50	0.45
18:AR:24:LYS:C	18:AR:26:ILE:H	2.19	0.45
54:B3:54:LEU:O	54:B3:58:ILE:HD13	2.16	0.45
25:BA:2024:G:OP2	25:BA:2034:U:H4'	2.16	0.45
25:BA:2243:U:H2'	25:BA:2244:U:C6	2.52	0.45
25:BA:959:A:N3	25:BA:2457:U:O2'	2.44	0.45
27:BC:164:VAL:HG12	27:BC:173:LEU:HA	1.98	0.45
28:BD:125:TRP:CE3	28:BD:160:LYS:CG	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BL:131:ALA:O	36:BL:135:ILE:HG12	2.15	0.45
37:BM:29:GLY:N	37:BM:104:GLU:OE1	2.38	0.45
25:CA:1530:G:H22	25:CA:1542:U:H1'	1.81	0.45
25:CA:1786:A:H1'	25:CA:1938:A:N6	2.31	0.45
25:CA:2511:U:C5	25:CA:2512:C:C5	3.05	0.45
25:CA:2522:U:H2'	25:CA:2523:G:H5''	1.97	0.45
25:CA:812:C:H5''	25:CA:1250:G:O2'	2.16	0.45
40:CP:91:VAL:HG21	40:CP:96:LEU:CD2	2.47	0.45
45:CU:97:SER:OG	45:CU:98:ASN:ND2	2.49	0.45
1:DA:1513:A:H2'	1:DA:1514:G:C8	2.50	0.45
2:DB:188:ASP:OD1	2:DB:189:THR:N	2.43	0.45
2:DB:73:LYS:HD2	2:DB:76:ALA:HB3	1.98	0.45
3:DC:83:ASP:OD1	3:DC:84:VAL:N	2.50	0.45
21:DU:17:ARG:HA	21:DU:17:ARG:NE	2.31	0.45
1:AA:1048:G:H2'	1:AA:1050:G:C8	2.52	0.45
1:AA:767:A:O2'	1:AA:1524:C:O2	2.31	0.45
1:AA:17:U:H2'	1:AA:18:C:C6	2.51	0.45
1:AA:404:G:O6	4:AD:2:ALA:N	2.48	0.45
1:AA:96:U:O2'	1:AA:97:G:O5'	2.35	0.45
1:AA:96:U:O2'	1:AA:97:G:P	2.74	0.45
3:AC:193:TYR:C	3:AC:193:TYR:CD2	2.90	0.45
4:AD:37:ALA:N	4:AD:38:PRO:CD	2.80	0.45
9:AI:42:GLU:O	9:AI:44:ALA:N	2.48	0.45
10:AJ:42:LEU:HB3	10:AJ:71:LEU:HD13	1.96	0.45
15:AO:70:LEU:HD13	15:AO:78:TYR:CD1	2.51	0.45
18:AR:56:ALA:C	18:AR:58:ALA:H	2.20	0.45
1:AA:178:C:OP2	20:AT:60:ARG:NH2	2.49	0.45
22:AV:159:ASP:O	22:AV:160:ASP:HB3	2.16	0.45
22:AV:28:ILE:CD1	22:AV:30:THR:HG23	2.46	0.45
25:BA:2520:C:C6	25:BA:2567:G:H1'	2.51	0.45
25:BA:2528:U:O2'	25:BA:2530:A:OP1	2.18	0.45
27:BC:60:ALA:O	27:BC:62:ARG:NH2	2.48	0.45
28:BD:12:THR:HG21	40:BP:8:GLU:CG	2.46	0.45
25:BA:2091:C:H4'	48:BX:55:MET:HE3	1.98	0.45
25:BA:1000:A:O2'	50:BZ:10:ARG:NH1	2.50	0.45
31:CG:53:PRO:HG3	31:CG:61:TRP:CE3	2.52	0.45
38:CN:87:PHE:HE1	38:CN:116:VAL:HG22	1.82	0.45
45:CU:4:ILE:HG22	45:CU:5:ARG:N	2.31	0.45
1:DA:1505:G:H4'	1:DA:1506:U:H5''	1.98	0.45
1:DA:261:U:OP1	20:DT:71:LYS:NZ	2.48	0.45
1:DA:911:U:H2'	1:DA:912:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DB:40:ILE:HD12	2:DB:41:ILE:H	1.82	0.45
1:AA:768:A:H5'	1:AA:1524:C:H1'	1.99	0.45
4:AD:109:ALA:HB3	4:AD:113:GLU:HG2	1.99	0.45
5:AE:97:GLN:HB2	5:AE:124:LEU:CD1	2.46	0.45
9:AI:105:THR:HG22	9:AI:106:ARG:H	1.80	0.45
9:AI:46:MET:N	9:AI:46:MET:SD	2.80	0.45
10:AJ:32:THR:OG1	10:AJ:33:GLY:N	2.50	0.45
19:AS:45:ILE:C	19:AS:47:LEU:H	2.20	0.45
21:AU:12:PHE:CE2	21:AU:16:LEU:HD21	2.51	0.45
22:AV:61:GLU:HB2	22:AV:67:LYS:HG2	1.97	0.45
25:BA:1059:G:H5''	25:BA:1060:U:H2'	1.98	0.45
25:BA:1301:A:O2'	25:BA:1302:A:H3'	2.17	0.45
25:BA:1989:G:H2'	25:BA:1990:C:O4'	2.17	0.45
25:BA:570:G:H2'	25:BA:2030:A:N7	2.32	0.45
25:BA:2039:U:H2'	25:BA:2040:G:C8	2.51	0.45
25:BA:2422:C:H4'	25:BA:2423:U:OP1	2.16	0.45
25:BA:277:G:N3	25:BA:277:G:H3'	2.32	0.45
25:BA:2892:G:H5''	25:BA:2894:G:N2	2.31	0.45
25:BA:68:G:H2'	25:BA:69:C:O4'	2.16	0.45
32:BH:134:VAL:CG1	32:BH:138:VAL:HG21	2.47	0.45
32:BH:144:VAL:HG13	32:BH:145:ASN:N	2.32	0.45
32:BH:3:VAL:HA	32:BH:38:PRO:HA	1.97	0.45
25:BA:973:A:H5''	42:BR:81:LYS:CG	2.47	0.45
25:BA:973:A:H5''	42:BR:81:LYS:HG3	1.98	0.45
25:BA:1187:G:H5''	42:BR:83:TYR:CE1	2.51	0.45
49:BY:4:LYS:O	49:BY:7:ARG:NH1	2.49	0.45
51:C0:25:THR:O	51:C0:27:LEU:N	2.43	0.45
53:C2:18:PHE:HA	53:C2:43:THR:HG21	1.97	0.45
25:CA:1824:G:OP2	27:CC:52:HIS:NE2	2.39	0.45
41:CQ:89:ILE:HD13	41:CQ:93:ILE:HB	1.98	0.45
46:CV:6:ALA:HB1	46:CV:40:ILE:CG2	2.46	0.45
46:CV:77:VAL:HG23	46:CV:89:ILE:HG12	1.99	0.45
1:DA:1054:C:OP2	60:DA:1843:HOH:O	2.21	0.45
1:DA:9:G:C2	1:DA:10:A:C8	3.05	0.45
1:DA:496:A:H2'	1:DA:497:G:N7	2.31	0.45
1:DA:858:G:C2'	1:DA:859:G:H5'	2.46	0.45
2:DB:51:ASN:CG	2:DB:52:GLU:N	2.69	0.45
10:DJ:8:ILE:HG23	10:DJ:74:VAL:HB	1.98	0.45
1:AA:466:A:N6	1:AA:468:A:N7	2.63	0.45
3:AC:156:ARG:NH1	3:AC:156:ARG:HB3	2.31	0.45
19:AS:14:HIS:HA	19:AS:17:LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:B4:14:CYS:SG	55:B4:33:HIS:ND1	2.85	0.45
25:BA:1562:U:H2'	25:BA:1563:U:O4'	2.16	0.45
25:BA:587:C:O2	36:BL:33:ARG:NH2	2.44	0.45
27:BC:16:VAL:N	27:BC:203:VAL:CG1	2.80	0.45
28:BD:57:ALA:C	28:BD:59:ARG:H	2.18	0.45
32:BH:22:LYS:H	32:BH:22:LYS:CD	2.30	0.45
39:BO:53:THR:HB	39:BO:65:THR:CG2	2.47	0.45
25:CA:1071:G:H1'	25:CA:1089:A:H2'	1.98	0.45
25:CA:2407:A:OP1	60:CA:3561:HOH:O	2.21	0.45
25:CA:2543:G:C6	25:CA:2544:G:C6	3.05	0.45
25:CA:2648:G:N2	25:CA:2673:G:H1'	2.31	0.45
25:CA:2883:A:H5'	25:CA:2884:U:H5''	1.98	0.45
25:CA:996:A:H61	25:CA:1159:U:H3	1.65	0.45
28:CD:124:ARG:HA	28:CD:165:MET:CE	2.46	0.45
33:CI:32:VAL:HG22	33:CI:66:PHE:CZ	2.51	0.45
25:CA:327:G:N2	45:CU:67:SER:OG	2.49	0.45
1:DA:1076:U:N3	1:DA:1082:A:C2	2.85	0.45
1:DA:1288:A:N1	1:DA:1371:G:H1'	2.32	0.45
1:DA:309:A:H2'	1:DA:310:G:H8	1.82	0.45
1:DA:831:A:C5'	2:DB:21:ARG:HH12	2.29	0.45
6:DF:54:LEU:HD12	6:DF:55:HIS:N	2.32	0.45
7:DG:30:LEU:HD21	7:DG:42:ILE:HD11	1.98	0.45
9:DI:90:TYR:CD1	9:DI:94:LEU:HD21	2.52	0.45
11:DK:81:ASN:HB3	11:DK:106:ARG:HB3	1.98	0.45
1:AA:152:A:N6	1:AA:170:U:C2	2.85	0.45
1:AA:477:C:H2'	1:AA:478:A:C8	2.51	0.45
1:AA:401:C:O2'	1:AA:621:A:N3	2.37	0.45
8:AH:78:VAL:HG21	8:AH:125:ILE:HD11	1.99	0.45
16:AP:1:MET:CG	16:AP:2:VAL:N	2.79	0.45
25:BA:1833:C:C4	25:BA:1834:U:C5	3.05	0.45
25:BA:995:C:O2	34:BJ:3:THR:OG1	2.21	0.45
35:BK:76:VAL:HG12	40:BP:72:VAL:HG22	1.99	0.45
54:C3:22:LYS:HA	54:C3:47:ALA:O	2.17	0.45
25:CA:1171:G:C6	25:CA:1172:C:N4	2.85	0.45
25:CA:1269:A:N1	25:CA:2011:U:C5	2.84	0.45
25:CA:2880:C:N3	25:CA:2881:U:C5	2.85	0.45
34:CJ:44:TYR:HA	34:CJ:50:THR:HG21	1.98	0.45
38:CN:32:GLU:HA	38:CN:115:LEU:CD1	2.47	0.45
45:CU:38:ILE:HD12	45:CU:39:ASN:HB2	1.99	0.45
1:DA:1107:C:OP2	3:DC:172:ARG:NH1	2.50	0.45
1:DA:1054:C:H5'	1:DA:1196:A:N3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:182:A:C8	1:DA:184:G:C5	3.03	0.45
3:DC:67:THR:HA	3:DC:102:ASN:HB2	1.98	0.45
4:DD:9:LEU:HD12	4:DD:10:LYS:H	1.80	0.45
5:DE:96:MET:SD	5:DE:144:LEU:HD21	2.57	0.45
12:DL:25:GLU:HG2	12:DL:27:CYS:SG	2.57	0.45
12:DL:43:LYS:HG2	12:DL:44:LYS:HG2	1.98	0.45
13:DM:68:ASP:O	13:DM:71:ARG:N	2.50	0.45
14:DN:42:TRP:CZ3	14:DN:45:VAL:HG11	2.52	0.45
14:DN:81:ARG:HA	14:DN:84:VAL:CG1	2.47	0.45
15:DO:3:LEU:HD13	15:DO:8:THR:CG2	2.47	0.45
1:AA:1183:U:O2'	1:AA:1185:G:OP2	2.33	0.45
1:AA:1416:G:C3'	1:AA:1417:G:H5'	2.47	0.45
1:AA:201:G:C2	1:AA:217:C:O2	2.70	0.45
4:AD:19:LEU:HD12	4:AD:64:ILE:HA	1.97	0.45
7:AG:108:ALA:CB	7:AG:120:LEU:HD12	2.46	0.45
8:AH:96:MET:HB2	8:AH:99:LEU:O	2.17	0.45
9:AI:30:ILE:HD13	9:AI:38:TYR:CD2	2.51	0.45
1:AA:501:C:P	12:AL:121:ARG:NH2	2.90	0.45
14:AN:2:LYS:HZ2	14:AN:4:SER:H	1.65	0.45
25:BA:1028:A:N3	25:BA:2486:C:O2'	2.37	0.45
25:BA:1263:U:OP1	51:B0:12:ARG:NH1	2.49	0.45
25:BA:1361:G:C5	25:BA:1371:G:N2	2.85	0.45
25:BA:1415:U:C6	25:BA:1588:G:N1	2.85	0.45
25:BA:1433:A:N6	25:BA:1434:A:H62	2.14	0.45
25:BA:2629:U:O2'	25:BA:2630:G:OP2	2.34	0.45
25:BA:446:G:OP2	41:BQ:2:ARG:NH1	2.49	0.45
26:BB:3098:G:N1	46:BV:14:LYS:HG2	2.31	0.45
46:BV:29:ILE:H	46:BV:29:ILE:HD12	1.80	0.45
25:CA:1794:A:H1'	25:CA:1900:A:C2	2.52	0.45
25:CA:2297:A:O3'	30:CF:70:ARG:NH1	2.50	0.45
25:CA:2324:U:H3'	25:CA:2325:G:C5'	2.47	0.45
25:CA:2849:U:H4'	25:CA:2868:A:C2	2.51	0.45
25:CA:659:G:H4'	29:CE:95:LYS:CD	2.46	0.45
25:CA:1187:G:H5''	42:CR:83:TYR:CZ	2.52	0.45
43:CS:3:THR:HG21	43:CS:58:ALA:HB3	1.98	0.45
1:DA:1493:A:H5'	1:DA:1494:G:OP2	2.17	0.45
1:DA:435:A:C6	1:DA:436:C:C4	3.04	0.45
1:DA:973:G:OP1	10:DJ:59:LYS:NZ	2.38	0.45
3:DC:61:ALA:O	3:DC:63:SER:N	2.50	0.45
5:DE:70:ASN:N	5:DE:70:ASN:OD1	2.50	0.45
1:DA:1491:G:C3'	12:DL:44:LYS:HZ2	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1137:C:O2'	1:AA:1138:G:OP2	2.32	0.45
1:AA:242:G:C2	1:AA:245:U:C4	3.05	0.45
1:AA:463:U:H5'	1:AA:464:U:OP2	2.17	0.45
2:AB:183:VAL:HG11	2:AB:197:ASP:H	1.82	0.45
2:AB:50:PHE:O	2:AB:52:GLU:N	2.47	0.45
3:AC:152:GLU:CB	3:AC:167:TRP:HB3	2.47	0.45
13:AM:75:MET:SD	30:BF:111:ARG:NH2	2.90	0.45
25:BA:1378:A:O2'	25:BA:1380:G:OP2	2.34	0.45
25:BA:647:G:H2'	25:BA:648:G:O5'	2.17	0.45
25:BA:947:A:H2'	25:BA:948:C:C6	2.52	0.45
25:BA:61:C:C2	25:BA:94:A:C2	3.05	0.45
27:BC:57:HIS:CD2	27:BC:58:LYS:H	2.35	0.45
37:BM:26:VAL:HG11	37:BM:133:LYS:HA	1.99	0.45
25:BA:329:G:O6	45:BU:16:LYS:HG2	2.17	0.45
46:BV:6:ALA:HB3	46:BV:65:VAL:HG12	1.99	0.45
49:BY:21:LEU:HA	49:BY:25:GLN:HB3	1.98	0.45
25:CA:242:G:H5''	54:C3:63:TYR:CE2	2.52	0.45
25:CA:2027:G:C6	25:CA:2028:U:C4	3.05	0.45
25:CA:2436:G:O2'	25:CA:2437:G:H5'	2.16	0.45
58:CA:3166:PAR:H13	58:CA:3166:PAR:O62	2.17	0.45
27:CC:265:PHE:N	27:CC:265:PHE:CD1	2.83	0.45
28:CD:8:LYS:HE3	28:CD:193:VAL:HG23	1.99	0.45
30:CF:127:TYR:HB2	30:CF:155:ILE:CG1	2.47	0.45
1:DA:409:U:H2'	1:DA:410:G:C8	2.51	0.45
1:DA:74:A:H2'	1:DA:75:G:O4'	2.16	0.45
4:DD:99:ASP:O	4:DD:103:TYR:N	2.46	0.45
11:DK:84:VAL:HG13	11:DK:110:ILE:HA	1.99	0.45
12:DL:72:HIS:ND1	12:DL:74:LEU:HD12	2.32	0.45
13:DM:106:ALA:HB3	13:DM:110:LYS:HD3	1.99	0.45
1:DA:1318:A:H4'	19:DS:10:PHE:HZ	1.81	0.45
19:DS:63:THR:OG1	19:DS:64:ASP:N	2.38	0.45
1:AA:105:G:H2'	1:AA:106:C:O4'	2.17	0.45
1:AA:1124:G:P	10:AJ:37:ARG:CZ	3.05	0.45
1:AA:582:C:C2	1:AA:760:G:N1	2.85	0.45
11:AK:26:SER:O	11:AK:27:PHE:CB	2.65	0.45
15:AO:83:GLU:H	15:AO:83:GLU:CD	2.20	0.45
56:B5:136:LEU:CB	56:B5:139:ASN:C	2.85	0.45
25:BA:1026:G:H2'	25:BA:1027:A:C8	2.51	0.45
25:BA:1501:G:C2'	25:BA:1502:A:O5'	2.65	0.45
25:BA:1932:A:C2	25:BA:1969:A:C5	3.05	0.45
25:BA:364:C:H2'	25:BA:365:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:883:G:N1	25:BA:893:C:O2	2.50	0.45
26:BB:3094:A:C5	26:BB:3095:U:C4	3.05	0.45
27:BC:176:ARG:CZ	27:BC:176:ARG:N	2.80	0.45
25:BA:1568:G:H4'	27:BC:58:LYS:HB3	1.98	0.45
32:BH:93:SER:OG	32:BH:94:ILE:N	2.48	0.45
39:BO:41:ALA:O	39:BO:44:GLY:N	2.47	0.45
39:BO:53:THR:HG21	39:BO:65:THR:HG22	1.99	0.45
43:BS:59:GLU:HA	43:BS:64:ALA:CB	2.47	0.45
43:BS:73:LYS:CB	43:BS:106:VAL:CG1	2.94	0.45
46:BV:65:VAL:O	46:BV:68:LYS:N	2.39	0.45
25:CA:194:G:OP2	60:CA:3757:HOH:O	2.21	0.45
25:CA:1996:C:H4'	25:CA:1997:C:OP1	2.17	0.45
25:CA:2032:G:N1	25:CA:2572:A:C8	2.85	0.45
58:CA:3168:PAR:H51	58:CA:3168:PAR:H322	1.82	0.45
25:CA:605:G:C5	25:CA:606:U:C5	3.05	0.45
30:CF:1:ALA:HA	30:CF:96:TRP:CD1	2.52	0.45
40:CP:75:THR:O	40:CP:77:SER:N	2.49	0.45
40:CP:83:ILE:HD13	40:CP:84:SER:N	2.31	0.45
42:CR:46:GLU:CD	42:CR:46:GLU:C	2.75	0.45
1:DA:1299:A:O2'	1:DA:1301:U:O4'	2.21	0.45
1:DA:570:G:H2'	1:DA:571:U:C6	2.51	0.45
1:DA:599:C:H4'	8:DH:88:ARG:NH1	2.31	0.45
1:DA:821:G:H2'	1:DA:822:U:C6	2.52	0.45
3:DC:140:ASN:O	3:DC:141:ALA:CB	2.64	0.45
15:DO:76:ALA:O	15:DO:80:ARG:HG2	2.16	0.45
1:AA:1053:G:H4'	1:AA:1054:C:H5'	1.99	0.45
1:AA:1414:U:O2'	1:AA:1415:G:H5'	2.16	0.45
1:AA:982:U:H4'	1:AA:983:A:C5'	2.47	0.45
1:AA:428:G:H4'	4:AD:9:LEU:HD23	1.98	0.45
12:AL:75:GLN:HG2	22:AV:104:PRO:HG3	1.99	0.45
15:AO:81:LEU:N	15:AO:83:GLU:OE2	2.50	0.45
20:AT:48:GLN:HA	20:AT:51:PHE:HB3	1.99	0.45
22:AV:112:LYS:HG3	22:AV:113:ASP:N	2.32	0.45
25:BA:139:U:O4	44:BT:2:ILE:CB	2.62	0.45
25:BA:1844:C:H2'	25:BA:1845:G:H5''	1.99	0.45
25:BA:1769:U:O2'	25:BA:1958:C:OP1	2.32	0.45
25:BA:249:C:O2	36:BL:63:LYS:NZ	2.50	0.45
25:BA:2552:U:C2	25:BA:2554:U:H5'	2.52	0.45
25:BA:632:A:H2'	25:BA:633:A:C8	2.51	0.45
29:BE:154:ASP:HB3	29:BE:157:LEU:HB3	1.99	0.45
30:BF:70:ARG:HE	30:BF:71:LYS:HZ2	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BF:8:LYS:O	30:BF:10:GLU:N	2.48	0.45
31:BG:8:VAL:HG13	31:BG:49:LEU:HB2	1.99	0.45
34:BJ:42:ALA:O	41:BQ:63:ARG:HD2	2.17	0.45
38:BN:87:PHE:HB3	38:BN:94:TYR:CE1	2.51	0.45
25:CA:2472:G:H2'	25:CA:2475:C:H42	1.81	0.45
25:CA:587:C:N3	36:CL:33:ARG:NH2	2.65	0.45
32:CH:9:VAL:HG12	32:CH:35:LYS:HZ2	1.81	0.45
32:CH:97:ARG:NH2	32:CH:97:ARG:O	2.50	0.45
35:CK:39:ILE:HD12	35:CK:62:VAL:CG2	2.47	0.45
43:CS:5:ALA:HB3	43:CS:54:ALA:HB2	1.98	0.45
1:DA:1136:C:O2'	1:DA:1137:C:OP1	2.34	0.45
1:DA:1350:A:C2	1:DA:1351:U:C2	3.05	0.45
1:DA:1360:A:N6	1:DA:1361:G:N3	2.65	0.45
1:DA:50:A:N6	1:DA:361:G:C4'	2.80	0.45
1:DA:977:A:O2'	1:DA:981:U:N3	2.45	0.45
4:DD:9:LEU:CG	4:DD:10:LYS:N	2.80	0.45
5:DE:105:ILE:CG2	5:DE:112:ARG:HB2	2.47	0.45
5:DE:44:GLY:HA3	5:DE:74:VAL:HG21	1.99	0.45
7:DG:3:ARG:H	7:DG:5:ARG:CZ	2.29	0.45
8:DH:92:LEU:HD21	8:DH:116:ALA:HB1	1.98	0.45
12:DL:73:ASN:HD21	12:DL:104:CYS:HA	1.82	0.45
13:DM:114:LYS:HD2	13:DM:114:LYS:HA	1.83	0.45
24:DW:57:G:H2'	24:DW:58:A:H5'	1.99	0.45
1:AA:1140:C:O2'	1:AA:1141:C:OP2	2.30	0.44
4:AD:26:ARG:NH1	4:AD:31:LYS:HD3	2.32	0.44
5:AE:94:VAL:HG21	5:AE:140:THR:HG22	1.99	0.44
9:AI:9:THR:OG1	9:AI:10:GLY:N	2.48	0.44
12:AL:65:SER:CB	12:AL:82:ILE:HD11	2.48	0.44
12:AL:94:ARG:NH1	12:AL:95:TYR:CD2	2.85	0.44
13:AM:108:THR:HG22	13:AM:109:ARG:HG3	1.99	0.44
16:AP:52:LEU:HD23	16:AP:57:ILE:HD11	1.99	0.44
51:B0:53:VAL:O	51:B0:54:ILE:HG13	2.17	0.44
25:BA:1875:G:HO2'	25:BA:1876:A:P	2.39	0.44
25:BA:2059:A:C2	25:BA:2503:A:C6	3.05	0.44
26:BB:3112:G:H2'	26:BB:3113:C:C6	2.53	0.44
30:BF:7:TYR:HA	30:BF:11:VAL:HB	1.98	0.44
41:BQ:98:ALA:HB2	41:BQ:105:PHE:CD2	2.52	0.44
43:BS:22:ASP:HA	43:BS:25:ARG:HG3	1.99	0.44
44:BT:30:ILE:HG13	44:BT:85:VAL:HG13	1.99	0.44
45:BU:32:LYS:HZ2	45:BU:32:LYS:HB3	1.81	0.44
45:BU:5:ARG:O	45:BU:8:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:CA:1131:G:OP1	34:CJ:82:GLY:HA2	2.15	0.44
25:CA:1327:A:N6	25:CA:1328:A:C2	2.85	0.44
25:CA:1850:G:C6	25:CA:1851:U:C4	3.06	0.44
25:CA:2335:A:N6	25:CA:2337:G:H1'	2.32	0.44
25:CA:796:C:H2'	25:CA:797:G:H8	1.82	0.44
29:CE:118:LEU:HD11	29:CE:188:MET:SD	2.57	0.44
33:CI:102:ARG:HA	33:CI:105:LEU:HG	1.98	0.44
39:CO:7:ARG:HD2	39:CO:97:PHE:CE2	2.52	0.44
40:CP:17:PRO:HG2	40:CP:83:ILE:CD1	2.47	0.44
1:DA:1149:C:OP2	9:DI:11:ARG:NH1	2.49	0.44
2:DB:84:ALA:HB2	2:DB:218:ALA:HB2	1.98	0.44
6:DF:38:ARG:CZ	6:DF:96:VAL:CG2	2.95	0.44
12:DL:116:LYS:O	12:DL:117:TYR:CB	2.65	0.44
13:DM:22:ILE:HD11	13:DM:66:GLU:H	1.82	0.44
21:DU:24:GLU:CG	21:DU:25:LYS:H	2.31	0.44
1:AA:25:C:C4	1:AA:558:G:N2	2.85	0.44
1:AA:270:A:C5	1:AA:271:C:C4	3.06	0.44
1:AA:19:A:H5''	5:AE:91:GLY:HA3	1.98	0.44
14:AN:64:CYS:SG	14:AN:83:LYS:HE3	2.57	0.44
19:AS:34:TRP:N	19:AS:34:TRP:CD1	2.84	0.44
25:BA:1798:U:H5''	27:BC:269:ARG:HH22	1.82	0.44
25:BA:2144:G:O2'	25:BA:2146:C:OP2	2.30	0.44
25:BA:2231:U:C4	25:BA:2232:C:C5	3.05	0.44
25:BA:2557:G:H2'	25:BA:2558:C:C6	2.52	0.44
25:BA:2603:G:C5	25:BA:2604:U:C5	3.05	0.44
25:BA:2204:G:H4'	27:BC:149:LYS:HG3	1.99	0.44
31:BG:23:ILE:HD12	31:BG:24:THR:N	2.32	0.44
32:BH:122:LEU:HA	32:BH:124:THR:OG1	2.17	0.44
32:BH:72:ILE:HD13	32:BH:140:ALA:HA	1.99	0.44
39:BO:83:LEU:HA	39:BO:87:ILE:HG13	1.99	0.44
25:CA:1737:G:C4	25:CA:1738:G:N2	2.85	0.44
25:CA:832:U:H2'	25:CA:833:A:C8	2.52	0.44
30:CF:160:LYS:N	30:CF:164:GLU:OE2	2.50	0.44
36:CL:111:ILE:HD12	36:CL:111:ILE:N	2.32	0.44
45:CU:53:GLN:N	45:CU:54:PRO:CD	2.81	0.44
47:CW:21:VAL:HA	47:CW:36:VAL:HA	1.98	0.44
1:DA:260:G:H2'	1:DA:261:U:C6	2.52	0.44
1:DA:414:A:C6	1:DA:431:A:C2	3.06	0.44
1:DA:542:G:C2	1:DA:543:U:C6	3.05	0.44
1:DA:958:A:N6	1:DA:959:A:N1	2.66	0.44
2:DB:59:LYS:H	2:DB:61:ALA:H	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DC:172:ARG:HD2	3:DC:174:PRO:HG3	1.97	0.44
4:DD:46:PRO:O	4:DD:48:LEU:N	2.50	0.44
12:DL:90:LEU:HB2	12:DL:93:VAL:CG1	2.47	0.44
13:DM:85:CYS:SG	13:DM:88:GLY:N	2.90	0.44
14:AN:20:PHE:CG	14:AN:21:ALA:N	2.85	0.44
25:BA:2141:G:H2'	25:BA:2141:G:N3	2.33	0.44
25:BA:2394:C:OP2	54:B3:29:ARG:HD3	2.17	0.44
27:BC:246:PRO:HG2	27:BC:247:TRP:CE3	2.51	0.44
33:BI:121:ILE:HA	33:BI:124:MET:HB3	1.98	0.44
39:BO:31:THR:HG23	39:BO:32:PRO:CD	2.47	0.44
39:BO:82:ALA:HB1	39:BO:87:ILE:HG12	2.00	0.44
43:BS:73:LYS:HB2	43:BS:106:VAL:HG13	1.99	0.44
25:CA:1922:G:O6	58:CA:3167:PAR:C22	2.63	0.44
25:CA:2626:C:H2'	25:CA:2627:G:O4'	2.17	0.44
25:CA:475:C:N4	25:CA:476:G:C6	2.84	0.44
25:CA:84:A:H4'	45:CU:5:ARG:HD3	2.00	0.44
25:CA:885:C:O2'	25:CA:892:A:N7	2.50	0.44
26:CB:3017:C:H2'	26:CB:3018:G:O4'	2.17	0.44
29:CE:130:LYS:HB3	29:CE:133:LEU:HD11	1.99	0.44
36:CL:89:VAL:O	36:CL:94:THR:HG21	2.17	0.44
39:CO:18:LEU:CD1	39:CO:25:ARG:HD2	2.47	0.44
41:CQ:91:ARG:H	41:CQ:91:ARG:HG2	1.69	0.44
43:CS:21:ALA:O	43:CS:23:LEU:N	2.51	0.44
1:DA:1004:A:H2'	1:DA:1005:A:O4'	2.18	0.44
1:DA:1145:A:C2	1:DA:1147:C:N4	2.85	0.44
1:DA:1202:U:C5	1:DA:1203:C:C5	3.05	0.44
1:DA:532:A:N6	1:DA:1206:G:O2'	2.49	0.44
1:DA:129:A:H1'	1:DA:130:A:C8	2.52	0.44
1:DA:782:A:C2	1:DA:801:U:H1'	2.53	0.44
5:DE:122:ASN:CG	5:DE:123:VAL:H	2.21	0.44
7:DG:68:ASN:ND2	7:DG:128:ALA:O	2.49	0.44
12:DL:15:LYS:O	12:DL:17:ALA:N	2.51	0.44
1:DA:1358:U:P	14:DN:75:ARG:CZ	3.05	0.44
16:DP:46:LYS:NZ	16:DP:48:GLU:O	2.49	0.44
1:AA:1219:A:H2'	1:AA:1220:G:C8	2.53	0.44
1:AA:1494:G:C2	1:AA:1495:U:C6	3.06	0.44
1:AA:298:A:H2'	1:AA:299:G:O4'	2.18	0.44
4:AD:170:TRP:HB2	4:AD:184:ARG:HB2	1.98	0.44
4:AD:54:GLN:HB3	4:AD:58:LYS:NZ	2.33	0.44
8:AH:80:ARG:NH2	8:AH:82:GLY:H	2.16	0.44
14:AN:64:CYS:HB2	14:AN:80:SER:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AR:33:ILE:HD11	18:AR:63:ARG:NH2	2.31	0.44
19:AS:5:LEU:HD11	19:AS:10:PHE:HD2	1.82	0.44
25:BA:2020:A:H5'	51:B0:8:THR:CG2	2.48	0.44
54:B3:31:ILE:CD1	54:B3:35:LYS:HE3	2.47	0.44
25:BA:1073:A:H3'	25:BA:1074:G:H5''	1.99	0.44
25:BA:1794:A:H2'	25:BA:1795:C:H6	1.82	0.44
25:BA:2250:G:OP1	25:BA:2275:C:O2'	2.22	0.44
25:BA:2045:C:C2	25:BA:2624:G:C2	3.06	0.44
27:BC:48:ILE:O	27:BC:48:ILE:CD1	2.65	0.44
30:BF:107:VAL:HG13	30:BF:108:PRO:HD3	1.98	0.44
30:BF:135:ILE:HD11	30:BF:142:TYR:N	2.32	0.44
33:BI:106:GLN:NE2	33:BI:107:GLU:OE2	2.50	0.44
35:BK:99:ILE:HD13	35:BK:115:ILE:HG23	2.00	0.44
49:BY:28:LEU:HD21	49:BY:42:LEU:HB3	1.99	0.44
25:CA:1176:U:H2'	25:CA:1177:G:C8	2.51	0.44
25:CA:1359:A:C8	25:CA:1373:A:N1	2.86	0.44
25:CA:1675:C:H2'	25:CA:1676:A:O4'	2.17	0.44
25:CA:1893:C:C5	25:CA:1894:C:C5	3.05	0.44
25:CA:192:C:C6	25:CA:193:U:C6	3.06	0.44
25:CA:792:A:C8	25:CA:2440:C:C2	3.05	0.44
25:CA:2820:A:O2'	25:CA:2821:A:P	2.75	0.44
25:CA:849:A:N6	25:CA:928:A:H61	2.15	0.44
26:CB:3050:A:OP1	39:CO:68:LYS:N	2.38	0.44
27:CC:143:VAL:HB	27:CC:153:LEU:HB2	1.99	0.44
37:CM:8:LYS:HD3	37:CM:8:LYS:H	1.82	0.44
43:CS:17:VAL:HA	43:CS:43:ALA:HB1	1.99	0.44
47:CW:19:LEU:HB3	47:CW:37:ARG:HG2	1.99	0.44
1:DA:31:G:H22	1:DA:47:C:H4'	1.82	0.44
1:DA:92:U:H2'	1:DA:93:U:C6	2.51	0.44
3:DC:150:LYS:HG2	3:DC:201:TRP:CE3	2.52	0.44
7:DG:95:ARG:HA	7:DG:98:ALA:HB3	1.98	0.44
14:DN:3:GLN:NE2	60:DN:304:HOH:O	2.50	0.44
1:AA:1072:G:C6	1:AA:1104:G:C2	3.06	0.44
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.99	0.44
21:AU:17:ARG:NH2	21:AU:20:LYS:O	2.50	0.44
25:BA:1638:C:H4'	25:BA:2710:C:O2	2.17	0.44
25:BA:297:G:H5''	45:BU:84:PHE:HB2	1.99	0.44
32:BH:134:VAL:HG13	32:BH:138:VAL:HG21	1.99	0.44
32:BH:143:ILE:O	32:BH:144:VAL:HB	2.18	0.44
34:BJ:31:GLU:HG2	34:BJ:142:ILE:CG1	2.48	0.44
38:BN:53:THR:HG22	38:BN:94:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:BP:20:ARG:HH21	40:BP:20:ARG:CG	2.30	0.44
25:CA:2373:G:C6	25:CA:2374:C:C4	3.05	0.44
25:CA:2791:G:N2	25:CA:2806:C:H1'	2.33	0.44
25:CA:500:G:N2	25:CA:502:A:H3'	2.33	0.44
25:CA:725:G:C6	25:CA:726:G:N1	2.85	0.44
25:CA:784:G:C6	27:CC:227:VAL:HG21	2.51	0.44
32:CH:121:VAL:CG2	32:CH:128:HIS:CE1	3.00	0.44
34:CJ:65:THR:HG22	34:CJ:68:LYS:NZ	2.32	0.44
41:CQ:5:ARG:O	41:CQ:6:GLY:C	2.56	0.44
44:CT:68:LYS:HG2	44:CT:69:ARG:N	2.32	0.44
48:CX:31:ASN:HD21	48:CX:52:ALA:HB2	1.83	0.44
1:DA:1361:G:C5	1:DA:1362:A:N7	2.86	0.44
1:DA:1375:A:C5	1:DA:1376:U:C5	3.06	0.44
1:DA:381:C:H2'	1:DA:382:A:O4'	2.18	0.44
1:DA:642:A:C5	1:DA:643:C:C4	3.05	0.44
9:DI:57:MET:SD	9:DI:61:LEU:HG	2.57	0.44
16:DP:52:LEU:O	16:DP:53:ASP:HB2	2.17	0.44
1:AA:1040:U:H2'	1:AA:1041:G:C8	2.52	0.44
1:AA:1117:A:O3'	9:AI:106:ARG:NH1	2.49	0.44
1:AA:452:A:N6	1:AA:480:U:O2	2.51	0.44
1:AA:491:G:H2'	1:AA:492:C:C6	2.52	0.44
20:AT:55:GLN:N	20:AT:56:PRO:CD	2.81	0.44
25:BA:1501:G:H2'	25:BA:1502:A:O5'	2.17	0.44
25:BA:2394:C:P	54:B3:29:ARG:HH21	2.41	0.44
25:BA:572:A:C2	25:BA:2033:A:C2	3.06	0.44
25:BA:726:G:O2'	25:BA:727:A:OP2	2.34	0.44
30:BF:35:LEU:HD12	30:BF:153:ILE:HA	1.98	0.44
25:BA:2840:C:C5'	38:BN:53:THR:HG21	2.47	0.44
40:BP:20:ARG:CB	40:BP:20:ARG:HH21	2.31	0.44
25:CA:1060:U:H4'	25:CA:1061:U:H5'	1.99	0.44
25:CA:1141:U:H4'	25:CA:1142:A:O4'	2.18	0.44
25:CA:2130:U:O2'	25:CA:2158:A:N1	2.40	0.44
25:CA:962:G:H21	25:CA:2250:G:H1	1.65	0.44
25:CA:2285:C:OP2	52:C1:25:ASN:ND2	2.46	0.44
25:CA:2598:A:H5''	27:CC:233:GLY:HA3	1.99	0.44
25:CA:2728:U:OP2	58:CA:3166:PAR:H222	2.17	0.44
25:CA:569:U:O4	25:CA:570:G:C6	2.70	0.44
25:CA:585:G:H2'	25:CA:586:A:N7	2.33	0.44
25:CA:627:A:N1	25:CA:636:G:O2'	2.45	0.44
25:CA:7:G:H4'	34:CJ:15:TRP:CH2	2.53	0.44
25:CA:988:A:N6	50:CZ:13:ILE:HD11	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:CB:3061:G:C2	26:CB:3062:C:C2	3.06	0.44
34:CJ:32:LEU:C	34:CJ:36:LEU:HD12	2.38	0.44
36:CL:117:THR:OG1	36:CL:118:THR:N	2.51	0.44
38:CN:34:ILE:HG22	38:CN:113:ILE:CG2	2.48	0.44
40:CP:59:THR:OG1	40:CP:72:VAL:CG1	2.66	0.44
25:CA:139:U:H3	44:CT:2:ILE:CD1	2.28	0.44
1:DA:110:C:H2'	1:DA:111:G:O4'	2.17	0.44
1:DA:96:U:HO2'	1:DA:97:G:C5'	2.31	0.44
3:DC:153:VAL:HB	3:DC:198:VAL:HG13	1.99	0.44
4:DD:188:ARG:HG3	4:DD:189:SER:H	1.83	0.44
10:DJ:57:VAL:HG13	10:DJ:58:ASN:N	2.32	0.44
10:DJ:6:ILE:HG22	10:DJ:76:ILE:O	2.18	0.44
1:AA:1001:C:H2'	1:AA:1002:G:O4'	2.18	0.44
1:AA:829:G:H2'	1:AA:830:G:H5'	2.00	0.44
3:AC:60:PRO:O	3:AC:62:LYS:N	2.50	0.44
4:AD:9:LEU:HD13	4:AD:10:LYS:CB	2.47	0.44
1:AA:1309:G:P	13:AM:87:ARG:NH1	2.91	0.44
25:BA:1028:A:N6	25:BA:1125:G:H2'	2.33	0.44
25:BA:1300:G:O2'	25:BA:1635:A:OP1	2.31	0.44
25:BA:2410:G:C2	25:BA:2411:A:H1'	2.53	0.44
25:BA:265:A:H4'	25:BA:266:G:OP1	2.18	0.44
25:BA:31:C:O3'	25:BA:1238:G:C5'	2.65	0.44
25:BA:479:A:H4'	25:BA:480:A:OP1	2.16	0.44
25:BA:619:G:O6	60:BA:3292:HOH:O	2.20	0.44
27:BC:90:ILE:HD12	27:BC:102:TYR:CD1	2.52	0.44
25:BA:2314:A:H5''	30:BF:34:THR:HG21	2.00	0.44
34:BJ:4:PHE:O	41:BQ:63:ARG:NH2	2.45	0.44
37:BM:78:LEU:O	37:BM:79:ALA:CB	2.65	0.44
38:BN:54:LEU:HD12	38:BN:62:ASN:HD22	1.83	0.44
40:BP:95:LYS:HB3	40:BP:97:TYR:CE2	2.53	0.44
46:BV:14:LYS:O	46:BV:16:ALA:N	2.51	0.44
25:CA:1438:U:O2	25:CA:1555:G:N2	2.50	0.44
25:CA:1837:C:O2'	25:CA:1927:A:N3	2.35	0.44
25:CA:2413:G:C2	25:CA:2414:G:C8	3.06	0.44
25:CA:2514:U:H2'	25:CA:2515:C:C6	2.52	0.44
25:CA:2792:A:H3'	25:CA:2793:C:H5''	1.99	0.44
25:CA:555:G:N2	58:CA:3169:PAR:HN62	2.15	0.44
26:CB:3053:A:C2	26:CB:3054:G:C8	3.05	0.44
32:CH:84:ALA:HA	32:CH:90:LEU:HA	2.00	0.44
35:CK:102:PRO:HB3	35:CK:121:GLU:HB3	2.00	0.44
35:CK:118:LEU:HD23	35:CK:118:LEU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:CM:31:PHE:HB3	37:CM:130:PHE:CZ	2.53	0.44
43:CS:53:SER:O	43:CS:57:ASN:N	2.39	0.44
1:DA:411:A:C5	1:DA:429:U:C5	3.06	0.44
1:DA:613:C:C2	1:DA:628:G:N2	2.85	0.44
2:DB:69:PHE:HA	2:DB:162:PHE:O	2.18	0.44
3:DC:110:GLU:HG3	3:DC:144:LEU:HD23	2.00	0.44
3:DC:66:VAL:O	3:DC:67:THR:CB	2.65	0.44
4:DD:19:LEU:HB2	4:DD:21:LEU:HD22	2.00	0.44
13:DM:20:THR:O	13:DM:22:ILE:N	2.47	0.44
13:DM:31:LYS:HG3	13:DM:35:ALA:HB2	1.99	0.44
13:DM:2:ALA:HB2	13:DM:45:ILE:HD13	2.00	0.44
1:AA:1202:U:O4'	14:AN:69:ARG:CZ	2.65	0.44
1:AA:1237:C:H3'	1:AA:1336:C:H41	1.83	0.44
1:AA:148:G:N2	1:AA:175:C:O2	2.51	0.44
4:AD:14:ARG:HG2	4:AD:38:PRO:HB3	1.99	0.44
6:AF:39:LEU:HD13	6:AF:40:GLU:N	2.33	0.44
1:AA:1539:C:H5''	21:AU:18:ARG:HG3	2.00	0.44
22:AV:5:ASP:OD1	22:AV:5:ASP:N	2.51	0.44
24:AX:15:G:H2'	24:AX:16:U:C2	2.53	0.44
25:BA:1248:G:O2'	41:BQ:2:ARG:HA	2.17	0.44
25:BA:137:U:HO2'	25:BA:138:U:P	2.37	0.44
25:BA:2195:U:H2'	25:BA:2196:C:H6	1.83	0.44
25:BA:454:A:H4'	25:BA:455:C:OP2	2.18	0.44
25:BA:971:G:H2'	25:BA:972:A:O4'	2.18	0.44
30:BF:9:ASP:OD1	30:BF:10:GLU:N	2.51	0.44
32:BH:121:VAL:HG12	32:BH:122:LEU:N	2.32	0.44
25:CA:1663:G:C6	25:CA:1992:G:C8	3.05	0.44
25:CA:2591:C:H2'	25:CA:2592:G:H8	1.82	0.44
25:CA:2740:A:H2'	25:CA:2741:A:C8	2.53	0.44
25:CA:315:G:H2'	25:CA:316:C:O4'	2.18	0.44
25:CA:38:A:H2'	25:CA:39:G:O4'	2.18	0.44
25:CA:555:G:N2	58:CA:3169:PAR:C64	2.81	0.44
25:CA:735:A:N7	25:CA:761:A:H2	2.15	0.44
26:CB:3079:G:H2'	26:CB:3080:U:O4'	2.18	0.44
28:CD:155:VAL:HG12	28:CD:155:VAL:O	2.18	0.44
30:CF:3:LEU:C	30:CF:3:LEU:HD12	2.37	0.44
30:CF:62:GLN:HB3	30:CF:94:ARG:NH1	2.33	0.44
41:CQ:67:ALA:O	41:CQ:70:GLN:N	2.51	0.44
45:CU:11:ILE:HD11	45:CU:79:ALA:HB2	2.00	0.44
1:DA:1287:A:C6	1:DA:1288:A:C6	3.06	0.44
1:DA:17:U:H2'	1:DA:18:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:428:G:C5'	4:DD:9:LEU:HD11	2.48	0.44
2:DB:23:TRP:CZ3	2:DB:25:PRO:HA	2.52	0.44
1:DA:1347:G:C8	9:DI:109:ARG:HB3	2.53	0.44
13:DM:22:ILE:CD1	13:DM:66:GLU:HB2	2.48	0.44
21:DU:10:GLU:HB3	21:DU:11:PRO:HD2	2.00	0.44
18:DR:35:GLU:HB2	21:DU:19:PHE:HZ	1.83	0.44
1:AA:556:C:O2'	1:AA:557:G:H5'	2.17	0.44
1:AA:943:U:C2'	1:AA:944:G:H5'	2.48	0.44
8:AH:80:ARG:HH22	8:AH:82:GLY:H	1.64	0.44
10:AJ:74:VAL:HG13	10:AJ:75:ASP:N	2.33	0.44
13:AM:11:ASP:HA	13:AM:45:ILE:HG13	2.00	0.44
15:AO:49:ASP:OD2	15:AO:52:SER:OG	2.27	0.44
25:BA:1092:C:C5	25:BA:1093:G:H1'	2.53	0.44
25:BA:1816:C:H3'	27:BC:61:TYR:CE1	2.52	0.44
25:BA:197:A:C2	25:BA:198:C:H1'	2.52	0.44
25:BA:72:U:O4	49:BY:58:ASN:ND2	2.50	0.44
25:BA:322:A:P	29:BE:162:ARG:HH21	2.41	0.44
31:BG:23:ILE:HD13	31:BG:71:LEU:HD21	1.99	0.44
38:BN:103:ARG:HB2	38:BN:110:MET:HE3	2.00	0.44
45:BU:53:GLN:N	45:BU:54:PRO:HD2	2.33	0.44
25:CA:2119:A:O2'	25:CA:2120:G:P	2.76	0.44
25:CA:1999:C:H4'	25:CA:2723:C:O2	2.18	0.44
25:CA:2817:U:O2	25:CA:2836:U:H1'	2.17	0.44
27:CC:226:PRO:HA	27:CC:232:GLY:HA3	1.99	0.44
27:CC:230:PRO:HB2	27:CC:244:VAL:CG2	2.47	0.44
36:CL:35:HIS:C	36:CL:36:LYS:HG2	2.38	0.44
41:CQ:89:ILE:HD12	41:CQ:90:ASP:N	2.33	0.44
42:CR:49:ILE:HB	42:CR:51:VAL:O	2.18	0.44
6:DF:55:HIS:N	6:DF:55:HIS:ND1	2.65	0.44
8:DH:10:MET:HE1	8:DH:33:LYS:HA	1.99	0.44
12:DL:90:LEU:HD12	12:DL:90:LEU:N	2.32	0.44
19:DS:31:LEU:HD12	19:DS:32:ARG:H	1.83	0.44
1:AA:1279:G:H4'	1:AA:1280:A:OP1	2.18	0.43
1:AA:6:G:HO2'	1:AA:7:A:P	2.37	0.43
1:AA:791:G:C6	1:AA:792:A:N7	2.86	0.43
1:AA:908:A:C2	1:AA:909:A:C5	3.06	0.43
1:AA:938:A:C6	1:AA:939:G:C5	3.05	0.43
4:AD:187:GLU:OE2	4:AD:188:ARG:NH1	2.51	0.43
5:AE:44:GLY:HA2	5:AE:74:VAL:CG2	2.48	0.43
1:AA:1226:C:N4	13:AM:103:LYS:HD2	2.33	0.43
14:AN:82:ILE:HG23	14:AN:83:LYS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:AO:7:ALA:O	15:AO:8:THR:OG1	2.30	0.43
18:AR:41:PRO:O	18:AR:45:THR:HG22	2.17	0.43
25:BA:1061:U:C5'	33:BI:9:LYS:HD2	2.48	0.43
25:BA:1062:G:N2	25:BA:1077:A:C2	2.86	0.43
25:BA:1394:U:C4	25:BA:1395:A:C6	3.06	0.43
25:BA:2230:G:H2'	25:BA:2231:U:C6	2.53	0.43
25:BA:220:G:O2'	25:BA:233:A:N3	2.47	0.43
25:BA:2848:G:N3	25:BA:2867:G:C2	2.86	0.43
25:BA:31:C:O3'	25:BA:1238:G:H5''	2.17	0.43
25:BA:704:G:N3	25:BA:726:G:C2	2.86	0.43
26:BB:3053:A:C2	26:BB:3054:G:C8	3.06	0.43
30:BF:15:LEU:HD21	30:BF:168:LEU:HA	2.00	0.43
44:BT:39:THR:OG1	44:BT:40:LYS:N	2.50	0.43
49:BY:16:THR:O	49:BY:19:LEU:N	2.51	0.43
49:BY:5:GLU:HG3	49:BY:56:LEU:HD11	2.00	0.43
25:CA:2016:U:O2'	25:CA:2017:U:OP1	2.31	0.43
25:CA:2517:C:C5	25:CA:2542:A:C5	3.06	0.43
25:CA:301:G:H1'	25:CA:302:C:C6	2.53	0.43
25:CA:569:U:C4	25:CA:570:G:C6	3.05	0.43
28:CD:114:LYS:HE2	28:CD:196:ALA:CB	2.47	0.43
29:CE:105:LEU:HA	29:CE:108:ILE:HG23	2.00	0.43
25:CA:990:A:H61	42:CR:78:ARG:HH12	1.66	0.43
1:DA:691:G:H1	11:DK:53:ARG:NH2	2.16	0.43
8:DH:27:MET:HB3	8:DH:28:PRO:CD	2.49	0.43
9:DI:6:TYR:CZ	9:DI:89:GLU:HG2	2.53	0.43
12:DL:34:CYS:H	12:DL:55:VAL:HG23	1.83	0.43
1:DA:523:A:N1	12:DL:89:ASP:CB	2.81	0.43
25:CA:885:C:C3'	13:DM:92:ARG:HH22	2.31	0.43
20:DT:57:ILE:O	20:DT:61:GLN:HG2	2.18	0.43
1:AA:1190:G:OP1	3:AC:5:VAL:N	2.51	0.43
1:AA:246:A:C4	1:AA:279:A:N6	2.86	0.43
1:AA:292:G:N7	1:AA:293:G:H1'	2.34	0.43
1:AA:789:U:O2'	1:AA:791:G:N7	2.42	0.43
1:AA:844:G:N7	1:AA:846:G:O2'	2.45	0.43
2:AB:58:ASN:ND2	2:AB:220:THR:O	2.51	0.43
5:AE:13:GLU:HB3	5:AE:39:VAL:CG1	2.48	0.43
7:AG:91:VAL:HG21	7:AG:99:LEU:CD2	2.48	0.43
10:AJ:85:ASP:HA	10:AJ:88:MET:HE3	2.00	0.43
25:BA:1678:A:H2'	25:BA:1679:A:O4'	2.18	0.43
25:BA:1779:U:C5	25:BA:1784:A:N7	2.83	0.43
25:BA:605:G:N7	25:BA:606:U:C5	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:780:G:H21	25:BA:783:A:H62	1.66	0.43
13:AM:75:MET:SD	30:BF:109:ARG:NH1	2.91	0.43
25:BA:805:G:OP2	36:BL:41:ARG:HG2	2.18	0.43
40:BP:87:ARG:NH2	40:BP:109:ILE:O	2.44	0.43
46:BV:29:ILE:HD11	46:BV:88:HIS:HE1	1.83	0.43
49:BY:26:PHE:CE2	49:BY:30:MET:CE	3.01	0.43
25:CA:2741:A:H2'	25:CA:2742:G:O4'	2.18	0.43
25:CA:948:C:H2'	25:CA:949:G:H8	1.83	0.43
29:CE:3:LEU:HD12	29:CE:14:VAL:HG11	2.00	0.43
25:CA:2310:C:C4	30:CF:76:PHE:CE1	3.06	0.43
38:CN:117:ASP:O	38:CN:118:ARG:HB2	2.18	0.43
38:CN:3:HIS:O	38:CN:4:ARG:HB2	2.16	0.43
40:CP:17:PRO:CG	40:CP:83:ILE:HD11	2.48	0.43
1:DA:1097:C:H2'	1:DA:1098:C:C6	2.53	0.43
1:DA:1141:C:O2'	1:DA:1142:G:OP2	2.29	0.43
1:DA:1401:G:C2	1:DA:1402:C:H1'	2.53	0.43
2:DB:86:SER:HB2	2:DB:89:GLN:HE21	1.83	0.43
5:DE:100:SER:C	5:DE:102:GLY:H	2.22	0.43
5:DE:80:THR:HG23	5:DE:122:ASN:HD21	1.83	0.43
5:DE:81:LEU:HG	5:DE:147:MET:SD	2.58	0.43
7:DG:93:PRO:HA	7:DG:96:ARG:HB2	2.00	0.43
12:DL:43:LYS:O	12:DL:45:PRO:HD2	2.17	0.43
16:DP:42:ILE:O	16:DP:44:SER:N	2.41	0.43
20:DT:31:PHE:HE1	20:DT:57:ILE:HD13	1.83	0.43
18:DR:35:GLU:HB2	21:DU:19:PHE:CZ	2.52	0.43
1:AA:1492:A:O2'	1:AA:1493:A:O5'	2.35	0.43
1:AA:49:U:O4	1:AA:365:U:H5	2.02	0.43
2:AB:87:CYS:O	2:AB:89:GLN:N	2.51	0.43
4:AD:59:GLN:C	4:AD:60:LYS:HD2	2.38	0.43
7:AG:40:GLU:HA	7:AG:43:VAL:HG22	1.99	0.43
1:AA:826:C:H4'	8:AH:13:ARG:HD3	2.00	0.43
11:AK:23:ILE:HG23	11:AK:86:VAL:HA	2.00	0.43
12:AL:114:ARG:HB2	12:AL:119:VAL:HB	1.99	0.43
15:AO:19:ALA:C	15:AO:21:ASP:H	2.22	0.43
55:B4:30:GLU:O	55:B4:32:LYS:N	2.51	0.43
25:BA:1060:U:H4'	25:BA:1061:U:H5'	1.99	0.43
25:BA:1022:G:C5	25:BA:1140:C:C4	3.05	0.43
25:BA:1420:A:O2'	25:BA:1421:G:P	2.76	0.43
25:BA:2306:C:OP2	25:BA:2307:G:O2'	2.29	0.43
25:BA:2666:C:C5	25:BA:2667:C:C5	3.06	0.43
25:BA:545:U:C6	25:BA:547:A:H4'	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BC:15:VAL:CG1	27:BC:16:VAL:N	2.81	0.43
25:CA:1142:A:H4'	34:CJ:27:ARG:NH2	2.33	0.43
25:CA:184:C:O2	25:CA:213:A:C2	2.71	0.43
25:CA:1995:U:OP1	28:CD:128:ARG:CZ	2.67	0.43
25:CA:2345:G:H4'	25:CA:2346:A:C5'	2.49	0.43
25:CA:372:G:C4	48:CX:60:LYS:HE3	2.54	0.43
25:CA:77:G:H5''	49:CY:2:LYS:CD	2.47	0.43
29:CE:59:PRO:CG	29:CE:70:SER:HB2	2.47	0.43
30:CF:28:PRO:HB2	30:CF:168:LEU:CD1	2.48	0.43
1:DA:1014:A:N7	1:DA:1015:G:C6	2.87	0.43
1:DA:1140:C:O2'	1:DA:1141:C:P	2.77	0.43
1:DA:1372:U:OP1	9:DI:74:GLY:N	2.51	0.43
58:DA:1655:PAR:H322	58:DA:1655:PAR:H51	1.82	0.43
1:DA:8:A:O4'	5:DE:107:ALA:HA	2.18	0.43
2:DB:96:TRP:CH2	2:DB:172:ALA:HA	2.53	0.43
3:DC:121:THR:HG22	3:DC:122:SER:N	2.32	0.43
3:DC:71:ALA:O	3:DC:72:ARG:C	2.55	0.43
10:DJ:90:LEU:HG	10:DJ:91:ASP:N	2.33	0.43
21:DU:17:ARG:HG2	21:DU:20:LYS:NZ	2.33	0.43
1:AA:484:G:H4'	1:AA:485:U:C5'	2.48	0.43
1:AA:857:C:H2'	1:AA:858:G:O4'	2.19	0.43
7:AG:66:LEU:HA	7:AG:69:VAL:HG23	2.00	0.43
9:AI:84:THR:HG21	9:AI:103:PHE:CD2	2.53	0.43
12:AL:42:PRO:HB2	12:AL:89:ASP:HB3	2.00	0.43
54:B3:30:HIS:CE1	54:B3:31:ILE:HG23	2.53	0.43
25:BA:1661:G:C5	25:BA:1662:U:C5	3.07	0.43
25:BA:1707:G:H2'	25:BA:1708:C:O4'	2.18	0.43
25:BA:1753:G:N2	25:BA:1756:G:OP2	2.48	0.43
22:AV:130:ARG:NH1	25:BA:1945:G:O2'	2.46	0.43
25:BA:2578:G:OP2	25:BA:2578:G:H4'	2.17	0.43
25:BA:2799:A:C5	25:BA:2801:G:C8	3.06	0.43
28:BD:68:PHE:CD1	28:BD:75:ALA:HA	2.53	0.43
31:BG:24:THR:HG22	31:BG:25:ILE:N	2.33	0.43
39:BO:58:ILE:O	39:BO:62:LEU:CD1	2.66	0.43
43:BS:98:LYS:NZ	43:BS:98:LYS:HB2	2.34	0.43
49:BY:21:LEU:HA	49:BY:25:GLN:CB	2.49	0.43
25:CA:2821:A:OP2	38:CN:3:HIS:CE1	2.71	0.43
29:CE:59:PRO:HG2	29:CE:70:SER:CB	2.48	0.43
37:CM:96:ILE:HD12	37:CM:126:ILE:HD13	2.00	0.43
1:DA:1360:A:H2'	1:DA:1361:G:H5'	1.99	0.43
1:DA:407:U:C2	1:DA:408:A:C8	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:DE:131:THR:HG22	5:DE:132:ASN:N	2.33	0.43
8:DH:125:ILE:O	8:DH:125:ILE:HG13	2.19	0.43
3:AC:37:PHE:O	3:AC:38:LYS:CB	2.67	0.43
4:AD:191:LEU:O	4:AD:192:SER:CB	2.66	0.43
5:AE:79:GLY:O	5:AE:121:HIS:N	2.51	0.43
1:AA:1060:U:H5''	10:AJ:53:ILE:HD12	2.01	0.43
18:AR:45:THR:HG23	18:AR:47:THR:CG2	2.48	0.43
22:AV:135:ASP:O	22:AV:136:ALA:C	2.57	0.43
54:B3:31:ILE:CG1	54:B3:35:LYS:HE3	2.48	0.43
25:BA:1059:G:H3'	25:BA:1060:U:C6	2.52	0.43
25:BA:1099:G:C5'	33:BI:4:VAL:HG11	2.48	0.43
25:BA:1022:G:N2	25:BA:1142:A:C2	2.80	0.43
25:BA:1670:C:C4	25:BA:1671:U:N3	2.87	0.43
25:BA:1681:G:N3	25:BA:1762:A:H2'	2.34	0.43
25:BA:1832:C:N4	25:BA:1833:C:C4	2.86	0.43
25:BA:242:G:H5''	54:B3:63:TYR:CE2	2.54	0.43
25:BA:671:C:H6	25:BA:671:C:C5'	2.30	0.43
28:BD:129:THR:HG23	28:BD:130:GLN:O	2.17	0.43
28:BD:12:THR:HG22	28:BD:13:ARG:H	1.84	0.43
29:BE:196:VAL:O	29:BE:199:MET:N	2.52	0.43
37:BM:73:ILE:N	37:BM:73:ILE:HD12	2.33	0.43
38:BN:12:ARG:CZ	38:BN:20:MET:CE	2.97	0.43
44:BT:31:VAL:CG1	44:BT:84:TYR:CD2	3.01	0.43
55:C4:25:VAL:CG1	55:C4:35:GLN:HB2	2.48	0.43
25:CA:1078:U:O2'	25:CA:1088:A:OP1	2.29	0.43
25:CA:1531:C:H3'	25:CA:1532:A:H8	1.84	0.43
25:CA:2177:C:N4	25:CA:2178:C:N3	2.66	0.43
25:CA:322:A:H5'	25:CA:340:A:H1'	2.01	0.43
25:CA:453:A:H5''	60:CA:3245:HOH:O	2.18	0.43
25:CA:479:A:H4'	25:CA:480:A:OP1	2.18	0.43
25:CA:83:A:H2'	25:CA:84:A:C8	2.53	0.43
25:CA:2597:G:H5'	27:CC:240:GLY:HA3	2.00	0.43
28:CD:115:GLY:O	38:CN:3:HIS:NE2	2.50	0.43
32:CH:57:LYS:O	32:CH:59:ALA:N	2.45	0.43
35:CK:35:VAL:HG23	35:CK:36:GLY:H	1.83	0.43
36:CL:93:ASN:ND2	36:CL:93:ASN:O	2.52	0.43
1:DA:1031:C:H5''	1:DA:1032:G:OP1	2.17	0.43
1:DA:1134:G:O6	1:DA:1141:C:N4	2.45	0.43
1:DA:1361:G:C4	1:DA:1362:A:N7	2.86	0.43
1:DA:1361:G:N2	60:DA:1840:HOH:O	2.51	0.43
1:DA:1376:U:O4	7:DG:10:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:223:A:H2'	1:DA:224:U:C6	2.54	0.43
1:DA:235:C:H2'	1:DA:236:A:C8	2.53	0.43
3:DC:179:ARG:HD2	3:DC:206:GLU:HB3	2.00	0.43
9:DI:44:ALA:O	9:DI:47:VAL:HG13	2.18	0.43
11:DK:31:ILE:HG22	11:DK:46:THR:HA	1.99	0.43
12:DL:29:GLN:HB2	12:DL:82:ILE:O	2.19	0.43
12:DL:43:LYS:O	12:DL:45:PRO:CD	2.66	0.43
12:DL:55:VAL:HG12	12:DL:63:VAL:O	2.17	0.43
12:DL:99:ARG:HG3	12:DL:106:GLY:HA2	2.01	0.43
16:DP:67:ILE:HG22	16:DP:71:VAL:HG23	2.01	0.43
1:AA:1167:A:C5	1:AA:1169:A:N1	2.87	0.43
1:AA:1321:U:C5	1:AA:1322:C:C5	3.06	0.43
1:AA:1499:A:O2'	1:AA:1500:A:H5'	2.18	0.43
1:AA:483:C:H2'	1:AA:484:G:N7	2.33	0.43
1:AA:878:A:P	8:AH:80:ARG:HH21	2.40	0.43
4:AD:64:ILE:HD11	4:AD:65:TYR:CZ	2.52	0.43
9:AI:30:ILE:HD11	9:AI:38:TYR:HB2	2.01	0.43
12:AL:121:ARG:CZ	12:AL:121:ARG:HB3	2.48	0.43
12:AL:74:LEU:HD23	12:AL:104:CYS:HB2	1.99	0.43
14:AN:48:LEU:HD13	14:AN:49:GLN:HE21	1.82	0.43
19:AS:50:ALA:HA	19:AS:57:HIS:CD2	2.53	0.43
22:AV:129:VAL:HG12	22:AV:165:THR:HG23	2.01	0.43
25:BA:1019:U:H3	25:BA:1142:A:H62	1.67	0.43
25:BA:2306:C:H3'	25:BA:2307:G:H8	1.83	0.43
25:BA:2569:G:C2	25:BA:2570:G:C8	3.06	0.43
30:BF:48:LEU:H	30:BF:48:LEU:HD12	1.83	0.43
32:BH:80:ILE:HD13	32:BH:94:ILE:HG21	2.01	0.43
25:BA:1062:G:N2	33:BI:134:SER:OG	2.39	0.43
25:BA:1139:G:O3'	34:BJ:26:GLY:HA3	2.18	0.43
45:BU:38:ILE:HD12	45:BU:39:ASN:N	2.34	0.43
25:CA:1160:G:C6	25:CA:1161:C:N4	2.86	0.43
25:CA:137:U:O2	44:CT:1:MET:HE2	2.19	0.43
25:CA:2001:C:H4'	25:CA:2689:U:H2'	2.01	0.43
25:CA:2143:C:N3	25:CA:2148:G:N2	2.53	0.43
25:CA:2282:G:C4	25:CA:2425:A:N6	2.87	0.43
25:CA:529:A:C5	25:CA:2042:A:C2	3.06	0.43
25:CA:68:G:H2'	25:CA:69:C:O4'	2.19	0.43
28:CD:155:VAL:CG1	28:CD:155:VAL:O	2.65	0.43
25:CA:2311:A:H5'	30:CF:76:PHE:HE2	1.83	0.43
32:CH:9:VAL:HG22	32:CH:13:GLY:HA3	2.00	0.43
40:CP:33:GLU:OE1	40:CP:38:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:CT:37:ASP:OD1	44:CT:37:ASP:N	2.46	0.43
1:DA:1058:G:H2'	1:DA:1059:C:O4'	2.17	0.43
1:DA:1357:A:N6	1:DA:1363:A:C2	2.86	0.43
1:DA:982:U:H4'	1:DA:983:A:C5'	2.49	0.43
1:DA:71:A:H61	1:DA:99:C:H1'	1.82	0.43
4:DD:145:ILE:HG12	4:DD:150:LYS:HZ1	1.84	0.43
8:DH:41:LYS:HG3	8:DH:42:GLU:N	2.34	0.43
11:DK:79:ILE:HD13	11:DK:105:PHE:CE1	2.53	0.43
12:DL:50:ARG:HG2	12:DL:90:LEU:HD21	2.00	0.43
17:DQ:19:LYS:N	17:DQ:51:ASN:OD1	2.49	0.43
1:AA:321:A:H2'	1:AA:322:C:C6	2.54	0.43
1:AA:134:G:H1'	1:AA:325:A:C5	2.54	0.43
1:AA:386:C:C2'	1:AA:387:U:C5'	2.97	0.43
1:AA:908:A:H2'	1:AA:909:A:C8	2.54	0.43
3:AC:180:ALA:HB1	3:AC:203:PHE:CE1	2.53	0.43
13:AM:80:LEU:HA	13:AM:83:LEU:HD11	2.00	0.43
10:AJ:65:TYR:HB3	14:AN:96:LEU:CD1	2.48	0.43
21:AU:12:PHE:N	21:AU:12:PHE:CD1	2.84	0.43
22:AV:130:ARG:O	22:AV:133:ARG:HB3	2.19	0.43
25:BA:1064:C:H2'	25:BA:1064:C:O2	2.19	0.43
25:BA:1266:G:OP1	51:B0:15:ARG:NE	2.49	0.43
25:BA:1406:U:H2'	25:BA:1407:G:H8	1.84	0.43
25:BA:2844:G:C5	25:BA:2845:U:C5	3.06	0.43
25:BA:550:C:H5''	58:BA:3003:PAR:H532	2.00	0.43
28:BD:101:PHE:HD1	28:BD:104:VAL:HG11	1.83	0.43
30:BF:136:ILE:N	30:BF:136:ILE:CD1	2.81	0.43
30:BF:3:LEU:HD12	30:BF:6:TYR:HB3	2.01	0.43
30:BF:59:ILE:HG23	30:BF:137:PHE:CD2	2.54	0.43
31:BG:93:TYR:CD1	31:BG:106:LEU:HA	2.54	0.43
32:BH:48:GLU:O	32:BH:51:ARG:NH1	2.52	0.43
34:BJ:77:HIS:HD2	34:BJ:79:GLY:N	2.17	0.43
36:BL:136:GLU:O	36:BL:139:GLY:N	2.45	0.43
41:BQ:67:ALA:HB2	41:BQ:98:ALA:HB1	2.01	0.43
53:C2:5:PHE:CZ	53:C2:7:PRO:HB3	2.54	0.43
25:CA:1023:U:OP2	60:CA:3706:HOH:O	2.21	0.43
28:CD:103:ASP:N	28:CD:103:ASP:OD1	2.43	0.43
31:CG:102:ILE:HG22	31:CG:104:LEU:HD13	2.00	0.43
33:CI:121:ILE:O	33:CI:125:THR:OG1	2.30	0.43
25:CA:2706:A:O2'	38:CN:64:ARG:NH1	2.52	0.43
40:CP:105:LYS:HA	40:CP:108:ARG:HD3	2.00	0.43
42:CR:68:ARG:HG2	42:CR:92:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:CZ:26:LEU:HB2	50:CZ:28:LEU:CD1	2.49	0.43
1:DA:1061:G:N7	1:DA:1062:U:C5	2.87	0.43
1:DA:1178:G:C6	9:DI:99:ARG:NH2	2.86	0.43
1:DA:210:C:H4'	1:DA:211:G:C2	2.54	0.43
1:DA:235:C:HO2'	17:DQ:73:TRP:HZ3	1.62	0.43
1:DA:32:A:OP1	1:DA:398:U:H1'	2.18	0.43
1:DA:382:A:H2'	1:DA:383:A:C8	2.54	0.43
1:DA:96:U:C2'	1:DA:97:G:O5'	2.67	0.43
4:DD:110:THR:HG23	4:DD:113:GLU:H	1.84	0.43
1:DA:430:A:P	4:DD:9:LEU:HD23	2.58	0.43
8:DH:101:ILE:HG22	8:DH:129:VAL:CG2	2.47	0.43
9:DI:98:LEU:HA	9:DI:101:ALA:HB3	2.00	0.43
13:DM:34:LEU:HB3	13:DM:39:ILE:CD1	2.48	0.43
13:DM:69:LEU:HA	13:DM:72:GLU:HB2	2.00	0.43
14:DN:5:MET:SD	14:DN:8:ARG:NE	2.89	0.43
21:DU:40:LYS:H	21:DU:41:PRO:HD2	1.84	0.43
1:AA:1142:G:C4	1:AA:1143:G:H1'	2.54	0.43
1:AA:1160:G:HO2'	1:AA:1161:C:P	2.41	0.43
1:AA:185:U:H4'	20:AT:69:LYS:HE2	2.00	0.43
1:AA:448:A:C4	1:AA:487:A:C2	3.06	0.43
4:AD:58:LYS:HZ3	4:AD:203:LEU:HB3	1.82	0.43
17:AQ:68:SER:O	17:AQ:69:LYS:C	2.57	0.43
24:AX:63:G:H1'	52:B1:27:ARG:CD	2.48	0.43
53:B2:34:ARG:HH11	53:B2:42:LEU:HA	1.83	0.43
54:B3:35:LYS:HB2	54:B3:40:LYS:HE3	2.00	0.43
25:BA:1655:A:C8	25:BA:1656:C:C5	3.07	0.43
25:BA:321:U:OP2	29:BE:130:LYS:NZ	2.46	0.43
25:BA:80:G:N2	25:BA:81:G:H1'	2.34	0.43
27:BC:132:ARG:HH12	27:BC:169:ALA:HA	1.83	0.43
28:BD:113:SER:HB2	28:BD:168:GLU:H	1.84	0.43
31:BG:154:GLU:CG	31:BG:156:TYR:H	2.32	0.43
34:BJ:125:TYR:OH	34:BJ:131:ASN:OD1	2.34	0.43
36:BL:82:LEU:HD21	36:BL:135:ILE:CD1	2.48	0.43
51:C0:53:VAL:O	51:C0:54:ILE:HG13	2.19	0.43
25:CA:1028:A:N6	25:CA:1125:G:H2'	2.34	0.43
25:CA:140:C:O2'	25:CA:141:G:OP1	2.30	0.43
25:CA:1844:C:H5'	27:CC:253:GLY:O	2.19	0.43
25:CA:2221:G:C5	25:CA:2222:C:C5	3.07	0.43
25:CA:2290:G:N2	25:CA:2373:G:O2'	2.51	0.43
25:CA:2569:G:C2	25:CA:2570:G:C8	3.07	0.43
25:CA:2660:A:H2'	25:CA:2661:G:O4'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:CA:868:U:C4	25:CA:869:G:N7	2.86	0.43
25:CA:95:A:H4'	49:CY:38:GLN:O	2.19	0.43
30:CF:28:PRO:HB2	30:CF:168:LEU:HD11	2.01	0.43
36:CL:105:ILE:CG2	36:CL:106:GLU:N	2.82	0.43
49:CY:42:LEU:HA	49:CY:45:GLN:HG2	2.00	0.43
1:DA:1302:C:H41	13:DM:14:HIS:HB2	1.84	0.43
1:DA:1428:A:C2	1:DA:1473:G:C2	3.07	0.43
1:DA:1494:G:N7	58:DA:1654:PAR:H222	2.34	0.43
1:DA:246:A:N1	1:DA:278:G:O2'	2.39	0.43
1:DA:317:U:N3	1:DA:318:G:N7	2.66	0.43
1:DA:31:G:N2	1:DA:47:C:H4'	2.34	0.43
1:DA:523:A:N1	12:DL:89:ASP:HB2	2.33	0.43
1:DA:982:U:H4'	1:DA:983:A:H5'	2.00	0.43
4:DD:152:GLN:O	4:DD:154:ARG:N	2.52	0.43
4:DD:25:VAL:HG13	4:DD:26:ARG:HG2	1.99	0.43
7:DG:17:LYS:HG3	7:DG:18:PHE:N	2.33	0.43
8:DH:88:ARG:CZ	8:DH:122:GLY:C	2.87	0.43
11:DK:105:PHE:O	11:DK:107:ILE:N	2.44	0.43
10:DJ:65:TYR:HB3	14:DN:96:LEU:HD13	2.01	0.43
17:DQ:60:GLU:O	17:DQ:76:VAL:N	2.47	0.43
20:DT:28:MET:HE3	20:DT:66:LEU:HD11	2.01	0.43
1:AA:104:G:O2'	1:AA:105:G:H5'	2.19	0.43
1:AA:923:A:O2'	1:AA:1399:C:OP2	2.35	0.43
1:AA:1399:C:C2	1:AA:1502:A:N6	2.87	0.43
1:AA:501:C:H1'	1:AA:549:C:H1'	2.01	0.43
1:AA:560:A:OP2	1:AA:566:G:N2	2.52	0.43
1:AA:1160:G:H5''	2:AB:132:LYS:HD3	2.00	0.43
2:AB:30:PHE:N	2:AB:30:PHE:CD1	2.87	0.43
3:AC:57:ILE:HD11	3:AC:64:ILE:HG22	2.01	0.43
7:AG:15:ASP:HB3	7:AG:24:ALA:HB2	2.01	0.43
10:AJ:35:GLN:HG2	10:AJ:80:THR:HG22	2.00	0.43
11:AK:63:ALA:CB	11:AK:92:GLY:HA2	2.48	0.43
22:AV:28:ILE:HD11	22:AV:179:LYS:HE3	2.00	0.43
54:B3:61:LEU:HB3	54:B3:64:ALA:HB3	2.01	0.43
25:BA:2255:G:H5''	25:BA:2256:G:OP2	2.18	0.43
25:BA:2676:C:O2	25:BA:2732:G:N2	2.47	0.43
25:BA:1750:G:O2'	25:BA:2860:A:N1	2.42	0.43
28:BD:133:THR:HG23	28:BD:134:HIS:N	2.34	0.43
30:BF:90:LEU:HD13	30:BF:95:MET:CB	2.48	0.43
31:BG:27:GLY:HA3	31:BG:78:VAL:CG1	2.49	0.43
43:BS:59:GLU:HA	43:BS:64:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BB:3075:G:H1'	46:BV:29:ILE:CG1	2.49	0.43
46:BV:44:HIS:HE1	46:BV:85:LYS:HA	1.84	0.43
25:CA:1663:G:C6	25:CA:1992:G:N7	2.87	0.43
25:CA:2243:U:H2'	25:CA:2244:U:C6	2.54	0.43
25:CA:2377:A:N3	39:CO:92:PHE:CZ	2.87	0.43
25:CA:301:G:OP2	45:CU:81:ARG:NH1	2.43	0.43
25:CA:587:C:C6	25:CA:671:C:H1'	2.53	0.43
25:CA:874:G:N2	25:CA:904:G:C5	2.86	0.43
26:CB:3049:C:OP1	39:CO:101:GLY:HA3	2.19	0.43
27:CC:16:VAL:N	27:CC:203:VAL:HG22	2.34	0.43
32:CH:121:VAL:CG2	32:CH:128:HIS:NE2	2.82	0.43
32:CH:15:LEU:HG	32:CH:16:GLY:N	2.33	0.43
33:CI:36:GLU:HG2	33:CI:65:SER:HB2	2.00	0.43
39:CO:41:ALA:O	39:CO:43:ASN:N	2.51	0.43
1:DA:810:C:H2'	1:DA:811:C:O4'	2.19	0.43
2:DB:91:PHE:CE1	2:DB:150:GLY:HA2	2.53	0.43
4:DD:14:ARG:HG2	4:DD:14:ARG:HH11	1.84	0.43
4:DD:65:TYR:CD2	4:DD:94:LEU:HB3	2.54	0.43
5:DE:126:LYS:O	5:DE:127:ALA:HB2	2.18	0.43
5:DE:36:LEU:HD23	5:DE:133:PRO:HB2	2.00	0.43
13:DM:52:GLN:O	13:DM:55:THR:OG1	2.34	0.43
21:DU:21:ARG:NH1	23:DV:4:G:H1'	2.34	0.43
1:AA:1118:U:C4'	9:AI:106:ARG:NH2	2.81	0.43
1:AA:1157:A:C5	1:AA:1180:A:C6	3.07	0.43
1:AA:1243:C:H2'	1:AA:1244:G:H8	1.83	0.43
1:AA:500:G:O3'	12:AL:121:ARG:NH2	2.52	0.43
7:AG:4:ARG:HG3	7:AG:5:ARG:N	2.33	0.43
11:AK:79:ILE:O	11:AK:79:ILE:HG23	2.19	0.43
12:AL:24:LEU:HB2	12:AL:59:ASN:ND2	2.34	0.43
14:AN:53:ARG:O	14:AN:55:SER:N	2.52	0.43
1:AA:1015:G:OP1	19:AS:14:HIS:CD2	2.71	0.43
51:B0:30:ASP:HB3	51:B0:33:SER:HB3	2.00	0.43
55:B4:10:LEU:HD12	55:B4:33:HIS:CE1	2.54	0.43
25:BA:323:C:H6	25:BA:1205:A:N1	2.17	0.43
25:BA:1322:A:O3'	43:BS:84:ARG:NH2	2.52	0.43
25:BA:191:A:H2'	25:BA:192:C:C6	2.54	0.43
25:BA:1932:A:H2'	25:BA:1933:G:O4'	2.19	0.43
25:BA:2024:G:C5	25:BA:2025:C:C5	3.07	0.43
25:BA:309:A:H4'	45:BU:16:LYS:NZ	2.34	0.43
27:BC:106:PRO:HA	27:BC:194:VAL:HA	2.01	0.43
31:BG:37:ASN:C	31:BG:39:ALA:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BH:122:LEU:HA	32:BH:123:ARG:C	2.40	0.43
32:BH:26:ALA:O	32:BH:31:VAL:HG13	2.19	0.43
38:BN:28:LEU:O	38:BN:32:GLU:N	2.46	0.43
25:BA:1249:U:H5'	41:BQ:3:VAL:HG13	2.01	0.43
49:BY:18:LEU:HD12	49:BY:22:LEU:HD12	2.00	0.43
25:CA:1782:U:H2'	25:CA:2608:G:O2'	2.19	0.43
25:CA:2727:A:C6	25:CA:2728:U:O4	2.71	0.43
25:CA:983:A:C6	25:CA:984:A:C2	3.06	0.43
35:CK:108:ARG:HA	35:CK:116:ILE:CD1	2.49	0.43
40:CP:60:VAL:CG1	40:CP:73:PHE:HE1	2.31	0.43
40:CP:83:ILE:H	40:CP:83:ILE:HD12	1.84	0.43
25:CA:84:A:H4'	45:CU:5:ARG:NE	2.34	0.43
50:CZ:4:ILE:HD11	50:CZ:39:ASP:HA	2.01	0.43
1:DA:1096:C:O2	1:DA:1170:A:O2'	2.34	0.43
1:DA:1358:U:OP2	14:DN:75:ARG:NH1	2.52	0.43
1:DA:38:G:N1	1:DA:397:A:OP1	2.50	0.43
2:DB:127:ASP:N	2:DB:127:ASP:OD1	2.50	0.43
4:DD:145:ILE:HG12	4:DD:146:ARG:H	1.84	0.43
5:DE:89:HIS:CD2	5:DE:90:THR:HG23	2.53	0.43
9:DI:30:ILE:HA	9:DI:65:ILE:HG13	2.01	0.43
10:DJ:40:ILE:HB	10:DJ:73:LEU:O	2.19	0.43
1:AA:1083:U:C5	1:AA:1084:G:C5	3.07	0.42
1:AA:925:G:H1'	1:AA:1502:A:C4	2.54	0.42
1:AA:986:U:H2'	1:AA:987:G:O4'	2.19	0.42
14:AN:44:ALA:HA	14:AN:47:LYS:CE	2.49	0.42
1:AA:1360:A:OP2	14:AN:75:ARG:NH2	2.51	0.42
15:AO:78:TYR:HA	15:AO:81:LEU:HG	2.01	0.42
19:AS:44:MET:SD	19:AS:62:VAL:HG21	2.59	0.42
22:AV:28:ILE:CD1	22:AV:179:LYS:HE3	2.48	0.42
24:AX:7:A:C3'	24:AX:8:U:H5'	2.49	0.42
25:BA:1210:G:H4'	25:BA:1211:C:H5''	2.01	0.42
25:BA:1365:A:N3	25:BA:1365:A:H2'	2.34	0.42
25:BA:2116:G:H5'	25:BA:2117:A:P	2.59	0.42
25:BA:2680:U:O2'	25:BA:2681:C:P	2.76	0.42
25:BA:410:G:H5''	25:BA:411:G:H5'	2.01	0.42
25:BA:634:C:H2'	25:BA:635:C:H6	1.83	0.42
25:BA:2747:G:O2'	31:BG:66:THR:HG22	2.18	0.42
31:BG:49:LEU:HD13	31:BG:71:LEU:HD22	2.01	0.42
43:BS:69:LEU:HD22	43:BS:107:VAL:HG22	2.00	0.42
45:BU:11:ILE:HG22	45:BU:21:ARG:CB	2.49	0.42
46:BV:48:MET:O	46:BV:51:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:C2:12:ARG:NH2	53:C2:44:VAL:HG22	2.34	0.42
25:CA:1582:C:C2'	25:CA:1585:C:H42	2.31	0.42
25:CA:1979:U:H2'	25:CA:1980:G:H5'	2.01	0.42
25:CA:2198:A:C4	32:CH:29:PHE:HB2	2.54	0.42
25:CA:2207:C:C2	25:CA:2218:G:C2	3.07	0.42
25:CA:2230:G:H2'	25:CA:2231:U:C6	2.54	0.42
25:CA:2469:A:H4'	37:CM:55:ARG:HE	1.84	0.42
25:CA:273:G:O6	25:CA:364:C:N4	2.47	0.42
25:CA:720:U:H2'	25:CA:721:A:C8	2.54	0.42
25:CA:76:C:O2'	49:CY:52:ARG:HA	2.18	0.42
27:CC:170:TYR:HD1	27:CC:184:GLU:HA	1.84	0.42
41:CQ:39:ILE:CD1	42:CR:77:PHE:CD1	3.02	0.42
1:DA:1178:G:N2	1:DA:1181:G:OP2	2.52	0.42
1:DA:262:A:C6	1:DA:263:A:C6	3.07	0.42
1:DA:345:C:H5'	1:DA:346:G:C5	2.54	0.42
1:DA:432:A:H2'	1:DA:433:G:O4'	2.19	0.42
5:DE:104:GLY:HA2	5:DE:122:ASN:HA	2.00	0.42
8:DH:10:MET:HA	8:DH:13:ARG:HG2	2.00	0.42
1:AA:555:U:H2'	1:AA:556:C:C6	2.55	0.42
1:AA:575:G:H4'	1:AA:576:C:OP1	2.19	0.42
3:AC:22:TRP:CE2	14:AN:94:PRO:HG2	2.54	0.42
8:AH:53:GLY:HA2	8:AH:57:PRO:HA	2.01	0.42
8:AH:78:VAL:HG13	8:AH:79:SER:H	1.83	0.42
11:AK:88:GLY:H	11:AK:114:THR:CG2	2.31	0.42
19:AS:30:PRO:HA	19:AS:48:THR:HG21	2.00	0.42
22:AV:66:LEU:HB3	22:AV:101:VAL:HG23	2.00	0.42
25:BA:1214:A:H2'	25:BA:1215:G:O4'	2.19	0.42
25:BA:1417:C:O2'	25:BA:1587:G:O2'	2.08	0.42
25:BA:1798:U:OP2	27:BC:270:ARG:NH2	2.45	0.42
25:BA:1867:G:C2'	25:BA:1868:C:H5'	2.49	0.42
25:BA:563:A:C4	25:BA:2018:G:C2	3.07	0.42
25:BA:2213:U:H4'	25:BA:2214:C:OP2	2.19	0.42
25:BA:2231:U:C5	25:BA:2232:C:C5	3.07	0.42
25:BA:742:A:H2'	25:BA:743:A:C8	2.54	0.42
25:BA:747:U:C4	25:BA:2613:U:C4	3.07	0.42
28:BD:26:VAL:HB	28:BD:188:LEU:HD22	2.00	0.42
28:BD:49:GLN:HA	28:BD:81:GLU:HB3	2.00	0.42
29:BE:32:VAL:HG11	36:BL:6:LEU:CD1	2.49	0.42
30:BF:35:LEU:HD12	30:BF:153:ILE:HG22	2.00	0.42
25:BA:2299:U:P	30:BF:71:LYS:NZ	2.92	0.42
45:BU:84:PHE:CG	45:BU:85:ARG:N	2.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:CA:1731:G:H2'	25:CA:1732:C:H3'	2.00	0.42
25:CA:2344:U:H4'	25:CA:2345:G:OP1	2.19	0.42
25:CA:2796:U:H3	25:CA:2799:A:H61	1.66	0.42
25:CA:2843:G:H2'	25:CA:2844:G:O4'	2.19	0.42
25:CA:1922:G:C6	58:CA:3167:PAR:H221	2.53	0.42
31:CG:60:GLY:HA2	31:CG:63:GLN:HB2	2.01	0.42
32:CH:97:ARG:NE	32:CH:97:ARG:CA	2.82	0.42
35:CK:9:ASN:OD1	35:CK:18:ARG:NH1	2.52	0.42
36:CL:73:ILE:O	36:CL:73:ILE:HG23	2.20	0.42
38:CN:38:LEU:HB3	38:CN:39:PRO:CD	2.49	0.42
42:CR:49:ILE:HG22	42:CR:54:VAL:N	2.34	0.42
44:CT:19:LYS:O	44:CT:23:ALA:N	2.52	0.42
45:CU:35:VAL:HG22	45:CU:38:ILE:HG12	2.02	0.42
49:CY:17:GLU:HA	49:CY:20:ASN:HB2	2.02	0.42
1:DA:1326:U:C2	1:DA:1327:C:C5	3.07	0.42
2:DB:114:LEU:HB2	2:DB:144:LEU:HG	2.01	0.42
4:DD:117:LEU:O	4:DD:118:VAL:HB	2.19	0.42
4:DD:76:TYR:CE2	4:DD:204:TYR:HB3	2.53	0.42
5:DE:157:ARG:C	5:DE:159:LYS:N	2.73	0.42
10:DJ:44:THR:HG22	10:DJ:70:HIS:HA	2.01	0.42
15:DO:12:VAL:HA	15:DO:27:VAL:HG21	2.01	0.42
16:DP:5:ARG:HD2	16:DP:6:LEU:N	2.34	0.42
1:AA:1145:A:H1'	1:AA:1146:A:OP2	2.18	0.42
1:AA:1169:A:N6	1:AA:1170:A:N1	2.67	0.42
1:AA:1306:A:C6	1:AA:1307:U:C2	3.07	0.42
1:AA:22:G:H2'	1:AA:23:C:H6	1.85	0.42
1:AA:406:G:H2'	1:AA:407:U:H5'	2.00	0.42
1:AA:859:G:O2'	1:AA:860:A:P	2.77	0.42
1:AA:76:G:N2	1:AA:95:C:N3	2.66	0.42
12:AL:114:ARG:NH1	12:AL:119:VAL:O	2.50	0.42
14:AN:45:VAL:HG12	14:AN:46:LEU:HD23	2.01	0.42
15:AO:10:LYS:H	15:AO:10:LYS:CD	2.33	0.42
25:BA:1693:U:H4'	25:BA:1694:C:OP2	2.19	0.42
25:BA:2321:U:H5'	25:BA:2322:A:OP2	2.19	0.42
25:BA:588:U:H1'	29:BE:85:PHE:CD1	2.54	0.42
25:BA:679:C:H2'	25:BA:680:C:H6	1.84	0.42
25:BA:815:C:P	42:BR:85:LYS:NZ	2.92	0.42
25:BA:880:G:N2	25:BA:898:C:N3	2.66	0.42
27:BC:180:MET:O	27:BC:267:VAL:HG22	2.19	0.42
31:BG:66:THR:OG1	31:BG:67:ALA:N	2.53	0.42
32:BH:80:ILE:HD12	32:BH:82:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:BK:35:VAL:HG21	35:BK:69:VAL:HG13	2.00	0.42
54:C3:56:LEU:O	54:C3:57:VAL:HB	2.18	0.42
25:CA:1416:G:H1	25:CA:1582:C:H42	1.67	0.42
25:CA:1824:G:H21	27:CC:251:THR:CG2	2.32	0.42
25:CA:1869:G:C2	25:CA:1873:G:C6	3.07	0.42
25:CA:528:A:H2	25:CA:2043:C:C5'	2.32	0.42
25:CA:2299:U:OP1	30:CF:71:LYS:NZ	2.51	0.42
25:CA:2452:C:C4	25:CA:2453:A:C6	3.07	0.42
25:CA:627:A:H4'	25:CA:628:G:OP1	2.18	0.42
27:CC:203:VAL:O	27:CC:205:GLY:N	2.52	0.42
28:CD:29:VAL:HB	28:CD:98:VAL:HG22	2.01	0.42
36:CL:56:PRO:O	36:CL:59:ARG:N	2.48	0.42
41:CQ:75:TYR:OH	41:CQ:91:ARG:NH1	2.50	0.42
25:CA:998:C:P	41:CQ:91:ARG:NH2	2.93	0.42
1:DA:102:G:H2'	1:DA:103:U:H6	1.84	0.42
1:DA:33:A:H5'	1:DA:364:A:H1'	2.00	0.42
1:DA:779:C:H2'	1:DA:780:A:O4'	2.20	0.42
1:DA:980:C:C5	1:DA:981:U:C2	3.08	0.42
2:DB:108:ARG:O	2:DB:111:ILE:N	2.51	0.42
4:DD:123:ILE:HG12	4:DD:143:VAL:HB	2.01	0.42
4:DD:150:LYS:HE3	4:DD:150:LYS:HA	2.02	0.42
8:DH:87:LYS:HZ3	8:DH:92:LEU:HA	1.83	0.42
9:DI:130:ARG:HB3	9:DI:130:ARG:CZ	2.48	0.42
9:DI:46:MET:SD	9:DI:48:VAL:HG22	2.59	0.42
12:DL:30:LYS:O	12:DL:81:LEU:HD12	2.18	0.42
1:DA:579:A:O2'	15:DO:54:ARG:NH1	2.52	0.42
1:AA:1157:A:C6	1:AA:1180:A:C5	3.08	0.42
1:AA:983:A:H2	1:AA:1222:G:H22	1.67	0.42
1:AA:1352:C:H2'	1:AA:1353:G:C8	2.54	0.42
1:AA:681:A:H2'	1:AA:682:G:O4'	2.19	0.42
1:AA:866:C:C4	1:AA:867:G:H1'	2.55	0.42
2:AB:71:GLY:HA2	2:AB:164:ILE:HG22	2.02	0.42
3:AC:148:GLY:HA3	3:AC:172:ARG:O	2.19	0.42
4:AD:160:GLU:OE2	4:AD:161:LEU:N	2.52	0.42
7:AG:100:ALA:HB3	7:AG:103:TRP:CH2	2.49	0.42
17:AQ:30:LYS:HG2	17:AQ:37:PHE:CZ	2.54	0.42
21:AU:53:VAL:HG13	21:AU:54:LYS:N	2.34	0.42
51:B0:29:VAL:HA	51:B0:36:LYS:HA	2.01	0.42
54:B3:31:ILE:C	54:B3:31:ILE:HD12	2.39	0.42
54:B3:30:HIS:O	54:B3:31:ILE:HG13	2.19	0.42
25:BA:1256:G:OP1	29:BE:67:ARG:NH1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1370:C:H2'	25:BA:1371:G:O4'	2.19	0.42
25:BA:1505:A:H2'	25:BA:1506:U:O4'	2.19	0.42
25:BA:2250:G:H8	25:BA:2250:G:O5'	2.03	0.42
58:BA:3001:PAR:N21	58:BA:3001:PAR:O43	2.52	0.42
28:BD:54:ALA:HA	28:BD:76:GLY:HA2	2.02	0.42
29:BE:118:LEU:HD11	29:BE:188:MET:HG3	2.02	0.42
34:BJ:28:LEU:HD12	34:BJ:142:ILE:HG23	2.00	0.42
25:BA:1131:G:C8	34:BJ:77:HIS:CE1	3.07	0.42
36:BL:90:VAL:HG23	36:BL:120:VAL:CG2	2.49	0.42
39:BO:74:VAL:HA	39:BO:77:ALA:HB3	2.00	0.42
40:BP:47:ILE:HA	40:BP:96:LEU:CD1	2.50	0.42
46:BV:66:ASP:HB2	46:BV:68:LYS:HD2	2.01	0.42
47:BW:63:GLY:HA2	47:BW:83:GLU:HB3	2.02	0.42
25:CA:2097:A:C6	25:CA:2098:U:C4	3.07	0.42
25:CA:2358:A:C6	25:CA:2359:C:C2	3.07	0.42
25:CA:594:U:H2'	25:CA:595:C:C6	2.55	0.42
25:CA:587:C:C5	25:CA:671:C:H1'	2.55	0.42
25:CA:84:A:N1	25:CA:98:G:O2'	2.32	0.42
27:CC:9:SER:OG	27:CC:12:ARG:NE	2.53	0.42
32:CH:103:VAL:HA	32:CH:106:ALA:HB3	2.01	0.42
36:CL:111:ILE:CG2	36:CL:112:LEU:N	2.82	0.42
1:DA:1113:C:H2'	1:DA:1114:C:C6	2.54	0.42
1:DA:446:G:H2'	1:DA:446:G:N3	2.33	0.42
1:DA:858:G:O2'	1:DA:859:G:H5'	2.19	0.42
12:DL:75:GLN:CG	12:DL:76:GLU:N	2.82	0.42
18:DR:52:GLN:O	18:DR:54:GLN:N	2.46	0.42
19:DS:34:TRP:CD1	19:DS:52:HIS:CG	3.07	0.42
21:DU:40:LYS:C	21:DU:42:THR:N	2.72	0.42
21:DU:26:ALA:CB	23:DV:5:A:H5'	2.45	0.42
1:AA:104:G:C2'	1:AA:105:G:H5'	2.49	0.42
1:AA:1355:G:C5	1:AA:1368:A:C2	3.08	0.42
1:AA:181:A:H1'	1:AA:194:C:N4	2.34	0.42
6:AF:88:MET:HE3	6:AF:90:MET:HE1	1.99	0.42
13:AM:45:ILE:HA	13:AM:48:LEU:HG	2.01	0.42
19:AS:67:VAL:O	19:AS:69:HIS:N	2.50	0.42
25:BA:1141:U:H4'	25:BA:1142:A:O4'	2.20	0.42
25:BA:1726:C:N3	25:BA:1735:A:H2	2.17	0.42
25:BA:2152:G:H2'	25:BA:2152:G:N3	2.34	0.42
25:BA:747:U:C5	25:BA:2613:U:C5	3.07	0.42
25:BA:2868:A:C2	25:BA:2869:G:C4	3.07	0.42
25:BA:544:C:H3'	25:BA:545:U:N1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:799:G:C6	25:BA:800:A:C6	3.07	0.42
25:BA:2060:A:H3'	29:BE:63:LYS:HZ3	1.85	0.42
31:BG:34:ARG:HH11	31:BG:74:MET:CE	2.32	0.42
37:BM:19:GLY:O	37:BM:38:ARG:NH2	2.50	0.42
39:BO:31:THR:HG22	39:BO:33:ARG:N	2.34	0.42
41:BQ:109:VAL:HG12	41:BQ:113:LYS:HE3	2.02	0.42
43:BS:49:LYS:HA	43:BS:52:GLU:HG3	2.01	0.42
47:BW:67:PHE:CE2	47:BW:78:ILE:HD12	2.54	0.42
25:CA:1438:U:C5	25:CA:1552:A:C2	3.08	0.42
25:CA:1979:U:C2'	25:CA:1980:G:H5'	2.50	0.42
25:CA:2024:G:C6	25:CA:2025:C:C4	3.08	0.42
25:CA:2403:C:N3	25:CA:2404:U:C5	2.87	0.42
25:CA:2553:G:N3	25:CA:2583:G:H1'	2.33	0.42
25:CA:2646:C:H2'	25:CA:2647:U:O4'	2.19	0.42
25:CA:553:G:H2'	25:CA:554:U:O4'	2.20	0.42
25:CA:60:G:C8	25:CA:62:U:C6	3.06	0.42
25:CA:81:G:O2'	25:CA:295:G:O2'	2.28	0.42
25:CA:948:C:H2'	25:CA:949:G:C8	2.55	0.42
27:CC:106:PRO:HG2	27:CC:109:LEU:HD23	2.00	0.42
25:CA:1500:G:N2	27:CC:97:ASP:O	2.50	0.42
36:CL:110:VAL:O	36:CL:111:ILE:HB	2.19	0.42
36:CL:62:PRO:O	54:C3:12:ARG:CG	2.68	0.42
36:CL:90:VAL:HA	36:CL:94:THR:HG21	2.01	0.42
42:CR:14:VAL:HB	42:CR:98:ILE:HD13	2.02	0.42
1:DA:1412:C:H2'	1:DA:1413:A:C8	2.55	0.42
1:DA:163:C:H2'	1:DA:164:G:O4'	2.20	0.42
4:DD:61:VAL:HG22	4:DD:62:ARG:N	2.34	0.42
11:DK:52:PHE:CZ	11:DK:62:ALA:HA	2.54	0.42
1:AA:1463:U:H2'	1:AA:1464:U:C6	2.55	0.42
1:AA:269:C:H2'	1:AA:270:A:C8	2.54	0.42
1:AA:659:U:H2'	1:AA:660:C:C6	2.54	0.42
1:AA:792:A:H4'	1:AA:793:U:H5''	2.01	0.42
3:AC:156:ARG:HH22	3:AC:196:ILE:HG13	1.85	0.42
5:AE:106:ILE:HG13	5:AE:124:LEU:HB3	2.02	0.42
7:AG:100:ALA:O	7:AG:103:TRP:CZ2	2.70	0.42
8:AH:40:LEU:HB3	8:AH:46:ILE:HG12	2.01	0.42
1:AA:636:U:H5'	17:AQ:6:ARG:CZ	2.50	0.42
19:AS:36:ARG:O	19:AS:38:SER:N	2.48	0.42
56:B5:136:LEU:C	56:B5:140:PRO:N	2.73	0.42
25:BA:1045:C:C3'	25:BA:1046:A:H5'	2.50	0.42
25:BA:1055:G:C6	25:BA:1056:G:C4	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:31:C:O2'	25:BA:1238:G:H5'	2.20	0.42
25:BA:137:U:O2'	25:BA:138:U:P	2.77	0.42
25:BA:1585:C:H2'	25:BA:1586:A:O4'	2.20	0.42
25:BA:1593:A:H2'	25:BA:1594:U:O4'	2.20	0.42
25:BA:20:C:H2'	25:BA:21:A:H8	1.83	0.42
25:BA:2544:G:O2'	25:BA:2545:G:H5'	2.19	0.42
25:BA:898:C:C4	25:BA:899:A:C8	3.08	0.42
25:BA:995:C:H5'	25:BA:995:C:H6	1.84	0.42
25:BA:2223:G:O2'	27:BC:264:LYS:NZ	2.53	0.42
32:BH:118:PRO:O	32:BH:119:ASN:HB3	2.19	0.42
42:BR:16:GLU:HA	42:BR:98:ILE:HD11	2.02	0.42
49:BY:41:HIS:CE1	49:BY:42:LEU:HD13	2.55	0.42
25:CA:1070:A:O2'	25:CA:1097:U:O3'	2.38	0.42
25:CA:1450:G:C6	25:CA:1451:C:N4	2.88	0.42
25:CA:2060:A:O2'	25:CA:2061:G:OP2	2.36	0.42
25:CA:225:C:C4	25:CA:226:A:C8	3.08	0.42
25:CA:608:A:C6	25:CA:609:A:C6	3.08	0.42
25:CA:78:U:H2'	25:CA:79:C:C6	2.55	0.42
34:CJ:38:GLY:HA3	34:CJ:50:THR:HG23	2.01	0.42
34:CJ:3:THR:HG21	41:CQ:56:PHE:CE1	2.55	0.42
40:CP:13:LYS:H	40:CP:76:HIS:HD2	1.68	0.42
41:CQ:87:VAL:CG1	41:CQ:89:ILE:HG23	2.49	0.42
45:CU:85:ARG:NH2	45:CU:101:THR:OG1	2.53	0.42
50:CZ:11:SER:OG	50:CZ:13:ILE:HG23	2.20	0.42
1:DA:1000:A:C2	1:DA:1041:G:C2	3.08	0.42
1:DA:152:A:N6	1:DA:170:U:C2	2.87	0.42
1:DA:293:G:H2'	1:DA:294:U:H6	1.84	0.42
1:DA:793:U:C3'	1:DA:794:A:H5''	2.49	0.42
2:DB:47:VAL:HB	2:DB:48:PRO:CD	2.49	0.42
2:DB:54:LEU:HD12	2:DB:54:LEU:N	2.34	0.42
2:DB:82:ASP:O	2:DB:85:LEU:N	2.52	0.42
4:DD:22:LYS:O	4:DD:24:GLY:N	2.53	0.42
7:DG:111:ARG:NH2	7:DG:126:ASP:OD2	2.52	0.42
15:DO:85:LEU:HD11	15:DO:87:LEU:HD23	2.02	0.42
21:DU:26:ALA:C	21:DU:28:VAL:N	2.73	0.42
1:AA:601:G:C6	1:AA:602:A:C5	3.08	0.42
1:AA:878:A:OP1	8:AH:80:ARG:CZ	2.67	0.42
4:AD:68:LEU:O	4:AD:72:PHE:HB3	2.20	0.42
6:AF:81:ASN:C	6:AF:83:ALA:N	2.72	0.42
10:AJ:52:LEU:HD11	14:AN:81:ARG:CD	2.50	0.42
1:AA:1309:G:OP1	13:AM:87:ARG:CZ	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AP:21:VAL:HG11	16:AP:60:TRP:CD1	2.55	0.42
25:BA:1273:U:H5''	25:BA:1646:C:N4	2.34	0.42
25:BA:1355:G:C6	25:BA:1377:G:N2	2.88	0.42
25:BA:1794:A:H1'	25:BA:1900:A:N3	2.35	0.42
25:BA:1928:A:C8	25:BA:1928:A:H3'	2.54	0.42
25:BA:2024:G:C4	25:BA:2040:G:C2	3.08	0.42
25:BA:2479:U:OP1	25:BA:2537:U:H1'	2.20	0.42
25:BA:267:C:H2'	25:BA:268:C:C6	2.54	0.42
25:BA:34:U:HO2'	25:BA:35:G:P	2.43	0.42
25:BA:565:C:H2'	25:BA:566:U:O4'	2.20	0.42
25:BA:760:G:C2	25:BA:761:A:H1'	2.55	0.42
35:BK:35:VAL:CG1	35:BK:104:THR:HG21	2.50	0.42
35:BK:64:ARG:HD3	35:BK:79:PHE:CD2	2.55	0.42
25:CA:2420:C:H5''	52:C1:7:LYS:CE	2.49	0.42
53:C2:22:MET:HA	53:C2:28:ARG:HG2	2.01	0.42
25:CA:1000:A:H62	25:CA:1154:G:H2'	1.84	0.42
25:CA:1069:A:H4'	25:CA:1070:A:C8	2.55	0.42
25:CA:2081:U:H2'	25:CA:2082:A:C8	2.54	0.42
25:CA:215:G:O3'	25:CA:216:A:H4'	2.19	0.42
25:CA:2335:A:OP1	39:CO:13:ARG:NH2	2.53	0.42
25:CA:2469:A:O2'	37:CM:55:ARG:NH1	2.50	0.42
25:CA:747:U:C4	25:CA:2613:U:C4	3.07	0.42
25:CA:572:A:C2	25:CA:2033:A:C2	3.08	0.42
36:CL:110:VAL:CG2	36:CL:127:VAL:HA	2.49	0.42
37:CM:34:LYS:HB3	37:CM:129:THR:HG23	2.02	0.42
40:CP:60:VAL:HG12	40:CP:73:PHE:HE1	1.84	0.42
50:CZ:31:ILE:HD12	50:CZ:31:ILE:N	2.34	0.42
1:DA:709:U:H2'	1:DA:710:G:C8	2.55	0.42
2:DB:115:LYS:HZ2	2:DB:153:ASP:CG	2.22	0.42
4:DD:127:GLY:O	4:DD:128:ARG:CB	2.67	0.42
5:DE:114:VAL:CG2	5:DE:115:LEU:N	2.83	0.42
5:DE:156:LYS:HD2	8:DH:66:PHE:CZ	2.55	0.42
1:AA:1001:C:H2'	1:AA:1002:G:C1'	2.50	0.42
1:AA:1160:G:O2'	1:AA:1161:C:P	2.78	0.42
1:AA:179:A:C5	1:AA:180:U:C4	3.08	0.42
1:AA:389:A:C6	1:AA:390:U:H1'	2.55	0.42
3:AC:41:GLN:HG3	3:AC:42:TYR:CD2	2.54	0.42
4:AD:51:TYR:HA	4:AD:54:GLN:HB2	2.00	0.42
8:AH:10:MET:HG3	8:AH:27:MET:SD	2.60	0.42
8:AH:17:GLY:HA2	8:AH:22:LYS:CE	2.49	0.42
9:AI:28:ILE:HD11	9:AI:35:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:19:VAL:HG11	9:AI:83:ILE:HG13	2.02	0.42
11:AK:16:VAL:O	11:AK:17:SER:CB	2.66	0.42
12:AL:104:CYS:O	12:AL:105:SER:CB	2.67	0.42
12:AL:37:VAL:O	12:AL:37:VAL:HG23	2.20	0.42
12:AL:3:THR:HG22	12:AL:5:ASN:H	1.85	0.42
1:AA:982:U:H3'	14:AN:5:MET:HE1	2.02	0.42
15:AO:57:LEU:HD12	15:AO:58:ARG:N	2.35	0.42
18:AR:48:ARG:HD3	18:AR:48:ARG:H	1.85	0.42
19:AS:15:LEU:O	19:AS:18:LYS:HG3	2.19	0.42
22:AV:126:ARG:HG2	22:AV:169:ILE:CG1	2.49	0.42
25:BA:1275:A:C8	38:BN:16:HIS:ND1	2.88	0.42
25:BA:1433:A:N1	25:BA:1434:A:N6	2.67	0.42
25:BA:1773:A:H2'	25:BA:1774:C:C5'	2.50	0.42
25:BA:2004:G:H2'	25:BA:2005:A:O4'	2.19	0.42
25:BA:2030:A:C2	25:BA:2499:C:H5''	2.55	0.42
25:BA:2112:G:H2'	25:BA:2112:G:N3	2.35	0.42
25:BA:545:U:O2'	25:BA:547:A:H5'	2.18	0.42
29:BE:7:ASP:O	29:BE:9:GLN:N	2.53	0.42
30:BF:105:ILE:HG22	30:BF:106:ALA:H	1.84	0.42
25:BA:1223:G:OP2	42:BR:68:ARG:NH1	2.53	0.42
25:CA:1211:C:H3'	25:CA:1212:G:H5'	2.02	0.42
25:CA:137:U:OP2	25:CA:140:C:N4	2.53	0.42
25:CA:2376:A:N1	39:CO:92:PHE:HE2	2.18	0.42
25:CA:2418:A:HO2'	25:CA:2419:U:P	2.41	0.42
25:CA:2624:G:H2'	25:CA:2625:G:H5'	2.00	0.42
25:CA:637:A:N1	25:CA:651:G:O2'	2.38	0.42
25:CA:7:G:H4'	34:CJ:15:TRP:CZ2	2.55	0.42
27:CC:226:PRO:HD3	27:CC:233:GLY:HA2	2.01	0.42
30:CF:110:ILE:HD11	30:CF:113:PHE:HA	2.02	0.42
30:CF:45:ASP:N	30:CF:45:ASP:OD1	2.52	0.42
32:CH:88:GLY:HA3	32:CH:125:THR:HG22	2.01	0.42
33:CI:42:ASN:HA	33:CI:45:THR:HB	2.01	0.42
34:CJ:73:VAL:CG1	34:CJ:86:GLN:HG3	2.49	0.42
41:CQ:64:ILE:CD1	41:CQ:91:ARG:HB3	2.50	0.42
42:CR:21:ARG:HG3	42:CR:93:PHE:CD2	2.55	0.42
45:CU:6:ARG:HA	45:CU:24:VAL:HG23	2.02	0.42
45:CU:42:LYS:H	45:CU:42:LYS:HD3	1.83	0.42
1:DA:642:A:C6	1:DA:643:C:N3	2.88	0.42
1:DA:958:A:C6	19:DS:54:GLY:HA3	2.55	0.42
2:DB:174:LYS:O	2:DB:178:ASN:N	2.41	0.42
3:DC:42:TYR:OH	3:DC:90:VAL:HG11	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:DE:96:MET:HE2	5:DE:115:LEU:HD21	2.01	0.42
11:DK:63:ALA:CB	11:DK:92:GLY:HA3	2.50	0.42
11:DK:81:ASN:CB	11:DK:106:ARG:HB3	2.50	0.42
11:DK:84:VAL:CG1	11:DK:107:ILE:HD11	2.50	0.42
1:AA:1225:A:H2'	1:AA:1226:C:C6	2.54	0.42
1:AA:1490:U:OP2	58:AA:1672:PAR:H641	2.20	0.42
1:AA:453:G:H2'	1:AA:454:G:O4'	2.20	0.42
1:AA:930:C:C4	1:AA:931:C:C5	3.08	0.42
12:AL:42:PRO:CB	12:AL:89:ASP:HB3	2.50	0.42
25:BA:1094:U:N3	25:BA:1097:U:OP2	2.49	0.42
25:BA:139:U:O4	44:BT:2:ILE:N	2.47	0.42
25:BA:196:A:H2'	25:BA:196:A:N3	2.35	0.42
25:BA:416:U:H2'	25:BA:417:C:C6	2.54	0.42
25:BA:969:G:H2'	25:BA:970:U:H6	1.85	0.42
30:BF:107:VAL:HG13	30:BF:108:PRO:CD	2.50	0.42
32:BH:141:LYS:O	32:BH:142:VAL:HG13	2.20	0.42
32:BH:146:VAL:O	32:BH:147:VAL:HG22	2.19	0.42
32:BH:99:ILE:HD11	32:BH:130:VAL:HG21	2.01	0.42
35:BK:77:ILE:HG12	40:BP:71:ARG:CG	2.50	0.42
37:BM:34:LYS:HB2	37:BM:131:VAL:HG21	2.01	0.42
25:CA:132:G:N2	25:CA:148:U:C2	2.87	0.42
25:CA:2134:A:H62	25:CA:2157:G:H1'	1.85	0.42
25:CA:2292:U:H2'	25:CA:2293:G:C8	2.54	0.42
25:CA:2527:C:C4	25:CA:2528:U:C5	3.08	0.42
25:CA:627:A:C6	25:CA:637:A:C8	3.08	0.42
25:CA:671:C:H2'	25:CA:672:C:C6	2.55	0.42
25:CA:805:G:O4'	36:CL:38:GLN:CG	2.68	0.42
25:CA:817:C:H2'	25:CA:818:G:O4'	2.19	0.42
29:CE:127:GLU:HG2	29:CE:133:LEU:HD22	2.02	0.42
29:CE:181:ILE:O	29:CE:181:ILE:HG22	2.20	0.42
30:CF:7:TYR:HA	30:CF:11:VAL:HG22	2.02	0.42
30:CF:60:SER:HB2	30:CF:94:ARG:NH2	2.35	0.42
25:CA:2839:G:N2	38:CN:91:ALA:O	2.38	0.42
1:DA:110:C:C4	1:DA:111:G:C5	3.08	0.42
1:DA:1321:U:O3'	19:DS:78:ARG:NH1	2.52	0.42
1:DA:116:A:H61	1:DA:313:A:H1'	1.84	0.42
1:DA:49:U:O4	1:DA:365:U:H5	2.03	0.42
1:DA:683:G:H21	11:DK:40:ASN:HA	1.84	0.42
1:DA:74:A:H1'	1:DA:97:G:N2	2.34	0.42
2:DB:117:LEU:HD12	2:DB:117:LEU:O	2.19	0.42
2:DB:118:GLU:C	2:DB:120:GLN:H	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DB:81:LYS:HA	2:DB:85:LEU:HD13	2.02	0.42
3:DC:47:LEU:HB3	3:DC:50:ALA:HB3	2.01	0.42
4:DD:103:TYR:O	4:DD:106:GLY:N	2.51	0.42
6:DF:3:HIS:O	6:DF:92:THR:OG1	2.36	0.42
23:DV:8:U:H3'	23:DV:9:A:H5''	2.02	0.42
1:AA:1152:A:OP1	10:AJ:70:HIS:ND1	2.48	0.42
1:AA:620:C:H2'	1:AA:621:A:O4'	2.20	0.42
1:AA:859:G:HO2'	1:AA:860:A:P	2.41	0.42
3:AC:156:ARG:HD2	3:AC:193:TYR:CE2	2.55	0.42
4:AD:171:LEU:CB	4:AD:182:PHE:HA	2.50	0.42
5:AE:101:GLU:OE2	5:AE:103:THR:N	2.46	0.42
1:AA:1118:U:H5'	9:AI:106:ARG:CZ	2.50	0.42
13:AM:52:GLN:OE1	13:AM:52:GLN:N	2.53	0.42
1:AA:1310:G:O5'	13:AM:79:ARG:NH2	2.53	0.42
15:AO:11:ILE:HD11	15:AO:31:LEU:CD1	2.50	0.42
25:BA:1485:U:H2'	25:BA:1486:U:C6	2.54	0.42
25:BA:2140:G:N3	25:BA:2140:G:H2'	2.34	0.42
26:BB:3020:G:C6	26:BB:3064:G:C6	3.07	0.42
35:BK:97:THR:O	35:BK:98:ARG:HB2	2.19	0.42
37:BM:33:LEU:HD13	37:BM:117:PHE:HB3	2.02	0.42
40:BP:72:VAL:O	40:BP:72:VAL:HG23	2.20	0.42
25:CA:1232:G:C6	25:CA:1233:C:C4	3.08	0.42
25:CA:1416:G:HO2'	25:CA:1417:C:H6	1.66	0.42
25:CA:1730:C:H4'	25:CA:1731:G:O5'	2.20	0.42
25:CA:2004:G:OP2	60:CA:3794:HOH:O	2.22	0.42
25:CA:2204:G:C2	25:CA:2205:A:C8	3.07	0.42
25:CA:279:A:N6	25:CA:361:G:H1'	2.35	0.42
25:CA:536:G:P	58:CA:3169:PAR:H611	2.60	0.42
25:CA:794:A:H2'	25:CA:795:C:C6	2.55	0.42
25:CA:959:A:H62	37:CM:82:MET:HE3	1.85	0.42
27:CC:135:PRO:O	27:CC:138:SER:OG	2.38	0.42
35:CK:61:VAL:HG21	35:CK:112:PHE:CE1	2.54	0.42
36:CL:111:ILE:HG22	36:CL:112:LEU:N	2.34	0.42
42:CR:4:VAL:HB	42:CR:13:ARG:HB2	2.02	0.42
42:CR:71:LYS:HA	42:CR:89:HIS:O	2.20	0.42
42:CR:74:ILE:O	42:CR:86:GLN:HA	2.20	0.42
43:CS:69:LEU:HG	43:CS:107:VAL:CG2	2.50	0.42
44:CT:40:LYS:NZ	44:CT:59:ASN:HA	2.35	0.42
40:CP:105:LYS:NZ	1:DA:1432:G:OP2	2.40	0.42
1:DA:236:A:H2'	1:DA:237:G:O4'	2.20	0.42
1:DA:346:G:N3	1:DA:346:G:H3'	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:DE:125:ALA:O	5:DE:126:LYS:HB3	2.20	0.42
7:DG:138:ARG:CG	7:DG:139:GLU:N	2.83	0.42
9:DI:7:TYR:CG	9:DI:8:GLY:N	2.88	0.42
11:DK:113:VAL:O	11:DK:114:THR:C	2.57	0.42
23:DV:16:U:P	23:DV:16:U:H3'	2.60	0.42
1:AA:1028:C:O2	1:AA:1033:G:N2	2.41	0.41
1:AA:988:G:N2	1:AA:1217:C:O2	2.53	0.41
1:AA:519:C:O3'	22:AV:81:LYS:NZ	2.50	0.41
2:AB:101:LEU:N	2:AB:101:LEU:HD22	2.35	0.41
10:AJ:67:ILE:CD1	14:AN:96:LEU:HB2	2.50	0.41
11:AK:33:THR:CG2	11:AK:44:TRP:HE3	2.33	0.41
11:AK:50:SER:CB	25:BA:2146:C:H42	2.33	0.41
15:AO:33:THR:HG22	15:AO:63:ARG:HE	1.85	0.41
25:BA:1049:C:H1'	25:BA:1113:U:H4'	2.02	0.41
25:BA:1430:G:H2'	25:BA:1431:A:O4'	2.20	0.41
25:BA:2290:G:H2'	25:BA:2291:U:C6	2.55	0.41
25:BA:2365:G:H2'	25:BA:2366:A:C8	2.55	0.41
25:BA:2730:C:H2'	25:BA:2731:G:C8	2.55	0.41
25:BA:782:A:H4'	25:BA:783:A:O5'	2.20	0.41
25:BA:826:U:H2'	25:BA:828:U:O4'	2.19	0.41
27:BC:181:ARG:O	27:BC:181:ARG:HG3	2.20	0.41
25:BA:1813:G:H1'	27:BC:49:THR:OG1	2.20	0.41
28:BD:14:ILE:O	28:BD:22:ILE:HG23	2.20	0.41
32:BH:31:VAL:N	32:BH:32:PRO:CD	2.83	0.41
32:BH:3:VAL:CG1	32:BH:21:VAL:HG12	2.50	0.41
46:BV:29:ILE:HD13	46:BV:31:TYR:HE2	1.85	0.41
44:BT:8:LEU:HD13	49:BY:21:LEU:HB2	2.03	0.41
54:C3:44:ARG:N	54:C3:45:PRO:CD	2.82	0.41
25:CA:1131:G:O6	25:CA:2024:G:O2'	2.35	0.41
25:CA:1509:A:O2'	25:CA:1510:G:P	2.78	0.41
25:CA:1842:G:H2'	25:CA:1843:C:O4'	2.20	0.41
25:CA:2880:C:C2	25:CA:2881:U:C5	3.07	0.41
25:CA:547:A:H2'	25:CA:548:G:H5'	2.01	0.41
28:CD:56:LYS:HB2	28:CD:59:ARG:HG2	2.02	0.41
32:CH:121:VAL:CG2	32:CH:128:HIS:CG	2.95	0.41
42:CR:51:VAL:CG1	42:CR:52:PRO:HD2	2.50	0.41
46:CV:63:ILE:HD11	46:CV:72:VAL:HG11	2.01	0.41
25:CA:850:U:O2	50:CZ:46:MET:HE3	2.20	0.41
1:DA:407:U:H2'	1:DA:408:A:C8	2.54	0.41
1:DA:374:A:H5''	1:DA:452:A:C2	2.55	0.41
1:DA:499:A:H4'	1:DA:500:G:OP1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:633:G:H2'	1:DA:634:C:H6	1.84	0.41
1:DA:715:A:OP1	1:DA:805:C:O2'	2.30	0.41
4:DD:192:SER:HB3	4:DD:195:ILE:HG12	2.02	0.41
6:DF:18:VAL:HG12	6:DF:19:PRO:HD3	2.02	0.41
7:DG:5:ARG:O	7:DG:7:ILE:N	2.53	0.41
15:DO:26:GLU:OE1	15:DO:77:ARG:NE	2.52	0.41
21:DU:24:GLU:CD	21:DU:25:LYS:H	2.24	0.41
1:AA:204:G:H1'	1:AA:465:A:C2	2.55	0.41
1:AA:820:U:H4'	1:AA:821:G:OP2	2.20	0.41
3:AC:156:ARG:CA	3:AC:163:ALA:HA	2.49	0.41
13:AM:39:ILE:O	13:AM:41:GLU:N	2.50	0.41
16:AP:14:ARG:N	16:AP:15:PRO:HD3	2.36	0.41
17:AQ:69:LYS:HG3	17:AQ:69:LYS:O	2.20	0.41
19:AS:41:PHE:CD1	19:AS:41:PHE:N	2.87	0.41
56:B5:78:ALA:HA	56:B5:123:VAL:CB	2.50	0.41
25:BA:1720:U:H2'	25:BA:1721:G:O4'	2.20	0.41
31:BG:108:PHE:CE1	31:BG:151:ARG:CZ	3.04	0.41
32:BH:135:HIS:CE1	32:BH:138:VAL:HG21	2.55	0.41
33:BI:105:LEU:HD21	33:BI:129:GLU:HB2	2.02	0.41
35:BK:13:ASN:HD21	35:BK:97:THR:HG23	1.84	0.41
36:BL:81:ASP:CG	36:BL:100:ILE:HD11	2.40	0.41
38:BN:65:LEU:HD11	38:BN:69:ARG:CZ	2.51	0.41
41:BQ:57:ARG:O	41:BQ:61:ILE:HG12	2.21	0.41
47:BW:54:ASP:O	47:BW:55:HIS:HB2	2.20	0.41
25:CA:1071:G:H2'	25:CA:1072:C:C5'	2.50	0.41
25:CA:122:G:H2'	25:CA:123:G:O4'	2.20	0.41
25:CA:1672:A:N6	25:CA:1673:G:C6	2.87	0.41
25:CA:197:A:N6	25:CA:2430:A:H2'	2.34	0.41
25:CA:2589:A:C2	25:CA:2606:C:N3	2.88	0.41
25:CA:783:A:H8	25:CA:784:G:H4'	1.85	0.41
27:CC:35:LYS:HZ3	27:CC:37:SER:HG	1.68	0.41
31:CG:75:VAL:HG13	31:CG:76:ILE:N	2.35	0.41
34:CJ:140:LEU:HD12	34:CJ:141:ASP:N	2.35	0.41
39:CO:4:LYS:O	39:CO:7:ARG:NH1	2.53	0.41
1:DA:393:A:C2	1:DA:394:G:C8	3.08	0.41
1:DA:48:C:C3'	1:DA:49:U:H5''	2.49	0.41
2:DB:71:GLY:HA2	2:DB:164:ILE:CG2	2.50	0.41
4:DD:124:MET:HB3	4:DD:143:VAL:HA	2.02	0.41
8:DH:78:VAL:HG11	8:DH:125:ILE:HD11	2.02	0.41
11:DK:31:ILE:HG22	11:DK:46:THR:HB	2.02	0.41
19:DS:36:ARG:HB2	19:DS:72:GLY:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:DT:71:LYS:HD3	20:DT:75:HIS:CE1	2.55	0.41
21:DU:37:PHE:HB3	21:DU:41:PRO:CD	2.50	0.41
1:AA:1031:C:H5'	1:AA:1032:G:C4	2.56	0.41
1:AA:1290:G:H5''	7:AG:35:LYS:CE	2.50	0.41
1:AA:1522:U:H2'	1:AA:1523:G:H8	1.85	0.41
1:AA:327:A:C4	1:AA:329:A:C8	3.08	0.41
2:AB:39:HIS:N	2:AB:39:HIS:CD2	2.87	0.41
4:AD:8:LYS:HB3	4:AD:21:LEU:HD13	2.01	0.41
4:AD:91:LEU:CD1	4:AD:197:GLU:HG3	2.49	0.41
6:AF:11:HIS:HB2	6:AF:12:PRO:HD2	2.03	0.41
6:AF:67:PRO:O	6:AF:69:GLU:N	2.49	0.41
15:AO:82:ILE:HG13	15:AO:83:GLU:H	1.85	0.41
19:AS:12:ASP:OD1	19:AS:37:ARG:NH1	2.53	0.41
22:AV:55:LEU:HD22	22:AV:75:MET:CE	2.51	0.41
25:BA:1182:G:H2'	25:BA:1183:U:O4'	2.20	0.41
25:BA:1651:G:C2'	25:BA:1652:A:O5'	2.69	0.41
25:BA:1731:G:O2'	25:BA:1732:C:H2'	2.20	0.41
25:BA:1740:G:C5	25:BA:1741:C:C5	3.08	0.41
25:BA:2879:A:H4'	25:BA:2880:C:OP1	2.20	0.41
25:BA:298:G:P	45:BU:84:PHE:HB3	2.61	0.41
25:BA:414:C:H4'	25:BA:1879:C:O2	2.19	0.41
25:BA:715:A:H2'	25:BA:716:A:C8	2.56	0.41
25:BA:81:G:C6	25:BA:82:U:C2	3.09	0.41
28:BD:133:THR:CG2	28:BD:134:HIS:CD2	3.03	0.41
28:BD:2:ILE:HG13	28:BD:3:GLY:N	2.35	0.41
32:BH:90:LEU:C	32:BH:92:GLY:N	2.73	0.41
40:BP:27:VAL:HG12	40:BP:29:VAL:HG23	2.02	0.41
41:BQ:81:GLY:HA2	41:BQ:116:LEU:HD23	2.02	0.41
53:C2:30:VAL:HG22	53:C2:33:ARG:HH12	1.84	0.41
25:CA:1318:U:H2'	25:CA:1319:C:C6	2.55	0.41
25:CA:1670:C:C5	25:CA:1671:U:C4	3.08	0.41
25:CA:2324:U:H3'	25:CA:2325:G:H5''	2.02	0.41
25:CA:2377:A:H2'	25:CA:2378:A:C8	2.55	0.41
25:CA:2662:A:C5	25:CA:2663:G:H1'	2.56	0.41
32:CH:122:LEU:C	32:CH:124:THR:N	2.73	0.41
38:CN:55:ALA:HB1	38:CN:80:PHE:H	1.85	0.41
41:CQ:38:VAL:O	41:CQ:41:ALA:HB3	2.20	0.41
1:DA:1007:U:H3'	1:DA:1008:U:H5''	2.02	0.41
1:DA:28:A:O2'	1:DA:296:U:OP1	2.30	0.41
1:DA:404:G:C6	1:DA:405:U:C4	3.08	0.41
1:DA:427:U:C4	1:DA:428:G:C6	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:DB:71:GLY:HA2	2:DB:164:ILE:HG22	2.03	0.41
2:DB:27:MET:HE2	2:DB:30:PHE:HD2	1.86	0.41
4:DD:143:VAL:O	4:DD:143:VAL:HG23	2.20	0.41
5:DE:48:PHE:CD1	5:DE:141:ILE:HD13	2.56	0.41
6:DF:22:ILE:HG13	6:DF:23:GLU:N	2.34	0.41
8:DH:96:MET:HE2	8:DH:99:LEU:HG	2.03	0.41
11:DK:85:MET:O	11:DK:87:LYS:NZ	2.53	0.41
17:DQ:46:VAL:HG22	17:DQ:47:HIS:N	2.35	0.41
18:DR:34:THR:HG23	18:DR:36:SER:N	2.35	0.41
21:DU:9:ASN:N	21:DU:9:ASN:OD1	2.53	0.41
1:AA:557:G:C6	1:AA:558:G:C6	3.07	0.41
1:AA:673:A:C5'	6:AF:86:ARG:NH1	2.84	0.41
8:AH:55:THR:C	8:AH:57:PRO:HD3	2.41	0.41
11:AK:35:THR:HA	11:AK:41:ALA:HA	2.01	0.41
1:AA:952:U:C5	13:AM:103:LYS:HE2	2.55	0.41
13:AM:45:ILE:HA	13:AM:48:LEU:CD1	2.50	0.41
14:AN:72:GLY:HA3	14:AN:81:ARG:HD3	2.01	0.41
16:AP:6:LEU:HB2	16:AP:17:TYR:HB3	2.02	0.41
51:B0:37:HIS:HB3	51:B0:43:THR:HG22	2.01	0.41
25:BA:2082:A:H2'	25:BA:2083:G:O4'	2.21	0.41
25:BA:647:G:C2'	25:BA:648:G:O5'	2.67	0.41
25:BA:847:U:O2	25:BA:934:U:H1'	2.21	0.41
25:BA:945:A:C5	25:BA:2448:A:C2	3.08	0.41
28:BD:71:ALA:HB3	28:BD:73:VAL:HG13	2.01	0.41
25:BA:2298:A:H5''	30:BF:71:LYS:NZ	2.36	0.41
31:BG:154:GLU:HG2	31:BG:156:TYR:H	1.85	0.41
41:BQ:82:LEU:HG	41:BQ:87:VAL:HG11	2.02	0.41
25:CA:1141:U:OP2	34:CJ:65:THR:CG2	2.68	0.41
25:CA:2037:A:H2'	25:CA:2038:G:C8	2.55	0.41
25:CA:1853:A:N1	25:CA:2087:G:H1'	2.36	0.41
25:CA:2329:U:H2'	25:CA:2330:G:O4'	2.20	0.41
25:CA:2576:G:N3	25:CA:2576:G:H3'	2.35	0.41
25:CA:2624:G:C2'	25:CA:2625:G:H5'	2.50	0.41
28:CD:110:THR:HB	28:CD:202:ILE:HG12	2.00	0.41
33:CI:8:VAL:H	33:CI:58:ILE:HD12	1.85	0.41
38:CN:24:MET:HE2	38:CN:44:LEU:HB2	2.03	0.41
40:CP:31:VAL:HG12	40:CP:32:VAL:N	2.35	0.41
45:CU:96:LYS:O	45:CU:97:SER:CB	2.67	0.41
1:DA:604:G:C2	1:DA:635:A:C2	3.08	0.41
1:DA:844:G:H2'	1:DA:844:G:N3	2.36	0.41
3:DC:97:VAL:HG22	3:DC:98:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DD:98:LEU:HD22	4:DD:118:VAL:CG1	2.51	0.41
5:DE:96:MET:CE	5:DE:115:LEU:HD21	2.51	0.41
5:DE:96:MET:HA	5:DE:125:ALA:HA	2.01	0.41
6:DF:9:MET:HE1	18:DR:65:LEU:HA	2.02	0.41
8:DH:71:VAL:CG1	8:DH:72:VAL:N	2.84	0.41
13:DM:106:ALA:O	13:DM:108:THR:N	2.53	0.41
13:DM:19:LEU:O	13:DM:22:ILE:CG2	2.68	0.41
14:DN:73:PHE:HA	14:DN:80:SER:HA	2.02	0.41
24:DW:3:C:H2'	24:DW:4:C:C6	2.55	0.41
1:AA:1124:G:C2'	1:AA:1145:A:H62	2.34	0.41
1:AA:1240:U:OP1	7:AG:119:ARG:NH2	2.54	0.41
1:AA:1310:G:OP1	13:AM:79:ARG:NH2	2.53	0.41
1:AA:232:G:H1'	1:AA:262:A:N1	2.35	0.41
1:AA:469:C:C5	1:AA:470:C:C4	3.09	0.41
1:AA:738:C:C2'	1:AA:739:C:O5'	2.69	0.41
1:AA:739:C:C4	1:AA:740:U:C4	3.08	0.41
1:AA:818:G:O2'	1:AA:819:A:H5'	2.21	0.41
3:AC:38:LYS:HE3	3:AC:94:ILE:HD12	2.01	0.41
7:AG:103:TRP:HB2	7:AG:137:LYS:HD3	2.01	0.41
10:AJ:71:LEU:H	10:AJ:71:LEU:HD12	1.85	0.41
11:AK:34:ILE:HD11	11:AK:42:LEU:HG	2.03	0.41
13:AM:69:LEU:HA	13:AM:72:GLU:HG2	2.02	0.41
14:AN:27:LYS:HA	14:AN:30:ILE:CG1	2.46	0.41
18:AR:45:THR:HG23	18:AR:47:THR:HG23	2.02	0.41
51:B0:52:LYS:HE2	51:B0:55:ALA:HB2	2.02	0.41
52:B1:38:PHE:O	52:B1:39:ASP:CB	2.67	0.41
56:B5:136:LEU:HA	56:B5:139:ASN:CB	2.50	0.41
25:BA:1515:A:H1'	25:BA:1557:C:H1'	2.02	0.41
25:BA:2207:C:H2'	25:BA:2208:C:C6	2.56	0.41
25:BA:2484:G:P	37:BM:44:ARG:NH2	2.94	0.41
25:BA:593:U:H2'	25:BA:594:U:C6	2.56	0.41
25:BA:675:A:OP1	29:BE:58:LYS:NZ	2.53	0.41
25:BA:1500:G:O3'	27:BC:100:ARG:NH2	2.53	0.41
27:BC:30:ALA:HB3	27:BC:31:PRO:HD3	2.02	0.41
32:BH:72:ILE:HG21	32:BH:140:ALA:HB1	2.03	0.41
39:BO:38:GLN:HB3	39:BO:47:VAL:HG21	2.02	0.41
43:BS:29:VAL:HG21	43:BS:69:LEU:HB3	2.03	0.41
25:CA:2526:G:C2'	55:C4:1:MET:H1	2.32	0.41
25:CA:1097:U:H2'	25:CA:1098:A:H5'	2.03	0.41
25:CA:1245:G:H4'	29:CE:33:VAL:HG23	2.03	0.41
25:CA:13:A:N3	25:CA:15:G:C6	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:CA:2063:C:O2	25:CA:2450:A:N1	2.53	0.41
25:CA:60:G:C8	25:CA:62:U:H2'	2.55	0.41
26:CB:3078:A:OP2	46:CV:18:ARG:NH2	2.53	0.41
30:CF:57:ALA:HB2	30:CF:64:PRO:HD3	2.03	0.41
34:CJ:16:TYR:HB3	34:CJ:140:LEU:HB2	2.01	0.41
38:CN:44:LEU:HA	38:CN:47:VAL:HG12	2.03	0.41
40:CP:75:THR:C	40:CP:77:SER:H	2.23	0.41
1:DA:1179:A:H2'	1:DA:1180:A:O4'	2.20	0.41
1:DA:487:A:C8	1:DA:488:C:C5	3.08	0.41
1:DA:619:U:H3	4:DD:131:ASN:HB3	1.85	0.41
1:DA:728:A:C6	1:DA:729:A:C6	3.08	0.41
1:DA:766:A:H2'	1:DA:767:A:O4'	2.20	0.41
2:DB:154:MET:SD	2:DB:158:PRO:HG3	2.60	0.41
2:DB:90:PHE:CZ	2:DB:154:MET:HA	2.55	0.41
4:DD:25:VAL:HG22	4:DD:26:ARG:N	2.35	0.41
5:DE:72:ILE:HG12	5:DE:145:GLU:HB2	2.02	0.41
9:DI:10:GLY:HA2	9:DI:81:HIS:ND1	2.35	0.41
11:DK:79:ILE:HD12	11:DK:80:LYS:H	1.85	0.41
12:DL:9:ARG:O	12:DL:10:LYS:CB	2.67	0.41
13:DM:2:ALA:HA	13:DM:53:ILE:HD11	2.03	0.41
15:DO:29:VAL:O	15:DO:33:THR:HG23	2.21	0.41
1:AA:927:G:O2'	1:AA:1503:A:N7	2.38	0.41
1:AA:616:G:N2	1:AA:617:G:C4	2.88	0.41
2:AB:183:VAL:HG21	2:AB:197:ASP:CB	2.50	0.41
3:AC:134:MET:O	3:AC:137:ALA:N	2.50	0.41
3:AC:66:VAL:HG22	3:AC:67:THR:N	2.36	0.41
4:AD:171:LEU:HA	4:AD:182:PHE:HA	2.01	0.41
4:AD:58:LYS:HB3	4:AD:200:ILE:HG12	2.03	0.41
8:AH:69:LYS:HD2	8:AH:69:LYS:N	2.36	0.41
9:AI:55:VAL:HG11	9:AI:94:LEU:HD22	2.03	0.41
11:AK:129:VAL:HG12	23:AW:10:A:H4'	2.02	0.41
14:AN:42:TRP:H	14:AN:42:TRP:HE3	1.67	0.41
17:AQ:12:VAL:O	17:AQ:13:VAL:HB	2.21	0.41
21:AU:14:VAL:HG13	21:AU:16:LEU:HG	2.02	0.41
11:AK:126:LYS:C	21:AU:35:ARG:NH2	2.74	0.41
22:AV:108:GLU:C	22:AV:110:ARG:N	2.73	0.41
22:AV:150:SER:O	22:AV:151:GLU:C	2.58	0.41
25:BA:245:G:O6	54:B3:7:ARG:HD3	2.20	0.41
55:B4:13:ASN:OD1	55:B4:13:ASN:N	2.53	0.41
25:BA:1088:A:N3	25:BA:1088:A:H3'	2.36	0.41
25:BA:1326:U:O2'	25:BA:1327:A:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2221:G:C5	25:BA:2222:C:C5	3.09	0.41
25:BA:2391:G:O6	25:BA:2425:A:H8	2.03	0.41
25:BA:834:G:C6	25:BA:835:C:C4	3.07	0.41
27:BC:250:GLN:HB3	27:BC:254:LYS:HB2	2.02	0.41
35:BK:4:GLU:O	35:BK:5:GLN:HB2	2.20	0.41
25:BA:459:U:HO2'	44:BT:73:ARG:NH1	2.14	0.41
25:CA:1033:U:C4	25:CA:2750:A:C2	3.09	0.41
25:CA:1241:A:H2'	25:CA:1241:A:N3	2.35	0.41
25:CA:2327:A:H3'	25:CA:2328:A:C8	2.55	0.41
25:CA:2657:A:O2'	31:CG:159:LYS:NZ	2.50	0.41
25:CA:2841:C:H2'	25:CA:2842:G:C8	2.56	0.41
25:CA:776:G:H4'	25:CA:777:G:O5'	2.20	0.41
25:CA:969:G:H2'	25:CA:970:U:C6	2.56	0.41
26:CB:3023:G:O6	26:CB:3060:C:N4	2.51	0.41
28:CD:155:VAL:O	28:CD:156:PHE:HB2	2.21	0.41
29:CE:121:VAL:HG21	29:CE:124:PHE:HB2	2.02	0.41
30:CF:32:LYS:HA	30:CF:95:MET:HE2	2.02	0.41
32:CH:30:LEU:HD23	32:CH:36:ALA:HB3	2.02	0.41
25:CA:1007:C:OP1	34:CJ:39:LYS:HD2	2.20	0.41
25:CA:2379:G:O3'	39:CO:17:LYS:NZ	2.53	0.41
35:CK:74:GLY:HA3	40:CP:74:GLN:HG3	2.03	0.41
25:CA:499:U:H4'	45:CU:42:LYS:HG2	2.03	0.41
49:CY:26:PHE:O	49:CY:29:ARG:HG2	2.20	0.41
49:CY:39:GLN:HB3	49:CY:42:LEU:HD13	2.03	0.41
1:DA:1033:G:N2	1:DA:1034:G:C4	2.88	0.41
1:DA:1333:A:H2'	1:DA:1334:G:O4'	2.20	0.41
1:DA:1461:G:H2'	1:DA:1462:C:O4'	2.20	0.41
1:DA:633:G:H2'	1:DA:634:C:C6	2.55	0.41
1:DA:649:A:H5''	1:DA:650:G:OP2	2.21	0.41
1:DA:588:G:C4	1:DA:753:A:C6	3.08	0.41
1:DA:872:A:N3	1:DA:872:A:H2'	2.35	0.41
2:DB:111:ILE:CD1	2:DB:151:ILE:CD1	2.98	0.41
2:DB:28:LYS:N	2:DB:29:PRO:HD2	2.35	0.41
4:DD:123:ILE:HG12	4:DD:124:MET:H	1.86	0.41
4:DD:20:PHE:HD1	4:DD:20:PHE:HA	1.79	0.41
5:DE:33:PHE:N	5:DE:33:PHE:CD1	2.88	0.41
11:DK:15:GLN:HA	11:DK:77:TYR:O	2.20	0.41
11:DK:22:HIS:CE1	11:DK:35:THR:HG21	2.56	0.41
1:DA:1491:G:H3'	12:DL:44:LYS:NZ	2.35	0.41
14:DN:73:PHE:C	14:DN:73:PHE:CD1	2.92	0.41
17:DQ:44:LEU:HD21	17:DQ:73:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:DS:29:LYS:HB2	19:DS:30:PRO:HD2	2.03	0.41
1:AA:1172:C:H2'	1:AA:1173:U:C6	2.55	0.41
1:AA:1315:U:H2'	1:AA:1316:G:O4'	2.21	0.41
1:AA:204:G:C3'	1:AA:205:A:H5''	2.49	0.41
1:AA:33:A:H2'	1:AA:34:C:H6	1.86	0.41
1:AA:66:A:C2	1:AA:67:C:C6	3.08	0.41
2:AB:164:ILE:HG12	2:AB:165:ASP:N	2.35	0.41
2:AB:55:ALA:O	2:AB:57:LEU:N	2.53	0.41
3:AC:22:TRP:CD1	3:AC:23:PHE:N	2.89	0.41
4:AD:118:VAL:HG13	4:AD:119:SER:N	2.36	0.41
4:AD:19:LEU:C	4:AD:19:LEU:CD2	2.89	0.41
4:AD:201:VAL:HG23	4:AD:202:GLU:N	2.35	0.41
6:AF:21:MET:HB2	6:AF:22:ILE:H	1.75	0.41
10:AJ:51:VAL:O	10:AJ:62:ARG:HA	2.20	0.41
11:AK:67:ALA:HB1	11:AK:100:LEU:CD2	2.50	0.41
11:AK:111:THR:HG23	21:AU:5:LYS:HD3	2.03	0.41
11:AK:75:LYS:HA	11:AK:75:LYS:HD2	1.95	0.41
13:AM:24:GLY:CA	13:AM:69:LEU:CD2	2.98	0.41
15:AO:63:ARG:NH1	15:AO:87:LEU:CD2	2.84	0.41
15:AO:89:ARG:NH1	15:AO:89:ARG:HB3	2.36	0.41
1:AA:261:U:C5	20:AT:74:ARG:CZ	3.03	0.41
22:AV:6:ILE:HD12	22:AV:139:LYS:HB2	2.03	0.41
25:BA:1079:C:H2'	25:BA:1080:A:H5'	2.02	0.41
25:BA:1741:C:C4	25:BA:1742:U:C5	3.08	0.41
25:BA:2286:G:OP2	52:B1:29:LYS:NZ	2.40	0.41
25:BA:2461:A:H1'	25:BA:2492:U:C2	2.55	0.41
25:BA:2498:C:P	60:BA:3689:HOH:O	2.78	0.41
25:BA:244:A:C2	25:BA:255:A:C4	3.09	0.41
58:BA:3004:PAR:N21	58:BA:3004:PAR:H531	2.36	0.41
25:BA:507:A:H5''	25:BA:509:C:O4'	2.20	0.41
25:BA:574:A:H4'	25:BA:575:A:O5'	2.21	0.41
25:BA:796:C:H2'	25:BA:797:G:C8	2.55	0.41
27:BC:194:VAL:HG22	27:BC:195:GLY:N	2.36	0.41
29:BE:21:ARG:N	29:BE:110:SER:HG	2.18	0.41
30:BF:33:ILE:O	30:BF:90:LEU:HD11	2.21	0.41
36:BL:2:ARG:O	36:BL:2:ARG:HG2	2.21	0.41
37:BM:96:ILE:HG21	37:BM:126:ILE:CD1	2.51	0.41
38:BN:70:THR:HG22	38:BN:71:ARG:N	2.35	0.41
48:BX:32:LEU:HD13	48:BX:49:ARG:NE	2.35	0.41
25:CA:1085:A:C6	25:CA:1086:A:N6	2.88	0.41
25:CA:1415:U:C2	25:CA:1588:G:N2	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:CA:2543:G:H2'	25:CA:2544:G:C8	2.56	0.41
25:CA:2845:U:H2'	25:CA:2846:G:C8	2.56	0.41
25:CA:35:G:C2'	25:CA:36:G:O5'	2.69	0.41
26:CB:3024:G:C5'	26:CB:3025:U:H5	2.34	0.41
27:CC:12:ARG:HA	27:CC:15:VAL:HG23	2.02	0.41
30:CF:28:PRO:HA	30:CF:158:THR:HB	2.02	0.41
30:CF:9:ASP:N	30:CF:9:ASP:OD1	2.53	0.41
40:CP:47:ILE:HD13	40:CP:61:ARG:HB2	2.02	0.41
45:CU:32:LYS:HB3	45:CU:63:ALA:HB1	2.02	0.41
46:CV:81:PRO:HD2	46:CV:83:LYS:CE	2.51	0.41
1:DA:1446:A:H2'	1:DA:1446:A:N3	2.35	0.41
1:DA:505:G:C6	1:DA:535:A:C2	3.08	0.41
1:DA:577:G:C2	1:DA:578:C:C6	3.09	0.41
2:DB:120:GLN:N	2:DB:120:GLN:OE1	2.53	0.41
2:DB:133:GLU:O	2:DB:137:ARG:HB2	2.21	0.41
1:DA:439:U:O2'	4:DD:131:ASN:OD1	2.39	0.41
5:DE:137:VAL:O	5:DE:137:VAL:HG13	2.20	0.41
5:DE:14:LYS:HZ1	5:DE:112:ARG:HH22	1.67	0.41
7:DG:132:GLY:H	7:DG:135:VAL:HG12	1.85	0.41
13:DM:4:ILE:C	13:DM:6:GLY:H	2.23	0.41
18:DR:52:GLN:C	18:DR:54:GLN:N	2.74	0.41
19:DS:42:PRO:O	19:DS:44:MET:N	2.54	0.41
23:DV:4:G:H2'	23:DV:5:A:H5'	2.02	0.41
1:AA:1137:C:HO2'	1:AA:1138:G:P	2.43	0.41
1:AA:955:U:H1'	1:AA:1227:A:H62	1.84	0.41
1:AA:1237:C:OP1	60:AA:1864:HOH:O	2.22	0.41
1:AA:669:G:OP1	15:AO:48:LYS:NZ	2.44	0.41
1:AA:955:U:H2'	1:AA:956:U:O4'	2.20	0.41
2:AB:32:PHE:CG	2:AB:32:PHE:O	2.74	0.41
5:AE:38:VAL:CG1	5:AE:117:VAL:HG11	2.51	0.41
6:AF:70:VAL:HG23	6:AF:71:ILE:H	1.86	0.41
10:AJ:40:ILE:HG13	10:AJ:73:LEU:HD11	2.01	0.41
14:AN:44:ALA:HA	14:AN:47:LYS:HE2	2.02	0.41
21:AU:40:LYS:HE3	21:AU:40:LYS:H	1.86	0.41
22:AV:70:VAL:CG1	22:AV:75:MET:CE	2.99	0.41
23:AW:10:A:O2'	23:AW:11:A:P	2.79	0.41
25:BA:1223:G:N2	25:BA:1226:A:OP2	2.47	0.41
25:BA:1488:C:N3	25:BA:1502:A:C2	2.89	0.41
25:BA:1952:A:C6	25:BA:1953:A:C6	3.09	0.41
25:BA:1995:U:H5''	25:BA:1996:C:O5'	2.20	0.41
25:BA:2187:U:C4	25:BA:2188:U:N3	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2728:U:O2'	25:BA:2729:G:O5'	2.38	0.41
25:BA:674:G:H1'	29:BE:69:ARG:HD3	2.02	0.41
30:BF:153:ILE:HD12	30:BF:154:THR:N	2.35	0.41
32:BH:124:THR:HG22	32:BH:125:THR:N	2.32	0.41
26:BB:3098:G:H1	46:BV:14:LYS:HG2	1.86	0.41
50:BZ:7:THR:HG23	50:BZ:34:THR:HB	2.02	0.41
25:CA:1315:C:C2	25:CA:1338:G:N2	2.89	0.41
25:CA:1865:U:C5	25:CA:1875:G:N1	2.89	0.41
25:CA:2078:C:C2	25:CA:2079:U:C6	3.09	0.41
25:CA:2297:A:N3	25:CA:2297:A:H2'	2.36	0.41
25:CA:747:U:C4	25:CA:2613:U:C5	3.09	0.41
25:CA:2899:A:C2	25:CA:2900:A:C4	3.09	0.41
25:CA:57:C:H2'	25:CA:58:G:O4'	2.21	0.41
27:CC:106:PRO:HB3	27:CC:141:HIS:NE2	2.36	0.41
30:CF:3:LEU:HD11	30:CF:99:PHE:CE1	2.56	0.41
31:CG:97:VAL:CG1	31:CG:98:LYS:N	2.83	0.41
33:CI:21:PRO:HB2	33:CI:22:PRO:HD3	2.03	0.41
34:CJ:84:ILE:O	34:CJ:84:ILE:HG23	2.21	0.41
25:CA:666:A:H4'	36:CL:48:ARG:CD	2.50	0.41
39:CO:17:LYS:O	39:CO:20:GLU:N	2.54	0.41
1:DA:1035:A:H2'	1:DA:1036:A:O4'	2.21	0.41
1:DA:977:A:N6	1:DA:1224:U:O4'	2.54	0.41
1:DA:1360:A:H62	1:DA:1361:G:N2	2.19	0.41
1:DA:1420:U:O4	58:DA:1655:PAR:H221	2.12	0.41
1:DA:551:U:C4	1:DA:552:U:C5	3.09	0.41
1:DA:723:U:O2'	1:DA:724:G:P	2.78	0.41
1:DA:980:C:C5'	1:DA:981:U:C5	3.03	0.41
1:DA:995:C:N3	1:DA:1046:A:O2'	2.46	0.41
2:DB:119:THR:O	2:DB:119:THR:HG22	2.21	0.41
2:DB:144:LEU:HB2	2:DB:148:LEU:CB	2.51	0.41
4:DD:170:TRP:CE2	4:DD:186:PRO:HD3	2.56	0.41
4:DD:26:ARG:NH2	4:DD:29:ASP:O	2.53	0.41
9:DI:87:LEU:HD21	9:DI:95:ARG:HH21	1.86	0.41
10:DJ:18:ILE:HG23	10:DJ:19:ASP:N	2.36	0.41
16:DP:6:LEU:HD12	16:DP:71:VAL:CG1	2.50	0.41
1:AA:1144:G:C2	1:AA:1145:A:N1	2.89	0.41
1:AA:1169:A:N6	1:AA:1170:A:C2	2.89	0.41
1:AA:1431:A:H2	1:AA:1469:C:H41	1.69	0.41
1:AA:1484:C:H2'	1:AA:1485:U:O4'	2.21	0.41
1:AA:406:G:N2	1:AA:437:U:C2	2.89	0.41
1:AA:625:U:H4'	16:AP:16:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:77:A:H2'	1:AA:78:A:H8	1.84	0.41
1:AA:859:G:H2'	1:AA:860:A:C8	2.56	0.41
3:AC:6:HIS:HD2	3:AC:9:GLY:N	2.19	0.41
4:AD:54:GLN:HB3	4:AD:58:LYS:HZ1	1.86	0.41
7:AG:136:LYS:O	7:AG:140:ASP:N	2.54	0.41
9:AI:55:VAL:HG11	9:AI:94:LEU:HB2	2.02	0.41
12:AL:52:VAL:HG22	12:AL:53:CYS:N	2.36	0.41
13:AM:85:CYS:SG	13:AM:87:ARG:N	2.93	0.41
15:AO:70:LEU:O	15:AO:73:LYS:N	2.49	0.41
18:AR:59:ILE:O	18:AR:63:ARG:HG2	2.21	0.41
53:B2:1:MET:N	53:B2:1:MET:CE	2.83	0.41
25:BA:1696:G:C6	25:BA:1697:G:C4	3.09	0.41
25:BA:2504:U:O5'	25:BA:2504:U:H6	2.04	0.41
25:BA:29:U:O5'	25:BA:29:U:H6	2.04	0.41
25:BA:44:A:H2'	25:BA:45:G:O4'	2.20	0.41
25:BA:519:U:H2'	25:BA:520:G:O4'	2.21	0.41
25:BA:532:A:N7	25:BA:2021:C:H2'	2.36	0.41
25:BA:548:G:O2'	25:BA:549:G:N2	2.54	0.41
25:BA:582:A:C6	25:BA:583:G:C6	3.09	0.41
29:BE:5:LEU:CD2	29:BE:121:VAL:HA	2.51	0.41
29:BE:129:PRO:HB3	29:BE:159:LEU:HD11	2.03	0.41
32:BH:4:ILE:HD13	32:BH:18:GLN:CB	2.50	0.41
41:BQ:40:LYS:HG2	41:BQ:41:ALA:N	2.35	0.41
41:BQ:87:VAL:HA	42:BR:49:ILE:HG21	2.03	0.41
44:BT:51:PHE:O	44:BT:52:GLU:C	2.59	0.41
45:BU:24:VAL:HG13	45:BU:33:VAL:CG2	2.51	0.41
54:C3:27:ASN:ND2	54:C3:39:ARG:HH11	2.18	0.41
25:CA:1243:C:C4	25:CA:1244:A:N7	2.89	0.41
25:CA:2235:G:H2'	25:CA:2236:U:O4'	2.20	0.41
25:CA:2820:A:HO2'	25:CA:2821:A:P	2.43	0.41
25:CA:656:G:H2'	25:CA:657:U:O4'	2.20	0.41
25:CA:800:A:H4'	25:CA:801:G:O5'	2.19	0.41
25:CA:84:A:H4'	45:CU:5:ARG:CD	2.51	0.41
25:CA:861:A:C2	25:CA:917:A:C4	3.09	0.41
30:CF:160:LYS:H	30:CF:160:LYS:HG3	1.75	0.41
31:CG:126:THR:HG22	31:CG:127:GLN:H	1.86	0.41
25:CA:2377:A:N3	39:CO:92:PHE:CE2	2.89	0.41
43:CS:37:THR:HB	43:CS:38:TYR:CD2	2.56	0.41
44:CT:18:GLU:O	44:CT:22:THR:HG22	2.21	0.41
1:DA:1051:C:H2'	1:DA:1052:U:C6	2.56	0.41
1:DA:1134:G:C6	1:DA:1135:U:C6	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:1465:A:H2'	1:DA:1466:C:C6	2.55	0.41
25:CA:1689:A:H4'	1:DA:1475:G:H4'	2.03	0.41
1:DA:232:G:H1'	1:DA:262:A:N1	2.36	0.41
1:DA:294:U:C2	1:DA:295:C:C5	3.08	0.41
1:DA:33:A:H2'	1:DA:34:C:C6	2.56	0.41
1:DA:355:C:C2	1:DA:356:A:C8	3.08	0.41
5:DE:83:HIS:CE1	5:DE:147:MET:CE	3.03	0.41
5:DE:18:VAL:HG22	5:DE:19:ASN:N	2.36	0.41
15:DO:3:LEU:HD13	15:DO:8:THR:HG23	2.02	0.41
19:DS:80:TYR:CD1	19:DS:81:ARG:N	2.88	0.41
21:DU:19:PHE:N	21:DU:22:SER:OG	2.53	0.41
1:AA:179:A:C6	1:AA:180:U:N3	2.88	0.41
1:AA:260:G:H2'	1:AA:261:U:C6	2.56	0.41
1:AA:809:G:C2'	1:AA:810:C:O5'	2.69	0.41
3:AC:173:VAL:HG12	3:AC:175:LEU:HD12	2.03	0.41
3:AC:23:PHE:HE2	10:AJ:69:THR:HG23	1.85	0.41
4:AD:117:LEU:HD12	4:AD:122:ALA:HB3	2.03	0.41
4:AD:46:PRO:HB2	4:AD:48:LEU:CD2	2.51	0.41
7:AG:103:TRP:HB3	7:AG:137:LYS:HE3	2.03	0.41
12:AL:25:GLU:HB2	12:AL:27:CYS:SG	2.60	0.41
1:AA:1330:U:H4'	13:AM:23:TYR:CE1	2.56	0.41
1:AA:617:G:H4'	16:AP:46:LYS:HD2	2.02	0.41
19:AS:31:LEU:HD22	19:AS:49:ILE:HD12	2.02	0.41
22:AV:38:LEU:C	22:AV:40:GLY:H	2.24	0.41
22:AV:81:LYS:HA	22:AV:84:MET:HG2	2.03	0.41
23:AW:10:A:C4	23:AW:11:A:C8	3.09	0.41
56:B5:136:LEU:C	56:B5:139:ASN:CA	2.89	0.41
25:BA:1109:C:N4	25:BA:1110:G:N1	2.68	0.41
25:BA:195:A:H2'	25:BA:198:C:N4	2.36	0.41
25:BA:2286:G:O6	52:B1:22:THR:OG1	2.24	0.41
25:BA:2512:C:H1'	28:BD:145:SER:O	2.21	0.41
25:BA:779:U:P	27:BC:48:ILE:HG13	2.61	0.41
25:BA:842:U:H2'	25:BA:843:G:O4'	2.20	0.41
29:BE:125:SER:OG	29:BE:154:ASP:OD2	2.39	0.41
31:BG:79:THR:HG22	31:BG:80:GLU:N	2.36	0.41
25:BA:910:A:C4	37:BM:13:HIS:CE1	3.09	0.41
38:BN:38:LEU:HB3	38:BN:39:PRO:HD3	2.03	0.41
38:BN:47:VAL:O	38:BN:51:LEU:HD23	2.21	0.41
25:CA:1847:A:O2'	25:CA:1848:A:P	2.78	0.41
25:CA:2209:G:C2	25:CA:2216:G:C2	3.08	0.41
25:CA:2513:A:H2'	25:CA:2513:A:N3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:CA:36:G:N3	25:CA:450:G:O2'	2.54	0.41
25:CA:541:A:H2'	25:CA:542:C:O4'	2.21	0.41
25:CA:549:G:OP2	25:CA:549:G:H3'	2.21	0.41
25:CA:927:A:H2'	25:CA:928:A:O4'	2.21	0.41
25:CA:1827:U:OP2	27:CC:220:ARG:NH1	2.53	0.41
28:CD:110:THR:HG21	28:CD:169:ARG:CZ	2.51	0.41
31:CG:4:ALA:HB2	31:CG:65:GLY:HA2	2.02	0.41
33:CI:73:PRO:HB2	33:CI:74:PRO:HD2	2.02	0.41
35:CK:103:VAL:HG21	35:CK:115:ILE:HD11	2.03	0.41
40:CP:54:LEU:HD12	40:CP:76:HIS:HB2	2.03	0.41
25:CA:559:G:H1'	41:CQ:55:GLN:NE2	2.36	0.41
45:CU:2:ALA:HB3	45:CU:5:ARG:HD2	2.02	0.41
44:CT:14:PRO:HD2	49:CY:33:ALA:CB	2.51	0.41
1:DA:243:A:C2	1:DA:246:A:C8	3.09	0.41
1:DA:709:U:H2'	1:DA:710:G:H8	1.86	0.41
1:DA:966:G:C4	24:DW:34:G:H4'	2.56	0.41
2:DB:162:PHE:HA	2:DB:184:PHE:O	2.20	0.41
4:DD:25:VAL:HG22	4:DD:26:ARG:H	1.86	0.41
5:DE:111:MET:O	5:DE:115:LEU:HD22	2.21	0.41
9:DI:130:ARG:OXT	9:DI:130:ARG:CG	2.68	0.41
10:DJ:87:LEU:O	10:DJ:90:LEU:HD23	2.21	0.41
1:DA:1223:C:P	19:DS:78:ARG:HH21	2.44	0.41
19:DS:6:LYS:HG2	19:DS:7:LYS:N	2.36	0.41
1:AA:1305:G:H21	1:AA:1332:A:H2	1.67	0.41
1:AA:671:G:H4'	6:AF:79:ARG:CZ	2.51	0.41
1:AA:913:A:H4'	1:AA:914:A:OP1	2.21	0.41
1:AA:946:A:H2'	1:AA:947:G:C8	2.55	0.41
2:AB:16:PHE:HB2	2:AB:17:GLY:H	1.79	0.41
4:AD:113:GLU:N	4:AD:113:GLU:CD	2.74	0.41
4:AD:56:ARG:CZ	4:AD:60:LYS:CE	2.98	0.41
5:AE:94:VAL:HG22	5:AE:95:PHE:N	2.36	0.41
1:AA:1307:U:O2'	13:AM:109:ARG:HD3	2.21	0.41
15:AO:17:ARG:NH1	15:AO:21:ASP:OD1	2.54	0.41
15:AO:32:LEU:HD13	15:AO:63:ARG:HB2	2.02	0.41
15:AO:78:TYR:CD1	15:AO:78:TYR:N	2.89	0.41
25:BA:1067:A:N3	25:BA:1067:A:H2'	2.36	0.41
25:BA:1176:U:H2'	25:BA:1177:G:C8	2.56	0.41
25:BA:1181:U:H2'	25:BA:1182:G:H8	1.86	0.41
25:BA:1316:U:H2'	25:BA:1317:G:C8	2.56	0.41
25:BA:1678:A:C2'	25:BA:1679:A:H5'	2.51	0.41
25:BA:172:A:H2'	25:BA:173:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1841:U:H2'	25:BA:1842:G:H8	1.86	0.41
25:BA:1996:C:H4'	25:BA:1997:C:OP1	2.21	0.41
25:BA:2807:U:H1'	25:BA:2892:G:N2	2.36	0.41
25:BA:939:G:C6	25:BA:940:G:C5	3.09	0.41
26:BB:3104:A:H2'	26:BB:3105:G:O4'	2.20	0.41
27:BC:128:THR:CG2	27:BC:190:THR:OG1	2.69	0.41
28:BD:104:VAL:O	28:BD:105:LYS:HB2	2.21	0.41
29:BE:35:TYR:CE2	29:BE:176:ASP:HB2	2.56	0.41
33:BI:23:VAL:HG22	33:BI:24:GLY:N	2.36	0.41
35:BK:108:ARG:HA	35:BK:116:ILE:HD11	2.02	0.41
25:BA:2822:G:O6	38:BN:2:ARG:HD3	2.21	0.41
43:BS:49:LYS:HA	43:BS:52:GLU:CG	2.51	0.41
43:BS:33:LEU:HD11	43:BS:51:LEU:HG	2.03	0.41
45:BU:41:VAL:O	45:BU:59:GLU:HA	2.21	0.41
25:CA:1093:G:OP1	31:CG:171:LYS:NZ	2.51	0.41
25:CA:1172:C:N4	25:CA:1173:U:C2	2.89	0.41
25:CA:1171:G:N2	25:CA:1179:G:C6	2.88	0.41
25:CA:1324:G:H1'	25:CA:1616:A:N6	2.36	0.41
25:CA:1608:A:C5	25:CA:1611:C:C4	3.09	0.41
25:CA:1794:A:H2'	25:CA:1795:C:H6	1.85	0.41
25:CA:2449:U:O2'	25:CA:2501:C:N4	2.52	0.41
25:CA:2709:G:OP1	38:CN:18:GLN:NE2	2.46	0.41
25:CA:661:A:H2'	25:CA:662:G:O4'	2.21	0.41
25:CA:686:U:O2'	53:C2:5:PHE:HA	2.21	0.41
36:CL:92:LEU:HG	36:CL:93:ASN:N	2.36	0.41
25:CA:871:U:H5''	37:CM:68:PHE:CZ	2.56	0.41
42:CR:51:VAL:HG12	42:CR:52:PRO:CD	2.51	0.41
45:CU:76:THR:HB	45:CU:78:LYS:HG2	2.03	0.41
49:CY:50:VAL:O	49:CY:53:VAL:N	2.54	0.41
1:DA:407:U:H2'	1:DA:408:A:H8	1.86	0.41
1:DA:451:A:C8	1:DA:452:A:C6	3.09	0.41
1:DA:509:A:P	60:DA:1760:HOH:O	2.79	0.41
1:DA:50:A:N6	1:DA:361:G:H4'	2.35	0.41
1:DA:57:G:C5	1:DA:58:C:C4	3.09	0.41
1:DA:958:A:C6	1:DA:959:A:N1	2.89	0.41
5:DE:36:LEU:HD21	5:DE:137:VAL:HG11	2.03	0.41
9:DI:23:PRO:HA	9:DI:61:LEU:HB3	2.02	0.41
16:DP:5:ARG:O	16:DP:20:VAL:N	2.47	0.41
1:AA:838:G:C2	1:AA:849:G:N3	2.89	0.40
1:AA:866:C:H4'	1:AA:919:A:H5'	2.03	0.40
1:AA:77:A:N6	1:AA:91:U:O4	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:968:A:H4'	1:AA:969:A:OP2	2.21	0.40
4:AD:19:LEU:HD13	4:AD:21:LEU:HG	2.03	0.40
7:AG:27:VAL:CG2	7:AG:40:GLU:HB3	2.51	0.40
14:AN:49:GLN:HA	14:AN:49:GLN:NE2	2.36	0.40
22:AV:65:THR:HG22	22:AV:66:LEU:H	1.86	0.40
22:AV:70:VAL:HG11	22:AV:75:MET:CE	2.51	0.40
25:BA:1093:G:O2'	25:BA:1099:G:N1	2.47	0.40
25:BA:1500:G:C2'	25:BA:1501:G:H5'	2.51	0.40
25:BA:1850:G:C6	25:BA:1851:U:C4	3.10	0.40
25:BA:1885:A:H2'	25:BA:1886:U:O4'	2.21	0.40
25:BA:2211:A:O2'	25:BA:2212:A:P	2.78	0.40
25:BA:2348:U:H2'	25:BA:2349:G:O4'	2.21	0.40
25:BA:2352:A:N1	47:BW:32:GLY:HA3	2.36	0.40
25:BA:2507:C:C2	25:BA:2508:G:C8	3.08	0.40
25:BA:2592:G:C6	25:BA:2593:U:C4	3.10	0.40
25:BA:2755:C:O2'	25:BA:2756:U:H2'	2.21	0.40
25:BA:2774:C:H2'	25:BA:2775:G:O4'	2.20	0.40
25:BA:2884:U:C6	51:B0:39:ARG:NH1	2.88	0.40
25:BA:340:A:H2'	25:BA:341:C:O4'	2.22	0.40
15:AO:89:ARG:NH2	25:BA:716:A:OP2	2.52	0.40
28:BD:186:LEU:HD21	40:BP:3:ILE:HG21	2.03	0.40
34:BJ:70:THR:HG23	34:BJ:71:ASP:OD2	2.21	0.40
41:BQ:75:TYR:C	41:BQ:75:TYR:CD1	2.95	0.40
48:BX:29:LEU:HD12	48:BX:29:LEU:N	2.35	0.40
25:CA:1425:G:N1	25:CA:1426:G:C2	2.90	0.40
25:CA:1813:G:N3	27:CC:49:THR:HG21	2.37	0.40
25:CA:2573:C:OP1	60:CA:3708:HOH:O	2.22	0.40
25:CA:559:G:H2'	25:CA:560:C:O4'	2.21	0.40
25:CA:588:U:H2'	25:CA:589:U:C6	2.55	0.40
25:CA:1655:A:H4'	28:CD:119:ALA:HA	2.02	0.40
25:CA:600:G:H1'	29:CE:100:MET:CG	2.51	0.40
35:CK:112:PHE:O	35:CK:113:MET:C	2.59	0.40
38:CN:87:PHE:CE1	38:CN:116:VAL:HG22	2.56	0.40
39:CO:62:LEU:HD23	39:CO:65:THR:HA	2.02	0.40
42:CR:39:LEU:O	42:CR:49:ILE:HG23	2.21	0.40
7:AG:70:ARG:HH12	1:DA:1029:U:H5''	1.86	0.40
1:DA:1118:U:H1'	1:DA:1179:A:C5	2.57	0.40
1:DA:1361:G:H2'	1:DA:1362:A:H5'	2.03	0.40
1:DA:264:C:H2'	1:DA:265:G:O4'	2.21	0.40
1:DA:453:G:N1	1:DA:480:U:O2	2.54	0.40
1:DA:676:A:H1'	11:DK:117:PRO:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DD:7:PRO:HB3	4:DD:9:LEU:CD2	2.51	0.40
6:DF:90:MET:SD	18:DR:61:ARG:NH1	2.93	0.40
21:DU:4:ILE:N	21:DU:4:ILE:HD13	2.36	0.40
1:AA:1118:U:H1'	1:AA:1179:A:C4	2.56	0.40
1:AA:1330:U:O4	1:AA:1331:G:N1	2.54	0.40
1:AA:307:C:C5	1:AA:308:C:C5	3.10	0.40
1:AA:64:G:C8	1:AA:99:C:N4	2.89	0.40
3:AC:124:LEU:HA	3:AC:128:VAL:HG22	2.03	0.40
4:AD:52:GLY:HA2	4:AD:55:LEU:HD12	2.03	0.40
10:AJ:40:ILE:CG1	10:AJ:73:LEU:HD21	2.52	0.40
13:AM:80:LEU:HD21	13:AM:85:CYS:SG	2.61	0.40
14:AN:66:GLN:HB2	14:AN:83:LYS:HE2	2.03	0.40
25:BA:591:U:H1'	54:B3:1:PRO:HD2	2.01	0.40
55:B4:36:ARG:CG	55:B4:37:GLN:N	2.84	0.40
25:BA:1551:A:N6	60:BA:3637:HOH:O	2.54	0.40
25:BA:1661:G:C6	25:BA:1662:U:C4	3.10	0.40
25:BA:1967:C:H2'	25:BA:1968:G:H5'	2.03	0.40
25:BA:2287:A:C4	25:BA:2289:G:C8	3.09	0.40
25:BA:2675:A:N1	25:BA:2676:C:C2	2.89	0.40
25:BA:2675:A:C2	25:BA:2676:C:C2	3.09	0.40
27:BC:77:VAL:HG21	27:BC:109:LEU:HD22	2.03	0.40
27:BC:174:ARG:HG2	27:BC:174:ARG:O	2.20	0.40
27:BC:225:ASN:HB3	27:BC:226:PRO:HD2	2.04	0.40
28:BD:9:VAL:CG2	28:BD:26:VAL:HG22	2.50	0.40
30:BF:16:MET:SD	30:BF:21:TYR:HB2	2.62	0.40
40:BP:30:TRP:CE2	40:BP:39:LEU:CD1	3.05	0.40
40:BP:91:VAL:CG1	40:BP:92:ARG:N	2.83	0.40
25:CA:1022:G:N2	25:CA:1142:A:C2	2.89	0.40
25:CA:117:G:C6	25:CA:119:A:N6	2.89	0.40
25:CA:1188:U:O2'	25:CA:1189:A:H5'	2.22	0.40
25:CA:1423:G:H2'	25:CA:1424:G:O4'	2.21	0.40
25:CA:1531:C:C6	25:CA:1532:A:C8	3.09	0.40
25:CA:163:C:H2'	25:CA:164:C:O4'	2.21	0.40
25:CA:2045:C:H5''	51:C0:14:MET:SD	2.61	0.40
25:CA:2259:U:H2'	25:CA:2260:C:H6	1.86	0.40
25:CA:2284:A:C2'	25:CA:2285:C:O5'	2.69	0.40
25:CA:2261:C:H1'	25:CA:2388:A:N3	2.36	0.40
25:CA:2436:G:C2'	25:CA:2437:G:H5'	2.52	0.40
25:CA:247:G:N7	25:CA:249:C:C2	2.90	0.40
25:CA:2582:G:C2	25:CA:2583:G:C8	3.09	0.40
25:CA:265:A:H4'	25:CA:266:G:OP1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:CA:2792:A:N6	25:CA:2793:C:C4	2.89	0.40
25:CA:2803:G:C2	25:CA:2804:U:C4	3.09	0.40
25:CA:89:A:C6	25:CA:90:U:C4	3.09	0.40
25:CA:906:U:O2'	37:CM:66:ARG:NH2	2.54	0.40
25:CA:2821:A:P	28:CD:115:GLY:H	2.44	0.40
33:CI:100:ILE:HG12	33:CI:105:LEU:HD21	2.02	0.40
44:CT:2:ILE:HG22	44:CT:4:GLU:CA	2.48	0.40
1:DA:1314:C:N4	19:DS:4:SER:OG	2.54	0.40
1:DA:723:U:O2'	1:DA:724:G:OP2	2.35	0.40
1:DA:920:U:H2'	1:DA:921:U:C6	2.57	0.40
3:DC:42:TYR:CZ	3:DC:90:VAL:HG11	2.56	0.40
4:DD:10:LYS:O	4:DD:12:SER:N	2.54	0.40
4:DD:21:LEU:N	4:DD:21:LEU:HD23	2.36	0.40
4:DD:4:TYR:CE2	4:DD:11:LEU:HD21	2.57	0.40
9:DI:13:LYS:HE2	9:DI:111:VAL:H	1.85	0.40
10:DJ:24:GLU:HG3	10:DJ:90:LEU:HD12	2.03	0.40
11:DK:108:THR:HG23	11:DK:109:ASN:HB3	2.03	0.40
11:DK:52:PHE:HZ	11:DK:62:ALA:HA	1.86	0.40
13:DM:77:ILE:O	13:DM:78:LYS:C	2.59	0.40
16:DP:39:PHE:C	16:DP:39:PHE:CD1	2.93	0.40
1:AA:1014:A:N7	1:AA:1015:G:C6	2.89	0.40
1:AA:328:C:C2'	1:AA:328:C:O2	2.70	0.40
1:AA:410:G:C2	1:AA:429:U:C5	3.10	0.40
1:AA:42:G:C6	1:AA:43:C:C4	3.09	0.40
1:AA:441:A:C2	1:AA:497:G:C6	3.10	0.40
1:AA:68:G:H5'	1:AA:171:A:O2'	2.21	0.40
1:AA:96:U:H1'	1:AA:97:G:H5'	2.02	0.40
3:AC:66:VAL:CG1	3:AC:101:ILE:HA	2.52	0.40
3:AC:152:GLU:HB3	3:AC:167:TRP:HB3	2.03	0.40
3:AC:57:ILE:HD11	3:AC:64:ILE:CG2	2.52	0.40
11:AK:16:VAL:HG23	11:AK:77:TYR:CD1	2.56	0.40
12:AL:15:LYS:H	12:AL:15:LYS:HD2	1.85	0.40
17:AQ:5:ILE:HG13	17:AQ:6:ARG:N	2.37	0.40
19:AS:18:LYS:CD	19:AS:31:LEU:HD21	2.51	0.40
22:AV:108:GLU:C	22:AV:110:ARG:H	2.22	0.40
25:BA:1068:G:O2'	25:BA:1096:A:H4'	2.21	0.40
25:BA:1071:G:H4'	25:BA:1089:A:OP2	2.21	0.40
25:BA:1075:C:H2'	25:BA:1076:C:C6	2.56	0.40
25:BA:1352:U:H2'	25:BA:1353:A:H5'	2.04	0.40
25:BA:1601:G:C5	25:BA:1602:U:C4	3.10	0.40
25:BA:1662:U:O2'	25:BA:2687:U:H5''	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:563:A:C6	25:BA:2018:G:C4	3.10	0.40
25:BA:2024:G:C4	25:BA:2025:C:C6	3.10	0.40
25:BA:2143:C:N4	25:BA:2148:G:O6	2.54	0.40
25:BA:2771:C:H2'	25:BA:2772:C:H6	1.86	0.40
26:BB:3118:C:N4	26:BB:3119:A:N6	2.69	0.40
32:BH:3:VAL:HG12	32:BH:21:VAL:HG12	2.02	0.40
36:BL:87:GLY:O	36:BL:89:VAL:N	2.46	0.40
43:BS:98:LYS:HZ2	43:BS:98:LYS:HB2	1.86	0.40
25:CA:1199:U:H2'	25:CA:1200:C:C6	2.55	0.40
25:CA:2362:C:H2'	25:CA:2363:G:O4'	2.20	0.40
25:CA:2396:G:C2	25:CA:2421:G:C2	3.09	0.40
25:CA:2577:A:H5''	25:CA:2578:G:H5'	2.03	0.40
25:CA:2746:U:C2'	25:CA:2747:G:H5'	2.52	0.40
25:CA:2720:U:C6	25:CA:2872:A:N6	2.89	0.40
25:CA:838:C:O2'	25:CA:839:U:H5'	2.22	0.40
27:CC:242:HIS:O	27:CC:244:VAL:HG13	2.21	0.40
31:CG:95:ALA:HB1	31:CG:130:ILE:HD11	2.04	0.40
35:CK:99:ILE:CD1	35:CK:115:ILE:HB	2.52	0.40
37:CM:64:TRP:O	37:CM:65:ILE:HG13	2.20	0.40
39:CO:79:ALA:HB1	39:CO:113:ALA:HB3	2.03	0.40
42:CR:51:VAL:HG12	42:CR:52:PRO:N	2.35	0.40
49:CY:56:LEU:HD13	49:CY:56:LEU:HA	1.97	0.40
1:DA:355:C:O2'	1:DA:388:G:N3	2.46	0.40
2:DB:164:ILE:HG12	2:DB:165:ASP:H	1.87	0.40
3:DC:152:GLU:HG2	3:DC:167:TRP:HB2	2.04	0.40
4:DD:192:SER:O	4:DD:193:ALA:HB3	2.21	0.40
8:DH:15:ARG:HB2	8:DH:75:ILE:CG2	2.51	0.40
9:DI:54:LEU:O	9:DI:55:VAL:HG13	2.22	0.40
9:DI:84:THR:HG21	9:DI:103:PHE:HB2	2.04	0.40
25:CA:2253:G:N2	24:DW:74:C:C4	2.90	0.40
1:AA:1279:G:H3'	1:AA:1279:G:N3	2.36	0.40
1:AA:1313:U:P	19:AS:6:LYS:HG2	2.62	0.40
1:AA:1399:C:C4	1:AA:1401:G:C2	3.09	0.40
1:AA:1411:C:H2'	1:AA:1412:C:C6	2.56	0.40
1:AA:1524:C:H2'	1:AA:1525:G:O4'	2.21	0.40
1:AA:227:G:H2'	1:AA:228:A:O4'	2.22	0.40
1:AA:437:U:C4	1:AA:438:U:C5	3.10	0.40
1:AA:767:A:H2'	1:AA:768:A:O4'	2.21	0.40
1:AA:834:U:N3	1:AA:835:U:C4	2.90	0.40
1:AA:937:A:C2'	1:AA:938:A:H5'	2.51	0.40
1:AA:939:G:OP1	7:AG:95:ARG:NH2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:135:LEU:O	2:AB:139:ARG:N	2.50	0.40
4:AD:19:LEU:HD21	4:AD:111:ARG:CD	2.51	0.40
9:AI:114:LYS:HE2	9:AI:118:LEU:O	2.21	0.40
12:AL:104:CYS:O	12:AL:105:SER:OG	2.33	0.40
1:AA:552:U:H4'	12:AL:84:GLY:O	2.21	0.40
13:AM:4:ILE:HG23	13:AM:5:ALA:N	2.36	0.40
15:AO:14:GLU:HG3	15:AO:84:ARG:NH2	2.36	0.40
18:AR:22:ASP:OD1	18:AR:23:TYR:N	2.54	0.40
20:AT:46:ALA:HA	20:AT:49:LYS:HB3	2.04	0.40
22:AV:12:VAL:HG23	22:AV:13:ARG:N	2.36	0.40
22:AV:83:ILE:HG13	22:AV:84:MET:N	2.36	0.40
24:AX:52:G:H1'	24:AX:63:G:N2	2.36	0.40
25:BA:1205:A:H4'	25:BA:1206:G:OP2	2.21	0.40
25:BA:1508:A:O2'	25:BA:1509:A:O4'	2.30	0.40
25:BA:2080:A:OP1	48:BX:19:HIS:CE1	2.74	0.40
25:BA:2461:A:H2'	25:BA:2462:C:C6	2.57	0.40
25:BA:2472:G:H2'	25:BA:2475:C:H42	1.86	0.40
25:BA:275:C:H2'	25:BA:276:U:H4'	2.02	0.40
25:BA:416:U:H2'	25:BA:417:C:O4'	2.22	0.40
25:BA:57:C:H2'	25:BA:58:G:O4'	2.22	0.40
25:BA:948:C:H1'	25:BA:984:A:O2'	2.22	0.40
32:BH:123:ARG:HE	32:BH:123:ARG:N	2.16	0.40
33:BI:133:ARG:HA	33:BI:137:LEU:CD1	2.51	0.40
36:BL:122:VAL:HB	36:BL:142:ILE:HG22	2.02	0.40
38:BN:53:THR:O	38:BN:56:LYS:HB2	2.21	0.40
41:BQ:27:ARG:HH22	41:BQ:40:LYS:HE2	1.85	0.40
41:BQ:67:ALA:O	41:BQ:71:ASN:ND2	2.55	0.40
25:CA:1207:C:N3	25:CA:1208:C:C5	2.90	0.40
25:CA:1336:A:C2	25:CA:1337:G:C4	3.09	0.40
25:CA:1711:A:C2	25:CA:1748:C:C2	3.10	0.40
25:CA:740:C:H5''	25:CA:1784:A:OP1	2.21	0.40
25:CA:203:A:H3'	25:CA:204:A:H2'	2.03	0.40
25:CA:2115:G:H2'	25:CA:2117:A:N7	2.37	0.40
25:CA:2283:C:C2'	25:CA:2284:A:H5'	2.51	0.40
25:CA:2403:C:C2	25:CA:2404:U:C6	3.09	0.40
25:CA:2479:U:OP1	25:CA:2537:U:H1'	2.22	0.40
25:CA:2680:U:C2	25:CA:2681:C:C5	3.09	0.40
25:CA:674:G:H1'	29:CE:69:ARG:HD3	2.02	0.40
25:CA:846:U:HO2'	25:CA:847:U:P	2.44	0.40
25:CA:970:U:H1'	25:CA:985:C:OP1	2.21	0.40
25:CA:1816:C:H3'	27:CC:61:TYR:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:CF:48:LEU:HD21	30:CF:147:ARG:HE	1.86	0.40
34:CJ:14:ASP:OD1	34:CJ:14:ASP:N	2.54	0.40
40:CP:83:ILE:CD1	40:CP:83:ILE:C	2.89	0.40
45:CU:15:GLY:C	45:CU:17:ASP:H	2.23	0.40
1:DA:1088:G:C6	1:DA:1089:G:C5	3.10	0.40
1:DA:1417:G:C6	1:DA:1482:G:C6	3.10	0.40
1:DA:1490:U:OP2	58:DA:1654:PAR:C64	2.70	0.40
3:DC:22:TRP:CD1	3:DC:59:ARG:HB2	2.56	0.40
4:DD:125:VAL:HG13	4:DD:126:ASN:H	1.86	0.40
4:DD:118:VAL:O	4:DD:131:ASN:HA	2.22	0.40
1:DA:620:C:H1'	4:DD:132:ILE:HD13	2.03	0.40
4:DD:176:GLY:C	4:DD:178:MET:N	2.74	0.40
6:DF:18:VAL:CG1	6:DF:19:PRO:HD3	2.51	0.40
7:DG:23:LEU:HA	7:DG:26:PHE:HB3	2.03	0.40
7:DG:76:LYS:O	7:DG:87:VAL:HG22	2.22	0.40
1:DA:35:G:N2	12:DL:115:SER:OG	2.42	0.40
12:DL:24:LEU:HG	12:DL:25:GLU:N	2.36	0.40
13:DM:53:ILE:CG2	13:DM:54:ASP:N	2.84	0.40
1:AA:374:A:C5'	1:AA:452:A:C2	3.04	0.40
1:AA:406:G:N2	1:AA:437:U:O2	2.54	0.40
1:AA:437:U:C4	1:AA:438:U:H5	2.39	0.40
1:AA:619:U:O2'	4:AD:128:ARG:NH2	2.55	0.40
1:AA:1190:G:O2'	3:AC:3:GLN:HG2	2.21	0.40
5:AE:153:VAL:HG13	5:AE:154:ALA:N	2.37	0.40
7:AG:60:GLU:HA	7:AG:63:GLU:HB3	2.03	0.40
11:AK:16:VAL:HG23	11:AK:77:TYR:CE1	2.57	0.40
12:AL:102:LEU:C	12:AL:102:LEU:HD12	2.42	0.40
17:AQ:45:HIS:HB2	17:AQ:71:LYS:HB3	2.04	0.40
19:AS:50:ALA:HB1	19:AS:57:HIS:CG	2.56	0.40
55:B4:27:CYS:HB2	55:B4:33:HIS:HB2	2.03	0.40
25:BA:1932:A:C2	25:BA:1969:A:C6	3.10	0.40
25:BA:2280:G:C2	25:BA:2281:A:C8	3.09	0.40
25:BA:2680:U:HO2'	25:BA:2681:C:P	2.44	0.40
25:BA:399:U:H5''	48:BX:56:ARG:NH1	2.37	0.40
28:BD:170:VAL:HG12	28:BD:171:THR:N	2.36	0.40
28:BD:82:PHE:CD1	28:BD:82:PHE:N	2.89	0.40
31:BG:21:GLN:HG3	31:BG:36:LEU:HB2	2.04	0.40
31:BG:71:LEU:HG	31:BG:74:MET:HE3	2.03	0.40
34:BJ:130:HIS:HD2	34:BJ:132:HIS:H	1.70	0.40
40:BP:50:ARG:HG2	40:BP:50:ARG:O	2.22	0.40
40:BP:13:LYS:NZ	40:BP:75:THR:O	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BS:88:ARG:HG3	43:BS:94:ASP:OD2	2.22	0.40
55:C4:10:LEU:HD13	55:C4:33:HIS:CD2	2.56	0.40
25:CA:1208:C:C2	25:CA:1209:U:C6	3.10	0.40
25:CA:1269:A:H2'	25:CA:1270:C:C6	2.57	0.40
25:CA:1608:A:C8	25:CA:1611:C:N4	2.90	0.40
25:CA:1685:C:H2'	25:CA:1686:C:H6	1.86	0.40
25:CA:1721:G:H2'	25:CA:1737:G:N2	2.36	0.40
25:CA:1881:C:H2'	25:CA:1882:U:O4'	2.21	0.40
25:CA:563:A:C6	25:CA:2018:G:C4	3.09	0.40
25:CA:2104:C:N4	25:CA:2185:U:O4	2.54	0.40
25:CA:2308:G:O6	25:CA:2311:A:C8	2.74	0.40
25:CA:364:C:H2'	25:CA:365:U:C6	2.57	0.40
25:CA:465:G:H2'	25:CA:466:A:C8	2.56	0.40
25:CA:748:G:H2'	25:CA:750:A:OP2	2.21	0.40
25:CA:883:G:N2	25:CA:894:U:C2	2.90	0.40
25:CA:998:C:OP2	41:CQ:91:ARG:NH2	2.55	0.40
26:CB:3046:A:C5	26:CB:3047:C:C4	3.10	0.40
27:CC:250:GLN:NE2	27:CC:252:LYS:O	2.50	0.40
27:CC:74:PRO:O	27:CC:96:LYS:HG2	2.21	0.40
37:CM:75:GLU:HB2	37:CM:90:GLU:HG3	2.03	0.40
43:CS:10:ALA:O	43:CS:12:SER:N	2.50	0.40
1:DA:109:A:C6	1:DA:326:G:C5	3.10	0.40
1:DA:1106:G:H2'	1:DA:1107:C:C6	2.57	0.40
1:DA:1496:C:H2'	1:DA:1497:G:O4'	2.21	0.40
1:DA:39:G:H2'	1:DA:40:C:H6	1.86	0.40
1:DA:448:A:C8	1:DA:487:A:N1	2.89	0.40
1:DA:401:C:H1'	1:DA:622:A:H1'	2.04	0.40
3:DC:66:VAL:HG12	3:DC:67:THR:N	2.36	0.40
4:DD:123:ILE:HG23	4:DD:124:MET:N	2.37	0.40
1:DA:560:A:C6	5:DE:128:TYR:CE2	3.10	0.40
7:DG:60:GLU:C	7:DG:62:PHE:H	2.25	0.40
11:DK:23:ILE:HB	11:DK:96:THR:HG21	2.03	0.40
1:DA:981:U:OP1	14:DN:12:ARG:NH1	2.55	0.40
23:DV:10:A:C4	23:DV:11:A:N7	2.90	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:358:U:OP1	32:CH:123:ARG:NH2[4_455]	1.91	0.29



## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/241 (90%)	120 (56%)	54 (25%)	42 (19%)	0	0
2	DB	216/241 (90%)	130 (60%)	50 (23%)	36 (17%)	0	0
3	AC	204/233 (88%)	148 (72%)	34 (17%)	22 (11%)	0	2
3	DC	204/233 (88%)	154 (76%)	33 (16%)	17 (8%)	1	4
4	AD	203/206 (98%)	115 (57%)	55 (27%)	33 (16%)	0	1
4	DD	203/206 (98%)	111 (55%)	41 (20%)	51 (25%)	0	0
5	AE	148/167 (89%)	116 (78%)	19 (13%)	13 (9%)	1	3
5	DE	148/167 (89%)	106 (72%)	25 (17%)	17 (12%)	0	2
6	AF	98/135 (73%)	62 (63%)	22 (22%)	14 (14%)	0	1
6	DF	98/135 (73%)	74 (76%)	11 (11%)	13 (13%)	0	1
7	AG	149/179 (83%)	88 (59%)	43 (29%)	18 (12%)	0	1
7	DG	149/179 (83%)	112 (75%)	24 (16%)	13 (9%)	1	3
8	AH	127/130 (98%)	92 (72%)	27 (21%)	8 (6%)	1	7
8	DH	127/130 (98%)	97 (76%)	14 (11%)	16 (13%)	0	1
9	AI	125/130 (96%)	84 (67%)	28 (22%)	13 (10%)	0	2
9	DI	125/130 (96%)	83 (66%)	23 (18%)	19 (15%)	0	1
10	AJ	96/103 (93%)	60 (62%)	22 (23%)	14 (15%)	0	1
10	DJ	96/103 (93%)	71 (74%)	17 (18%)	8 (8%)	1	4
11	AK	115/129 (89%)	67 (58%)	30 (26%)	18 (16%)	0	1
11	DK	115/129 (89%)	85 (74%)	17 (15%)	13 (11%)	0	2
12	AL	121/124 (98%)	94 (78%)	14 (12%)	13 (11%)	0	2
12	DL	121/124 (98%)	72 (60%)	32 (26%)	17 (14%)	0	1
13	AM	112/118 (95%)	63 (56%)	29 (26%)	20 (18%)	0	0
13	DM	112/118 (95%)	71 (63%)	26 (23%)	15 (13%)	0	1
14	AN	92/101 (91%)	65 (71%)	18 (20%)	9 (10%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	DN	92/101 (91%)	63 (68%)	15 (16%)	14 (15%)	0	1
15	AO	86/89 (97%)	65 (76%)	17 (20%)	4 (5%)	2	14
15	DO	86/89 (97%)	66 (77%)	14 (16%)	6 (7%)	1	6
16	AP	80/82 (98%)	48 (60%)	26 (32%)	6 (8%)	1	5
16	DP	80/82 (98%)	48 (60%)	25 (31%)	7 (9%)	1	3
17	AQ	78/84 (93%)	55 (70%)	11 (14%)	12 (15%)	0	1
17	DQ	78/84 (93%)	47 (60%)	21 (27%)	10 (13%)	0	1
18	AR	53/75 (71%)	37 (70%)	9 (17%)	7 (13%)	0	1
18	DR	53/75 (71%)	38 (72%)	7 (13%)	8 (15%)	0	1
19	AS	77/92 (84%)	45 (58%)	17 (22%)	15 (20%)	0	0
19	DS	77/92 (84%)	53 (69%)	16 (21%)	8 (10%)	0	2
20	AT	83/87 (95%)	69 (83%)	6 (7%)	8 (10%)	0	3
20	DT	83/87 (95%)	62 (75%)	15 (18%)	6 (7%)	1	5
21	AU	49/71 (69%)	20 (41%)	16 (33%)	13 (26%)	0	0
21	DU	49/71 (69%)	25 (51%)	9 (18%)	15 (31%)	0	0
22	AV	181/185 (98%)	137 (76%)	30 (17%)	14 (8%)	1	5
27	BC	269/273 (98%)	216 (80%)	37 (14%)	16 (6%)	1	9
27	CC	269/273 (98%)	214 (80%)	41 (15%)	14 (5%)	2	12
28	BD	207/209 (99%)	176 (85%)	22 (11%)	9 (4%)	2	15
28	CD	207/209 (99%)	170 (82%)	25 (12%)	12 (6%)	1	10
29	BE	199/201 (99%)	160 (80%)	30 (15%)	9 (4%)	2	14
29	CE	199/201 (99%)	156 (78%)	31 (16%)	12 (6%)	1	9
30	BF	175/179 (98%)	127 (73%)	32 (18%)	16 (9%)	1	3
30	CF	175/179 (98%)	122 (70%)	37 (21%)	16 (9%)	1	3
31	BG	174/177 (98%)	133 (76%)	29 (17%)	12 (7%)	1	6
31	CG	174/177 (98%)	135 (78%)	27 (16%)	12 (7%)	1	6
32	BH	147/149 (99%)	84 (57%)	40 (27%)	23 (16%)	0	1
32	CH	147/149 (99%)	93 (63%)	36 (24%)	18 (12%)	0	1
33	BI	139/142 (98%)	77 (55%)	37 (27%)	25 (18%)	0	0
33	CI	139/142 (98%)	84 (60%)	39 (28%)	16 (12%)	0	2
34	BJ	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	CJ	140/142 (99%)	123 (88%)	13 (9%)	4 (3%)	4	24
35	BK	120/123 (98%)	99 (82%)	10 (8%)	11 (9%)	1	3
35	CK	120/123 (98%)	92 (77%)	22 (18%)	6 (5%)	2	12
36	BL	141/144 (98%)	114 (81%)	15 (11%)	12 (8%)	1	4
36	CL	141/144 (98%)	98 (70%)	29 (21%)	14 (10%)	0	2
37	BM	134/136 (98%)	110 (82%)	16 (12%)	8 (6%)	1	9
37	CM	134/136 (98%)	109 (81%)	17 (13%)	8 (6%)	1	9
38	BN	118/127 (93%)	98 (83%)	14 (12%)	6 (5%)	2	12
38	CN	118/127 (93%)	83 (70%)	32 (27%)	3 (2%)	5	28
39	BO	114/117 (97%)	90 (79%)	18 (16%)	6 (5%)	2	11
39	CO	114/117 (97%)	80 (70%)	23 (20%)	11 (10%)	0	3
40	BP	112/115 (97%)	94 (84%)	15 (13%)	3 (3%)	5	26
40	CP	112/115 (97%)	91 (81%)	16 (14%)	5 (4%)	2	14
41	BQ	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	17	55
41	CQ	115/118 (98%)	99 (86%)	13 (11%)	3 (3%)	5	27
42	BR	101/103 (98%)	89 (88%)	7 (7%)	5 (5%)	2	12
42	CR	101/103 (98%)	76 (75%)	18 (18%)	7 (7%)	1	6
43	BS	108/110 (98%)	96 (89%)	10 (9%)	2 (2%)	8	36
43	CS	108/110 (98%)	82 (76%)	16 (15%)	10 (9%)	0	3
44	BT	91/100 (91%)	72 (79%)	11 (12%)	8 (9%)	1	3
44	CT	91/100 (91%)	72 (79%)	11 (12%)	8 (9%)	1	3
45	BU	100/104 (96%)	79 (79%)	14 (14%)	7 (7%)	1	6
45	CU	100/104 (96%)	67 (67%)	23 (23%)	10 (10%)	0	2
46	BV	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
46	CV	92/94 (98%)	74 (80%)	14 (15%)	4 (4%)	2	15
47	BW	74/85 (87%)	60 (81%)	9 (12%)	5 (7%)	1	6
47	CW	73/85 (86%)	60 (82%)	10 (14%)	3 (4%)	3	16
48	BX	75/78 (96%)	62 (83%)	9 (12%)	4 (5%)	2	11
48	CX	75/78 (96%)	63 (84%)	10 (13%)	2 (3%)	5	26
49	BY	61/63 (97%)	46 (75%)	9 (15%)	6 (10%)	0	2
49	CY	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	BZ	56/59 (95%)	45 (80%)	11 (20%)	0	100	100
50	CZ	56/59 (95%)	47 (84%)	9 (16%)	0	100	100
51	B0	54/57 (95%)	45 (83%)	4 (7%)	5 (9%)	0	3
51	C0	54/57 (95%)	42 (78%)	4 (7%)	8 (15%)	0	1
52	B1	48/55 (87%)	31 (65%)	12 (25%)	5 (10%)	0	2
52	C1	48/55 (87%)	37 (77%)	11 (23%)	0	100	100
53	B2	44/46 (96%)	37 (84%)	6 (14%)	1 (2%)	6	30
53	C2	44/46 (96%)	38 (86%)	4 (9%)	2 (4%)	2	14
54	B3	62/65 (95%)	51 (82%)	7 (11%)	4 (6%)	1	7
54	C3	62/65 (95%)	52 (84%)	8 (13%)	2 (3%)	4	22
55	B4	36/38 (95%)	31 (86%)	3 (8%)	2 (6%)	2	10
55	C4	36/38 (95%)	30 (83%)	5 (14%)	1 (3%)	5	25
56	B5	183/228 (80%)	80 (44%)	66 (36%)	37 (20%)	0	0
All	All	11599/12383 (94%)	8463 (73%)	2041 (18%)	1095 (9%)	0	3

All (1095) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	23	TRP
2	AB	31	ILE
2	AB	34	ALA
2	AB	52	GLU
2	AB	73	LYS
2	AB	74	ARG
2	AB	87	CYS
2	AB	88	ASP
2	AB	95	ARG
2	AB	101	LEU
2	AB	102	THR
2	AB	107	VAL
2	AB	120	GLN
2	AB	127	ASP
2	AB	134	ALA
2	AB	150	GLY
2	AB	158	PRO
2	AB	164	ILE
2	AB	182	PRO

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Mol	Chain	Res	Type
2	AB	194	ASP
2	AB	201	PRO
3	AC	38	LYS
3	AC	66	VAL
3	AC	129	MET
3	AC	160	ALA
3	AC	166	GLU
4	AD	3	ARG
4	AD	4	TYR
4	AD	9	LEU
4	AD	20	PHE
4	AD	24	GLY
4	AD	33	LYS
4	AD	42	GLY
4	AD	43	ALA
4	AD	101	VAL
4	AD	125	VAL
4	AD	151	LYS
4	AD	154	ARG
4	AD	166	GLU
4	AD	182	PHE
4	AD	188	ARG
4	AD	192	SER
5	AE	26	LYS
5	AE	135	ASN
5	AE	158	GLY
6	AF	22	ILE
6	AF	33	GLU
6	AF	64	VAL
6	AF	70	VAL
6	AF	91	ARG
6	AF	92	THR
6	AF	99	ALA
7	AG	59	LEU
7	AG	67	GLU
7	AG	151	PHE
8	AH	54	ASP
8	AH	67	GLN
8	AH	74	SER
8	AH	110	VAL
8	AH	111	MET
9	AI	31	ASN

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Mol	Chain	Res	Type
9	AI	54	LEU
9	AI	91	ASP
9	AI	106	ARG
9	AI	107	ASP
10	AJ	57	VAL
10	AJ	61	ALA
10	AJ	74	VAL
10	AJ	100	ILE
11	AK	27	PHE
11	AK	30	THR
11	AK	41	ALA
11	AK	45	ALA
11	AK	53	ARG
11	AK	55	SER
11	AK	77	TYR
11	AK	79	ILE
11	AK	119	ASN
12	AL	24	LEU
12	AL	25	GLU
12	AL	58	THR
12	AL	102	LEU
13	AM	4	ILE
13	AM	7	ILE
13	AM	12	HIS
13	AM	37	ALA
13	AM	41	GLU
13	AM	66	GLU
13	AM	92	ARG
13	AM	97	VAL
13	AM	112	PRO
14	AN	46	LEU
14	AN	56	SER
15	AO	14	GLU
15	AO	20	ASN
15	AO	47	LYS
16	AP	24	SER
16	AP	47	GLU
16	AP	63	GLN
17	AQ	12	VAL
17	AQ	13	VAL
17	AQ	17	MET
17	AQ	19	LYS

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Mol	Chain	Res	Type
17	AQ	68	SER
17	AQ	70	THR
17	AQ	82	ALA
18	AR	28	THR
18	AR	29	LEU
19	AS	37	ARG
19	AS	43	ASN
19	AS	44	MET
20	AT	4	ILE
20	AT	6	SER
20	AT	67	ILE
20	AT	85	LYS
21	AU	8	GLU
21	AU	10	GLU
21	AU	12	PHE
21	AU	21	ARG
21	AU	25	LYS
21	AU	53	VAL
22	AV	49	PRO
22	AV	113	ASP
22	AV	147	LYS
27	BC	5	CYS
27	BC	123	ILE
27	BC	133	ASN
28	BD	102	ALA
28	BD	105	LYS
28	BD	113	SER
28	BD	152	PRO
30	BF	9	ASP
30	BF	46	LYS
30	BF	84	ILE
30	BF	93	GLU
30	BF	153	ILE
30	BF	154	THR
32	BH	3	VAL
32	BH	14	SER
32	BH	28	ASN
32	BH	41	LYS
32	BH	63	ALA
32	BH	71	LYS
32	BH	72	ILE
32	BH	91	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	BH	120	GLY
32	BH	138	VAL
32	BH	144	VAL
33	BI	7	TYR
33	BI	133	ARG
34	BJ	81	ILE
35	BK	29	HIS
35	BK	35	VAL
35	BK	98	ARG
36	BL	30	THR
36	BL	94	THR
37	BM	8	LYS
38	BN	118	ARG
39	BO	54	VAL
39	BO	88	LYS
42	BR	51	VAL
43	BS	64	ALA
44	BT	2	ILE
44	BT	4	GLU
44	BT	52	GLU
44	BT	70	HIS
45	BU	16	LYS
45	BU	84	PHE
45	BU	85	ARG
47	BW	28	SER
47	BW	50	GLY
48	BX	2	ARG
48	BX	42	GLU
49	BY	57	LEU
51	B0	25	THR
52	B1	4	ILE
53	B2	44	VAL
54	B3	31	ILE
54	B3	32	LEU
56	B5	21	THR
56	B5	52	ARG
56	B5	68	LEU
56	B5	80	GLY
56	B5	126	LYS
56	B5	130	ILE
56	B5	133	PRO
56	B5	149	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
56	B5	156	ILE
56	B5	174	PRO
56	B5	212	VAL
56	B5	220	PRO
27	CC	9	SER
27	CC	133	ASN
27	CC	260	LYS
28	CD	98	VAL
28	CD	105	LYS
28	CD	152	PRO
28	CD	181	ASP
29	CE	18	THR
30	CF	92	GLY
30	CF	93	GLU
30	CF	101	ARG
30	CF	113	PHE
30	CF	117	SER
30	CF	144	LYS
31	CG	45	ALA
31	CG	117	PRO
32	CH	3	VAL
32	CH	9	VAL
32	CH	96	THR
32	CH	113	SER
32	CH	120	GLY
32	CH	121	VAL
32	CH	123	ARG
32	CH	130	VAL
33	CI	20	SER
33	CI	89	SER
33	CI	108	ILE
33	CI	109	ALA
33	CI	128	ILE
34	CJ	81	ILE
35	CK	35	VAL
36	CL	30	THR
36	CL	111	ILE
36	CL	116	VAL
36	CL	124	GLY
37	CM	3	GLN
37	CM	65	ILE
38	CN	118	ARG

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Mol	Chain	Res	Type
38	CN	119	SER
39	CO	6	ALA
39	CO	30	ARG
39	CO	57	ALA
39	CO	100	HIS
39	CO	113	ALA
40	CP	9	GLN
40	CP	10	GLU
40	CP	84	SER
41	CQ	86	SER
43	CS	47	VAL
43	CS	64	ALA
43	CS	67	ASP
43	CS	68	ASP
44	CT	4	GLU
44	CT	5	GLU
45	CU	16	LYS
45	CU	42	LYS
46	CV	9	ARG
46	CV	66	ASP
48	CX	32	LEU
49	CY	7	ARG
49	CY	25	GLN
49	CY	57	LEU
51	C0	3	GLN
51	C0	25	THR
2	DB	15	HIS
2	DB	21	ARG
2	DB	23	TRP
2	DB	45	LYS
2	DB	58	ASN
2	DB	64	LYS
2	DB	86	SER
2	DB	87	CYS
2	DB	152	LYS
2	DB	164	ILE
2	DB	193	PRO
2	DB	208	ARG
2	DB	222	ARG
3	DC	67	THR
3	DC	75	ILE
3	DC	156	ARG

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Mol	Chain	Res	Type
4	DD	9	LEU
4	DD	10	LYS
4	DD	24	GLY
4	DD	29	ASP
4	DD	42	GLY
4	DD	43	ALA
4	DD	47	ARG
4	DD	111	ARG
4	DD	121	LYS
4	DD	128	ARG
4	DD	134	SER
4	DD	139	PRO
4	DD	145	ILE
4	DD	153	SER
4	DD	174	ASP
4	DD	178	MET
4	DD	184	ARG
4	DD	186	PRO
5	DE	108	GLY
5	DE	111	MET
5	DE	123	VAL
5	DE	127	ALA
6	DF	78	PHE
6	DF	91	ARG
6	DF	92	THR
7	DG	23	LEU
7	DG	57	SER
7	DG	128	ALA
8	DH	21	ASN
8	DH	69	LYS
8	DH	87	LYS
8	DH	103	VAL
8	DH	126	ILE
9	DI	36	GLU
9	DI	43	THR
9	DI	55	VAL
9	DI	60	LYS
9	DI	86	ALA
9	DI	87	LEU
9	DI	90	TYR
9	DI	116	VAL
10	DJ	36	VAL

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Mol	Chain	Res	Type
10	DJ	57	VAL
11	DK	15	GLN
11	DK	52	PHE
11	DK	57	LYS
11	DK	80	LYS
11	DK	107	ILE
11	DK	127	ARG
12	DL	3	THR
12	DL	10	LYS
12	DL	16	VAL
12	DL	24	LEU
12	DL	26	ALA
12	DL	44	LYS
12	DL	89	ASP
12	DL	117	TYR
13	DM	14	HIS
13	DM	16	VAL
13	DM	77	ILE
13	DM	78	LYS
13	DM	107	ARG
14	DN	25	GLU
14	DN	28	ALA
14	DN	42	TRP
14	DN	81	ARG
15	DO	20	ASN
16	DP	25	ARG
16	DP	37	GLY
16	DP	45	GLU
16	DP	53	ASP
17	DQ	12	VAL
17	DQ	13	VAL
17	DQ	21	ILE
17	DQ	50	ASN
17	DQ	63	GLU
18	DR	21	ILE
18	DR	26	ILE
19	DS	6	LYS
19	DS	30	PRO
19	DS	77	THR
20	DT	4	ILE
20	DT	79	LEU
21	DU	10	GLU

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Mol	Chain	Res	Type
21	DU	23	CYS
2	AB	13	GLY
2	AB	16	PHE
2	AB	38	VAL
2	AB	51	ASN
2	AB	67	ILE
2	AB	92	VAL
2	AB	98	GLY
2	AB	183	VAL
2	AB	190	ASN
2	AB	193	PRO
3	AC	14	ILE
3	AC	61	ALA
3	AC	95	ALA
3	AC	96	GLY
3	AC	141	ALA
3	AC	145	GLY
3	AC	146	ALA
3	AC	157	LEU
3	AC	159	GLY
3	AC	190	HIS
3	AC	206	GLU
4	AD	5	LEU
4	AD	35	GLU
4	AD	58	LYS
4	AD	169	THR
4	AD	191	LEU
5	AE	71	MET
5	AE	78	ASN
5	AE	134	ILE
6	AF	43	GLY
7	AG	82	GLY
7	AG	103	TRP
7	AG	113	ASP
7	AG	133	THR
7	AG	149	LYS
7	AG	150	ALA
8	AH	63	LEU
9	AI	43	THR
9	AI	58	VAL
9	AI	105	THR
10	AJ	79	PRO

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Mol	Chain	Res	Type
10	AJ	92	LEU
11	AK	50	SER
11	AK	52	PHE
11	AK	82	LEU
11	AK	126	LYS
12	AL	19	SER
12	AL	43	LYS
12	AL	93	VAL
12	AL	103	ASP
13	AM	27	LYS
13	AM	96	PRO
14	AN	16	ALA
14	AN	48	LEU
16	AP	42	ILE
17	AQ	6	ARG
17	AQ	9	GLN
17	AQ	50	ASN
19	AS	5	LEU
19	AS	28	LYS
19	AS	31	LEU
19	AS	45	ILE
19	AS	49	ILE
19	AS	67	VAL
20	AT	7	ALA
20	AT	47	ALA
21	AU	9	ASN
21	AU	37	PHE
22	AV	55	LEU
22	AV	72	ASP
22	AV	99	ILE
22	AV	183	LEU
27	BC	167	ASP
27	BC	171	VAL
27	BC	176	ARG
27	BC	235	GLU
27	BC	259	ASN
28	BD	2	ILE
28	BD	58	ASN
28	BD	94	GLN
29	BE	4	VAL
29	BE	155	GLU
30	BF	38	GLY

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Mol	Chain	Res	Type
30	BF	88	VAL
30	BF	112	ASP
31	BG	14	VAL
31	BG	99	GLY
31	BG	151	ARG
32	BH	29	PHE
32	BH	121	VAL
32	BH	134	VAL
32	BH	142	VAL
33	BI	28	GLY
33	BI	39	LYS
33	BI	82	ALA
33	BI	92	PRO
34	BJ	6	ALA
34	BJ	30	THR
35	BK	50	GLY
35	BK	89	ASN
35	BK	91	SER
35	BK	118	LEU
36	BL	15	ALA
36	BL	69	ARG
36	BL	81	ASP
36	BL	82	LEU
36	BL	93	ASN
36	BL	112	LEU
37	BM	79	ALA
39	BO	27	VAL
39	BO	51	ALA
42	BR	16	GLU
42	BR	48	LYS
42	BR	57	GLY
43	BS	74	ILE
44	BT	92	ASN
45	BU	15	GLY
47	BW	9	ARG
49	BY	15	ASN
51	B0	3	GLN
51	B0	31	LYS
55	B4	31	PRO
56	B5	129	ARG
56	B5	134	ARG
56	B5	135	GLY

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Mol	Chain	Res	Type
56	B5	140	PRO
56	B5	142	ALA
56	B5	171	ILE
56	B5	172	HIS
56	B5	189	ILE
56	B5	205	LYS
56	B5	214	VAL
27	CC	121	ALA
27	CC	195	GLY
28	CD	87	GLY
28	CD	90	PHE
28	CD	103	ASP
28	CD	104	VAL
28	CD	206	ALA
29	CE	6	LYS
29	CE	7	ASP
29	CE	9	GLN
29	CE	49	ARG
29	CE	61	ARG
30	CF	26	GLN
30	CF	94	ARG
30	CF	96	TRP
30	CF	176	PHE
32	CH	14	SER
32	CH	15	LEU
32	CH	57	LYS
32	CH	83	LYS
33	CI	65	SER
33	CI	87	SER
35	CK	73	ASP
35	CK	108	ARG
36	CL	17	LYS
36	CL	114	GLY
37	CM	59	ARG
37	CM	81	ARG
38	CN	3	HIS
39	CO	5	SER
39	CO	68	LYS
39	CO	112	GLU
40	CP	110	LYS
41	CQ	6	GLY
41	CQ	85	ALA

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Mol	Chain	Res	Type
42	CR	46	GLU
42	CR	56	GLY
42	CR	57	GLY
42	CR	79	ARG
43	CS	59	GLU
43	CS	62	ASP
44	CT	37	ASP
44	CT	58	VAL
44	CT	88	LYS
45	CU	40	LEU
45	CU	55	GLY
45	CU	97	SER
47	CW	54	ASP
48	CX	46	VAL
49	CY	6	LEU
51	C0	53	VAL
51	C0	54	ILE
53	C2	45	SER
55	C4	6	SER
2	DB	19	GLN
2	DB	46	THR
2	DB	59	LYS
2	DB	74	ARG
2	DB	75	ALA
2	DB	95	ARG
2	DB	97	LEU
2	DB	130	THR
2	DB	143	LYS
2	DB	147	SER
2	DB	201	PRO
3	DC	3	GLN
3	DC	12	LEU
3	DC	74	GLY
3	DC	78	GLY
3	DC	141	ALA
3	DC	196	ILE
4	DD	23	SER
4	DD	25	VAL
4	DD	33	LYS
4	DD	34	ILE
4	DD	35	GLU
4	DD	140	ASN

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Mol	Chain	Res	Type
4	DD	147	GLU
4	DD	162	ALA
4	DD	173	VAL
4	DD	179	GLU
4	DD	188	ARG
4	DD	189	SER
4	DD	190	ASP
5	DE	126	LYS
5	DE	157	ARG
5	DE	158	GLY
6	DF	14	GLN
6	DF	38	ARG
6	DF	54	LEU
6	DF	56	LYS
6	DF	77	THR
7	DG	5	ARG
7	DG	16	PRO
7	DG	58	GLU
8	DH	20	ALA
8	DH	39	VAL
8	DH	40	LEU
8	DH	44	GLY
8	DH	70	ALA
8	DH	71	VAL
8	DH	89	LYS
9	DI	26	GLY
9	DI	34	SER
9	DI	53	GLU
9	DI	57	MET
9	DI	58	VAL
9	DI	94	LEU
10	DJ	29	ALA
10	DJ	89	ARG
11	DK	73	ALA
11	DK	78	GLY
12	DL	12	ARG
12	DL	107	VAL
12	DL	122	PRO
13	DM	38	GLY
13	DM	39	ILE
13	DM	66	GLU
13	DM	67	GLY

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Mol	Chain	Res	Type
13	DM	98	ARG
14	DN	18	LYS
14	DN	21	ALA
14	DN	24	ALA
14	DN	27	LYS
14	DN	49	GLN
15	DO	47	LYS
15	DO	73	LYS
16	DP	44	SER
17	DQ	10	GLY
17	DQ	68	SER
17	DQ	70	THR
18	DR	30	LYS
18	DR	47	THR
18	DR	49	ALA
19	DS	5	LEU
19	DS	16	LEU
19	DS	43	ASN
20	DT	69	LYS
20	DT	78	ASN
21	DU	8	GLU
21	DU	9	ASN
21	DU	13	ASP
21	DU	25	LYS
21	DU	33	ARG
21	DU	35	ARG
2	AB	77	SER
2	AB	89	GLN
2	AB	147	SER
2	AB	152	LYS
2	AB	206	ALA
3	AC	36	ASP
3	AC	62	LYS
3	AC	67	THR
4	AD	10	LYS
4	AD	82	LEU
4	AD	168	PRO
5	AE	12	GLN
5	AE	45	ARG
5	AE	103	THR
7	AG	54	SER
7	AG	77	SER

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Mol	Chain	Res	Type
7	AG	121	ALA
7	AG	128	ALA
8	AH	64	LYS
9	AI	13	LYS
9	AI	96	SER
10	AJ	36	VAL
10	AJ	93	ALA
12	AL	105	SER
12	AL	123	LYS
13	AM	14	HIS
13	AM	40	ALA
13	AM	44	LYS
15	AO	3	LEU
16	AP	28	ARG
18	AR	25	ASP
18	AR	30	LYS
18	AR	54	GLN
19	AS	70	LYS
20	AT	5	LYS
20	AT	34	LYS
21	AU	22	SER
21	AU	26	ALA
22	AV	86	SER
22	AV	110	ARG
27	BC	73	ILE
27	BC	195	GLY
29	BE	152	GLU
29	BE	173	THR
30	BF	40	GLY
30	BF	117	SER
30	BF	175	PRO
31	BG	166	GLU
32	BH	12	LEU
32	BH	16	GLY
32	BH	62	LEU
32	BH	146	VAL
33	BI	9	LYS
33	BI	11	GLN
33	BI	18	ASN
33	BI	20	SER
33	BI	30	GLN
33	BI	62	ALA

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Mol	Chain	Res	Type
33	BI	83	ALA
33	BI	89	SER
33	BI	109	ALA
33	BI	110	GLN
35	BK	90	ASN
36	BL	88	GLY
37	BM	24	THR
37	BM	81	ARG
37	BM	133	LYS
38	BN	106	ASP
39	BO	13	ARG
40	BP	75	THR
40	BP	104	GLY
44	BT	72	GLN
47	BW	29	VAL
48	BX	22	ASN
49	BY	22	LEU
52	B1	16	THR
56	B5	61	THR
56	B5	70	LYS
56	B5	150	GLY
56	B5	184	LYS
56	B5	201	PRO
56	B5	211	SER
56	B5	215	THR
27	CC	156	SER
27	CC	197	ALA
27	CC	257	ARG
28	CD	36	GLN
29	CE	171	ASP
30	CF	20	ASN
30	CF	149	ARG
31	CG	11	PRO
31	CG	58	ALA
31	CG	174	LYS
32	CH	59	ALA
32	CH	122	LEU
32	CH	135	HIS
33	CI	19	PRO
33	CI	96	LYS
33	CI	116	MET
36	CL	12	SER

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Mol	Chain	Res	Type
36	CL	15	ALA
36	CL	54	GLN
36	CL	62	PRO
36	CL	115	GLU
39	CO	45	SER
42	CR	53	PHE
43	CS	63	GLY
43	CS	66	ILE
43	CS	80	PRO
44	CT	17	SER
45	CU	88	ASP
47	CW	53	ARG
51	C0	52	LYS
2	DB	22	TYR
2	DB	36	ASN
2	DB	57	LEU
2	DB	73	LYS
2	DB	194	ASP
2	DB	207	ILE
3	DC	80	LYS
4	DD	26	ARG
4	DD	30	THR
4	DD	62	ARG
4	DD	110	THR
4	DD	123	ILE
4	DD	151	LYS
4	DD	181	THR
4	DD	183	LYS
4	DD	192	SER
5	DE	99	ALA
5	DE	131	THR
6	DF	53	LYS
6	DF	93	LYS
7	DG	7	ILE
7	DG	24	ALA
7	DG	62	PHE
7	DG	94	VAL
8	DH	83	LEU
8	DH	96	MET
10	DJ	35	GLN
10	DJ	75	ASP
10	DJ	95	GLY

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Mol	Chain	Res	Type
11	DK	125	LYS
11	DK	126	LYS
12	DL	34	CYS
12	DL	51	LYS
12	DL	88	LYS
12	DL	104	CYS
13	DM	11	ASP
13	DM	21	SER
14	DN	62	ASN
15	DO	19	ALA
16	DP	50	THR
17	DQ	20	SER
20	DT	86	LEU
21	DU	29	LEU
21	DU	38	TYR
2	AB	11	LYS
2	AB	39	HIS
2	AB	68	LEU
2	AB	160	ALA
2	AB	170	HIS
3	AC	3	GLN
4	AD	7	PRO
4	AD	28	ILE
4	AD	31	LYS
4	AD	102	VAL
4	AD	153	SER
4	AD	193	ALA
5	AE	143	GLY
6	AF	16	GLU
6	AF	21	MET
6	AF	93	LYS
6	AF	94	HIS
8	AH	96	MET
9	AI	6	TYR
10	AJ	6	ILE
10	AJ	34	ALA
10	AJ	58	ASN
10	AJ	91	ASP
11	AK	72	ASP
11	AK	75	LYS
11	AK	91	PRO
12	AL	44	LYS

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Mol	Chain	Res	Type
13	AM	23	TYR
13	AM	113	ARG
14	AN	62	ASN
14	AN	69	ARG
17	AQ	69	LYS
17	AQ	80	GLU
18	AR	57	ARG
19	AS	47	LEU
21	AU	34	ARG
22	AV	97	SER
22	AV	106	LEU
27	BC	150	GLY
28	BD	178	VAL
29	BE	86	ALA
29	BE	158	PHE
30	BF	173	ASP
30	BF	174	PHE
31	BG	11	PRO
31	BG	12	ALA
31	BG	79	THR
32	BH	147	VAL
33	BI	41	PHE
33	BI	49	GLU
33	BI	51	GLY
33	BI	59	THR
36	BL	99	ASN
36	BL	115	GLU
37	BM	26	VAL
37	BM	69	PRO
38	BN	72	ASP
38	BN	116	VAL
39	BO	53	THR
45	BU	36	GLU
47	BW	55	HIS
49	BY	2	LYS
49	BY	25	GLN
49	BY	61	ALA
51	B0	26	SER
52	B1	31	GLU
52	B1	32	LYS
52	B1	39	ASP
56	B5	35	ALA

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Mol	Chain	Res	Type
56	B5	217	THR
27	CC	51	ARG
27	CC	235	GLU
28	CD	156	PHE
28	CD	162	ALA
29	CE	129	PRO
33	CI	83	ALA
34	CJ	21	THR
34	CJ	25	LEU
35	CK	93	GLN
36	CL	36	LYS
37	CM	8	LYS
37	CM	108	VAL
39	CO	101	GLY
42	CR	84	ARG
45	CU	18	LYS
47	CW	35	ILE
51	C0	26	SER
51	C0	49	ARG
2	DB	176	ALA
3	DC	23	PHE
3	DC	66	VAL
3	DC	98	PRO
4	DD	13	ARG
4	DD	46	PRO
4	DD	76	TYR
4	DD	143	VAL
4	DD	144	SER
5	DE	12	GLN
5	DE	100	SER
5	DE	137	VAL
6	DF	99	ALA
8	DH	32	LEU
9	DI	9	THR
9	DI	75	GLN
9	DI	89	GLU
9	DI	129	LYS
10	DJ	90	LEU
11	DK	56	ARG
14	DN	48	LEU
14	DN	99	ALA
14	DN	100	SER

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Mol	Chain	Res	Type
15	DO	30	ALA
16	DP	5	ARG
18	DR	48	ARG
18	DR	53	ARG
21	DU	12	PHE
21	DU	40	LYS
2	AB	56	GLU
3	AC	139	GLN
4	AD	23	SER
4	AD	32	CYS
5	AE	24	THR
6	AF	14	GLN
7	AG	79	ARG
7	AG	81	GLY
7	AG	127	ALA
9	AI	55	VAL
10	AJ	62	ARG
12	AL	94	ARG
13	AM	74	SER
16	AP	49	GLY
18	AR	27	ALA
19	AS	9	PRO
19	AS	13	LEU
19	AS	22	ALA
21	AU	35	ARG
27	BC	104	LEU
28	BD	86	GLU
29	BE	8	ALA
29	BE	61	ARG
30	BF	45	ASP
31	BG	159	LYS
33	BI	64	ARG
33	BI	114	ALA
34	BJ	25	LEU
34	BJ	82	GLY
35	BK	119	ALA
36	BL	87	GLY
41	BQ	52	ARG
42	BR	8	GLY
44	BT	88	LYS
45	BU	98	ASN
48	BX	60	LYS

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Mol	Chain	Res	Type
55	B4	30	GLU
56	B5	180	PHE
27	CC	122	ALA
29	CE	8	ALA
29	CE	83	VAL
30	CF	25	MET
30	CF	71	LYS
31	CG	173	ALA
32	CH	112	LYS
39	CO	42	PRO
40	CP	83	ILE
42	CR	28	ALA
43	CS	65	ASP
44	CT	27	SER
46	CV	14	LYS
49	CY	12	GLU
51	C0	55	ALA
53	C2	12	ARG
2	DB	11	LYS
2	DB	34	ALA
2	DB	35	ARG
3	DC	8	ASN
3	DC	146	ALA
3	DC	166	GLU
4	DD	166	GLU
5	DE	103	THR
5	DE	132	ASN
6	DF	26	THR
7	DG	130	ASN
9	DI	121	ALA
11	DK	91	PRO
11	DK	119	ASN
13	DM	65	VAL
15	DO	18	ASP
18	DR	46	GLY
19	DS	42	PRO
19	DS	53	ASN
20	DT	8	LYS
21	DU	52	ALA
3	AC	178	LEU
4	AD	17	THR
7	AG	15	ASP

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Mol	Chain	Res	Type
11	AK	15	GLN
12	AL	90	LEU
13	AM	83	LEU
14	AN	65	ARG
22	AV	47	GLY
22	AV	50	THR
22	AV	151	GLU
27	BC	164	VAL
29	BE	62	GLN
32	BH	8	LYS
33	BI	19	PRO
33	BI	97	VAL
35	BK	106	GLU
38	BN	52	ILE
38	BN	98	LEU
40	BP	16	VAL
54	B3	6	VAL
56	B5	182	PRO
27	CC	130	PRO
29	CE	196	VAL
32	CH	108	VAL
33	CI	92	PRO
33	CI	102	ARG
34	CJ	122	LEU
35	CK	72	PRO
36	CL	10	GLU
36	CL	103	ILE
45	CU	51	LEU
45	CU	54	PRO
2	DB	42	ASN
2	DB	98	GLY
4	DD	185	LYS
6	DF	44	ARG
12	DL	85	GLY
12	DL	119	VAL
13	DM	43	VAL
14	DN	32	ASP
17	DQ	66	PRO
21	DU	22	SER
6	AF	7	VAL
13	AM	25	VAL
30	BF	105	ILE

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Mol	Chain	Res	Type
37	BM	125	PRO
51	B0	54	ILE
54	B3	17	GLY
56	B5	43	VAL
30	CF	148	VAL
30	CF	175	PRO
31	CG	101	VAL
32	CH	118	PRO
45	CU	53	GLN
54	C3	31	ILE
4	DD	61	VAL
4	DD	125	VAL
5	DE	109	GLY
7	DG	6	VAL
7	DG	8	GLY
13	DM	4	ILE
21	DU	53	VAL
5	AE	105	ILE
5	AE	120	VAL
27	BC	234	GLY
31	BG	111	PRO
44	BT	71	GLY
27	CC	125	PRO
31	CG	20	GLY
31	CG	91	VAL
31	CG	161	VAL
33	CI	8	VAL
35	CK	119	ALA
37	CM	77	PRO
37	CM	80	VAL
44	CT	2	ILE
4	DD	101	VAL
8	DH	68	GLY
7	AG	6	VAL
14	AN	45	VAL
27	BC	48	ILE
31	BG	16	VAL
31	BG	81	GLY
31	BG	117	PRO
32	BH	143	ILE
56	B5	132	GLY
29	CE	76	PRO

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Mol	Chain	Res	Type
31	CG	14	VAL
31	CG	81	GLY
33	CI	28	GLY
46	CV	81	PRO
4	DD	37	ALA
5	DE	25	VAL
5	DE	105	ILE
9	AI	30	ILE
10	AJ	39	PRO
11	AK	89	PRO
14	AN	68	GLY
19	AS	42	PRO
21	AU	40	LYS
27	BC	108	GLY
32	BH	9	VAL
33	BI	23	VAL
34	BJ	96	ARG
35	BK	48	PRO
56	B5	153	ILE
33	CI	136	GLY
54	C3	57	VAL
3	DC	15	VAL
13	AM	65	VAL
45	BU	54	PRO
56	B5	77	ILE
27	CC	243	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/199 (90%)	145 (81%)	35 (19%)	1	7
2	DB	180/199 (90%)	142 (79%)	38 (21%)	1	5
3	AC	170/190 (90%)	138 (81%)	32 (19%)	1	8
3	DC	170/190 (90%)	140 (82%)	30 (18%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	172/173 (99%)	126 (73%)	46 (27%)	0	2
4	DD	172/173 (99%)	130 (76%)	42 (24%)	0	3
5	AE	113/126 (90%)	91 (80%)	22 (20%)	1	7
5	DE	113/126 (90%)	89 (79%)	24 (21%)	1	5
6	AF	87/116 (75%)	68 (78%)	19 (22%)	1	5
6	DF	87/116 (75%)	70 (80%)	17 (20%)	1	7
7	AG	124/147 (84%)	101 (82%)	23 (18%)	1	8
7	DG	124/147 (84%)	106 (86%)	18 (14%)	3	15
8	AH	104/105 (99%)	85 (82%)	19 (18%)	1	9
8	DH	104/105 (99%)	87 (84%)	17 (16%)	2	11
9	AI	105/107 (98%)	78 (74%)	27 (26%)	0	3
9	DI	105/107 (98%)	82 (78%)	23 (22%)	1	5
10	AJ	86/90 (96%)	66 (77%)	20 (23%)	1	4
10	DJ	86/90 (96%)	67 (78%)	19 (22%)	1	4
11	AK	90/99 (91%)	72 (80%)	18 (20%)	1	7
11	DK	90/99 (91%)	75 (83%)	15 (17%)	2	11
12	AL	103/104 (99%)	74 (72%)	29 (28%)	0	2
12	DL	103/104 (99%)	82 (80%)	21 (20%)	1	6
13	AM	92/96 (96%)	68 (74%)	24 (26%)	0	2
13	DM	92/96 (96%)	74 (80%)	18 (20%)	1	7
14	AN	79/84 (94%)	60 (76%)	19 (24%)	0	3
14	DN	79/84 (94%)	59 (75%)	20 (25%)	0	3
15	AO	76/77 (99%)	59 (78%)	17 (22%)	1	4
15	DO	76/77 (99%)	60 (79%)	16 (21%)	1	5
16	AP	65/65 (100%)	47 (72%)	18 (28%)	0	2
16	DP	65/65 (100%)	51 (78%)	14 (22%)	1	5
17	AQ	74/78 (95%)	61 (82%)	13 (18%)	2	10
17	DQ	74/78 (95%)	54 (73%)	20 (27%)	0	2
18	AR	48/65 (74%)	33 (69%)	15 (31%)	0	1
18	DR	48/65 (74%)	36 (75%)	12 (25%)	0	3
19	AS	70/79 (89%)	47 (67%)	23 (33%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	DS	70/79 (89%)	56 (80%)	14 (20%)	1	7
20	AT	65/66 (98%)	48 (74%)	17 (26%)	0	2
20	DT	65/66 (98%)	51 (78%)	14 (22%)	1	5
21	AU	44/61 (72%)	31 (70%)	13 (30%)	0	1
21	DU	44/61 (72%)	30 (68%)	14 (32%)	0	1
22	AV	157/160 (98%)	128 (82%)	29 (18%)	1	8
27	BC	216/218 (99%)	173 (80%)	43 (20%)	1	7
27	CC	216/218 (99%)	176 (82%)	40 (18%)	1	8
28	BD	164/164 (100%)	131 (80%)	33 (20%)	1	6
28	CD	164/164 (100%)	135 (82%)	29 (18%)	2	9
29	BE	165/165 (100%)	142 (86%)	23 (14%)	3	16
29	CE	165/165 (100%)	137 (83%)	28 (17%)	2	10
30	BF	148/150 (99%)	118 (80%)	30 (20%)	1	6
30	CF	148/150 (99%)	125 (84%)	23 (16%)	2	13
31	BG	137/138 (99%)	109 (80%)	28 (20%)	1	6
31	CG	137/138 (99%)	112 (82%)	25 (18%)	1	9
32	BH	113/114 (99%)	90 (80%)	23 (20%)	1	6
32	CH	113/114 (99%)	85 (75%)	28 (25%)	0	3
33	BI	109/110 (99%)	94 (86%)	15 (14%)	3	17
33	CI	109/110 (99%)	96 (88%)	13 (12%)	5	22
34	BJ	116/116 (100%)	98 (84%)	18 (16%)	2	13
34	CJ	116/116 (100%)	97 (84%)	19 (16%)	2	11
35	BK	103/104 (99%)	86 (84%)	17 (16%)	2	11
35	CK	103/104 (99%)	79 (77%)	24 (23%)	1	4
36	BL	102/103 (99%)	78 (76%)	24 (24%)	1	3
36	CL	102/103 (99%)	82 (80%)	20 (20%)	1	7
37	BM	109/109 (100%)	96 (88%)	13 (12%)	5	22
37	CM	109/109 (100%)	90 (83%)	19 (17%)	2	10
38	BN	100/103 (97%)	80 (80%)	20 (20%)	1	7
38	CN	100/103 (97%)	91 (91%)	9 (9%)	9	35
39	BO	86/87 (99%)	65 (76%)	21 (24%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	CO	86/87 (99%)	63 (73%)	23 (27%)	0	2
40	BP	99/100 (99%)	78 (79%)	21 (21%)	1	5
40	CP	99/100 (99%)	86 (87%)	13 (13%)	4	18
41	BQ	89/90 (99%)	77 (86%)	12 (14%)	4	17
41	CQ	89/90 (99%)	74 (83%)	15 (17%)	2	11
42	BR	84/84 (100%)	74 (88%)	10 (12%)	5	22
42	CR	84/84 (100%)	73 (87%)	11 (13%)	4	18
43	BS	93/93 (100%)	77 (83%)	16 (17%)	2	10
43	CS	93/93 (100%)	72 (77%)	21 (23%)	1	4
44	BT	80/84 (95%)	65 (81%)	15 (19%)	1	8
44	CT	80/84 (95%)	66 (82%)	14 (18%)	2	10
45	BU	83/85 (98%)	63 (76%)	20 (24%)	0	3
45	CU	83/85 (98%)	67 (81%)	16 (19%)	1	8
46	BV	78/78 (100%)	68 (87%)	10 (13%)	4	19
46	CV	78/78 (100%)	63 (81%)	15 (19%)	1	8
47	BW	57/63 (90%)	46 (81%)	11 (19%)	1	8
47	CW	56/63 (89%)	48 (86%)	8 (14%)	3	15
48	BX	67/68 (98%)	55 (82%)	12 (18%)	2	9
48	CX	67/68 (98%)	55 (82%)	12 (18%)	2	9
49	BY	55/55 (100%)	43 (78%)	12 (22%)	1	5
49	CY	55/55 (100%)	45 (82%)	10 (18%)	1	9
50	BZ	48/49 (98%)	40 (83%)	8 (17%)	2	11
50	CZ	48/49 (98%)	40 (83%)	8 (17%)	2	11
51	B0	47/48 (98%)	44 (94%)	3 (6%)	17	51
51	C0	47/48 (98%)	41 (87%)	6 (13%)	4	19
52	B1	45/49 (92%)	39 (87%)	6 (13%)	4	17
52	C1	45/49 (92%)	38 (84%)	7 (16%)	2	13
53	B2	38/38 (100%)	31 (82%)	7 (18%)	1	9
53	C2	38/38 (100%)	31 (82%)	7 (18%)	1	9
54	B3	51/52 (98%)	43 (84%)	8 (16%)	2	13
54	C3	51/52 (98%)	42 (82%)	9 (18%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	B4	34/34 (100%)	26 (76%)	8 (24%)	1	3
55	C4	34/34 (100%)	27 (79%)	7 (21%)	1	6
56	B5	61/180 (34%)	52 (85%)	9 (15%)	3	14
All	All	9543/10096 (94%)	7684 (80%)	1859 (20%)	1	7

All (1859) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	10	LEU
2	AB	19	GLN
2	AB	23	TRP
2	AB	24	ASN
2	AB	30	PHE
2	AB	32	PHE
2	AB	36	ASN
2	AB	37	LYS
2	AB	39	HIS
2	AB	41	ILE
2	AB	50	PHE
2	AB	54	LEU
2	AB	56	GLU
2	AB	91	PHE
2	AB	96	TRP
2	AB	100	MET
2	AB	101	LEU
2	AB	104	TRP
2	AB	105	LYS
2	AB	107	VAL
2	AB	117	LEU
2	AB	127	ASP
2	AB	141	LEU
2	AB	147	SER
2	AB	148	LEU
2	AB	151	ILE
2	AB	154	MET
2	AB	159	ASP
2	AB	164	ILE
2	AB	169	GLU
2	AB	179	LEU
2	AB	186	ILE
2	AB	197	ASP

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Mol	Chain	Res	Type
2	AB	207	ILE
2	AB	222	ARG
3	AC	3	GLN
3	AC	11	ARG
3	AC	16	LYS
3	AC	21	THR
3	AC	33	LEU
3	AC	39	VAL
3	AC	47	LEU
3	AC	52	VAL
3	AC	56	VAL
3	AC	62	LYS
3	AC	64	ILE
3	AC	66	VAL
3	AC	82	GLU
3	AC	84	VAL
3	AC	97	VAL
3	AC	101	ILE
3	AC	102	ASN
3	AC	107	ARG
3	AC	115	LEU
3	AC	126	ARG
3	AC	128	VAL
3	AC	140	ASN
3	AC	144	LEU
3	AC	162	ILE
3	AC	165	THR
3	AC	166	GLU
3	AC	169	ARG
3	AC	170	GLU
3	AC	175	LEU
3	AC	176	HIS
3	AC	178	LEU
3	AC	193	TYR
4	AD	5	LEU
4	AD	9	LEU
4	AD	12	SER
4	AD	14	ARG
4	AD	19	LEU
4	AD	20	PHE
4	AD	23	SER
4	AD	32	CYS

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Mol	Chain	Res	Type
4	AD	34	ILE
4	AD	49	SER
4	AD	50	ASP
4	AD	54	GLN
4	AD	55	LEU
4	AD	58	LYS
4	AD	61	VAL
4	AD	64	ILE
4	AD	72	PHE
4	AD	77	LYS
4	AD	82	LEU
4	AD	89	ASN
4	AD	90	LEU
4	AD	93	LEU
4	AD	94	LEU
4	AD	97	ARG
4	AD	102	VAL
4	AD	104	ARG
4	AD	111	ARG
4	AD	113	GLU
4	AD	115	ARG
4	AD	116	GLN
4	AD	132	ILE
4	AD	146	ARG
4	AD	147	GLU
4	AD	153	SER
4	AD	159	LEU
4	AD	160	GLU
4	AD	161	LEU
4	AD	163	GLU
4	AD	164	GLN
4	AD	165	ARG
4	AD	171	LEU
4	AD	188	ARG
4	AD	189	SER
4	AD	190	ASP
4	AD	198	HIS
4	AD	203	LEU
5	AE	12	GLN
5	AE	32	SER
5	AE	39	VAL
5	AE	43	ASN

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Mol	Chain	Res	Type
5	AE	46	VAL
5	AE	54	ARG
5	AE	56	VAL
5	AE	61	GLN
5	AE	77	ASN
5	AE	78	ASN
5	AE	80	THR
5	AE	82	GLN
5	AE	83	HIS
5	AE	114	VAL
5	AE	116	GLU
5	AE	120	VAL
5	AE	123	VAL
5	AE	124	LEU
5	AE	135	ASN
5	AE	144	LEU
5	AE	148	ASN
5	AE	157	ARG
6	AF	16	GLU
6	AF	18	VAL
6	AF	21	MET
6	AF	23	GLU
6	AF	36	ILE
6	AF	37	HIS
6	AF	41	ASP
6	AF	42	TRP
6	AF	44	ARG
6	AF	45	ARG
6	AF	54	LEU
6	AF	63	ASN
6	AF	71	ILE
6	AF	72	ASP
6	AF	86	ARG
6	AF	88	MET
6	AF	90	MET
6	AF	96	VAL
6	AF	97	THR
7	AG	13	LEU
7	AG	15	ASP
7	AG	27	VAL
7	AG	29	ILE
7	AG	31	MET

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Mol	Chain	Res	Type
7	AG	41	SER
7	AG	45	SER
7	AG	48	GLU
7	AG	50	LEU
7	AG	54	SER
7	AG	58	GLU
7	AG	59	LEU
7	AG	68	ASN
7	AG	84	THR
7	AG	85	TYR
7	AG	99	LEU
7	AG	101	MET
7	AG	102	ARG
7	AG	106	GLU
7	AG	120	LEU
7	AG	123	GLU
7	AG	124	LEU
7	AG	139	GLU
8	AH	11	LEU
8	AH	18	GLN
8	AH	25	VAL
8	AH	27	MET
8	AH	61	LEU
8	AH	64	LYS
8	AH	78	VAL
8	AH	80	ARG
8	AH	87	LYS
8	AH	89	LYS
8	AH	92	LEU
8	AH	99	LEU
8	AH	103	VAL
8	AH	108	LYS
8	AH	112	THR
8	AH	117	ARG
8	AH	118	GLN
8	AH	121	LEU
8	AH	125	ILE
9	AI	4	ASN
9	AI	6	TYR
9	AI	7	TYR
9	AI	11	ARG
9	AI	12	ARG

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Mol	Chain	Res	Type
9	AI	18	ARG
9	AI	21	ILE
9	AI	34	SER
9	AI	39	PHE
9	AI	42	GLU
9	AI	46	MET
9	AI	56	ASP
9	AI	61	LEU
9	AI	80	ARG
9	AI	87	LEU
9	AI	88	MET
9	AI	93	SER
9	AI	95	ARG
9	AI	98	LEU
9	AI	106	ARG
9	AI	109	ARG
9	AI	110	GLN
9	AI	113	ARG
9	AI	114	LYS
9	AI	118	LEU
9	AI	127	PHE
9	AI	128	SER
10	AJ	10	LEU
10	AJ	20	GLN
10	AJ	26	VAL
10	AJ	31	ARG
10	AJ	32	THR
10	AJ	35	GLN
10	AJ	36	VAL
10	AJ	37	ARG
10	AJ	40	ILE
10	AJ	42	LEU
10	AJ	44	THR
10	AJ	49	PHE
10	AJ	50	THR
10	AJ	71	LEU
10	AJ	74	VAL
10	AJ	80	THR
10	AJ	84	VAL
10	AJ	88	MET
10	AJ	92	LEU
10	AJ	100	ILE

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Mol	Chain	Res	Type
11	AK	15	GLN
11	AK	18	ASP
11	AK	20	VAL
11	AK	34	ILE
11	AK	42	LEU
11	AK	46	THR
11	AK	57	LYS
11	AK	59	THR
11	AK	77	TYR
11	AK	85	MET
11	AK	94	GLU
11	AK	95	SER
11	AK	110	ILE
11	AK	111	THR
11	AK	113	VAL
11	AK	118	HIS
11	AK	125	LYS
11	AK	128	ARG
12	AL	3	THR
12	AL	5	ASN
12	AL	15	LYS
12	AL	16	VAL
12	AL	18	LYS
12	AL	29	GLN
12	AL	43	LYS
12	AL	51	LYS
12	AL	56	ARG
12	AL	57	LEU
12	AL	62	GLU
12	AL	63	VAL
12	AL	64	THR
12	AL	67	ILE
12	AL	73	ASN
12	AL	74	LEU
12	AL	75	GLN
12	AL	76	GLU
12	AL	83	ARG
12	AL	87	VAL
12	AL	90	LEU
12	AL	94	ARG
12	AL	95	TYR
12	AL	98	VAL

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Mol	Chain	Res	Type
12	AL	103	ASP
12	AL	104	CYS
12	AL	110	ARG
12	AL	111	LYS
12	AL	121	ARG
13	AM	19	LEU
13	AM	22	ILE
13	AM	23	TYR
13	AM	28	THR
13	AM	30	SER
13	AM	34	LEU
13	AM	43	VAL
13	AM	48	LEU
13	AM	52	GLN
13	AM	57	ARG
13	AM	58	ASP
13	AM	63	PHE
13	AM	70	ARG
13	AM	71	ARG
13	AM	79	ARG
13	AM	83	LEU
13	AM	90	ARG
13	AM	98	ARG
13	AM	101	ARG
13	AM	104	THR
13	AM	105	ASN
13	AM	109	ARG
13	AM	113	ARG
13	AM	114	LYS
14	AN	3	GLN
14	AN	6	LYS
14	AN	10	VAL
14	AN	12	ARG
14	AN	13	VAL
14	AN	15	LEU
14	AN	20	PHE
14	AN	22	LYS
14	AN	46	LEU
14	AN	48	LEU
14	AN	51	LEU
14	AN	59	ARG
14	AN	63	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	AN	64	CYS
14	AN	79	LEU
14	AN	89	MET
14	AN	92	GLU
14	AN	93	ILE
14	AN	96	LEU
15	AO	10	LYS
15	AO	20	ASN
15	AO	22	THR
15	AO	27	VAL
15	AO	35	GLN
15	AO	47	LYS
15	AO	56	LEU
15	AO	58	ARG
15	AO	66	LEU
15	AO	67	LEU
15	AO	70	LEU
15	AO	72	ARG
15	AO	78	TYR
15	AO	82	ILE
15	AO	83	GLU
15	AO	84	ARG
15	AO	88	ARG
16	AP	1	MET
16	AP	2	VAL
16	AP	3	THR
16	AP	6	LEU
16	AP	18	GLN
16	AP	21	VAL
16	AP	29	ASN
16	AP	35	ARG
16	AP	47	GLU
16	AP	50	THR
16	AP	51	ARG
16	AP	52	LEU
16	AP	66	THR
16	AP	67	ILE
16	AP	69	ASP
16	AP	70	ARG
16	AP	77	GLU
16	AP	78	VAL
17	AQ	4	LYS

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Mol	Chain	Res	Type
17	AQ	11	ARG
17	AQ	27	ARG
17	AQ	28	PHE
17	AQ	36	LYS
17	AQ	40	ARG
17	AQ	43	LYS
17	AQ	52	GLU
17	AQ	58	VAL
17	AQ	62	ARG
17	AQ	70	THR
17	AQ	74	THR
17	AQ	76	VAL
18	AR	20	GLU
18	AR	25	ASP
18	AR	28	THR
18	AR	33	ILE
18	AR	38	LYS
18	AR	47	THR
18	AR	48	ARG
18	AR	50	LYS
18	AR	54	GLN
18	AR	59	ILE
18	AR	61	ARG
18	AR	63	ARG
18	AR	65	LEU
18	AR	67	LEU
18	AR	68	LEU
19	AS	4	SER
19	AS	5	LEU
19	AS	6	LYS
19	AS	15	LEU
19	AS	16	LEU
19	AS	18	LYS
19	AS	21	LYS
19	AS	24	GLU
19	AS	27	ASP
19	AS	28	LYS
19	AS	31	LEU
19	AS	32	ARG
19	AS	34	TRP
19	AS	36	ARG
19	AS	41	PHE

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Mol	Chain	Res	Type
19	AS	48	THR
19	AS	55	ARG
19	AS	56	GLN
19	AS	57	HIS
19	AS	60	VAL
19	AS	63	THR
19	AS	70	LYS
19	AS	71	LEU
20	AT	3	ASN
20	AT	6	SER
20	AT	10	ARG
20	AT	15	GLU
20	AT	27	MET
20	AT	30	THR
20	AT	40	GLU
20	AT	51	PHE
20	AT	55	GLN
20	AT	60	ARG
20	AT	61	GLN
20	AT	67	ILE
20	AT	69	LYS
20	AT	70	ASN
20	AT	71	LYS
20	AT	74	ARG
20	AT	86	LEU
21	AU	4	ILE
21	AU	7	ARG
21	AU	10	GLU
21	AU	12	PHE
21	AU	16	LEU
21	AU	21	ARG
21	AU	29	LEU
21	AU	32	VAL
21	AU	35	ARG
21	AU	37	PHE
21	AU	38	TYR
21	AU	40	LYS
21	AU	49	LYS
22	AV	4	SER
22	AV	16	LYS
22	AV	17	CYS
22	AV	19	GLU

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Mol	Chain	Res	Type
22	AV	26	SER
22	AV	36	SER
22	AV	39	ASP
22	AV	45	TYR
22	AV	55	LEU
22	AV	59	THR
22	AV	65	THR
22	AV	75	MET
22	AV	83	ILE
22	AV	84	MET
22	AV	101	VAL
22	AV	106	LEU
22	AV	109	GLU
22	AV	131	ASN
22	AV	143	LEU
22	AV	145	LYS
22	AV	146	ASP
22	AV	150	SER
22	AV	156	ARG
22	AV	159	ASP
22	AV	160	ASP
22	AV	161	VAL
22	AV	176	LEU
22	AV	179	LYS
22	AV	183	LEU
27	BC	6	LYS
27	BC	9	SER
27	BC	12	ARG
27	BC	17	LYS
27	BC	19	VAL
27	BC	24	HIS
27	BC	32	LEU
27	BC	33	LEU
27	BC	35	LYS
27	BC	45	ASN
27	BC	48	ILE
27	BC	51	ARG
27	BC	107	LYS
27	BC	109	LEU
27	BC	110	LYS
27	BC	116	GLN
27	BC	119	VAL

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Mol	Chain	Res	Type
27	BC	120	ASP
27	BC	128	THR
27	BC	138	SER
27	BC	142	ASN
27	BC	144	GLU
27	BC	159	THR
27	BC	162	GLN
27	BC	173	LEU
27	BC	174	ARG
27	BC	175	LEU
27	BC	176	ARG
27	BC	177	SER
27	BC	180	MET
27	BC	201	LEU
27	BC	212	TRP
27	BC	216	ARG
27	BC	220	ARG
27	BC	222	THR
27	BC	244	VAL
27	BC	249	VAL
27	BC	250	GLN
27	BC	257	ARG
27	BC	258	SER
27	BC	260	LYS
27	BC	263	ASP
27	BC	269	ARG
28	BD	4	LEU
28	BD	9	VAL
28	BD	18	ASP
28	BD	22	ILE
28	BD	26	VAL
28	BD	28	GLU
28	BD	33	ARG
28	BD	35	THR
28	BD	46	ARG
28	BD	60	VAL
28	BD	67	HIS
28	BD	73	VAL
28	BD	74	GLU
28	BD	91	THR
28	BD	92	VAL
28	BD	98	VAL

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Mol	Chain	Res	Type
28	BD	104	VAL
28	BD	118	PHE
28	BD	128	ARG
28	BD	129	THR
28	BD	133	THR
28	BD	140	HIS
28	BD	150	GLN
28	BD	159	LYS
28	BD	160	LYS
28	BD	164	GLN
28	BD	165	MET
28	BD	169	ARG
28	BD	177	VAL
28	BD	187	LEU
28	BD	197	THR
28	BD	199	SER
28	BD	202	ILE
29	BE	5	LEU
29	BE	6	LYS
29	BE	7	ASP
29	BE	9	GLN
29	BE	27	LEU
29	BE	40	ARG
29	BE	46	GLN
29	BE	48	THR
29	BE	49	ARG
29	BE	51	GLU
29	BE	91	ASP
29	BE	94	GLN
29	BE	112	LEU
29	BE	114	ARG
29	BE	115	GLN
29	BE	120	VAL
29	BE	145	ASP
29	BE	159	LEU
29	BE	162	ARG
29	BE	163	ASN
29	BE	164	LEU
29	BE	166	LYS
29	BE	181	ILE
30	BF	15	LEU
30	BF	29	ARG

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Mol	Chain	Res	Type
30	BF	34	THR
30	BF	35	LEU
30	BF	41	GLU
30	BF	48	LEU
30	BF	51	ASN
30	BF	56	LEU
30	BF	71	LYS
30	BF	78	ILE
30	BF	80	GLN
30	BF	89	THR
30	BF	90	LEU
30	BF	91	ARG
30	BF	93	GLU
30	BF	94	ARG
30	BF	95	MET
30	BF	103	ILE
30	BF	104	THR
30	BF	112	ASP
30	BF	113	PHE
30	BF	121	PHE
30	BF	124	ARG
30	BF	126	ASN
30	BF	129	MET
30	BF	136	ILE
30	BF	143	ASP
30	BF	152	ASP
30	BF	162	ASP
30	BF	163	GLU
31	BG	2	ARG
31	BG	14	VAL
31	BG	16	VAL
31	BG	23	ILE
31	BG	31	GLU
31	BG	32	LEU
31	BG	38	ASP
31	BG	41	GLU
31	BG	42	VAL
31	BG	48	THR
31	BG	71	LEU
31	BG	73	SER
31	BG	87	GLN
31	BG	94	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	BG	103	ASN
31	BG	104	LEU
31	BG	105	SER
31	BG	106	LEU
31	BG	121	THR
31	BG	126	THR
31	BG	130	ILE
31	BG	138	GLN
31	BG	151	ARG
31	BG	154	GLU
31	BG	161	VAL
31	BG	165	ASP
31	BG	167	VAL
31	BG	170	THR
32	BH	6	LEU
32	BH	7	ASP
32	BH	8	LYS
32	BH	12	LEU
32	BH	18	GLN
32	BH	19	VAL
32	BH	22	LYS
32	BH	25	TYR
32	BH	31	VAL
32	BH	35	LYS
32	BH	37	VAL
32	BH	44	ILE
32	BH	51	ARG
32	BH	70	GLU
32	BH	77	THR
32	BH	82	SER
32	BH	90	LEU
32	BH	91	PHE
32	BH	110	VAL
32	BH	116	ARG
32	BH	123	ARG
32	BH	138	VAL
32	BH	142	VAL
33	BI	8	VAL
33	BI	9	LYS
33	BI	32	VAL
33	BI	35	MET
33	BI	37	PHE

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Mol	Chain	Res	Type
33	BI	61	TYR
33	BI	81	LYS
33	BI	85	ILE
33	BI	91	LYS
33	BI	95	ASP
33	BI	97	VAL
33	BI	104	GLN
33	BI	111	THR
33	BI	115	ASP
33	BI	126	ARG
34	BJ	2	LYS
34	BJ	5	THR
34	BJ	7	LYS
34	BJ	9	GLU
34	BJ	11	VAL
34	BJ	34	ARG
34	BJ	40	HIS
34	BJ	68	LYS
34	BJ	73	VAL
34	BJ	80	HIS
34	BJ	84	ILE
34	BJ	95	ARG
34	BJ	103	ILE
34	BJ	111	LYS
34	BJ	114	LEU
34	BJ	119	PHE
34	BJ	135	GLN
34	BJ	139	VAL
35	BK	2	ILE
35	BK	17	ARG
35	BK	18	ARG
35	BK	19	VAL
35	BK	22	ILE
35	BK	24	VAL
35	BK	25	LEU
35	BK	49	ARG
35	BK	58	LEU
35	BK	67	LYS
35	BK	76	VAL
35	BK	91	SER
35	BK	95	ILE
35	BK	103	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	BK	111	LYS
35	BK	116	ILE
35	BK	118	LEU
36	BL	3	LEU
36	BL	4	ASN
36	BL	6	LEU
36	BL	19	LEU
36	BL	21	ARG
36	BL	27	LEU
36	BL	29	LYS
36	BL	36	LYS
36	BL	39	LYS
36	BL	41	ARG
36	BL	46	VAL
36	BL	59	ARG
36	BL	61	LEU
36	BL	67	THR
36	BL	91	ASP
36	BL	94	THR
36	BL	100	ILE
36	BL	104	GLN
36	BL	110	VAL
36	BL	112	LEU
36	BL	117	THR
36	BL	118	THR
36	BL	126	ARG
36	BL	132	ARG
37	BM	5	LYS
37	BM	14	LYS
37	BM	22	GLN
37	BM	25	ASP
37	BM	27	SER
37	BM	36	VAL
37	BM	44	ARG
37	BM	58	LYS
37	BM	81	ARG
37	BM	100	LYS
37	BM	115	GLU
37	BM	119	LEU
37	BM	128	THR
38	BN	1	MET
38	BN	2	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
38	BN	6	SER
38	BN	14	SER
38	BN	27	SER
38	BN	28	LEU
38	BN	33	ILE
38	BN	51	LEU
38	BN	57	THR
38	BN	69	ARG
38	BN	70	THR
38	BN	71	ARG
38	BN	75	ILE
38	BN	76	VAL
38	BN	81	ASN
38	BN	89	SER
38	BN	113	ILE
38	BN	116	VAL
38	BN	117	ASP
38	BN	118	ARG
39	BO	3	LYS
39	BO	8	ILE
39	BO	16	ARG
39	BO	21	LEU
39	BO	24	THR
39	BO	26	LEU
39	BO	28	VAL
39	BO	31	THR
39	BO	38	GLN
39	BO	48	LEU
39	BO	53	THR
39	BO	63	LYS
39	BO	65	THR
39	BO	78	VAL
39	BO	80	GLU
39	BO	84	GLU
39	BO	85	LYS
39	BO	103	VAL
39	BO	112	GLU
39	BO	115	LEU
39	BO	116	GLN
40	BP	4	ILE
40	BP	9	GLN
40	BP	16	VAL

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Mol	Chain	Res	Type
40	BP	18	SER
40	BP	20	ARG
40	BP	25	VAL
40	BP	28	LYS
40	BP	30	TRP
40	BP	49	ILE
40	BP	67	GLU
40	BP	71	ARG
40	BP	77	SER
40	BP	83	ILE
40	BP	84	SER
40	BP	88	ARG
40	BP	96	LEU
40	BP	99	LEU
40	BP	102	ARG
40	BP	110	LYS
40	BP	113	LEU
40	BP	114	ASN
41	BQ	2	ARG
41	BQ	3	VAL
41	BQ	4	LYS
41	BQ	5	ARG
41	BQ	7	VAL
41	BQ	17	LEU
41	BQ	40	LYS
41	BQ	50	ARG
41	BQ	59	LEU
41	BQ	82	LEU
41	BQ	91	ARG
41	BQ	99	VAL
42	BR	6	GLN
42	BR	32	THR
42	BR	46	GLU
42	BR	54	VAL
42	BR	58	VAL
42	BR	59	ILE
42	BR	71	LYS
42	BR	72	VAL
42	BR	79	ARG
42	BR	102	SER
43	BS	1	MET
43	BS	4	ILE

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Mol	Chain	Res	Type
43	BS	7	HIS
43	BS	13	SER
43	BS	19	LEU
43	BS	27	LYS
43	BS	46	LEU
43	BS	59	GLU
43	BS	81	SER
43	BS	84	ARG
43	BS	85	ILE
43	BS	97	LEU
43	BS	98	LYS
43	BS	99	ARG
43	BS	104	THR
43	BS	106	VAL
44	BT	3	ARG
44	BT	5	GLU
44	BT	17	SER
44	BT	31	VAL
44	BT	32	LEU
44	BT	37	ASP
44	BT	39	THR
44	BT	44	LYS
44	BT	50	LEU
44	BT	63	VAL
44	BT	64	LYS
44	BT	67	VAL
44	BT	73	ARG
44	BT	76	ARG
44	BT	79	ASP
45	BU	8	ASP
45	BU	13	LEU
45	BU	16	LYS
45	BU	21	ARG
45	BU	30	SER
45	BU	34	ILE
45	BU	38	ILE
45	BU	42	LYS
45	BU	46	LYS
45	BU	48	VAL
45	BU	51	LEU
45	BU	52	ASN
45	BU	67	SER

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Mol	Chain	Res	Type
45	BU	81	ARG
45	BU	84	PHE
45	BU	85	ARG
45	BU	88	ASP
45	BU	96	LYS
45	BU	98	ASN
45	BU	99	SER
46	BV	3	THR
46	BV	14	LYS
46	BV	24	ASN
46	BV	26	PHE
46	BV	29	ILE
46	BV	58	SER
46	BV	64	VAL
46	BV	65	VAL
46	BV	69	GLU
46	BV	82	TYR
47	BW	12	ARG
47	BW	29	VAL
47	BW	30	LEU
47	BW	48	ASN
47	BW	51	CYS
47	BW	54	ASP
47	BW	69	VAL
47	BW	75	ARG
47	BW	76	LYS
47	BW	80	ILE
47	BW	83	GLU
48	BX	2	ARG
48	BX	4	CYS
48	BX	10	ARG
48	BX	19	HIS
48	BX	29	LEU
48	BX	40	GLU
48	BX	42	GLU
48	BX	44	ARG
48	BX	45	PHE
48	BX	53	LYS
48	BX	65	THR
48	BX	76	LYS
49	BY	7	ARG
49	BY	8	GLU

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Mol	Chain	Res	Type
49	BY	10	SER
49	BY	14	LEU
49	BY	16	THR
49	BY	18	LEU
49	BY	22	LEU
49	BY	23	ARG
49	BY	53	VAL
49	BY	56	LEU
49	BY	57	LEU
49	BY	59	GLU
50	BZ	2	LYS
50	BZ	3	THR
50	BZ	10	ARG
50	BZ	23	LEU
50	BZ	34	THR
50	BZ	36	GLU
50	BZ	44	ARG
50	BZ	56	VAL
51	B0	21	LEU
51	B0	22	THR
51	B0	39	ARG
52	B1	16	THR
52	B1	24	LYS
52	B1	29	LYS
52	B1	36	LYS
52	B1	45	HIS
52	B1	46	VAL
53	B2	1	MET
53	B2	4	THR
53	B2	15	SER
53	B2	24	THR
53	B2	25	LYS
53	B2	42	LEU
53	B2	43	THR
54	B3	7	ARG
54	B3	22	LYS
54	B3	29	ARG
54	B3	30	HIS
54	B3	31	ILE
54	B3	34	LYS
54	B3	46	LYS
54	B3	61	LEU

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Mol	Chain	Res	Type
55	B4	9	LYS
55	B4	11	CYS
55	B4	13	ASN
55	B4	16	ILE
55	B4	23	ILE
55	B4	27	CYS
55	B4	30	GLU
55	B4	32	LYS
56	B5	46	LYS
56	B5	47	LEU
56	B5	50	ASP
56	B5	54	SER
56	B5	59	ARG
56	B5	68	LEU
56	B5	77	ILE
56	B5	85	GLU
56	B5	93	TYR
27	CC	2	VAL
27	CC	17	LYS
27	CC	23	LEU
27	CC	47	ARG
27	CC	50	THR
27	CC	51	ARG
27	CC	52	HIS
27	CC	62	ARG
27	CC	73	ILE
27	CC	87	SER
27	CC	97	ASP
27	CC	101	ARG
27	CC	103	ILE
27	CC	109	LEU
27	CC	113	ASP
27	CC	116	GLN
27	CC	124	LYS
27	CC	128	THR
27	CC	129	LEU
27	CC	133	ASN
27	CC	134	ILE
27	CC	138	SER
27	CC	142	ASN
27	CC	159	THR
27	CC	161	VAL

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Mol	Chain	Res	Type
27	CC	162	GLN
27	CC	175	LEU
27	CC	176	ARG
27	CC	180	MET
27	CC	181	ARG
27	CC	183	VAL
27	CC	190	THR
27	CC	202	ARG
27	CC	211	ARG
27	CC	212	TRP
27	CC	216	ARG
27	CC	245	THR
27	CC	254	LYS
27	CC	257	ARG
27	CC	264	LYS
28	CD	2	ILE
28	CD	4	LEU
28	CD	16	THR
28	CD	27	ILE
28	CD	32	ASN
28	CD	33	ARG
28	CD	39	ASP
28	CD	43	ASP
28	CD	58	ASN
28	CD	67	HIS
28	CD	77	ARG
28	CD	79	LEU
28	CD	83	ARG
28	CD	84	LEU
28	CD	86	GLU
28	CD	98	VAL
28	CD	103	ASP
28	CD	104	VAL
28	CD	105	LYS
28	CD	116	LYS
28	CD	118	PHE
28	CD	121	THR
28	CD	123	LYS
28	CD	131	ASP
28	CD	150	GLN
28	CD	157	LYS
28	CD	177	VAL

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Mol	Chain	Res	Type
28	CD	178	VAL
28	CD	197	THR
29	CE	7	ASP
29	CE	12	LEU
29	CE	40	ARG
29	CE	53	THR
29	CE	63	LYS
29	CE	65	THR
29	CE	67	ARG
29	CE	69	ARG
29	CE	73	ILE
29	CE	74	LYS
29	CE	77	ILE
29	CE	78	TRP
29	CE	79	ARG
29	CE	91	ASP
29	CE	95	LYS
29	CE	96	VAL
29	CE	108	ILE
29	CE	114	ARG
29	CE	116	ASP
29	CE	125	SER
29	CE	127	GLU
29	CE	131	THR
29	CE	133	LEU
29	CE	152	GLU
29	CE	165	HIS
29	CE	167	VAL
29	CE	170	ARG
29	CE	173	THR
30	CF	2	LYS
30	CF	3	LEU
30	CF	24	VAL
30	CF	26	GLN
30	CF	31	GLU
30	CF	34	THR
30	CF	36	ASN
30	CF	47	LYS
30	CF	65	LEU
30	CF	68	LYS
30	CF	78	ILE
30	CF	84	ILE

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Mol	Chain	Res	Type
30	CF	90	LEU
30	CF	91	ARG
30	CF	96	TRP
30	CF	104	THR
30	CF	107	VAL
30	CF	127	TYR
30	CF	129	MET
30	CF	141	ASP
30	CF	149	ARG
30	CF	160	LYS
30	CF	162	ASP
31	CG	10	VAL
31	CG	14	VAL
31	CG	15	ASP
31	CG	16	VAL
31	CG	24	THR
31	CG	25	ILE
31	CG	32	LEU
31	CG	46	ASP
31	CG	49	LEU
31	CG	61	TRP
31	CG	68	ARG
31	CG	70	LEU
31	CG	71	LEU
31	CG	73	SER
31	CG	79	THR
31	CG	83	THR
31	CG	86	LEU
31	CG	110	HIS
31	CG	126	THR
31	CG	129	GLU
31	CG	138	GLN
31	CG	140	ILE
31	CG	148	ARG
31	CG	162	ARG
31	CG	168	VAL
32	CH	8	LYS
32	CH	12	LEU
32	CH	14	SER
32	CH	29	PHE
32	CH	50	ARG
32	CH	54	LEU

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Mol	Chain	Res	Type
32	CH	57	LYS
32	CH	62	LEU
32	CH	72	ILE
32	CH	73	ASN
32	CH	75	LEU
32	CH	76	GLU
32	CH	83	LYS
32	CH	89	LYS
32	CH	90	LEU
32	CH	96	THR
32	CH	97	ARG
32	CH	98	ASP
32	CH	104	THR
32	CH	119	ASN
32	CH	127	GLU
32	CH	129	GLU
32	CH	135	HIS
32	CH	138	VAL
32	CH	142	VAL
32	CH	143	ILE
32	CH	145	ASN
32	CH	149	GLU
33	CI	4	VAL
33	CI	8	VAL
33	CI	12	VAL
33	CI	18	ASN
33	CI	38	CYS
33	CI	39	LYS
33	CI	42	ASN
33	CI	72	THR
33	CI	78	LEU
33	CI	95	ASP
33	CI	104	GLN
33	CI	115	ASP
33	CI	140	GLU
34	CJ	2	LYS
34	CJ	14	ASP
34	CJ	17	VAL
34	CJ	30	THR
34	CJ	36	LEU
34	CJ	39	LYS
34	CJ	40	HIS

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Mol	Chain	Res	Type
34	CJ	48	VAL
34	CJ	56	VAL
34	CJ	61	LYS
34	CJ	69	ARG
34	CJ	81	ILE
34	CJ	84	ILE
34	CJ	98	GLU
34	CJ	99	ARG
34	CJ	111	LYS
34	CJ	120	ARG
34	CJ	138	GLN
34	CJ	140	LEU
35	CK	2	ILE
35	CK	9	ASN
35	CK	23	LYS
35	CK	24	VAL
35	CK	25	LEU
35	CK	38	ILE
35	CK	49	ARG
35	CK	57	VAL
35	CK	58	LEU
35	CK	63	VAL
35	CK	70	ARG
35	CK	71	ARG
35	CK	82	ASN
35	CK	86	LEU
35	CK	88	ASN
35	CK	95	ILE
35	CK	103	VAL
35	CK	109	SER
35	CK	114	LYS
35	CK	115	ILE
35	CK	116	ILE
35	CK	117	SER
35	CK	118	LEU
35	CK	121	GLU
36	CL	3	LEU
36	CL	21	ARG
36	CL	23	ILE
36	CL	36	LYS
36	CL	38	GLN
36	CL	46	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	CL	48	ARG
36	CL	64	PHE
36	CL	66	PHE
36	CL	67	THR
36	CL	73	ILE
36	CL	74	THR
36	CL	82	LEU
36	CL	86	GLU
36	CL	91	ASP
36	CL	92	LEU
36	CL	115	GLU
36	CL	123	ARG
36	CL	125	LEU
36	CL	142	ILE
37	CM	8	LYS
37	CM	10	ARG
37	CM	18	ARG
37	CM	25	ASP
37	CM	31	PHE
37	CM	33	LEU
37	CM	42	THR
37	CM	45	GLN
37	CM	50	ARG
37	CM	55	ARG
37	CM	64	TRP
37	CM	67	VAL
37	CM	74	THR
37	CM	76	LYS
37	CM	114	ARG
37	CM	119	LEU
37	CM	126	ILE
37	CM	128	THR
37	CM	135	VAL
38	CN	4	ARG
38	CN	15	SER
38	CN	35	LYS
38	CN	38	LEU
38	CN	57	THR
38	CN	82	GLU
38	CN	90	ARG
38	CN	96	ARG
38	CN	102	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	CO	5	SER
39	CO	8	ILE
39	CO	10	ARG
39	CO	12	THR
39	CO	15	ARG
39	CO	16	ARG
39	CO	17	LYS
39	CO	35	ILE
39	CO	36	TYR
39	CO	38	GLN
39	CO	39	VAL
39	CO	46	GLU
39	CO	53	THR
39	CO	67	ASN
39	CO	76	LYS
39	CO	83	LEU
39	CO	84	GLU
39	CO	91	SER
39	CO	93	ASP
39	CO	94	ARG
39	CO	100	HIS
39	CO	102	ARG
39	CO	106	LEU
40	CP	7	LEU
40	CP	10	GLU
40	CP	14	GLN
40	CP	28	LYS
40	CP	38	ARG
40	CP	64	SER
40	CP	72	VAL
40	CP	83	ILE
40	CP	93	LYS
40	CP	95	LYS
40	CP	102	ARG
40	CP	108	ARG
40	CP	113	LEU
41	CQ	3	VAL
41	CQ	5	ARG
41	CQ	7	VAL
41	CQ	12	ARG
41	CQ	14	LYS
41	CQ	29	ARG

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Mol	Chain	Res	Type
41	CQ	39	ILE
41	CQ	50	ARG
41	CQ	57	ARG
41	CQ	86	SER
41	CQ	89	ILE
41	CQ	91	ARG
41	CQ	93	ILE
41	CQ	99	VAL
41	CQ	111	LYS
42	CR	12	HIS
42	CR	15	SER
42	CR	19	THR
42	CR	22	LEU
42	CR	25	LEU
42	CR	41	ILE
42	CR	46	GLU
42	CR	48	LYS
42	CR	80	ARG
42	CR	84	ARG
42	CR	91	GLN
43	CS	3	THR
43	CS	4	ILE
43	CS	13	SER
43	CS	17	VAL
43	CS	20	VAL
43	CS	23	LEU
43	CS	33	LEU
43	CS	42	LYS
43	CS	46	LEU
43	CS	59	GLU
43	CS	65	ASP
43	CS	67	ASP
43	CS	85	ILE
43	CS	86	MET
43	CS	88	ARG
43	CS	90	LYS
43	CS	92	ARG
43	CS	97	LEU
43	CS	98	LYS
43	CS	100	THR
43	CS	104	THR
44	CT	3	ARG

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Mol	Chain	Res	Type
44	CT	7	LEU
44	CT	8	LEU
44	CT	19	LYS
44	CT	36	LYS
44	CT	55	VAL
44	CT	60	THR
44	CT	61	LEU
44	CT	62	VAL
44	CT	63	VAL
44	CT	69	ARG
44	CT	76	ARG
44	CT	91	GLN
44	CT	93	LEU
45	CU	8	ASP
45	CU	14	THR
45	CU	25	LYS
45	CU	27	VAL
45	CU	29	SER
45	CU	30	SER
45	CU	35	VAL
45	CU	38	ILE
45	CU	42	LYS
45	CU	44	HIS
45	CU	52	ASN
45	CU	60	LYS
45	CU	71	ILE
45	CU	73	ASN
45	CU	76	THR
45	CU	92	VAL
46	CV	12	GLN
46	CV	17	SER
46	CV	38	LEU
46	CV	41	GLU
46	CV	42	LEU
46	CV	43	ASP
46	CV	46	LYS
46	CV	56	PHE
46	CV	69	GLU
46	CV	71	LYS
46	CV	72	VAL
46	CV	79	ARG
46	CV	83	LYS

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Mol	Chain	Res	Type
46	CV	86	LEU
46	CV	93	ARG
47	CW	15	GLU
47	CW	18	ARG
47	CW	19	LEU
47	CW	34	ILE
47	CW	37	ARG
47	CW	41	THR
47	CW	56	THR
47	CW	68	GLU
48	CX	3	VAL
48	CX	4	CYS
48	CX	7	THR
48	CX	10	ARG
48	CX	24	THR
48	CX	34	SER
48	CX	43	LYS
48	CX	53	LYS
48	CX	56	ARG
48	CX	58	ILE
48	CX	65	THR
48	CX	73	ARG
49	CY	1	MET
49	CY	7	ARG
49	CY	13	GLU
49	CY	18	LEU
49	CY	21	LEU
49	CY	30	MET
49	CY	48	ARG
49	CY	52	ARG
49	CY	55	THR
49	CY	56	LEU
50	CZ	4	ILE
50	CZ	10	ARG
50	CZ	13	ILE
50	CZ	33	HIS
50	CZ	40	THR
50	CZ	43	ILE
50	CZ	46	MET
50	CZ	51	SER
51	C0	2	VAL
51	C0	37	HIS

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Mol	Chain	Res	Type
51	C0	39	ARG
51	C0	45	ASP
51	C0	53	VAL
51	C0	56	LYS
52	C1	9	LYS
52	C1	22	THR
52	C1	24	LYS
52	C1	26	LYS
52	C1	27	ARG
52	C1	31	GLU
52	C1	43	ARG
53	C2	1	MET
53	C2	10	LEU
53	C2	11	LYS
53	C2	14	ARG
53	C2	24	THR
53	C2	34	ARG
53	C2	39	ARG
54	C3	5	THR
54	C3	6	VAL
54	C3	12	ARG
54	C3	13	PHE
54	C3	23	HIS
54	C3	27	ASN
54	C3	28	LEU
54	C3	40	LYS
54	C3	41	ARG
55	C4	2	LYS
55	C4	4	ARG
55	C4	10	LEU
55	C4	11	CYS
55	C4	24	ARG
55	C4	32	LYS
55	C4	36	ARG
2	DB	10	LEU
2	DB	14	VAL
2	DB	15	HIS
2	DB	16	PHE
2	DB	19	GLN
2	DB	26	LYS
2	DB	27	MET
2	DB	40	ILE

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Mol	Chain	Res	Type
2	DB	49	MET
2	DB	51	ASN
2	DB	57	LEU
2	DB	72	THR
2	DB	73	LYS
2	DB	74	ARG
2	DB	80	VAL
2	DB	85	LEU
2	DB	88	ASP
2	DB	91	PHE
2	DB	95	ARG
2	DB	114	LEU
2	DB	116	ASP
2	DB	123	ASP
2	DB	131	LYS
2	DB	133	GLU
2	DB	141	LEU
2	DB	144	LEU
2	DB	157	LEU
2	DB	161	LEU
2	DB	175	GLU
2	DB	179	LEU
2	DB	191	SER
2	DB	197	ASP
2	DB	205	ASP
2	DB	207	ILE
2	DB	214	LEU
2	DB	217	VAL
2	DB	220	THR
2	DB	222	ARG
3	DC	4	LYS
3	DC	5	VAL
3	DC	11	ARG
3	DC	16	LYS
3	DC	37	PHE
3	DC	39	VAL
3	DC	44	THR
3	DC	55	ILE
3	DC	57	ILE
3	DC	59	ARG
3	DC	63	SER
3	DC	76	VAL

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Mol	Chain	Res	Type
3	DC	77	ILE
3	DC	97	VAL
3	DC	100	GLN
3	DC	111	LEU
3	DC	119	SER
3	DC	121	THR
3	DC	125	GLU
3	DC	150	LYS
3	DC	151	VAL
3	DC	153	VAL
3	DC	156	ARG
3	DC	162	ILE
3	DC	167	TRP
3	DC	176	HIS
3	DC	178	LEU
3	DC	185	ASN
3	DC	196	ILE
3	DC	198	VAL
4	DD	5	LEU
4	DD	9	LEU
4	DD	11	LEU
4	DD	17	THR
4	DD	20	PHE
4	DD	22	LYS
4	DD	28	ILE
4	DD	29	ASP
4	DD	47	ARG
4	DD	55	LEU
4	DD	59	GLN
4	DD	61	VAL
4	DD	71	GLN
4	DD	72	PHE
4	DD	78	GLU
4	DD	82	LEU
4	DD	83	LYS
4	DD	90	LEU
4	DD	91	LEU
4	DD	93	LEU
4	DD	99	ASP
4	DD	100	ASN
4	DD	115	ARG
4	DD	117	LEU

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Mol	Chain	Res	Type
4	DD	124	MET
4	DD	125	VAL
4	DD	128	ARG
4	DD	147	GLU
4	DD	150	LYS
4	DD	154	ARG
4	DD	161	LEU
4	DD	164	GLN
4	DD	171	LEU
4	DD	178	MET
4	DD	181	THR
4	DD	182	PHE
4	DD	188	ARG
4	DD	191	LEU
4	DD	196	ASN
4	DD	201	VAL
4	DD	203	LEU
4	DD	206	LYS
5	DE	13	GLU
5	DE	15	LEU
5	DE	29	ARG
5	DE	30	ILE
5	DE	50	TYR
5	DE	55	GLU
5	DE	64	MET
5	DE	65	GLU
5	DE	70	ASN
5	DE	80	THR
5	DE	93	ARG
5	DE	101	GLU
5	DE	112	ARG
5	DE	115	LEU
5	DE	117	VAL
5	DE	121	HIS
5	DE	124	LEU
5	DE	126	LYS
5	DE	137	VAL
5	DE	138	ARG
5	DE	141	ILE
5	DE	142	ASP
5	DE	149	SER
5	DE	151	GLU

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Mol	Chain	Res	Type
6	DF	5	GLU
6	DF	15	SER
6	DF	22	ILE
6	DF	39	LEU
6	DF	54	LEU
6	DF	55	HIS
6	DF	58	HIS
6	DF	61	LEU
6	DF	72	ASP
6	DF	80	PHE
6	DF	85	ILE
6	DF	86	ARG
6	DF	88	MET
6	DF	90	MET
6	DF	91	ARG
6	DF	94	HIS
6	DF	100	SER
7	DG	3	ARG
7	DG	5	ARG
7	DG	15	ASP
7	DG	21	GLU
7	DG	28	ASN
7	DG	42	ILE
7	DG	50	LEU
7	DG	63	GLU
7	DG	70	ARG
7	DG	72	THR
7	DG	75	VAL
7	DG	89	VAL
7	DG	96	ARG
7	DG	111	ARG
7	DG	118	LEU
7	DG	131	LYS
7	DG	140	ASP
7	DG	142	HIS
8	DH	7	ILE
8	DH	15	ARG
8	DH	38	ASN
8	DH	41	LYS
8	DH	43	GLU
8	DH	46	ILE
8	DH	56	LYS

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Mol	Chain	Res	Type
8	DH	63	LEU
8	DH	72	VAL
8	DH	77	ARG
8	DH	87	LYS
8	DH	88	ARG
8	DH	90	ASP
8	DH	92	LEU
8	DH	99	LEU
8	DH	113	ASP
8	DH	125	ILE
9	DI	15	SER
9	DI	21	ILE
9	DI	25	ASN
9	DI	28	ILE
9	DI	35	LEU
9	DI	39	PHE
9	DI	42	GLU
9	DI	46	MET
9	DI	47	VAL
9	DI	61	LEU
9	DI	84	THR
9	DI	85	ARG
9	DI	90	TYR
9	DI	95	ARG
9	DI	98	LEU
9	DI	99	ARG
9	DI	103	PHE
9	DI	106	ARG
9	DI	109	ARG
9	DI	110	GLN
9	DI	111	VAL
9	DI	129	LYS
9	DI	130	ARG
10	DJ	8	ILE
10	DJ	15	HIS
10	DJ	22	THR
10	DJ	25	ILE
10	DJ	26	VAL
10	DJ	37	ARG
10	DJ	42	LEU
10	DJ	45	ARG
10	DJ	46	LYS

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Mol	Chain	Res	Type
10	DJ	57	VAL
10	DJ	63	ASP
10	DJ	64	GLN
10	DJ	67	ILE
10	DJ	78	GLU
10	DJ	80	THR
10	DJ	81	GLU
10	DJ	87	LEU
10	DJ	90	LEU
10	DJ	96	VAL
11	DK	23	ILE
11	DK	33	THR
11	DK	46	THR
11	DK	59	THR
11	DK	76	GLU
11	DK	79	ILE
11	DK	83	GLU
11	DK	84	VAL
11	DK	87	LYS
11	DK	93	ARG
11	DK	96	THR
11	DK	109	ASN
11	DK	113	VAL
11	DK	127	ARG
11	DK	129	VAL
12	DL	5	ASN
12	DL	10	LYS
12	DL	14	ARG
12	DL	21	VAL
12	DL	29	GLN
12	DL	39	THR
12	DL	44	LYS
12	DL	50	ARG
12	DL	52	VAL
12	DL	56	ARG
12	DL	57	LEU
12	DL	58	THR
12	DL	74	LEU
12	DL	86	ARG
12	DL	87	VAL
12	DL	90	LEU
12	DL	98	VAL

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Mol	Chain	Res	Type
12	DL	99	ARG
12	DL	104	CYS
12	DL	109	ASP
12	DL	116	LYS
13	DM	12	HIS
13	DM	14	HIS
13	DM	22	ILE
13	DM	23	TYR
13	DM	25	VAL
13	DM	31	LYS
13	DM	41	GLU
13	DM	58	ASP
13	DM	68	ASP
13	DM	72	GLU
13	DM	75	MET
13	DM	80	LEU
13	DM	85	CYS
13	DM	91	HIS
13	DM	104	THR
13	DM	108	THR
13	DM	113	ARG
13	DM	114	LYS
14	DN	2	LYS
14	DN	3	GLN
14	DN	6	LYS
14	DN	10	VAL
14	DN	25	GLU
14	DN	27	LYS
14	DN	32	ASP
14	DN	41	ARG
14	DN	42	TRP
14	DN	45	VAL
14	DN	46	LEU
14	DN	48	LEU
14	DN	62	ASN
14	DN	65	ARG
14	DN	71	HIS
14	DN	73	PHE
14	DN	74	LEU
14	DN	75	ARG
14	DN	96	LEU
14	DN	100	SER

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Mol	Chain	Res	Type
15	DO	3	LEU
15	DO	5	THR
15	DO	14	GLU
15	DO	18	ASP
15	DO	25	THR
15	DO	26	GLU
15	DO	31	LEU
15	DO	32	LEU
15	DO	33	THR
15	DO	53	ARG
15	DO	62	GLN
15	DO	65	LYS
15	DO	67	LEU
15	DO	81	LEU
15	DO	87	LEU
15	DO	88	ARG
16	DP	1	MET
16	DP	2	VAL
16	DP	6	LEU
16	DP	8	ARG
16	DP	12	LYS
16	DP	18	GLN
16	DP	20	VAL
16	DP	25	ARG
16	DP	54	LEU
16	DP	56	ARG
16	DP	66	THR
16	DP	67	ILE
16	DP	69	ASP
16	DP	80	LYS
17	DQ	8	LEU
17	DQ	14	SER
17	DQ	17	MET
17	DQ	20	SER
17	DQ	27	ARG
17	DQ	40	ARG
17	DQ	41	THR
17	DQ	48	ASP
17	DQ	53	CYS
17	DQ	57	ASP
17	DQ	59	VAL
17	DQ	63	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	DQ	64	CYS
17	DQ	65	ARG
17	DQ	67	LEU
17	DQ	68	SER
17	DQ	70	THR
17	DQ	73	TRP
17	DQ	77	ARG
17	DQ	79	VAL
18	DR	22	ASP
18	DR	25	ASP
18	DR	26	ILE
18	DR	28	THR
18	DR	36	SER
18	DR	39	ILE
18	DR	40	VAL
18	DR	44	ILE
18	DR	51	TYR
18	DR	57	ARG
18	DR	59	ILE
18	DR	60	LYS
19	DS	5	LEU
19	DS	13	LEU
19	DS	14	HIS
19	DS	17	LYS
19	DS	19	VAL
19	DS	31	LEU
19	DS	33	THR
19	DS	39	THR
19	DS	40	ILE
19	DS	55	ARG
19	DS	57	HIS
19	DS	63	THR
19	DS	64	ASP
19	DS	69	HIS
20	DT	6	SER
20	DT	15	GLU
20	DT	18	ARG
20	DT	20	HIS
20	DT	24	ARG
20	DT	30	THR
20	DT	31	PHE
20	DT	48	GLN

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Mol	Chain	Res	Type
20	DT	51	PHE
20	DT	79	LEU
20	DT	82	GLN
20	DT	83	ILE
20	DT	84	ASN
20	DT	86	LEU
21	DU	4	ILE
21	DU	10	GLU
21	DU	12	PHE
21	DU	16	LEU
21	DU	17	ARG
21	DU	19	PHE
21	DU	20	LYS
21	DU	23	CYS
21	DU	28	VAL
21	DU	29	LEU
21	DU	34	ARG
21	DU	40	LYS
21	DU	43	THR
21	DU	49	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
3	AC	6	HIS
3	AC	190	HIS
4	AD	41	HIS
4	AD	54	GLN
4	AD	164	GLN
6	AF	37	HIS
8	AH	18	GLN
11	AK	22	HIS
14	AN	49	GLN
14	AN	71	HIS
15	AO	42	HIS
15	AO	46	HIS
15	AO	51	HIS
16	AP	40	ASN
19	AS	52	HIS
19	AS	57	HIS
20	AT	78	ASN
27	BC	57	HIS

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Mol	Chain	Res	Type
27	BC	85	ASN
27	BC	133	ASN
27	BC	196	ASN
27	BC	225	ASN
27	BC	242	HIS
29	BE	92	HIS
31	BG	21	GLN
32	BH	119	ASN
32	BH	128	HIS
33	BI	106	GLN
34	BJ	47	HIS
34	BJ	77	HIS
34	BJ	130	HIS
45	BU	44	HIS
46	BV	44	HIS
56	B5	44	HIS
56	B5	66	HIS
27	CC	24	HIS
27	CC	116	GLN
27	CC	229	HIS
28	CD	140	HIS
34	CJ	47	HIS
39	CO	100	HIS
40	CP	76	HIS
42	CR	89	HIS
43	CS	9	HIS
46	CV	80	HIS
48	CX	33	HIS
50	CZ	33	HIS
51	C0	40	HIS
51	C0	41	HIS
52	C1	45	HIS
2	DB	18	HIS
2	DB	39	HIS
2	DB	89	GLN
4	DD	74	ASN
5	DE	83	HIS
6	DF	37	HIS
6	DF	58	HIS
12	DL	77	HIS
13	DM	14	HIS
15	DO	51	HIS

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Mol	Chain	Res	Type
17	DQ	45	HIS
19	DS	14	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1542 (99%)	349 (22%)	15 (0%)
1	DA	1538/1542 (99%)	330 (21%)	17 (1%)
23	AW	14/16 (87%)	5 (35%)	0
23	DV	15/16 (93%)	6 (40%)	0
24	AX	75/76 (98%)	27 (36%)	6 (8%)
24	DW	75/76 (98%)	20 (26%)	0
25	BA	2896/2904 (99%)	590 (20%)	35 (1%)
25	CA	2895/2904 (99%)	618 (21%)	34 (1%)
26	BB	118/120 (98%)	16 (13%)	0
26	CB	117/120 (97%)	27 (23%)	0
All	All	9280/9316 (99%)	1988 (21%)	107 (1%)

All (1988) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	28	A
1	AA	30	U
1	AA	31	G
1	AA	32	A
1	AA	33	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	65	A
1	AA	70	U
1	AA	74	A
1	AA	75	G
1	AA	76	G
1	AA	80	A
1	AA	81	A

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Mol	Chain	Res	Type
1	AA	82	G
1	AA	83	C
1	AA	85	U
1	AA	86	G
1	AA	89	U
1	AA	90	C
1	AA	91	U
1	AA	92	U
1	AA	95	C
1	AA	96	U
1	AA	97	G
1	AA	100	G
1	AA	108	G
1	AA	109	A
1	AA	110	C
1	AA	111	G
1	AA	115	G
1	AA	116	A
1	AA	121	U
1	AA	122	G
1	AA	130	A
1	AA	131	A
1	AA	139	A
1	AA	144	G
1	AA	163	C
1	AA	164	G
1	AA	181	A
1	AA	182	A
1	AA	183	C
1	AA	189	A
1	AA	191	G
1	AA	195	A
1	AA	197	A
1	AA	199	A
1	AA	200	G
1	AA	205	A
1	AA	206	C
1	AA	209	U
1	AA	210	C
1	AA	211	G
1	AA	214	C
1	AA	226	G

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Mol	Chain	Res	Type
1	AA	240	G
1	AA	245	U
1	AA	247	G
1	AA	251	G
1	AA	262	A
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	301	G
1	AA	308	C
1	AA	320	A
1	AA	321	A
1	AA	327	A
1	AA	328	C
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	346	G
1	AA	347	G
1	AA	352	C
1	AA	354	G
1	AA	356	A
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	376	G
1	AA	382	A
1	AA	384	G
1	AA	387	U
1	AA	389	A
1	AA	390	U
1	AA	406	G
1	AA	408	A
1	AA	411	A
1	AA	412	A
1	AA	413	G
1	AA	418	C
1	AA	421	U
1	AA	422	C
1	AA	423	G
1	AA	424	G
1	AA	427	U

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Mol	Chain	Res	Type
1	AA	428	G
1	AA	429	U
1	AA	446	G
1	AA	458	U
1	AA	463	U
1	AA	465	A
1	AA	466	A
1	AA	467	U
1	AA	468	A
1	AA	469	C
1	AA	474	G
1	AA	481	G
1	AA	484	G
1	AA	485	U
1	AA	486	U
1	AA	495	A
1	AA	497	G
1	AA	505	G
1	AA	509	A
1	AA	511	C
1	AA	518	C
1	AA	519	C
1	AA	521	G
1	AA	524	G
1	AA	527	G
1	AA	532	A
1	AA	533	A
1	AA	545	C
1	AA	547	A
1	AA	550	G
1	AA	559	A
1	AA	562	U
1	AA	563	A
1	AA	564	C
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	579	A
1	AA	581	G
1	AA	591	U
1	AA	592	G

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Mol	Chain	Res	Type
1	AA	596	A
1	AA	607	A
1	AA	650	G
1	AA	653	U
1	AA	661	G
1	AA	665	A
1	AA	666	G
1	AA	667	G
1	AA	676	A
1	AA	682	G
1	AA	687	A
1	AA	702	A
1	AA	703	G
1	AA	704	A
1	AA	712	A
1	AA	721	G
1	AA	722	G
1	AA	723	U
1	AA	724	G
1	AA	725	G
1	AA	731	G
1	AA	739	C
1	AA	747	A
1	AA	748	G
1	AA	755	G
1	AA	773	G
1	AA	778	G
1	AA	786	G
1	AA	787	A
1	AA	792	A
1	AA	793	U
1	AA	794	A
1	AA	796	C
1	AA	815	A
1	AA	817	C
1	AA	828	U
1	AA	829	G
1	AA	830	G
1	AA	831	A
1	AA	832	G
1	AA	836	G
1	AA	840	C

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Mol	Chain	Res	Type
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	845	A
1	AA	846	G
1	AA	849	G
1	AA	859	G
1	AA	860	A
1	AA	873	A
1	AA	878	A
1	AA	887	G
1	AA	890	G
1	AA	898	G
1	AA	899	C
1	AA	914	A
1	AA	919	A
1	AA	922	G
1	AA	926	G
1	AA	927	G
1	AA	934	C
1	AA	936	C
1	AA	938	A
1	AA	960	U
1	AA	966	G
1	AA	968	A
1	AA	969	A
1	AA	973	G
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	983	A
1	AA	989	U
1	AA	991	U
1	AA	992	U
1	AA	993	G
1	AA	994	A
1	AA	998	C
1	AA	1001	C
1	AA	1002	G
1	AA	1004	A
1	AA	1006	G
1	AA	1007	U

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Mol	Chain	Res	Type
1	AA	1009	U
1	AA	1017	U
1	AA	1018	G
1	AA	1025	U
1	AA	1026	G
1	AA	1028	C
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	G
1	AA	1034	G
1	AA	1036	A
1	AA	1037	C
1	AA	1043	G
1	AA	1053	G
1	AA	1054	C
1	AA	1055	A
1	AA	1056	U
1	AA	1061	G
1	AA	1066	C
1	AA	1086	U
1	AA	1088	G
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1102	A
1	AA	1104	G
1	AA	1118	U
1	AA	1123	U
1	AA	1133	G
1	AA	1135	U
1	AA	1136	C
1	AA	1137	C
1	AA	1138	G
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1146	A
1	AA	1154	G
1	AA	1158	C
1	AA	1159	U
1	AA	1160	G

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Mol	Chain	Res	Type
1	AA	1161	C
1	AA	1167	A
1	AA	1168	U
1	AA	1169	A
1	AA	1183	U
1	AA	1184	G
1	AA	1196	A
1	AA	1197	A
1	AA	1201	A
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1227	A
1	AA	1238	A
1	AA	1239	A
1	AA	1241	G
1	AA	1250	A
1	AA	1256	A
1	AA	1258	G
1	AA	1279	G
1	AA	1280	A
1	AA	1286	U
1	AA	1287	A
1	AA	1288	A
1	AA	1293	C
1	AA	1300	G
1	AA	1305	G
1	AA	1308	U
1	AA	1312	G
1	AA	1314	C
1	AA	1317	C
1	AA	1318	A
1	AA	1319	A
1	AA	1322	C
1	AA	1323	G
1	AA	1328	C
1	AA	1332	A
1	AA	1335	U
1	AA	1336	C
1	AA	1338	G
1	AA	1340	A
1	AA	1344	C

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Mol	Chain	Res	Type
1	AA	1345	U
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1364	U
1	AA	1368	A
1	AA	1378	C
1	AA	1379	G
1	AA	1394	A
1	AA	1397	C
1	AA	1398	A
1	AA	1401	G
1	AA	1417	G
1	AA	1432	G
1	AA	1441	A
1	AA	1442	G
1	AA	1446	A
1	AA	1452	C
1	AA	1487	G
1	AA	1492	A
1	AA	1493	A
1	AA	1494	G
1	AA	1496	C
1	AA	1497	G
1	AA	1499	A
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1524	C
1	AA	1529	G
1	AA	1530	G
1	AA	1533	C
1	AA	1534	A
1	AA	1535	C
1	AA	1539	C
23	AW	3	G
23	AW	9	A
23	AW	10	A
23	AW	11	A
23	AW	16	U
24	AX	2	C
24	AX	3	C

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Mol	Chain	Res	Type
24	AX	4	C
24	AX	5	G
24	AX	8	U
24	AX	13	C
24	AX	16	U
24	AX	17	C
24	AX	19	G
24	AX	20	U
24	AX	21	A
24	AX	22	G
24	AX	44	G
24	AX	45	U
24	AX	48	C
24	AX	49	C
24	AX	55	U
24	AX	61	C
24	AX	64	A
24	AX	66	U
24	AX	67	C
24	AX	70	G
24	AX	71	G
24	AX	73	A
24	AX	74	C
24	AX	75	C
24	AX	76	A
25	BA	10	A
25	BA	12	U
25	BA	13	A
25	BA	14	A
25	BA	15	G
25	BA	23	G
25	BA	34	U
25	BA	35	G
25	BA	46	G
25	BA	49	A
25	BA	50	U
25	BA	58	G
25	BA	61	C
25	BA	63	A
25	BA	71	A
25	BA	74	A
25	BA	75	G

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Mol	Chain	Res	Type
25	BA	80	G
25	BA	91	A
25	BA	93	G
25	BA	101	A
25	BA	102	U
25	BA	103	A
25	BA	118	A
25	BA	119	A
25	BA	120	U
25	BA	137	U
25	BA	138	U
25	BA	139	U
25	BA	140	C
25	BA	141	G
25	BA	142	A
25	BA	181	A
25	BA	188	G
25	BA	191	A
25	BA	196	A
25	BA	215	G
25	BA	216	A
25	BA	222	A
25	BA	225	C
25	BA	245	G
25	BA	248	G
25	BA	250	G
25	BA	255	A
25	BA	264	C
25	BA	265	A
25	BA	266	G
25	BA	273	G
25	BA	276	U
25	BA	277	G
25	BA	291	G
25	BA	299	A
25	BA	302	C
25	BA	309	A
25	BA	311	A
25	BA	322	A
25	BA	323	C
25	BA	329	G
25	BA	330	A

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Mol	Chain	Res	Type
25	BA	331	C
25	BA	332	A
25	BA	350	G
25	BA	361	G
25	BA	367	G
25	BA	371	A
25	BA	372	G
25	BA	376	G
25	BA	380	G
25	BA	386	G
25	BA	396	G
25	BA	405	U
25	BA	406	G
25	BA	411	G
25	BA	412	A
25	BA	424	G
25	BA	442	G
25	BA	463	G
25	BA	464	U
25	BA	477	A
25	BA	478	A
25	BA	481	G
25	BA	490	C
25	BA	491	G
25	BA	505	A
25	BA	507	A
25	BA	508	A
25	BA	510	C
25	BA	529	A
25	BA	531	C
25	BA	532	A
25	BA	533	G
25	BA	538	A
25	BA	543	G
25	BA	544	C
25	BA	545	U
25	BA	546	U
25	BA	547	A
25	BA	548	G
25	BA	549	G
25	BA	550	C
25	BA	563	A

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Mol	Chain	Res	Type
25	BA	569	U
25	BA	573	U
25	BA	574	A
25	BA	575	A
25	BA	584	C
25	BA	586	A
25	BA	588	U
25	BA	603	A
25	BA	613	A
25	BA	614	A
25	BA	615	U
25	BA	622	G
25	BA	637	A
25	BA	645	C
25	BA	647	G
25	BA	648	G
25	BA	653	U
25	BA	654	A
25	BA	655	A
25	BA	664	G
25	BA	668	A
25	BA	671	C
25	BA	672	C
25	BA	686	U
25	BA	695	G
25	BA	715	A
25	BA	716	A
25	BA	717	C
25	BA	722	A
25	BA	730	A
25	BA	736	C
25	BA	747	U
25	BA	764	A
25	BA	765	C
25	BA	775	G
25	BA	776	G
25	BA	782	A
25	BA	784	G
25	BA	785	G
25	BA	792	A
25	BA	798	G
25	BA	805	G

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Mol	Chain	Res	Type
25	BA	812	C
25	BA	815	C
25	BA	816	C
25	BA	819	A
25	BA	827	U
25	BA	828	U
25	BA	830	G
25	BA	845	A
25	BA	846	U
25	BA	847	U
25	BA	858	G
25	BA	859	G
25	BA	867	C
25	BA	869	G
25	BA	878	A
25	BA	885	C
25	BA	893	C
25	BA	894	U
25	BA	896	A
25	BA	899	A
25	BA	910	A
25	BA	914	G
25	BA	915	C
25	BA	927	A
25	BA	928	A
25	BA	940	G
25	BA	941	A
25	BA	946	C
25	BA	953	G
25	BA	957	C
25	BA	958	U
25	BA	961	C
25	BA	974	G
25	BA	976	G
25	BA	982	C
25	BA	983	A
25	BA	984	A
25	BA	985	C
25	BA	990	A
25	BA	995	C
25	BA	996	A
25	BA	999	U

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Mol	Chain	Res	Type
25	BA	1012	U
25	BA	1013	C
25	BA	1017	G
25	BA	1022	G
25	BA	1023	U
25	BA	1026	G
25	BA	1027	A
25	BA	1033	U
25	BA	1040	A
25	BA	1046	A
25	BA	1047	G
25	BA	1055	G
25	BA	1061	U
25	BA	1062	G
25	BA	1063	G
25	BA	1065	U
25	BA	1066	U
25	BA	1070	A
25	BA	1071	G
25	BA	1072	C
25	BA	1073	A
25	BA	1074	G
25	BA	1075	C
25	BA	1082	U
25	BA	1083	U
25	BA	1084	A
25	BA	1088	A
25	BA	1092	C
25	BA	1093	G
25	BA	1094	U
25	BA	1098	A
25	BA	1099	G
25	BA	1103	A
25	BA	1112	G
25	BA	1115	G
25	BA	1122	G
25	BA	1132	U
25	BA	1133	A
25	BA	1135	C
25	BA	1136	G
25	BA	1139	G
25	BA	1142	A

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Mol	Chain	Res	Type
25	BA	1143	A
25	BA	1154	G
25	BA	1155	A
25	BA	1156	A
25	BA	1174	U
25	BA	1175	A
25	BA	1176	U
25	BA	1177	G
25	BA	1178	C
25	BA	1186	G
25	BA	1199	U
25	BA	1204	A
25	BA	1238	G
25	BA	1248	G
25	BA	1250	G
25	BA	1253	A
25	BA	1256	G
25	BA	1265	A
25	BA	1266	G
25	BA	1270	C
25	BA	1271	G
25	BA	1272	A
25	BA	1273	U
25	BA	1284	A
25	BA	1286	A
25	BA	1289	C
25	BA	1301	A
25	BA	1306	C
25	BA	1308	A
25	BA	1327	A
25	BA	1329	U
25	BA	1352	U
25	BA	1353	A
25	BA	1359	A
25	BA	1365	A
25	BA	1368	G
25	BA	1374	G
25	BA	1379	U
25	BA	1383	A
25	BA	1386	C
25	BA	1395	A
25	BA	1398	C

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Mol	Chain	Res	Type
25	BA	1399	C
25	BA	1411	U
25	BA	1416	G
25	BA	1419	A
25	BA	1420	A
25	BA	1421	G
25	BA	1428	C
25	BA	1437	C
25	BA	1449	G
25	BA	1450	G
25	BA	1451	C
25	BA	1452	G
25	BA	1453	A
25	BA	1455	G
25	BA	1461	C
25	BA	1482	G
25	BA	1490	A
25	BA	1493	C
25	BA	1497	U
25	BA	1502	A
25	BA	1504	A
25	BA	1505	A
25	BA	1508	A
25	BA	1509	A
25	BA	1510	G
25	BA	1515	A
25	BA	1533	C
25	BA	1534	U
25	BA	1535	A
25	BA	1536	C
25	BA	1537	G
25	BA	1547	C
25	BA	1548	A
25	BA	1554	U
25	BA	1559	U
25	BA	1560	G
25	BA	1565	C
25	BA	1566	A
25	BA	1569	A
25	BA	1578	U
25	BA	1583	A
25	BA	1584	U

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Mol	Chain	Res	Type
25	BA	1603	A
25	BA	1606	C
25	BA	1607	C
25	BA	1608	A
25	BA	1609	A
25	BA	1644	C
25	BA	1647	U
25	BA	1648	U
25	BA	1649	G
25	BA	1651	G
25	BA	1652	A
25	BA	1674	G
25	BA	1677	A
25	BA	1714	U
25	BA	1715	G
25	BA	1723	G
25	BA	1726	C
25	BA	1729	U
25	BA	1730	C
25	BA	1731	G
25	BA	1733	G
25	BA	1734	G
25	BA	1737	G
25	BA	1738	G
25	BA	1744	A
25	BA	1754	A
25	BA	1758	U
25	BA	1764	C
25	BA	1773	A
25	BA	1776	G
25	BA	1781	U
25	BA	1791	A
25	BA	1799	G
25	BA	1800	C
25	BA	1801	A
25	BA	1802	A
25	BA	1808	A
25	BA	1811	G
25	BA	1816	C
25	BA	1819	A
25	BA	1829	A
25	BA	1845	G

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Mol	Chain	Res	Type
25	BA	1846	G
25	BA	1847	A
25	BA	1849	G
25	BA	1853	A
25	BA	1868	C
25	BA	1869	G
25	BA	1870	C
25	BA	1872	A
25	BA	1873	G
25	BA	1874	C
25	BA	1876	A
25	BA	1882	U
25	BA	1903	G
25	BA	1906	G
25	BA	1910	G
25	BA	1913	A
25	BA	1914	C
25	BA	1927	A
25	BA	1928	A
25	BA	1929	G
25	BA	1930	G
25	BA	1937	A
25	BA	1938	A
25	BA	1945	G
25	BA	1952	A
25	BA	1955	U
25	BA	1960	A
25	BA	1965	C
25	BA	1967	C
25	BA	1970	A
25	BA	1971	U
25	BA	1972	G
25	BA	1975	G
25	BA	1976	U
25	BA	1991	U
25	BA	1993	U
25	BA	1995	U
25	BA	1996	C
25	BA	1997	C
25	BA	2002	G
25	BA	2018	G
25	BA	2019	A

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Mol	Chain	Res	Type
25	BA	2022	U
25	BA	2023	C
25	BA	2030	A
25	BA	2031	A
25	BA	2033	A
25	BA	2043	C
25	BA	2055	C
25	BA	2056	G
25	BA	2060	A
25	BA	2061	G
25	BA	2062	A
25	BA	2069	G
25	BA	2072	C
25	BA	2076	U
25	BA	2093	G
25	BA	2095	A
25	BA	2097	A
25	BA	2102	G
25	BA	2103	C
25	BA	2105	U
25	BA	2106	U
25	BA	2107	G
25	BA	2108	A
25	BA	2110	G
25	BA	2111	U
25	BA	2112	G
25	BA	2113	U
25	BA	2115	G
25	BA	2116	G
25	BA	2117	A
25	BA	2118	U
25	BA	2119	A
25	BA	2120	G
25	BA	2122	U
25	BA	2124	G
25	BA	2126	A
25	BA	2127	G
25	BA	2128	G
25	BA	2130	U
25	BA	2132	U
25	BA	2133	G
25	BA	2134	A

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Mol	Chain	Res	Type
25	BA	2136	G
25	BA	2138	G
25	BA	2142	A
25	BA	2146	C
25	BA	2147	A
25	BA	2149	U
25	BA	2150	C
25	BA	2152	G
25	BA	2153	C
25	BA	2154	A
25	BA	2156	G
25	BA	2159	G
25	BA	2160	C
25	BA	2161	C
25	BA	2162	G
25	BA	2163	A
25	BA	2164	C
25	BA	2165	C
25	BA	2166	U
25	BA	2167	U
25	BA	2169	A
25	BA	2170	A
25	BA	2171	A
25	BA	2172	U
25	BA	2184	A
25	BA	2186	G
25	BA	2187	U
25	BA	2190	G
25	BA	2197	U
25	BA	2198	A
25	BA	2203	U
25	BA	2204	G
25	BA	2210	U
25	BA	2211	A
25	BA	2212	A
25	BA	2213	U
25	BA	2225	A
25	BA	2238	G
25	BA	2239	G
25	BA	2243	U
25	BA	2250	G
25	BA	2255	G

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Mol	Chain	Res	Type
25	BA	2268	A
25	BA	2278	A
25	BA	2279	G
25	BA	2283	C
25	BA	2286	G
25	BA	2287	A
25	BA	2305	U
25	BA	2324	U
25	BA	2325	G
25	BA	2327	A
25	BA	2334	U
25	BA	2336	A
25	BA	2346	A
25	BA	2347	C
25	BA	2350	C
25	BA	2358	A
25	BA	2383	G
25	BA	2385	C
25	BA	2402	U
25	BA	2403	C
25	BA	2406	A
25	BA	2410	G
25	BA	2423	U
25	BA	2425	A
25	BA	2429	G
25	BA	2430	A
25	BA	2431	U
25	BA	2435	A
25	BA	2441	U
25	BA	2445	G
25	BA	2448	A
25	BA	2452	C
25	BA	2453	A
25	BA	2474	U
25	BA	2476	A
25	BA	2478	A
25	BA	2484	G
25	BA	2491	U
25	BA	2494	G
25	BA	2502	G
25	BA	2505	G
25	BA	2518	A

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Mol	Chain	Res	Type
25	BA	2520	C
25	BA	2529	G
25	BA	2530	A
25	BA	2546	U
25	BA	2549	G
25	BA	2550	G
25	BA	2554	U
25	BA	2566	A
25	BA	2567	G
25	BA	2572	A
25	BA	2573	C
25	BA	2576	G
25	BA	2578	G
25	BA	2582	G
25	BA	2585	U
25	BA	2586	U
25	BA	2599	G
25	BA	2603	G
25	BA	2605	U
25	BA	2609	U
25	BA	2613	U
25	BA	2615	U
25	BA	2621	G
25	BA	2629	U
25	BA	2630	G
25	BA	2634	A
25	BA	2654	A
25	BA	2661	G
25	BA	2663	G
25	BA	2681	C
25	BA	2689	U
25	BA	2690	U
25	BA	2714	G
25	BA	2726	A
25	BA	2729	G
25	BA	2733	A
25	BA	2744	G
25	BA	2748	A
25	BA	2757	A
25	BA	2765	A
25	BA	2777	G
25	BA	2778	A

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Mol	Chain	Res	Type
25	BA	2780	G
25	BA	2790	U
25	BA	2791	G
25	BA	2793	C
25	BA	2797	U
25	BA	2798	U
25	BA	2799	A
25	BA	2800	A
25	BA	2801	G
25	BA	2811	G
25	BA	2818	U
25	BA	2820	A
25	BA	2821	A
25	BA	2825	G
25	BA	2836	U
25	BA	2849	U
25	BA	2858	C
25	BA	2861	U
25	BA	2867	G
25	BA	2873	A
25	BA	2874	C
25	BA	2877	G
25	BA	2880	C
25	BA	2883	A
25	BA	2884	U
25	BA	2885	G
25	BA	2887	A
26	BB	3002	G
26	BB	3009	G
26	BB	3015	A
26	BB	3022	U
26	BB	3027	C
26	BB	3035	C
26	BB	3042	C
26	BB	3044	G
26	BB	3045	A
26	BB	3056	G
26	BB	3067	G
26	BB	3085	G
26	BB	3089	U
26	BB	3090	C
26	BB	3099	A

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Mol	Chain	Res	Type
26	BB	3109	A
25	CA	10	A
25	CA	12	U
25	CA	13	A
25	CA	15	G
25	CA	34	U
25	CA	35	G
25	CA	42	A
25	CA	46	G
25	CA	58	G
25	CA	63	A
25	CA	71	A
25	CA	74	A
25	CA	75	G
25	CA	80	G
25	CA	84	A
25	CA	85	G
25	CA	92	U
25	CA	94	A
25	CA	101	A
25	CA	110	G
25	CA	118	A
25	CA	119	A
25	CA	120	U
25	CA	137	U
25	CA	138	U
25	CA	139	U
25	CA	140	C
25	CA	141	G
25	CA	142	A
25	CA	160	A
25	CA	162	U
25	CA	181	A
25	CA	188	G
25	CA	196	A
25	CA	199	A
25	CA	215	G
25	CA	216	A
25	CA	221	A
25	CA	222	A
25	CA	248	G
25	CA	249	C

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Mol	Chain	Res	Type
25	CA	250	G
25	CA	254	G
25	CA	255	A
25	CA	264	C
25	CA	265	A
25	CA	266	G
25	CA	272	A
25	CA	273	G
25	CA	276	U
25	CA	278	A
25	CA	285	G
25	CA	299	A
25	CA	302	C
25	CA	303	G
25	CA	311	A
25	CA	329	G
25	CA	330	A
25	CA	333	G
25	CA	338	G
25	CA	343	C
25	CA	346	A
25	CA	361	G
25	CA	362	A
25	CA	367	G
25	CA	371	A
25	CA	372	G
25	CA	374	A
25	CA	381	G
25	CA	386	G
25	CA	391	A
25	CA	396	G
25	CA	404	A
25	CA	405	U
25	CA	411	G
25	CA	412	A
25	CA	424	G
25	CA	433	C
25	CA	435	C
25	CA	450	G
25	CA	454	A
25	CA	455	C
25	CA	473	G

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Mol	Chain	Res	Type
25	CA	480	A
25	CA	481	G
25	CA	490	C
25	CA	491	G
25	CA	496	G
25	CA	504	A
25	CA	505	A
25	CA	508	A
25	CA	510	C
25	CA	525	U
25	CA	526	A
25	CA	529	A
25	CA	531	C
25	CA	532	A
25	CA	533	G
25	CA	538	A
25	CA	543	G
25	CA	544	C
25	CA	546	U
25	CA	547	A
25	CA	548	G
25	CA	549	G
25	CA	550	C
25	CA	558	U
25	CA	563	A
25	CA	572	A
25	CA	573	U
25	CA	574	A
25	CA	575	A
25	CA	579	G
25	CA	586	A
25	CA	587	C
25	CA	588	U
25	CA	592	A
25	CA	601	C
25	CA	603	A
25	CA	613	A
25	CA	614	A
25	CA	615	U
25	CA	618	G
25	CA	620	G
25	CA	622	G

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Mol	Chain	Res	Type
25	CA	627	A
25	CA	628	G
25	CA	631	A
25	CA	637	A
25	CA	645	C
25	CA	646	U
25	CA	647	G
25	CA	648	G
25	CA	653	U
25	CA	654	A
25	CA	655	A
25	CA	663	G
25	CA	668	A
25	CA	670	A
25	CA	677	A
25	CA	682	G
25	CA	686	U
25	CA	714	U
25	CA	715	A
25	CA	717	C
25	CA	730	A
25	CA	747	U
25	CA	748	G
25	CA	749	A
25	CA	753	A
25	CA	762	U
25	CA	764	A
25	CA	765	C
25	CA	775	G
25	CA	776	G
25	CA	782	A
25	CA	784	G
25	CA	785	G
25	CA	790	U
25	CA	792	A
25	CA	795	C
25	CA	805	G
25	CA	812	C
25	CA	819	A
25	CA	827	U
25	CA	828	U
25	CA	830	G

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Mol	Chain	Res	Type
25	CA	843	G
25	CA	845	A
25	CA	846	U
25	CA	847	U
25	CA	858	G
25	CA	859	G
25	CA	866	A
25	CA	869	G
25	CA	884	U
25	CA	893	C
25	CA	894	U
25	CA	896	A
25	CA	897	C
25	CA	899	A
25	CA	907	G
25	CA	910	A
25	CA	931	U
25	CA	934	U
25	CA	940	G
25	CA	941	A
25	CA	945	A
25	CA	946	C
25	CA	957	C
25	CA	958	U
25	CA	961	C
25	CA	964	C
25	CA	965	C
25	CA	974	G
25	CA	983	A
25	CA	985	C
25	CA	990	A
25	CA	995	C
25	CA	996	A
25	CA	997	G
25	CA	999	U
25	CA	1005	C
25	CA	1012	U
25	CA	1013	C
25	CA	1017	G
25	CA	1022	G
25	CA	1025	G
25	CA	1027	A

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Mol	Chain	Res	Type
25	CA	1028	A
25	CA	1033	U
25	CA	1057	A
25	CA	1059	G
25	CA	1060	U
25	CA	1061	U
25	CA	1062	G
25	CA	1065	U
25	CA	1066	U
25	CA	1067	A
25	CA	1068	G
25	CA	1070	A
25	CA	1071	G
25	CA	1072	C
25	CA	1073	A
25	CA	1075	C
25	CA	1079	C
25	CA	1082	U
25	CA	1083	U
25	CA	1087	G
25	CA	1088	A
25	CA	1089	A
25	CA	1090	A
25	CA	1092	C
25	CA	1097	U
25	CA	1098	A
25	CA	1104	C
25	CA	1106	G
25	CA	1110	G
25	CA	1111	A
25	CA	1112	G
25	CA	1115	G
25	CA	1119	U
25	CA	1122	G
25	CA	1130	U
25	CA	1132	U
25	CA	1134	A
25	CA	1135	C
25	CA	1136	G
25	CA	1139	G
25	CA	1143	A
25	CA	1149	G

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Mol	Chain	Res	Type
25	CA	1156	A
25	CA	1172	C
25	CA	1173	U
25	CA	1174	U
25	CA	1175	A
25	CA	1176	U
25	CA	1177	G
25	CA	1186	G
25	CA	1211	C
25	CA	1227	G
25	CA	1232	G
25	CA	1236	G
25	CA	1237	A
25	CA	1248	G
25	CA	1253	A
25	CA	1256	G
25	CA	1262	A
25	CA	1266	G
25	CA	1268	A
25	CA	1269	A
25	CA	1271	G
25	CA	1272	A
25	CA	1273	U
25	CA	1294	U
25	CA	1300	G
25	CA	1301	A
25	CA	1313	U
25	CA	1317	G
25	CA	1321	A
25	CA	1340	U
25	CA	1344	U
25	CA	1345	C
25	CA	1346	G
25	CA	1352	U
25	CA	1365	A
25	CA	1368	G
25	CA	1371	G
25	CA	1379	U
25	CA	1380	G
25	CA	1383	A
25	CA	1395	A
25	CA	1403	A

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Mol	Chain	Res	Type
25	CA	1406	U
25	CA	1416	G
25	CA	1419	A
25	CA	1420	A
25	CA	1424	G
25	CA	1427	A
25	CA	1428	C
25	CA	1429	G
25	CA	1433	A
25	CA	1434	A
25	CA	1444	G
25	CA	1452	G
25	CA	1453	A
25	CA	1455	G
25	CA	1460	U
25	CA	1461	C
25	CA	1467	U
25	CA	1474	U
25	CA	1476	U
25	CA	1482	G
25	CA	1494	A
25	CA	1495	A
25	CA	1504	A
25	CA	1508	A
25	CA	1509	A
25	CA	1510	G
25	CA	1515	A
25	CA	1519	G
25	CA	1524	G
25	CA	1528	A
25	CA	1532	A
25	CA	1533	C
25	CA	1534	U
25	CA	1535	A
25	CA	1536	C
25	CA	1537	G
25	CA	1541	C
25	CA	1560	G
25	CA	1562	U
25	CA	1566	A
25	CA	1569	A
25	CA	1578	U

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Mol	Chain	Res	Type
25	CA	1581	G
25	CA	1582	C
25	CA	1585	C
25	CA	1586	A
25	CA	1607	C
25	CA	1608	A
25	CA	1610	A
25	CA	1647	U
25	CA	1648	U
25	CA	1649	G
25	CA	1651	G
25	CA	1654	A
25	CA	1661	G
25	CA	1664	A
25	CA	1674	G
25	CA	1677	A
25	CA	1714	U
25	CA	1715	G
25	CA	1729	U
25	CA	1730	C
25	CA	1731	G
25	CA	1732	C
25	CA	1735	A
25	CA	1737	G
25	CA	1738	G
25	CA	1739	A
25	CA	1757	A
25	CA	1764	C
25	CA	1765	U
25	CA	1772	A
25	CA	1773	A
25	CA	1775	U
25	CA	1791	A
25	CA	1800	C
25	CA	1801	A
25	CA	1803	A
25	CA	1808	A
25	CA	1809	A
25	CA	1811	G
25	CA	1816	C
25	CA	1819	A
25	CA	1829	A

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Mol	Chain	Res	Type
25	CA	1830	C
25	CA	1836	C
25	CA	1839	G
25	CA	1847	A
25	CA	1848	A
25	CA	1858	A
25	CA	1859	U
25	CA	1867	G
25	CA	1869	G
25	CA	1870	C
25	CA	1872	A
25	CA	1873	G
25	CA	1885	A
25	CA	1906	G
25	CA	1908	C
25	CA	1913	A
25	CA	1915	U
25	CA	1930	G
25	CA	1937	A
25	CA	1938	A
25	CA	1955	U
25	CA	1961	C
25	CA	1964	G
25	CA	1965	C
25	CA	1967	C
25	CA	1970	A
25	CA	1971	U
25	CA	1972	G
25	CA	1980	G
25	CA	1991	U
25	CA	1993	U
25	CA	1995	U
25	CA	1996	C
25	CA	1997	C
25	CA	2017	U
25	CA	2020	A
25	CA	2023	C
25	CA	2025	C
25	CA	2026	U
25	CA	2031	A
25	CA	2033	A
25	CA	2034	U

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Mol	Chain	Res	Type
25	CA	2043	C
25	CA	2049	G
25	CA	2051	A
25	CA	2055	C
25	CA	2056	G
25	CA	2060	A
25	CA	2061	G
25	CA	2062	A
25	CA	2069	G
25	CA	2070	A
25	CA	2072	C
25	CA	2080	A
25	CA	2081	U
25	CA	2093	G
25	CA	2095	A
25	CA	2096	C
25	CA	2101	A
25	CA	2109	U
25	CA	2110	G
25	CA	2111	U
25	CA	2112	G
25	CA	2113	U
25	CA	2115	G
25	CA	2117	A
25	CA	2118	U
25	CA	2119	A
25	CA	2120	G
25	CA	2122	U
25	CA	2123	G
25	CA	2125	G
25	CA	2126	A
25	CA	2127	G
25	CA	2128	G
25	CA	2131	U
25	CA	2132	U
25	CA	2133	G
25	CA	2138	G
25	CA	2139	U
25	CA	2144	G
25	CA	2146	C
25	CA	2147	A
25	CA	2158	A

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Mol	Chain	Res	Type
25	CA	2159	G
25	CA	2160	C
25	CA	2161	C
25	CA	2163	A
25	CA	2164	C
25	CA	2165	C
25	CA	2167	U
25	CA	2169	A
25	CA	2171	A
25	CA	2172	U
25	CA	2173	A
25	CA	2184	A
25	CA	2185	U
25	CA	2189	U
25	CA	2190	G
25	CA	2191	A
25	CA	2195	U
25	CA	2198	A
25	CA	2204	G
25	CA	2211	A
25	CA	2212	A
25	CA	2213	U
25	CA	2214	C
25	CA	2225	A
25	CA	2238	G
25	CA	2239	G
25	CA	2250	G
25	CA	2268	A
25	CA	2278	A
25	CA	2283	C
25	CA	2286	G
25	CA	2287	A
25	CA	2288	A
25	CA	2289	G
25	CA	2297	A
25	CA	2298	A
25	CA	2299	U
25	CA	2304	G
25	CA	2305	U
25	CA	2307	G
25	CA	2308	G
25	CA	2309	A

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Mol	Chain	Res	Type
25	CA	2311	A
25	CA	2312	U
25	CA	2320	U
25	CA	2321	U
25	CA	2322	A
25	CA	2325	G
25	CA	2327	A
25	CA	2331	G
25	CA	2333	A
25	CA	2334	U
25	CA	2343	U
25	CA	2347	C
25	CA	2350	C
25	CA	2358	A
25	CA	2378	A
25	CA	2383	G
25	CA	2385	C
25	CA	2392	A
25	CA	2402	U
25	CA	2403	C
25	CA	2406	A
25	CA	2419	U
25	CA	2422	C
25	CA	2423	U
25	CA	2425	A
25	CA	2426	A
25	CA	2429	G
25	CA	2430	A
25	CA	2431	U
25	CA	2433	A
25	CA	2434	A
25	CA	2435	A
25	CA	2441	U
25	CA	2445	G
25	CA	2448	A
25	CA	2473	U
25	CA	2476	A
25	CA	2484	G
25	CA	2491	U
25	CA	2498	C
25	CA	2502	G
25	CA	2505	G

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Mol	Chain	Res	Type
25	CA	2513	A
25	CA	2518	A
25	CA	2520	C
25	CA	2523	G
25	CA	2524	G
25	CA	2529	G
25	CA	2534	A
25	CA	2535	G
25	CA	2546	U
25	CA	2547	A
25	CA	2554	U
25	CA	2566	A
25	CA	2567	G
25	CA	2569	G
25	CA	2572	A
25	CA	2573	C
25	CA	2582	G
25	CA	2585	U
25	CA	2586	U
25	CA	2602	A
25	CA	2603	G
25	CA	2604	U
25	CA	2608	G
25	CA	2609	U
25	CA	2611	C
25	CA	2613	U
25	CA	2629	U
25	CA	2646	C
25	CA	2661	G
25	CA	2663	G
25	CA	2681	C
25	CA	2689	U
25	CA	2690	U
25	CA	2704	C
25	CA	2716	C
25	CA	2718	G
25	CA	2720	U
25	CA	2721	A
25	CA	2726	A
25	CA	2729	G
25	CA	2744	G
25	CA	2748	A

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Mol	Chain	Res	Type
25	CA	2749	A
25	CA	2751	G
25	CA	2755	C
25	CA	2757	A
25	CA	2758	A
25	CA	2762	C
25	CA	2778	A
25	CA	2791	G
25	CA	2792	A
25	CA	2793	C
25	CA	2818	U
25	CA	2820	A
25	CA	2821	A
25	CA	2833	U
25	CA	2834	G
25	CA	2835	A
25	CA	2836	U
25	CA	2849	U
25	CA	2861	U
25	CA	2863	C
25	CA	2867	G
25	CA	2873	A
25	CA	2880	C
25	CA	2883	A
25	CA	2884	U
25	CA	2886	A
25	CA	2891	U
25	CA	2893	A
25	CA	2894	G
25	CA	2895	G
25	CA	2903	U
26	CB	3008	C
26	CB	3009	G
26	CB	3011	C
26	CB	3013	G
26	CB	3015	A
26	CB	3016	G
26	CB	3024	G
26	CB	3027	C
26	CB	3035	C
26	CB	3041	G
26	CB	3042	C

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Mol	Chain	Res	Type
26	CB	3044	G
26	CB	3047	C
26	CB	3049	C
26	CB	3050	A
26	CB	3051	G
26	CB	3056	G
26	CB	3067	G
26	CB	3085	G
26	CB	3088	C
26	CB	3089	U
26	CB	3090	C
26	CB	3091	C
26	CB	3099	A
26	CB	3109	A
26	CB	3116	G
26	CB	3118	C
1	DA	3	A
1	DA	4	U
1	DA	6	G
1	DA	9	G
1	DA	31	G
1	DA	32	A
1	DA	33	A
1	DA	39	G
1	DA	44	A
1	DA	47	C
1	DA	48	C
1	DA	49	U
1	DA	50	A
1	DA	51	A
1	DA	54	C
1	DA	70	U
1	DA	71	A
1	DA	75	G
1	DA	77	A
1	DA	83	C
1	DA	84	U
1	DA	85	U
1	DA	87	C
1	DA	92	U
1	DA	94	G
1	DA	97	G

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Mol	Chain	Res	Type
1	DA	98	A
1	DA	106	C
1	DA	108	G
1	DA	110	C
1	DA	111	G
1	DA	115	G
1	DA	120	A
1	DA	121	U
1	DA	122	G
1	DA	130	A
1	DA	131	A
1	DA	132	C
1	DA	134	G
1	DA	143	A
1	DA	156	C
1	DA	163	C
1	DA	168	G
1	DA	177	G
1	DA	181	A
1	DA	183	C
1	DA	189	A
1	DA	199	A
1	DA	204	G
1	DA	205	A
1	DA	206	C
1	DA	209	U
1	DA	210	C
1	DA	211	G
1	DA	212	G
1	DA	240	G
1	DA	245	U
1	DA	247	G
1	DA	249	U
1	DA	251	G
1	DA	253	A
1	DA	254	G
1	DA	262	A
1	DA	266	G
1	DA	267	C
1	DA	279	A
1	DA	289	G
1	DA	293	G

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Mol	Chain	Res	Type
1	DA	321	A
1	DA	328	C
1	DA	346	G
1	DA	347	G
1	DA	351	G
1	DA	352	C
1	DA	354	G
1	DA	356	A
1	DA	359	G
1	DA	367	U
1	DA	368	U
1	DA	372	C
1	DA	373	A
1	DA	382	A
1	DA	384	G
1	DA	388	G
1	DA	392	C
1	DA	398	U
1	DA	406	G
1	DA	411	A
1	DA	414	A
1	DA	421	U
1	DA	423	G
1	DA	428	G
1	DA	429	U
1	DA	430	A
1	DA	437	U
1	DA	446	G
1	DA	451	A
1	DA	452	A
1	DA	463	U
1	DA	466	A
1	DA	467	U
1	DA	468	A
1	DA	469	C
1	DA	474	G
1	DA	481	G
1	DA	484	G
1	DA	485	U
1	DA	486	U
1	DA	495	A
1	DA	500	G

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Mol	Chain	Res	Type
1	DA	508	U
1	DA	511	C
1	DA	518	C
1	DA	519	C
1	DA	524	G
1	DA	526	C
1	DA	529	G
1	DA	530	G
1	DA	532	A
1	DA	533	A
1	DA	547	A
1	DA	550	G
1	DA	561	U
1	DA	562	U
1	DA	564	C
1	DA	571	U
1	DA	572	A
1	DA	573	A
1	DA	576	C
1	DA	577	G
1	DA	579	A
1	DA	596	A
1	DA	599	C
1	DA	600	A
1	DA	615	G
1	DA	619	U
1	DA	639	G
1	DA	649	A
1	DA	650	G
1	DA	653	U
1	DA	661	G
1	DA	665	A
1	DA	695	A
1	DA	703	G
1	DA	710	G
1	DA	723	U
1	DA	724	G
1	DA	731	G
1	DA	733	G
1	DA	734	G
1	DA	742	G
1	DA	747	A

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Mol	Chain	Res	Type
1	DA	748	G
1	DA	750	C
1	DA	755	G
1	DA	764	C
1	DA	765	G
1	DA	777	A
1	DA	778	G
1	DA	792	A
1	DA	793	U
1	DA	794	A
1	DA	811	C
1	DA	814	A
1	DA	815	A
1	DA	817	C
1	DA	819	A
1	DA	820	U
1	DA	821	G
1	DA	828	U
1	DA	832	G
1	DA	841	C
1	DA	842	U
1	DA	843	U
1	DA	844	G
1	DA	845	A
1	DA	846	G
1	DA	849	G
1	DA	859	G
1	DA	887	G
1	DA	914	A
1	DA	922	G
1	DA	933	G
1	DA	934	C
1	DA	935	A
1	DA	945	G
1	DA	958	A
1	DA	960	U
1	DA	961	U
1	DA	969	A
1	DA	972	C
1	DA	975	A
1	DA	976	G
1	DA	977	A

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Mol	Chain	Res	Type
1	DA	980	C
1	DA	981	U
1	DA	983	A
1	DA	992	U
1	DA	993	G
1	DA	1004	A
1	DA	1005	A
1	DA	1006	G
1	DA	1007	U
1	DA	1008	U
1	DA	1009	U
1	DA	1018	G
1	DA	1019	A
1	DA	1021	A
1	DA	1022	A
1	DA	1025	U
1	DA	1026	G
1	DA	1027	C
1	DA	1028	C
1	DA	1030	U
1	DA	1032	G
1	DA	1033	G
1	DA	1036	A
1	DA	1043	G
1	DA	1065	U
1	DA	1069	C
1	DA	1070	U
1	DA	1073	U
1	DA	1080	A
1	DA	1086	U
1	DA	1087	G
1	DA	1088	G
1	DA	1092	A
1	DA	1094	G
1	DA	1095	U
1	DA	1101	A
1	DA	1102	A
1	DA	1123	U
1	DA	1125	U
1	DA	1126	U
1	DA	1127	G
1	DA	1133	G

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Mol	Chain	Res	Type
1	DA	1135	U
1	DA	1136	C
1	DA	1137	C
1	DA	1138	G
1	DA	1139	G
1	DA	1140	C
1	DA	1141	C
1	DA	1142	G
1	DA	1143	G
1	DA	1146	A
1	DA	1158	C
1	DA	1159	U
1	DA	1168	U
1	DA	1181	G
1	DA	1183	U
1	DA	1184	G
1	DA	1191	A
1	DA	1196	A
1	DA	1197	A
1	DA	1201	A
1	DA	1212	U
1	DA	1213	A
1	DA	1227	A
1	DA	1233	G
1	DA	1238	A
1	DA	1240	U
1	DA	1241	G
1	DA	1245	C
1	DA	1250	A
1	DA	1253	G
1	DA	1256	A
1	DA	1257	A
1	DA	1260	G
1	DA	1261	A
1	DA	1275	A
1	DA	1280	A
1	DA	1282	C
1	DA	1286	U
1	DA	1287	A
1	DA	1293	C
1	DA	1299	A
1	DA	1300	G

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Mol	Chain	Res	Type
1	DA	1302	C
1	DA	1305	G
1	DA	1308	U
1	DA	1317	C
1	DA	1318	A
1	DA	1319	A
1	DA	1320	C
1	DA	1321	U
1	DA	1322	C
1	DA	1326	U
1	DA	1336	C
1	DA	1338	G
1	DA	1346	A
1	DA	1353	G
1	DA	1362	A
1	DA	1363	A
1	DA	1364	U
1	DA	1368	A
1	DA	1370	G
1	DA	1378	C
1	DA	1379	G
1	DA	1402	C
1	DA	1414	U
1	DA	1419	G
1	DA	1433	A
1	DA	1434	A
1	DA	1441	A
1	DA	1442	G
1	DA	1446	A
1	DA	1452	C
1	DA	1454	G
1	DA	1457	G
1	DA	1461	G
1	DA	1463	U
1	DA	1478	U
1	DA	1487	G
1	DA	1492	A
1	DA	1494	G
1	DA	1497	G
1	DA	1499	A
1	DA	1503	A
1	DA	1506	U

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Mol	Chain	Res	Type
1	DA	1517	G
1	DA	1519	A
1	DA	1520	C
1	DA	1529	G
1	DA	1530	G
1	DA	1531	A
1	DA	1534	A
1	DA	1535	C
1	DA	1536	C
1	DA	1540	U
23	DV	5	A
23	DV	7	G
23	DV	9	A
23	DV	10	A
23	DV	11	A
23	DV	16	U
24	DW	17	C
24	DW	18	G
24	DW	19	G
24	DW	20	U
24	DW	21	A
24	DW	22	G
24	DW	33	U
24	DW	35	A
24	DW	36	A
24	DW	37	A
24	DW	44	G
24	DW	45	U
24	DW	46	G
24	DW	47	U
24	DW	48	C
24	DW	52	G
24	DW	53	G
24	DW	60	U
24	DW	62	C
24	DW	76	A

All (107) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	79	G
1	AA	115	G

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Mol	Chain	Res	Type
1	AA	351	G
1	AA	702	A
1	AA	738	C
1	AA	819	A
1	AA	859	G
1	AA	1145	A
1	AA	1211	U
1	AA	1279	G
1	AA	1299	A
1	AA	1317	C
1	AA	1377	A
1	AA	1493	A
1	AA	1533	C
24	AX	4	C
24	AX	44	G
24	AX	47	U
24	AX	72	C
24	AX	73	A
24	AX	75	C
25	BA	60	G
25	BA	139	U
25	BA	190	A
25	BA	265	A
25	BA	477	A
25	BA	544	C
25	BA	647	G
25	BA	715	A
25	BA	746	U
25	BA	764	A
25	BA	784	G
25	BA	859	G
25	BA	892	A
25	BA	984	A
25	BA	1358	G
25	BA	1378	A
25	BA	1420	A
25	BA	1452	G
25	BA	1501	G
25	BA	1606	C
25	BA	1617	C
25	BA	1757	A
25	BA	1875	G

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Mol	Chain	Res	Type
25	BA	1928	A
25	BA	2116	G
25	BA	2159	G
25	BA	2211	A
25	BA	2324	U
25	BA	2326	C
25	BA	2406	A
25	BA	2422	C
25	BA	2549	G
25	BA	2680	U
25	BA	2756	U
25	BA	2873	A
25	CA	271	G
25	CA	310	A
25	CA	404	A
25	CA	479	A
25	CA	509	C
25	CA	546	U
25	CA	669	G
25	CA	748	G
25	CA	764	A
25	CA	784	G
25	CA	846	U
25	CA	984	A
25	CA	1089	A
25	CA	1288	G
25	CA	1378	A
25	CA	1606	C
25	CA	1730	C
25	CA	1738	G
25	CA	1802	A
25	CA	1847	A
25	CA	1905	C
25	CA	2016	U
25	CA	2211	A
25	CA	2282	G
25	CA	2311	A
25	CA	2326	C
25	CA	2418	A
25	CA	2425	A
25	CA	2680	U
25	CA	2703	C

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Mol	Chain	Res	Type
25	CA	2748	A
25	CA	2756	U
25	CA	2790	U
25	CA	2820	A
1	DA	96	U
1	DA	114	U
1	DA	346	G
1	DA	421	U
1	DA	429	U
1	DA	484	G
1	DA	652	U
1	DA	709	U
1	DA	723	U
1	DA	841	C
1	DA	1069	C
1	DA	1079	G
1	DA	1101	A
1	DA	1134	G
1	DA	1145	A
1	DA	1281	C
1	DA	1286	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 510 ligands modelled in this entry, 497 are monoatomic - leaving 13 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	PAR	CA	3169	-	45,45,45	0.49	0	64,67,67	0.95	4 (6%)
58	PAR	BA	3002	-	45,45,45	0.79	1 (2%)	64,67,67	0.99	3 (4%)
58	PAR	CA	3168	-	45,45,45	0.54	0	64,67,67	1.33	5 (7%)
58	PAR	CA	3166	-	45,45,45	0.49	0	64,67,67	0.95	4 (6%)
58	PAR	BA	3001	-	45,45,45	0.71	0	64,67,67	1.04	5 (7%)
58	PAR	BA	3005	-	45,45,45	0.54	0	64,67,67	1.10	4 (6%)
58	PAR	BA	3004	-	45,45,45	0.71	0	64,67,67	1.05	5 (7%)
58	PAR	AA	1672	-	45,45,45	0.77	0	64,67,67	1.14	4 (6%)
58	PAR	BA	3003	-	45,45,45	0.74	0	64,67,67	1.08	5 (7%)
58	PAR	CA	3167	-	45,45,45	0.57	0	64,67,67	0.89	3 (4%)
58	PAR	DA	1654	-	45,45,45	0.53	0	64,67,67	0.83	2 (3%)
58	PAR	CA	3170	-	45,45,45	0.50	0	64,67,67	0.94	4 (6%)
58	PAR	DA	1655	-	45,45,45	0.50	0	64,67,67	0.92	3 (4%)

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	PAR	CA	3169	-	-	4/18/94/94	0/4/4/4
58	PAR	BA	3002	-	-	6/18/94/94	0/4/4/4
58	PAR	CA	3168	-	-	1/18/94/94	0/4/4/4
58	PAR	CA	3166	-	-	2/18/94/94	0/4/4/4
58	PAR	BA	3001	-	-	6/18/94/94	0/4/4/4
58	PAR	BA	3005	-	-	7/18/94/94	0/4/4/4
58	PAR	BA	3004	-	-	7/18/94/94	0/4/4/4
58	PAR	AA	1672	-	-	8/18/94/94	0/4/4/4
58	PAR	BA	3003	-	-	8/18/94/94	0/4/4/4
58	PAR	CA	3167	-	-	3/18/94/94	0/4/4/4
58	PAR	DA	1654	-	-	1/18/94/94	0/4/4/4
58	PAR	CA	3170	-	-	3/18/94/94	0/4/4/4
58	PAR	DA	1655	-	-	3/18/94/94	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	BA	3002	PAR	C13-C23	-2.04	1.50	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	CA	3168	PAR	C14-O33-C33	-4.52	106.77	117.96
58	CA	3168	PAR	C11-O11-C42	-4.50	106.83	117.96
58	CA	3168	PAR	C13-O52-C52	-4.48	106.88	117.96
58	BA	3004	PAR	O52-C13-O43	-3.78	107.33	111.43
58	BA	3005	PAR	C13-O52-C52	-3.61	109.03	117.96
58	CA	3170	PAR	C13-C23-C33	3.28	106.04	102.10
58	DA	1655	PAR	C13-C23-C33	3.22	105.97	102.10
58	CA	3166	PAR	C13-C23-C33	3.16	105.91	102.10
58	CA	3168	PAR	C11-O51-C51	-3.14	107.52	113.69
58	CA	3169	PAR	C13-C23-C33	3.13	105.87	102.10
58	AA	1672	PAR	C14-O33-C33	-3.11	110.28	117.96
58	CA	3168	PAR	C14-O54-C54	-3.04	107.71	113.69
58	BA	3003	PAR	C22-C12-C62	2.98	114.54	110.04
58	BA	3005	PAR	C11-O11-C42	-2.82	110.98	117.96
58	BA	3004	PAR	O54-C54-C64	2.81	111.23	106.01
58	CA	3167	PAR	C13-C23-C33	2.72	105.37	102.10
58	BA	3001	PAR	O52-C13-O43	-2.60	108.61	111.43
58	BA	3003	PAR	C52-C62-C12	2.53	115.81	109.63
58	CA	3166	PAR	C14-O33-C33	-2.50	111.78	117.96
58	CA	3169	PAR	C13-O52-C52	-2.50	111.79	117.96
58	CA	3169	PAR	C11-O11-C42	-2.49	111.80	117.96
58	CA	3169	PAR	C14-O33-C33	-2.49	111.81	117.96
58	CA	3166	PAR	C11-O11-C42	-2.48	111.83	117.96
58	CA	3166	PAR	C13-O52-C52	-2.47	111.85	117.96
58	BA	3005	PAR	O52-C13-C23	2.47	113.07	107.96
58	DA	1655	PAR	C14-O33-C33	-2.45	111.91	117.96
58	BA	3004	PAR	C14-O33-C33	-2.41	112.00	117.96
58	BA	3003	PAR	O54-C54-C64	2.39	110.45	106.01
58	AA	1672	PAR	C13-O52-C52	-2.34	112.16	117.96
58	BA	3005	PAR	C31-C41-C51	2.30	114.33	110.24
58	BA	3001	PAR	C11-O11-C42	-2.27	112.34	117.96
58	CA	3170	PAR	O43-C13-C23	2.26	107.89	104.98
58	BA	3001	PAR	C14-O33-C33	-2.22	112.46	117.96
58	BA	3001	PAR	C61-C51-C41	-2.21	107.82	113.00
58	BA	3002	PAR	C22-C12-C62	-2.20	106.72	110.04
58	BA	3004	PAR	C64-C54-C44	-2.14	108.89	113.10
58	BA	3002	PAR	C13-O52-C52	-2.14	112.67	117.96
58	BA	3002	PAR	O52-C13-C23	2.14	112.39	107.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	CA	3167	PAR	C14-O33-C33	-2.12	112.72	117.96
58	BA	3001	PAR	O11-C42-C52	2.12	112.86	107.48
58	CA	3167	PAR	O43-C13-C23	2.12	107.71	104.98
58	BA	3003	PAR	C62-C12-N12	-2.11	106.79	110.97
58	AA	1672	PAR	C22-C12-C62	-2.11	106.85	110.04
58	BA	3004	PAR	O43-C13-C23	2.11	107.69	104.98
58	DA	1654	PAR	C13-O52-C52	-2.10	112.77	117.96
58	DA	1655	PAR	C13-O52-C52	-2.07	112.85	117.96
58	DA	1654	PAR	O54-C54-C64	2.06	109.85	106.01
58	CA	3170	PAR	O54-C54-C64	2.05	109.83	106.01
58	CA	3170	PAR	C14-O33-C33	-2.05	112.89	117.96
58	BA	3003	PAR	O52-C13-O43	-2.05	109.21	111.43
58	AA	1672	PAR	O52-C13-C23	2.05	112.20	107.96

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BA	3003	PAR	C23-C13-O52-C52
58	BA	3003	PAR	O43-C13-O52-C52
58	BA	3003	PAR	C24-C14-O33-C33
58	BA	3003	PAR	C44-C54-C64-N64
58	BA	3003	PAR	O54-C54-C64-N64
58	CA	3169	PAR	O54-C54-C64-N64
58	BA	3004	PAR	C23-C13-O52-C52
58	BA	3004	PAR	O43-C13-O52-C52
58	BA	3004	PAR	C24-C14-O33-C33
58	BA	3005	PAR	C23-C13-O52-C52
58	BA	3001	PAR	C23-C13-O52-C52
58	BA	3001	PAR	C24-C14-O33-C33
58	CA	3169	PAR	C52-C42-O11-C11
58	AA	1672	PAR	O51-C51-C61-O61
58	AA	1672	PAR	C41-C51-C61-O61
58	BA	3005	PAR	C33-C43-C53-O53
58	BA	3003	PAR	O51-C51-C61-O61
58	BA	3003	PAR	C41-C51-C61-O61
58	BA	3005	PAR	O43-C43-C53-O53
58	BA	3001	PAR	O54-C14-O33-C33
58	CA	3170	PAR	O54-C14-O33-C33
58	BA	3004	PAR	O54-C14-O33-C33
58	CA	3170	PAR	O43-C13-O52-C52
58	BA	3001	PAR	O43-C13-O52-C52

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Mol	Chain	Res	Type	Atoms
58	CA	3166	PAR	O51-C51-C61-O61
58	DA	1655	PAR	O54-C14-O33-C33
58	AA	1672	PAR	O43-C43-C53-O53
58	BA	3004	PAR	C42-C52-O52-C13
58	BA	3004	PAR	C62-C52-O52-C13
58	CA	3167	PAR	O43-C13-O52-C52
58	AA	1672	PAR	O43-C13-O52-C52
58	BA	3005	PAR	O43-C13-O52-C52
58	AA	1672	PAR	C33-C43-C53-O53
58	DA	1655	PAR	C23-C13-O52-C52
58	CA	3167	PAR	C23-C13-O52-C52
58	BA	3002	PAR	C23-C13-O52-C52
58	AA	1672	PAR	C23-C13-O52-C52
58	CA	3170	PAR	C23-C13-O52-C52
58	BA	3002	PAR	O54-C54-C64-N64
58	AA	1672	PAR	O54-C54-C64-N64
58	BA	3005	PAR	O54-C54-C64-N64
58	CA	3168	PAR	O54-C14-O33-C33
58	BA	3005	PAR	O51-C11-O11-C42
58	BA	3002	PAR	O54-C14-O33-C33
58	CA	3169	PAR	O54-C14-O33-C33
58	CA	3166	PAR	O54-C14-O33-C33
58	BA	3002	PAR	O43-C43-C53-O53
58	BA	3005	PAR	C44-C54-C64-N64
58	BA	3002	PAR	C52-C42-O11-C11
58	AA	1672	PAR	C52-C42-O11-C11
58	BA	3001	PAR	C41-C51-C61-O61
58	DA	1655	PAR	O43-C13-O52-C52
58	BA	3002	PAR	C33-C43-C53-O53
58	BA	3003	PAR	C23-C33-O33-C14
58	CA	3167	PAR	C43-C33-O33-C14
58	BA	3001	PAR	C43-C33-O33-C14
58	BA	3004	PAR	C21-C11-O11-C42
58	CA	3169	PAR	C62-C52-O52-C13
58	DA	1654	PAR	C52-C42-O11-C11

There are no ring outliers.

13 monomers are involved in 106 short contacts:

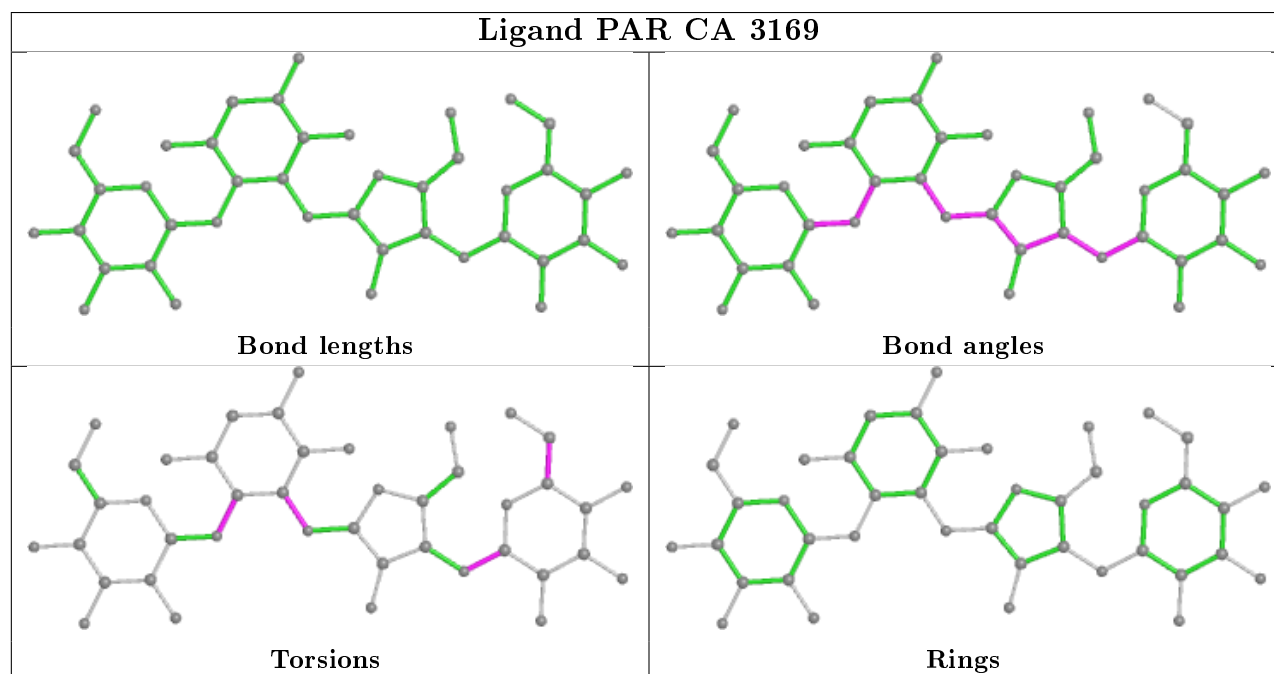
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	CA	3169	PAR	20	0
58	BA	3002	PAR	2	0

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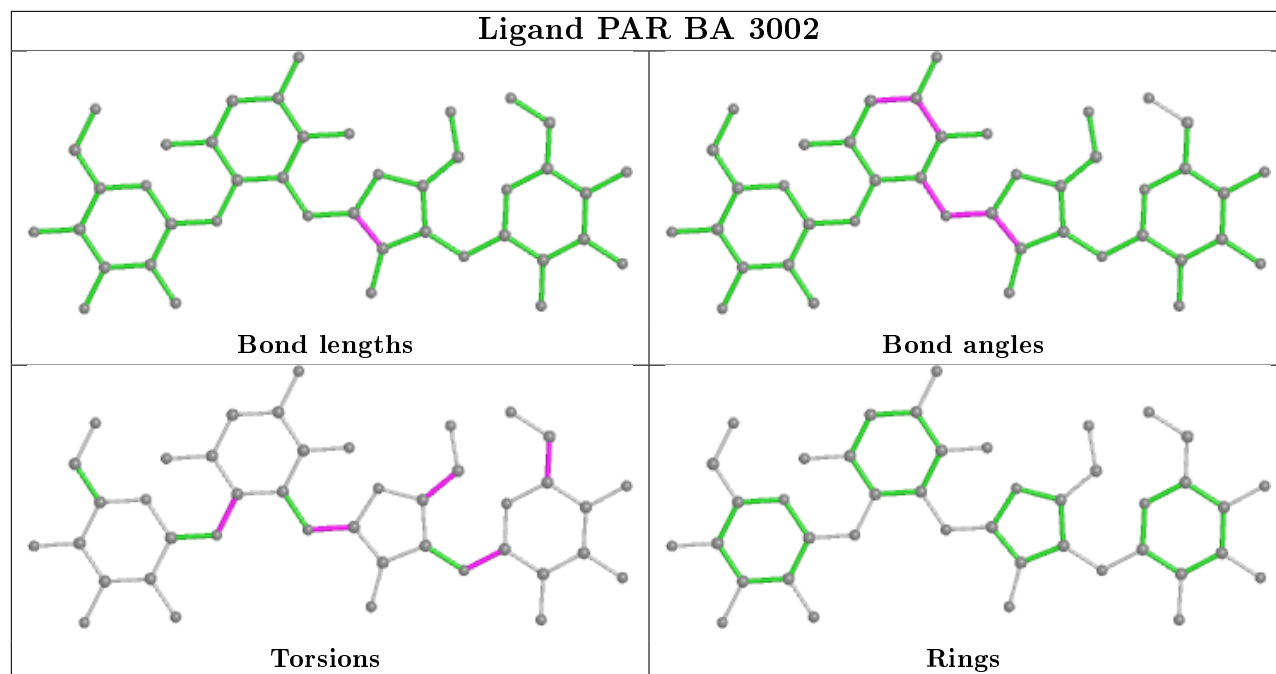
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	CA	3168	PAR	5	0
58	CA	3166	PAR	14	0
58	BA	3001	PAR	3	0
58	BA	3005	PAR	21	0
58	BA	3004	PAR	3	0
58	AA	1672	PAR	9	0
58	BA	3003	PAR	4	0
58	CA	3167	PAR	7	0
58	DA	1654	PAR	5	0
58	CA	3170	PAR	5	0
58	DA	1655	PAR	8	0

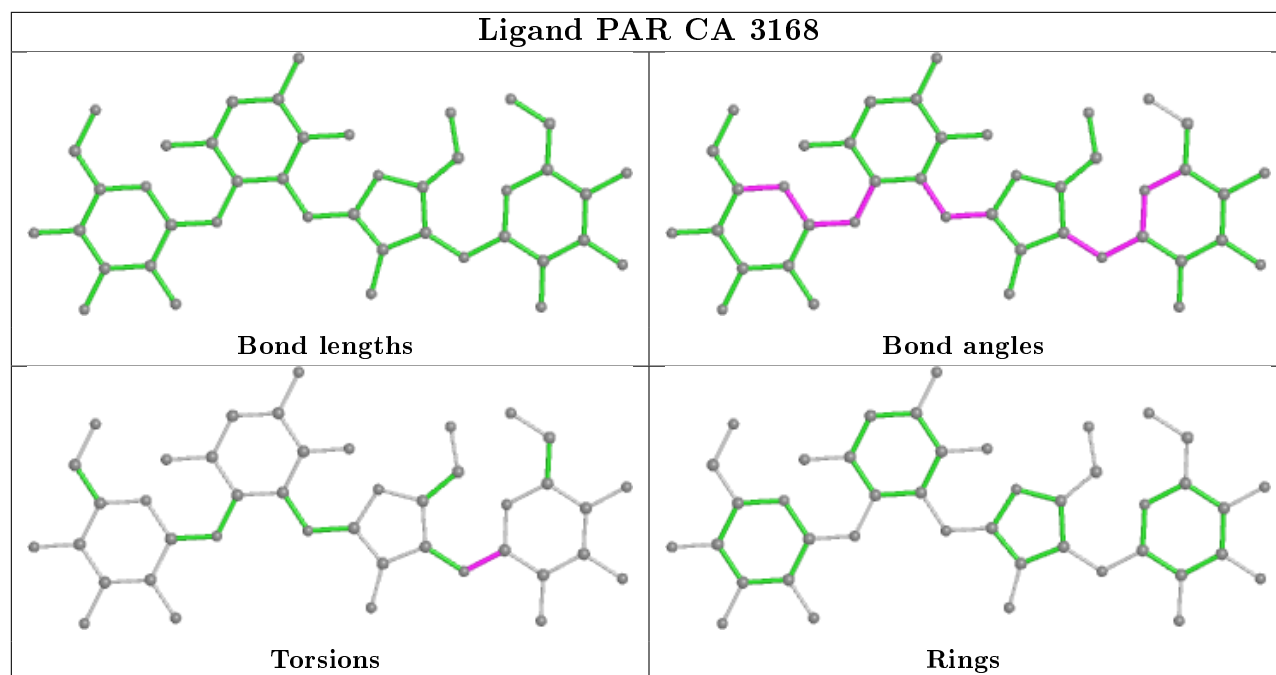
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



## Ligand PAR BA 3002

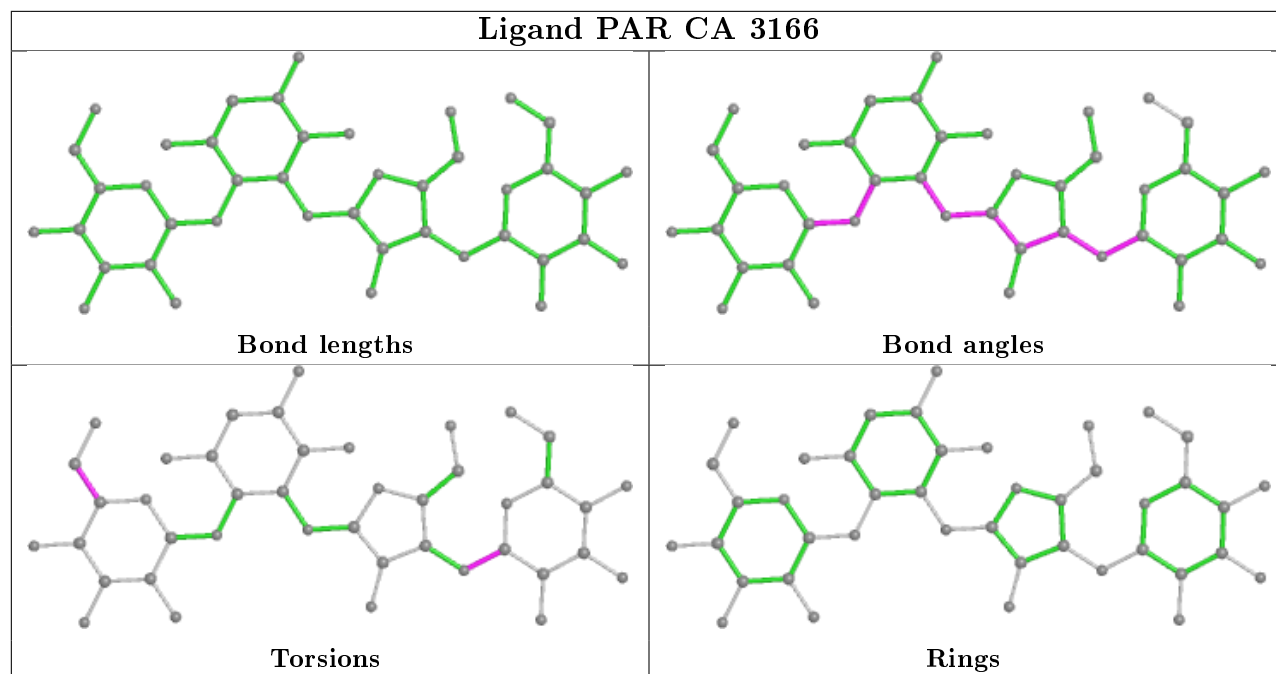


## Ligand PAR CA 3168

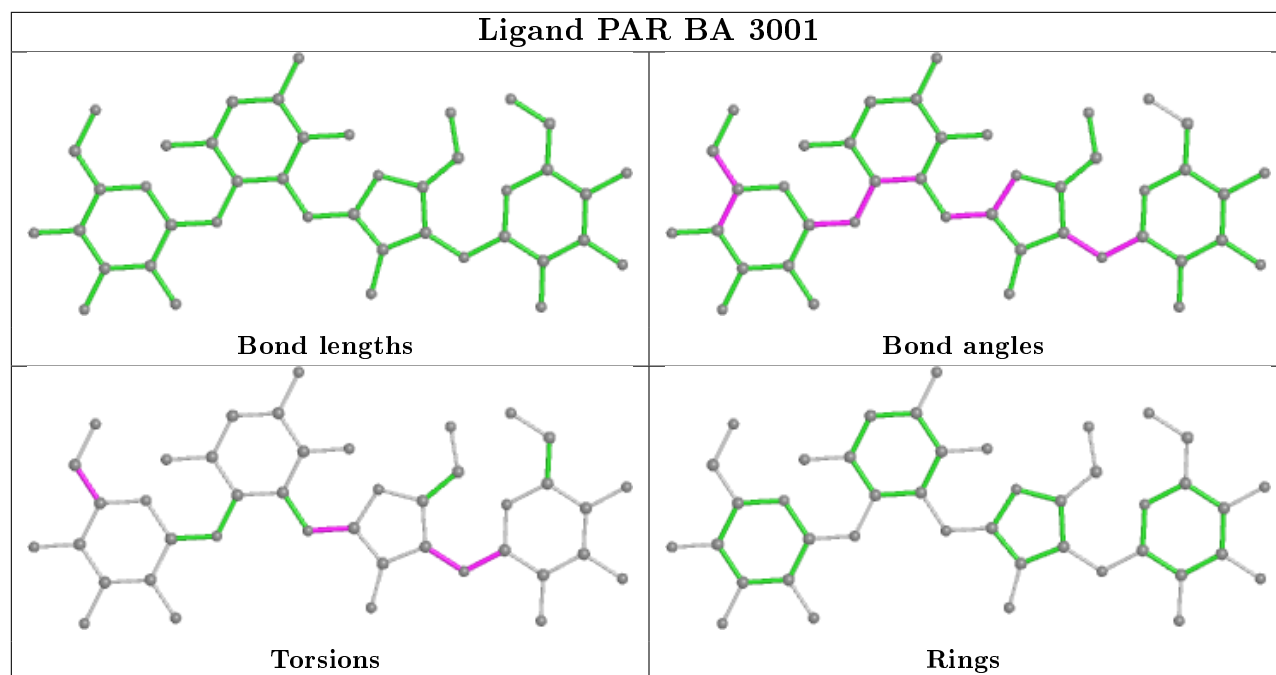




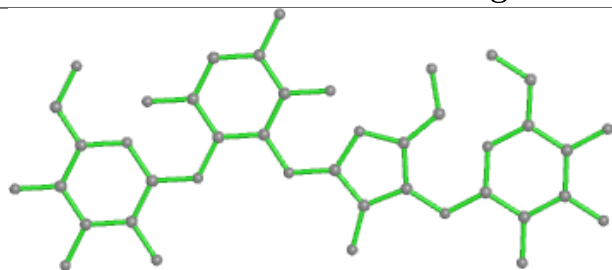
## Ligand PAR CA 3166



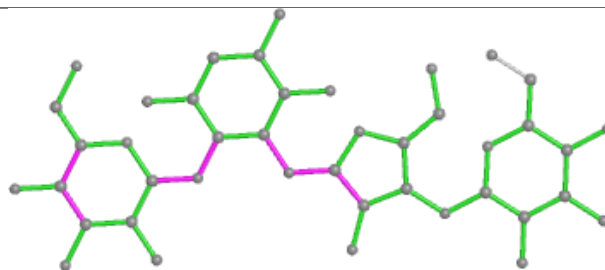
## Ligand PAR BA 3001



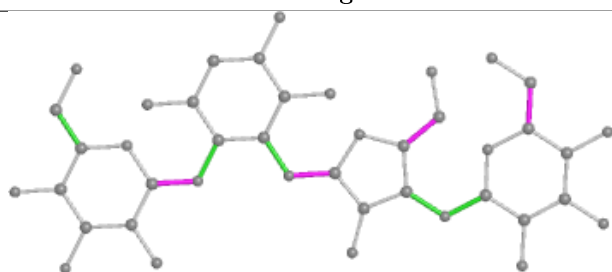
## Ligand PAR BA 3005



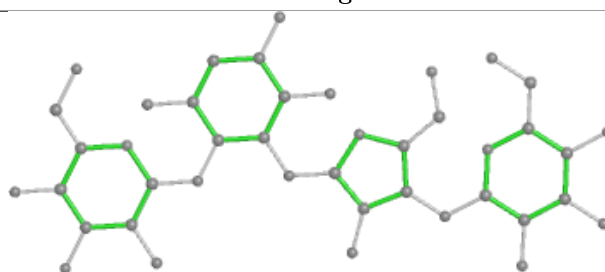
Bond lengths



Bond angles

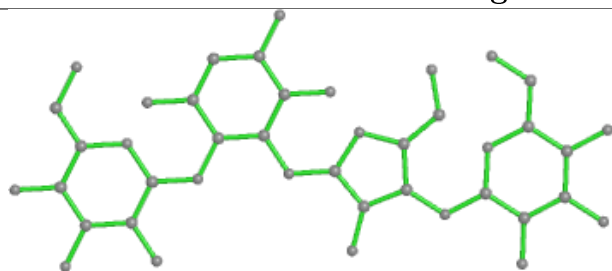


Torsions

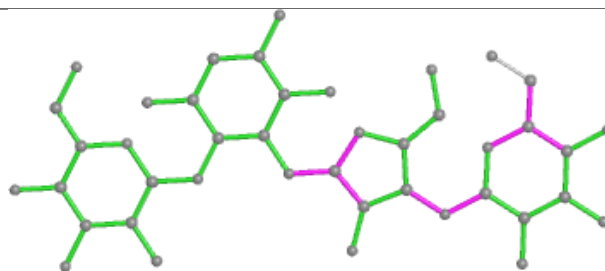


Rings

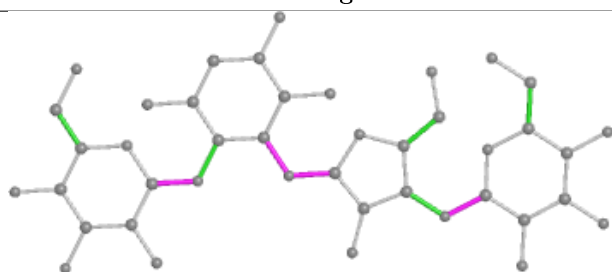
## Ligand PAR BA 3004



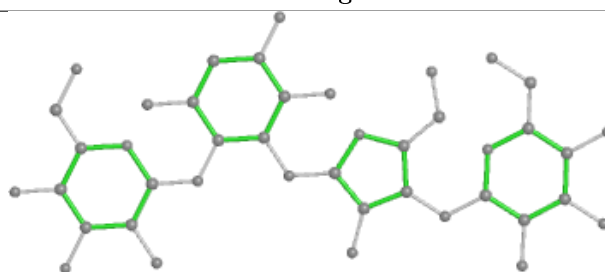
Bond lengths



Bond angles

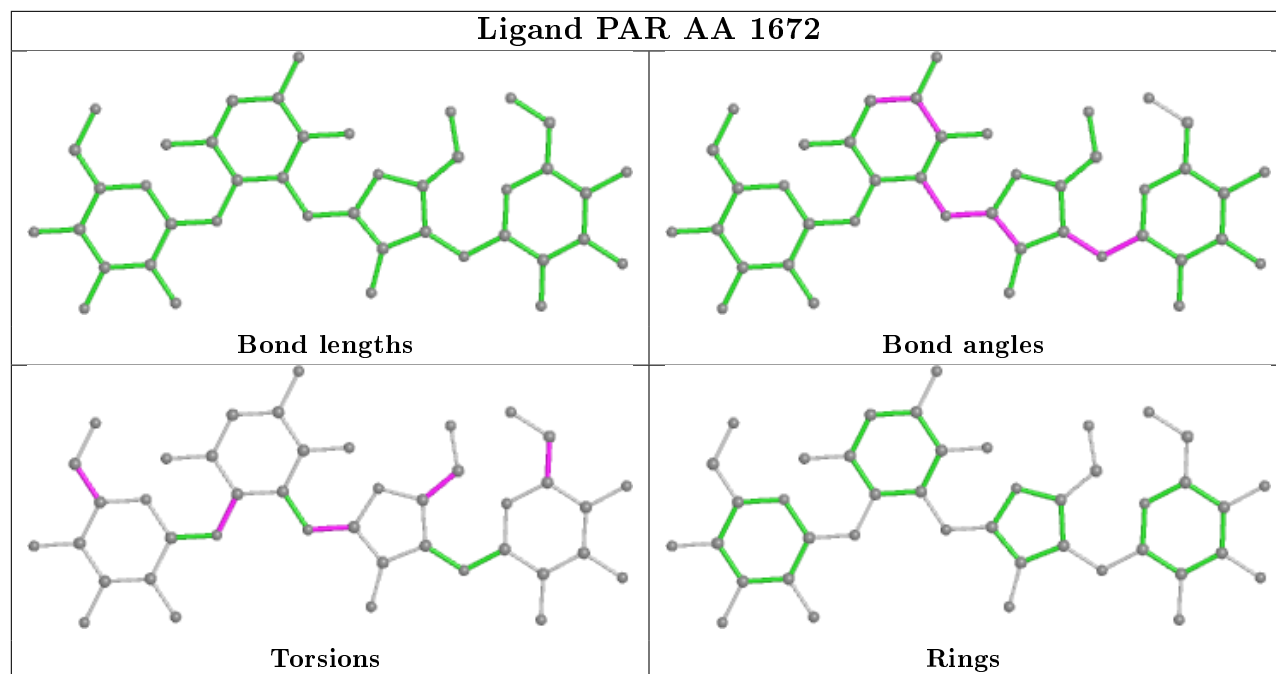


Torsions

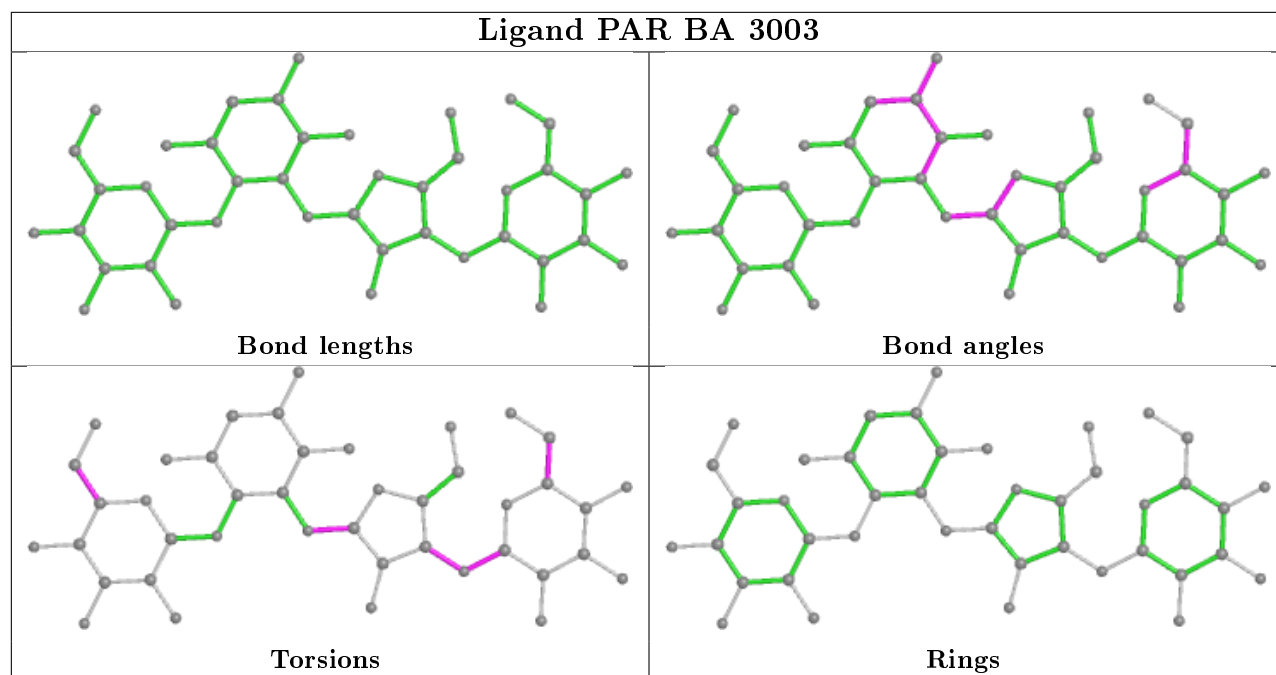


Rings

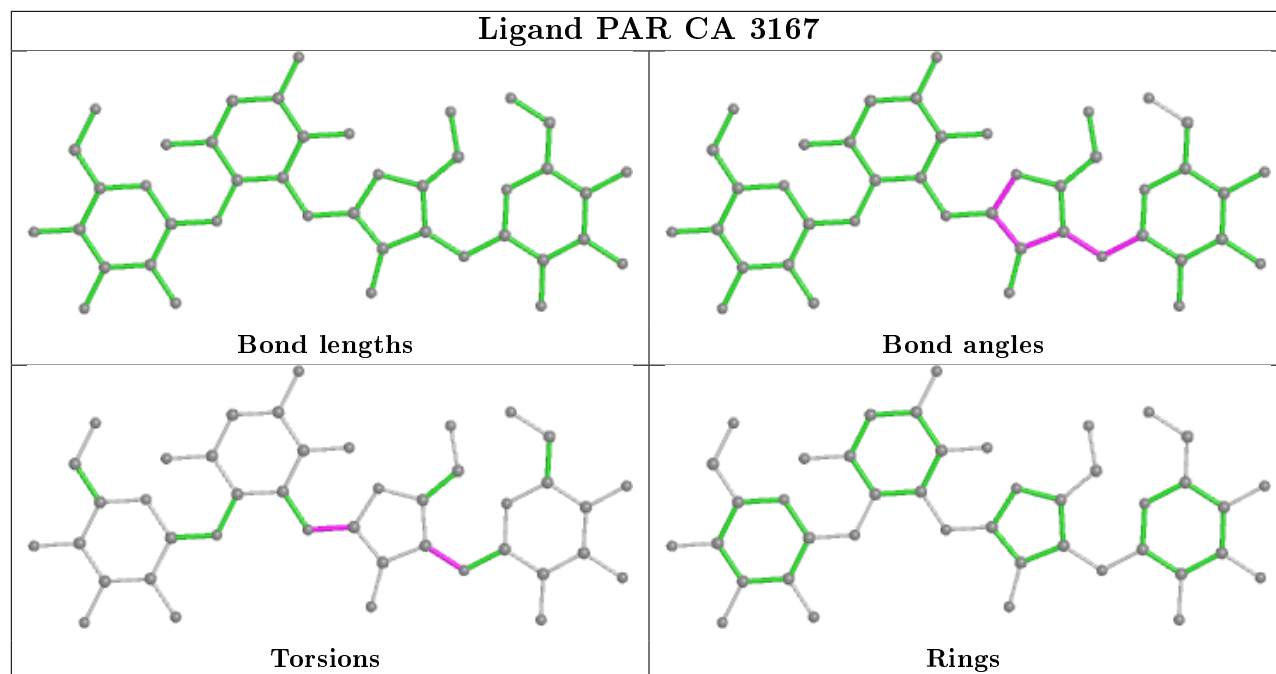
## Ligand PAR AA 1672



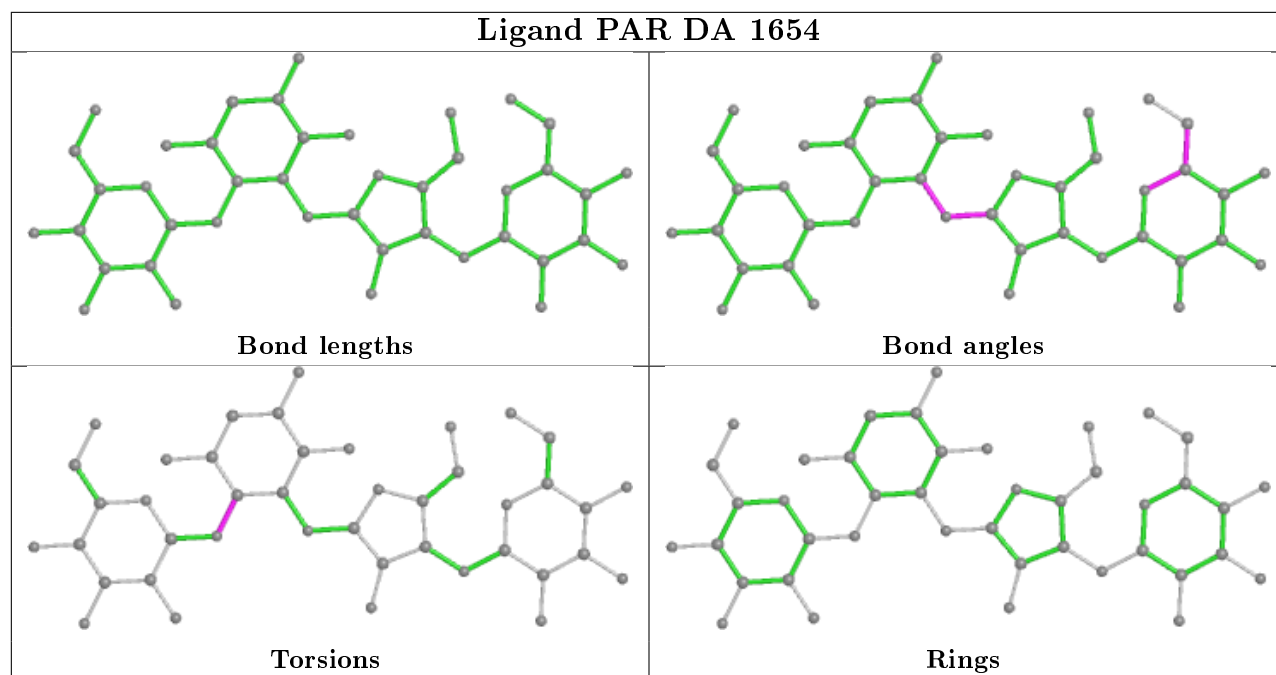
## Ligand PAR BA 3003

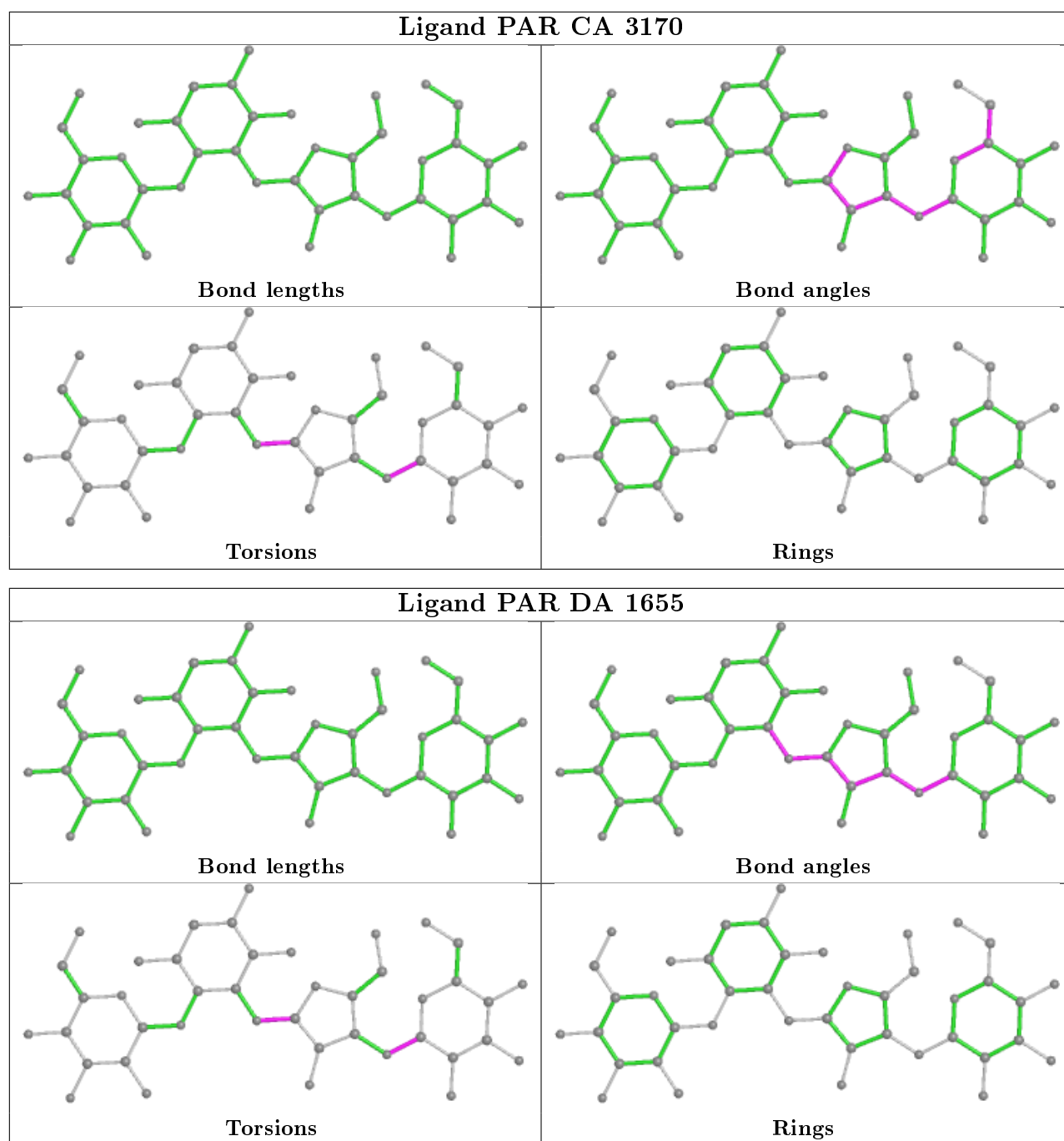


## Ligand PAR CA 3167



## Ligand PAR DA 1654





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1538/1542 (99%)	-0.65	2 (0%) 95 89	44, 86, 166, 303	0
1	DA	1539/1542 (99%)	-0.63	1 (0%) 95 89	47, 85, 145, 285	0
2	AB	218/241 (90%)	0.80	28 (12%) 3 1	64, 133, 196, 238	0
2	DB	218/241 (90%)	0.48	14 (6%) 19 6	68, 115, 176, 210	0
3	AC	206/233 (88%)	-0.44	0 100 100	44, 77, 114, 170	0
3	DC	206/233 (88%)	-0.17	0 100 100	49, 90, 145, 213	0
4	AD	205/206 (99%)	0.03	7 (3%) 45 19	62, 104, 170, 243	0
4	DD	205/206 (99%)	0.01	9 (4%) 34 13	47, 92, 166, 215	0
5	AE	150/167 (89%)	-0.16	1 (0%) 87 69	53, 81, 124, 222	0
5	DE	150/167 (89%)	-0.39	0 100 100	44, 79, 132, 171	0
6	AF	100/135 (74%)	-0.11	1 (1%) 82 59	67, 122, 177, 211	0
6	DF	100/135 (74%)	-0.27	2 (2%) 65 36	50, 94, 135, 153	0
7	AG	151/179 (84%)	0.18	8 (5%) 26 10	62, 119, 169, 239	0
7	DG	151/179 (84%)	-0.05	4 (2%) 56 27	61, 104, 150, 211	0
8	AH	129/130 (99%)	-0.05	3 (2%) 60 31	59, 92, 136, 159	0
8	DH	129/130 (99%)	-0.20	2 (1%) 72 44	49, 84, 119, 174	0
9	AI	127/130 (97%)	0.34	9 (7%) 16 5	57, 108, 158, 215	0
9	DI	127/130 (97%)	0.23	5 (3%) 39 15	70, 116, 174, 197	0
10	AJ	98/103 (95%)	0.47	9 (9%) 9 3	57, 111, 175, 216	0
10	DJ	98/103 (95%)	-0.03	3 (3%) 49 21	65, 111, 168, 200	0
11	AK	117/129 (90%)	0.36	12 (10%) 6 2	58, 108, 177, 232	0
11	DK	117/129 (90%)	-0.20	4 (3%) 45 19	47, 75, 131, 186	0
12	AL	123/124 (99%)	-0.23	3 (2%) 59 30	33, 65, 115, 216	0
12	DL	123/124 (99%)	0.05	1 (0%) 86 65	33, 71, 115, 205	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	114/118 (96%)	0.70	11 (9%) 8 2	73, 132, 191, 263	0
13	DM	114/118 (96%)	0.35	9 (7%) 12 4	92, 135, 174, 254	0
14	AN	96/101 (95%)	0.05	4 (4%) 36 14	59, 95, 188, 237	0
14	DN	96/101 (95%)	0.05	2 (2%) 63 34	62, 104, 164, 215	0
15	AO	88/89 (98%)	0.10	3 (3%) 45 19	60, 102, 166, 216	0
15	DO	88/89 (98%)	-0.10	2 (2%) 60 31	55, 85, 131, 156	0
16	AP	82/82 (100%)	0.40	6 (7%) 15 4	61, 86, 144, 198	0
16	DP	82/82 (100%)	0.43	6 (7%) 15 4	53, 79, 141, 227	0
17	AQ	80/84 (95%)	0.29	5 (6%) 20 6	52, 97, 152, 198	0
17	DQ	80/84 (95%)	0.51	6 (7%) 14 4	58, 96, 161, 233	0
18	AR	55/75 (73%)	0.02	2 (3%) 42 17	57, 97, 151, 178	0
18	DR	55/75 (73%)	-0.25	2 (3%) 42 17	57, 83, 134, 176	0
19	AS	79/92 (85%)	0.77	9 (11%) 5 1	91, 129, 184, 223	0
19	DS	79/92 (85%)	0.80	9 (11%) 5 1	83, 129, 181, 234	0
20	AT	85/87 (97%)	0.25	3 (3%) 44 18	54, 92, 134, 194	0
20	DT	85/87 (97%)	0.16	2 (2%) 59 30	64, 96, 132, 179	0
21	AU	51/71 (71%)	0.09	0 100 100	67, 117, 167, 203	0
21	DU	51/71 (71%)	-0.17	2 (3%) 39 15	54, 105, 159, 224	0
22	AV	183/185 (98%)	-0.13	3 (1%) 72 44	20, 86, 171, 232	0
23	AW	15/16 (93%)	-0.19	0 100 100	57, 128, 176, 205	0
23	DV	16/16 (100%)	-0.30	1 (6%) 20 6	44, 99, 143, 191	0
24	AX	76/76 (100%)	0.38	8 (10%) 6 2	44, 167, 277, 328	0
24	DW	76/76 (100%)	-0.48	0 100 100	51, 93, 135, 164	0
25	BA	2897/2904 (99%)	-0.44	94 (3%) 47 20	22, 52, 194, 368	0
25	CA	2897/2904 (99%)	-0.51	46 (1%) 72 44	37, 75, 205, 328	0
26	BB	119/120 (99%)	-0.82	0 100 100	41, 71, 101, 165	0
26	CB	118/120 (98%)	-0.81	0 100 100	63, 118, 153, 186	0
27	BC	271/273 (99%)	-0.46	0 100 100	32, 60, 94, 149	0
27	CC	271/273 (99%)	-0.34	1 (0%) 92 79	38, 73, 106, 185	0
28	BD	209/209 (100%)	-0.53	0 100 100	21, 45, 77, 170	0
28	CD	209/209 (100%)	-0.37	0 100 100	41, 68, 109, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	BE	201/201 (100%)	-0.34	0 100 100	23, 56, 105, 161	0
29	CE	201/201 (100%)	-0.18	0 100 100	32, 79, 125, 175	0
30	BF	177/179 (98%)	0.48	15 (8%) 10 3	44, 104, 177, 231	0
30	CF	177/179 (98%)	0.90	33 (18%) 1 0	87, 140, 202, 243	0
31	BG	176/177 (99%)	-0.15	3 (1%) 70 41	32, 72, 114, 158	0
31	CG	176/177 (99%)	0.40	7 (3%) 38 15	72, 112, 153, 195	0
32	BH	149/149 (100%)	0.25	7 (4%) 31 11	28, 118, 177, 265	0
32	CH	149/149 (100%)	0.57	14 (9%) 8 3	28, 133, 188, 220	0
33	BI	141/142 (99%)	2.88	81 (57%) 0 0	118, 197, 266, 320	0
33	CI	141/142 (99%)	3.46	92 (65%) 0 0	137, 210, 253, 292	0
34	BJ	142/142 (100%)	-0.57	0 100 100	21, 44, 79, 102	0
34	CJ	142/142 (100%)	-0.31	0 100 100	37, 65, 99, 167	0
35	BK	122/123 (99%)	-0.59	0 100 100	23, 49, 77, 104	0
35	CK	122/123 (99%)	-0.25	0 100 100	42, 69, 112, 148	0
36	BL	143/144 (99%)	-0.51	0 100 100	24, 54, 83, 118	0
36	CL	143/144 (99%)	-0.15	2 (1%) 75 49	39, 82, 125, 180	0
37	BM	136/136 (100%)	-0.48	0 100 100	27, 51, 89, 121	0
37	CM	136/136 (100%)	0.19	4 (2%) 51 23	44, 78, 106, 141	0
38	BN	120/127 (94%)	-0.58	0 100 100	22, 47, 71, 156	0
38	CN	120/127 (94%)	-0.20	1 (0%) 86 65	46, 76, 103, 191	0
39	BO	116/117 (99%)	-0.17	0 100 100	37, 67, 99, 123	0
39	CO	116/117 (99%)	0.48	8 (6%) 16 5	70, 122, 164, 201	0
40	BP	114/115 (99%)	-0.52	2 (1%) 68 40	30, 56, 99, 206	0
40	CP	114/115 (99%)	-0.32	0 100 100	45, 77, 116, 140	0
41	BQ	117/118 (99%)	-0.63	0 100 100	15, 39, 71, 91	0
41	CQ	117/118 (99%)	-0.42	0 100 100	32, 61, 85, 114	0
42	BR	103/103 (100%)	-0.48	0 100 100	21, 52, 87, 118	0
42	CR	103/103 (100%)	-0.36	1 (0%) 82 59	32, 73, 108, 171	0
43	BS	110/110 (100%)	-0.47	0 100 100	20, 44, 76, 117	0
43	CS	110/110 (100%)	-0.37	0 100 100	31, 65, 103, 140	0
44	BT	93/100 (93%)	-0.10	1 (1%) 80 56	43, 60, 126, 213	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	CT	93/100 (93%)	0.06	2 (2%) 62 33	56, 94, 142, 202	0
45	BU	102/104 (98%)	-0.41	0 100 100	33, 61, 118, 185	0
45	CU	102/104 (98%)	0.42	9 (8%) 10 3	56, 90, 177, 215	0
46	BV	94/94 (100%)	-0.29	1 (1%) 80 56	41, 71, 109, 127	0
46	CV	94/94 (100%)	0.10	1 (1%) 80 56	66, 110, 151, 196	0
47	BW	76/85 (89%)	-0.41	1 (1%) 77 51	32, 54, 92, 126	0
47	CW	75/85 (88%)	0.14	1 (1%) 77 51	46, 82, 120, 146	0
48	BX	77/78 (98%)	-0.31	0 100 100	39, 59, 101, 111	0
48	CX	77/78 (98%)	-0.08	2 (2%) 56 27	38, 82, 121, 150	0
49	BY	63/63 (100%)	-0.17	3 (4%) 30 11	39, 69, 114, 179	0
49	CY	63/63 (100%)	0.29	3 (4%) 30 11	66, 103, 165, 221	0
50	BZ	58/59 (98%)	-0.33	0 100 100	30, 47, 75, 106	0
50	CZ	58/59 (98%)	-0.21	1 (1%) 70 41	45, 73, 112, 188	0
51	B0	56/57 (98%)	-0.62	0 100 100	22, 46, 94, 143	0
51	C0	56/57 (98%)	-0.33	1 (1%) 68 40	37, 73, 117, 194	0
52	B1	50/55 (90%)	2.19	17 (34%) 0 0	76, 105, 185, 196	0
52	C1	50/55 (90%)	1.02	7 (14%) 2 1	79, 109, 138, 164	0
53	B2	46/46 (100%)	-0.38	1 (2%) 62 33	27, 45, 76, 155	0
53	C2	46/46 (100%)	-0.23	0 100 100	39, 68, 92, 151	0
54	B3	64/65 (98%)	-0.42	0 100 100	27, 48, 74, 122	0
54	C3	64/65 (98%)	-0.29	0 100 100	38, 69, 96, 109	0
55	B4	38/38 (100%)	-0.33	0 100 100	29, 52, 91, 122	0
55	C4	38/38 (100%)	0.01	0 100 100	47, 83, 109, 119	0
56	B5	191/228 (83%)	5.27	155 (81%) 0 0	28, 219, 264, 311	0
All	All	21100/21699 (97%)	-0.17	840 (3%) 38 15	15, 80, 183, 368	0

All (840) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
56	B5	222	VAL	25.3
33	CI	1	ALA	21.4
56	B5	38	ASP	20.9
56	B5	223	ARG	19.9
56	B5	105	ASP	19.8

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Mol	Chain	Res	Type	RSRZ
25	BA	2140	G	18.5
56	B5	165	ASN	18.1
56	B5	221	SER	17.3
56	B5	41	VAL	16.5
12	AL	124	ALA	15.6
33	BI	1	ALA	15.4
56	B5	218	MET	14.6
56	B5	216	THR	14.6
56	B5	193	ILE	14.3
33	BI	13	ALA	13.9
56	B5	215	THR	13.7
56	B5	198	ALA	13.6
12	DL	124	ALA	13.2
56	B5	220	PRO	13.0
56	B5	206	GLY	12.9
56	B5	224	ILE	12.9
33	CI	66	PHE	12.8
25	BA	2141	G	12.8
56	B5	199	HIS	12.5
56	B5	183	GLU	12.5
33	CI	5	GLN	12.4
33	CI	58	ILE	12.2
33	CI	59	THR	12.1
33	BI	12	VAL	12.1
56	B5	62	VAL	11.8
33	CI	30	GLN	11.3
45	CU	53	GLN	11.0
52	B1	52	LYS	10.7
25	BA	2177	C	10.4
52	B1	4	ILE	10.4
33	BI	20	SER	10.2
56	B5	166	ASP	10.0
25	BA	2176	A	10.0
25	BA	2157	G	10.0
56	B5	155	GLU	10.0
33	BI	2	LYS	9.7
56	B5	188	ASN	9.6
33	CI	2	LYS	9.5
56	B5	92	ASP	9.5
33	BI	11	GLN	9.4
25	BA	2174	C	9.4
33	CI	35	MET	9.4

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Mol	Chain	Res	Type	RSRZ
25	BA	2105	U	9.4
33	BI	14	ALA	9.3
33	CI	40	ALA	9.3
25	BA	2117	A	9.2
25	BA	2173	A	9.1
33	BI	7	TYR	9.0
33	BI	21	PRO	8.6
56	B5	101	GLN	8.6
25	BA	2163	A	8.6
56	B5	54	SER	8.6
25	BA	2126	A	8.6
25	BA	2127	G	8.6
25	BA	2111	U	8.5
56	B5	46	LYS	8.4
56	B5	25	ALA	8.3
56	B5	42	GLU	8.2
25	BA	2169	A	8.2
33	CI	52	LEU	8.2
56	B5	201	PRO	8.1
56	B5	21	THR	8.0
25	BA	2148	G	8.0
2	AB	156	GLY	7.9
56	B5	146	GLY	7.9
33	CI	6	ALA	7.9
33	CI	65	SER	7.9
56	B5	171	ILE	7.8
56	B5	217	THR	7.8
56	B5	194	ARG	7.8
56	B5	162	GLU	7.7
56	B5	202	GLU	7.6
25	BA	2134	A	7.6
56	B5	104	LEU	7.6
25	BA	2120	G	7.6
56	B5	196	LEU	7.5
56	B5	187	ASP	7.5
56	B5	209	LEU	7.4
25	CA	2141	G	7.4
25	CA	2172	U	7.4
25	BA	2180	U	7.4
56	B5	106	GLY	7.3
45	CU	48	VAL	7.3
25	BA	2165	C	7.2

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Mol	Chain	Res	Type	RSRZ
33	BI	25	PRO	7.2
56	B5	67	GLY	7.1
2	DB	9	MET	7.1
25	BA	2154	A	7.1
33	CI	82	ALA	7.1
25	BA	2162	G	7.0
56	B5	48	GLY	7.0
56	B5	181	PRO	6.9
56	B5	91	ALA	6.9
33	BI	45	THR	6.9
56	B5	47	LEU	6.9
56	B5	164	ARG	6.9
33	CI	63	ASP	6.9
25	BA	2155	U	6.8
56	B5	189	ILE	6.8
56	B5	37	PHE	6.8
56	B5	121	GLY	6.7
33	BI	139	VAL	6.7
33	CI	34	ILE	6.7
25	BA	2125	G	6.7
33	BI	3	LYS	6.7
16	DP	81	ALA	6.7
56	B5	208	PHE	6.6
56	B5	74	VAL	6.6
56	B5	195	ALA	6.5
25	BA	2110	G	6.5
25	BA	2128	G	6.5
33	CI	60	VAL	6.5
56	B5	180	PHE	6.5
25	BA	2153	C	6.5
50	CZ	1	ALA	6.4
33	CI	13	ALA	6.4
25	BA	2175	C	6.3
39	CO	114	GLY	6.3
25	BA	2178	C	6.3
56	B5	179	SER	6.3
56	B5	158	ALA	6.3
33	BI	94	LYS	6.3
33	CI	26	ALA	6.2
33	BI	70	THR	6.2
56	B5	122	ALA	6.2
56	B5	72	VAL	6.1

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Mol	Chain	Res	Type	RSRZ
19	DS	3	ARG	6.1
33	CI	67	THR	6.1
4	AD	28	ILE	6.1
33	CI	25	PRO	6.1
33	BI	15	GLY	6.0
13	AM	73	ILE	6.0
25	BA	2107	G	6.0
25	BA	2158	A	6.0
56	B5	219	GLY	6.0
56	B5	86	ALA	6.0
33	CI	85	ILE	6.0
16	DP	47	GLU	5.9
30	BF	115	GLY	5.9
52	B1	51	ALA	5.9
33	CI	53	PRO	5.9
33	BI	138	VAL	5.9
33	CI	31	GLY	5.9
56	B5	154	ARG	5.9
25	BA	2115	G	5.8
56	B5	63	SER	5.8
45	CU	45	GLN	5.8
25	BA	2138	G	5.8
56	B5	26	ALA	5.8
56	B5	128	GLY	5.8
33	CI	11	GLN	5.8
56	B5	192	PHE	5.8
25	BA	2136	G	5.7
33	CI	83	ALA	5.7
33	CI	12	VAL	5.7
25	CA	2142	A	5.7
13	AM	74	SER	5.7
56	B5	214	VAL	5.7
33	BI	6	ALA	5.7
25	CA	1175	A	5.7
56	B5	207	THR	5.6
25	BA	2150	C	5.6
56	B5	197	GLU	5.6
56	B5	204	ALA	5.6
56	B5	109	ASP	5.6
2	AB	9	MET	5.6
30	BF	106	ALA	5.6
47	CW	83	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
33	CI	39	LYS	5.5
25	BA	2143	C	5.5
56	B5	39	GLU	5.5
56	B5	24	GLU	5.4
2	AB	155	GLY	5.4
10	AJ	30	LYS	5.4
33	BI	19	PRO	5.3
56	B5	78	ALA	5.3
56	B5	182	PRO	5.3
51	C0	26	SER	5.3
25	BA	2142	A	5.3
16	AP	80	LYS	5.3
33	CI	95	ASP	5.3
7	DG	8	GLY	5.3
52	B1	3	GLY	5.3
25	BA	846	U	5.3
56	B5	22	ILE	5.2
17	AQ	83	VAL	5.2
25	BA	2135	A	5.2
25	BA	2156	G	5.2
7	AG	85	TYR	5.2
30	CF	92	GLY	5.2
33	BI	68	PHE	5.2
25	CA	613	A	5.2
56	B5	184	LYS	5.2
56	B5	66	HIS	5.1
24	AX	72	C	5.1
33	CI	37	PHE	5.1
56	B5	175	VAL	5.1
56	B5	210	ARG	5.1
7	AG	59	LEU	5.1
2	AB	166	ALA	5.1
10	AJ	33	GLY	5.1
24	AX	73	A	5.0
33	CI	10	LEU	5.0
33	CI	21	PRO	5.0
10	AJ	34	ALA	5.0
56	B5	213	TYR	5.0
33	BI	8	VAL	5.0
56	B5	100	ILE	5.0
25	BA	2118	U	5.0
56	B5	147	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
56	B5	176	GLY	5.0
13	AM	115	PRO	5.0
56	B5	205	LYS	5.0
2	DB	132	LYS	4.9
25	BA	2144	G	4.9
56	B5	156	ILE	4.9
56	B5	161	ILE	4.9
56	B5	168	THR	4.9
25	BA	2108	A	4.9
33	CI	15	GLY	4.9
33	CI	32	VAL	4.8
33	CI	33	ASN	4.8
25	BA	2116	G	4.8
33	BI	91	LYS	4.8
25	BA	546	U	4.8
49	CY	22	LEU	4.8
4	DD	28	ILE	4.8
56	B5	144	THR	4.8
11	DK	13	ARG	4.8
56	B5	75	LEU	4.8
33	CI	29	GLN	4.7
33	BI	113	ALA	4.7
45	CU	49	PRO	4.7
8	AH	2	SER	4.7
4	DD	24	GLY	4.7
25	BA	2172	U	4.7
56	B5	211	SER	4.7
56	B5	93	TYR	4.7
19	DS	13	LEU	4.7
52	B1	13	SER	4.6
25	CA	2112	G	4.6
56	B5	200	LYS	4.6
33	CI	38	CYS	4.6
48	CX	76	LYS	4.6
17	DQ	50	ASN	4.6
25	BA	2119	A	4.6
25	BA	2171	A	4.5
25	BA	2114	A	4.5
33	CI	114	ALA	4.5
38	CN	120	GLU	4.5
33	CI	14	ALA	4.5
33	BI	5	GLN	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
56	B5	68	LEU	4.4
56	B5	96	GLY	4.4
56	B5	145	VAL	4.4
56	B5	71	GLN	4.4
33	BI	65	SER	4.4
25	CA	2131	U	4.4
16	AP	81	ALA	4.4
33	BI	16	MET	4.4
25	BA	2104	C	4.4
25	BA	2124	G	4.4
33	BI	92	PRO	4.4
33	BI	77	VAL	4.3
10	AJ	31	ARG	4.3
33	CI	81	LYS	4.3
19	DS	68	GLY	4.3
13	DM	7	ILE	4.3
49	BY	63	ALA	4.3
4	AD	151	LYS	4.3
16	DP	80	LYS	4.3
25	BA	2188	U	4.3
25	CA	2123	G	4.3
45	CU	47	PRO	4.3
25	CA	2118	U	4.3
12	AL	25	GLU	4.2
33	CI	51	GLY	4.2
56	B5	143	GLY	4.2
14	DN	20	PHE	4.2
56	B5	110	PHE	4.2
56	B5	83	ILE	4.2
25	BA	2159	G	4.2
33	CI	42	ASN	4.2
30	CF	111	ARG	4.2
25	CA	2144	G	4.2
33	CI	19	PRO	4.2
10	AJ	102	LEU	4.2
25	BA	2123	G	4.2
33	CI	86	LYS	4.2
56	B5	212	VAL	4.2
56	B5	185	LEU	4.1
33	CI	16	MET	4.1
33	CI	20	SER	4.1
56	B5	44	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
19	AS	46	GLY	4.1
25	BA	2152	G	4.1
33	CI	28	GLY	4.1
56	B5	174	PRO	4.1
32	CH	136	SER	4.0
56	B5	178	ALA	4.0
33	BI	58	ILE	4.0
25	CA	2132	U	4.0
25	BA	2184	A	4.0
56	B5	133	PRO	4.0
33	BI	66	PHE	4.0
33	BI	105	LEU	4.0
33	BI	108	ILE	4.0
32	BH	149	GLU	4.0
9	AI	41	ARG	4.0
25	BA	2151	U	3.9
14	AN	29	ILE	3.9
25	BA	2129	C	3.9
39	CO	51	ALA	3.9
13	AM	71	ARG	3.9
56	B5	80	GLY	3.9
24	AX	19	G	3.9
30	BF	109	ARG	3.9
31	CG	9	VAL	3.9
33	CI	113	ALA	3.9
56	B5	76	ALA	3.9
33	CI	64	ARG	3.9
25	BA	2186	G	3.9
56	B5	203	GLY	3.9
25	BA	2109	U	3.9
25	BA	2112	G	3.8
16	AP	47	GLU	3.8
4	AD	27	ALA	3.8
33	BI	78	LEU	3.8
33	BI	22	PRO	3.8
25	BA	2147	A	3.8
33	BI	83	ALA	3.8
56	B5	84	LYS	3.8
56	B5	163	PHE	3.8
56	B5	99	ILE	3.8
33	CI	68	PHE	3.8
19	AS	30	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
56	B5	45	ALA	3.8
30	CF	131	VAL	3.8
33	BI	33	ASN	3.8
8	DH	2	SER	3.8
33	BI	57	VAL	3.8
14	DN	29	ILE	3.7
2	DB	88	ASP	3.7
25	BA	2181	U	3.7
40	BP	114	ASN	3.7
33	BI	67	THR	3.7
19	AS	65	GLU	3.7
19	DS	65	GLU	3.7
33	BI	54	ILE	3.7
2	AB	157	LEU	3.7
10	AJ	36	VAL	3.7
25	BA	2145	C	3.7
19	AS	74	PHE	3.7
7	AG	152	ALA	3.7
33	CI	56	VAL	3.6
56	B5	50	ASP	3.6
56	B5	169	GLY	3.6
56	B5	186	ALA	3.6
56	B5	135	GLY	3.6
2	AB	28	LYS	3.6
56	B5	53	ARG	3.5
33	CI	48	ILE	3.5
11	AK	126	LYS	3.5
33	BI	32	VAL	3.5
45	CU	52	ASN	3.5
33	BI	95	ASP	3.5
52	B1	29	LYS	3.5
2	DB	119	THR	3.5
33	BI	52	LEU	3.5
56	B5	23	ASP	3.5
52	B1	25	ASN	3.5
33	CI	44	LYS	3.5
25	CA	2129	C	3.5
30	CF	132	ARG	3.5
56	B5	36	LYS	3.5
33	BI	100	ILE	3.5
33	CI	43	ALA	3.5
56	B5	153	ILE	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
33	BI	96	LYS	3.4
33	BI	24	GLY	3.4
32	CH	1	MET	3.4
30	CF	116	LEU	3.4
33	CI	84	GLY	3.4
25	CA	2103	C	3.4
33	BI	141	ASP	3.4
32	BH	85	GLY	3.4
33	BI	98	GLY	3.4
33	CI	139	VAL	3.3
33	BI	48	ILE	3.3
17	DQ	71	LYS	3.3
2	DB	206	ALA	3.3
19	DS	41	PHE	3.3
25	CA	2104	C	3.3
25	BA	2170	A	3.3
30	BF	84	ILE	3.3
56	B5	191	ALA	3.3
25	CA	2152	G	3.3
30	BF	72	SER	3.3
11	DK	129	VAL	3.3
25	BA	2132	U	3.3
25	CA	546	U	3.3
2	AB	67	ILE	3.3
56	B5	190	ARG	3.3
30	CF	97	GLU	3.3
33	BI	97	VAL	3.3
45	CU	46	LYS	3.3
33	BI	53	PRO	3.3
49	CY	63	ALA	3.3
20	AT	86	LEU	3.3
7	AG	80	VAL	3.3
2	AB	189	THR	3.3
25	BA	1847	A	3.2
25	CA	2127	G	3.2
56	B5	69	GLY	3.2
33	CI	61	TYR	3.2
18	AR	67	LEU	3.2
25	BA	1175	A	3.2
5	AE	51	GLY	3.2
20	DT	85	LYS	3.2
25	BA	2106	U	3.2

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Mol	Chain	Res	Type	RSRZ
25	CA	2109	U	3.2
11	AK	45	ALA	3.2
30	CF	17	THR	3.2
2	AB	89	GLN	3.2
33	BI	87	SER	3.2
25	BA	2102	G	3.2
11	AK	77	TYR	3.2
20	AT	68	HIS	3.2
25	CA	2182	U	3.2
25	BA	2133	G	3.2
32	CH	94	ILE	3.2
33	CI	80	LYS	3.2
56	B5	89	ALA	3.2
25	BA	2137	U	3.2
25	CA	2146	C	3.2
56	B5	65	PRO	3.2
32	CH	16	GLY	3.2
30	CF	23	SER	3.2
33	CI	17	ALA	3.2
39	CO	37	ALA	3.2
56	B5	142	ALA	3.2
30	CF	114	ARG	3.1
14	AN	20	PHE	3.1
25	CA	2153	C	3.1
25	CA	2181	U	3.1
37	CM	32	GLY	3.1
12	AL	123	LYS	3.1
2	AB	62	SER	3.1
33	BI	60	VAL	3.1
1	AA	86	G	3.1
25	BA	2100	G	3.1
23	DV	9	A	3.1
32	CH	18	GLN	3.1
2	AB	88	ASP	3.1
33	CI	62	ALA	3.1
2	DB	213	TYR	3.1
33	CI	111	THR	3.1
56	B5	40	THR	3.1
19	AS	71	LEU	3.1
25	CA	2111	U	3.1
33	BI	59	THR	3.1
2	AB	39	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
2	DB	15	HIS	3.1
19	AS	56	GLN	3.0
33	BI	55	PRO	3.0
49	BY	62	GLY	3.0
33	CI	27	LEU	3.0
56	B5	43	VAL	3.0
4	AD	162	ALA	3.0
25	CA	2110	G	3.0
33	BI	26	ALA	3.0
33	BI	88	GLY	3.0
33	CI	136	GLY	3.0
33	CI	77	VAL	3.0
10	AJ	87	LEU	3.0
33	CI	47	SER	3.0
42	CR	50	GLY	3.0
56	B5	129	ARG	3.0
2	AB	29	PRO	3.0
56	B5	134	ARG	3.0
56	B5	97	GLU	3.0
25	BA	1065	U	3.0
11	DK	126	LYS	3.0
30	CF	96	TRP	3.0
49	CY	62	GLY	3.0
30	CF	113	PHE	3.0
24	AX	3	C	3.0
10	DJ	102	LEU	3.0
25	CA	2157	G	3.0
4	AD	163	GLU	3.0
56	B5	120	MET	2.9
25	CA	2174	C	2.9
56	B5	56	GLN	2.9
30	CF	149	ARG	2.9
56	B5	19	VAL	2.9
32	CH	142	VAL	2.9
30	CF	82	TYR	2.9
30	CF	62	GLN	2.9
25	BA	2164	C	2.9
25	CA	2168	G	2.9
2	AB	30	PHE	2.9
4	DD	27	ALA	2.9
11	AK	13	ARG	2.9
30	CF	129	MET	2.9

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Mol	Chain	Res	Type	RSRZ
30	CF	175	PRO	2.9
25	CA	896	A	2.9
11	AK	79	ILE	2.9
33	BI	80	LYS	2.9
30	BF	146	ASP	2.9
18	DR	48	ARG	2.9
32	CH	20	ASN	2.9
32	CH	110	VAL	2.9
52	C1	28	THR	2.9
16	DP	22	ALA	2.9
11	AK	74	VAL	2.8
30	CF	117	SER	2.8
33	BI	75	ALA	2.8
33	CI	117	THR	2.8
56	B5	157	LYS	2.8
17	AQ	6	ARG	2.8
33	BI	93	ASN	2.8
25	BA	2146	C	2.8
21	DU	27	GLY	2.8
8	DH	122	GLY	2.8
25	CA	1728	C	2.8
33	CI	55	PRO	2.8
33	CI	87	SER	2.8
56	B5	95	GLY	2.8
30	CF	24	VAL	2.8
19	DS	64	ASP	2.8
33	BI	46	ASP	2.8
33	CI	141	ASP	2.8
17	DQ	4	LYS	2.8
25	CA	2117	A	2.8
30	CF	22	ASN	2.8
56	B5	73	ARG	2.8
7	DG	6	VAL	2.8
30	BF	45	ASP	2.8
25	BA	2161	C	2.8
4	DD	25	VAL	2.8
52	B1	50	GLU	2.8
2	AB	153	ASP	2.8
49	BY	23	ARG	2.8
19	AS	61	PHE	2.8
13	DM	12	HIS	2.8
22	AV	45	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
33	BI	130	GLY	2.8
33	BI	4	VAL	2.8
52	B1	26	LYS	2.8
9	DI	39	PHE	2.8
37	CM	27	SER	2.8
25	CA	2156	G	2.8
39	CO	36	TYR	2.8
33	CI	4	VAL	2.8
25	BA	2101	A	2.8
30	BF	70	ARG	2.8
39	CO	89	ASP	2.8
25	CA	2106	U	2.7
33	CI	74	PRO	2.7
52	B1	6	GLU	2.7
11	AK	44	TRP	2.7
6	DF	96	VAL	2.7
25	BA	140	C	2.7
33	BI	114	ALA	2.7
33	BI	18	ASN	2.7
24	AX	56	C	2.7
8	AH	3	MET	2.7
33	CI	109	ALA	2.7
11	AK	125	LYS	2.7
44	BT	4	GLU	2.7
56	B5	148	ASN	2.7
52	B1	22	THR	2.7
30	CF	121	PHE	2.7
33	CI	97	VAL	2.7
45	CU	50	ALA	2.7
32	CH	19	VAL	2.7
33	CI	36	GLU	2.7
56	B5	151	GLU	2.7
33	CI	46	ASP	2.7
4	DD	147	GLU	2.7
30	BF	112	ASP	2.7
25	CA	2148	G	2.7
33	CI	24	GLY	2.7
9	AI	108	ALA	2.7
31	CG	51	PHE	2.6
56	B5	61	THR	2.6
10	DJ	35	GLN	2.6
52	C1	51	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
25	CA	2124	G	2.6
33	BI	90	GLY	2.6
33	CI	137	LEU	2.6
25	BA	2189	U	2.6
46	CV	3	THR	2.6
6	AF	8	PHE	2.6
2	AB	51	ASN	2.6
25	BA	2149	U	2.6
25	BA	2182	U	2.6
30	CF	86	CYS	2.6
33	CI	91	LYS	2.6
30	CF	37	MET	2.6
56	B5	70	LYS	2.6
25	BA	1171	G	2.6
13	AM	69	LEU	2.6
25	CA	140	C	2.6
33	BI	10	LEU	2.6
19	DS	44	MET	2.6
2	AB	32	PHE	2.5
30	BF	41	GLU	2.5
25	BA	2185	U	2.5
33	CI	57	VAL	2.5
13	AM	53	ILE	2.5
2	AB	66	LYS	2.5
22	AV	42	VAL	2.5
25	BA	2103	C	2.5
52	B1	12	SER	2.5
56	B5	125	SER	2.5
45	CU	23	LYS	2.5
2	AB	18	HIS	2.5
17	DQ	23	VAL	2.5
52	C1	37	LYS	2.5
14	AN	32	ASP	2.5
25	BA	2190	G	2.5
15	AO	89	ARG	2.5
31	BG	130	ILE	2.5
31	CG	52	GLY	2.5
32	BH	12	LEU	2.5
33	BI	116	MET	2.5
15	AO	75	VAL	2.5
25	CA	2173	A	2.5
9	AI	17	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
33	CI	78	LEU	2.5
25	CA	846	U	2.5
1	DA	82	G	2.5
48	CX	77	TYR	2.5
11	DK	15	GLN	2.5
13	DM	113	ARG	2.5
17	AQ	27	ARG	2.5
2	AB	38	VAL	2.5
56	B5	35	ALA	2.5
56	B5	51	PRO	2.5
33	CI	93	ASN	2.5
30	CF	19	PHE	2.5
10	DJ	6	ILE	2.5
25	CA	2133	G	2.5
56	B5	103	ILE	2.5
7	AG	144	MET	2.4
25	BA	2179	C	2.4
19	DS	72	GLY	2.4
33	BI	23	VAL	2.4
30	CF	93	GLU	2.4
31	BG	176	LYS	2.4
30	BF	1	ALA	2.4
44	CT	83	ALA	2.4
33	CI	76	ALA	2.4
31	CG	106	LEU	2.4
37	CM	31	PHE	2.4
2	AB	74	ARG	2.4
4	DD	151	LYS	2.4
9	AI	51	PRO	2.4
13	AM	34	LEU	2.4
56	B5	127	LEU	2.4
21	DU	45	ARG	2.4
2	AB	212	LEU	2.4
33	BI	86	LYS	2.4
56	B5	55	ASP	2.4
25	BA	2168	G	2.4
52	C1	30	PRO	2.4
20	DT	4	ILE	2.4
2	AB	70	VAL	2.4
33	BI	29	GLN	2.4
9	DI	9	THR	2.4
13	DM	13	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
56	B5	150	GLY	2.4
9	DI	38	TYR	2.4
33	CI	50	LYS	2.4
53	B2	46	LYS	2.4
31	CG	130	ILE	2.4
24	AX	55	U	2.3
7	AG	79	ARG	2.3
4	AD	107	PHE	2.3
11	AK	43	GLY	2.3
33	BI	30	GLN	2.3
39	CO	52	SER	2.3
2	DB	148	LEU	2.3
32	CH	38	PRO	2.3
32	CH	34	GLY	2.3
33	CI	22	PRO	2.3
33	CI	69	VAL	2.3
30	CF	16	MET	2.3
4	DD	184	ARG	2.3
33	BI	103	ALA	2.3
56	B5	94	VAL	2.3
56	B5	90	GLY	2.3
33	BI	82	ALA	2.3
13	AM	21	SER	2.3
30	CF	170	ALA	2.3
13	DM	43	VAL	2.3
11	AK	49	GLY	2.3
39	CO	88	LYS	2.3
4	DD	36	GLN	2.3
25	CA	2130	U	2.3
9	AI	20	PHE	2.3
25	CA	2145	C	2.3
25	BA	1174	U	2.3
47	BW	8	THR	2.3
6	DF	1	MET	2.3
46	BV	63	ILE	2.3
30	CF	99	PHE	2.3
7	DG	84	THR	2.3
25	CA	1174	U	2.3
30	CF	85	GLY	2.3
30	CF	130	GLY	2.3
25	CA	2147	A	2.3
52	C1	10	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
17	AQ	9	GLN	2.3
20	AT	87	ALA	2.3
33	CI	98	GLY	2.2
25	BA	138	U	2.2
16	DP	52	LEU	2.2
10	AJ	76	ILE	2.2
13	DM	4	ILE	2.2
33	CI	45	THR	2.2
25	BA	2187	U	2.2
33	CI	23	VAL	2.2
33	BI	115	ASP	2.2
52	B1	46	VAL	2.2
13	AM	18	ALA	2.2
15	DO	89	ARG	2.2
32	CH	140	ALA	2.2
30	CF	146	ASP	2.2
32	BH	34	GLY	2.2
16	AP	44	SER	2.2
2	AB	40	ILE	2.2
2	AB	17	GLY	2.2
2	DB	167	ASP	2.2
9	AI	9	THR	2.2
52	B1	11	VAL	2.2
56	B5	49	ILE	2.2
16	DP	48	GLU	2.2
25	BA	2121	G	2.2
25	CA	1870	C	2.2
33	BI	49	GLU	2.2
56	B5	139	ASN	2.2
33	CI	41	PHE	2.2
19	AS	58	VAL	2.2
30	BF	110	ILE	2.2
40	BP	1	SER	2.2
13	DM	58	ASP	2.2
32	CH	17	ASP	2.2
39	CO	50	ALA	2.2
33	BI	79	LEU	2.2
11	AK	129	VAL	2.2
14	AN	25	GLU	2.2
8	AH	128	TYR	2.2
2	AB	31	ILE	2.2
9	DI	43	THR	2.2

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Mol	Chain	Res	Type	RSRZ
10	AJ	49	PHE	2.2
2	DB	87	CYS	2.2
9	DI	91	ASP	2.2
56	B5	123	VAL	2.2
56	B5	52	ARG	2.2
18	DR	55	LEU	2.2
33	BI	47	SER	2.2
1	AA	1032	G	2.2
17	DQ	43	LYS	2.2
33	BI	51	GLY	2.2
33	BI	64	ARG	2.2
2	AB	117	LEU	2.1
15	AO	87	LEU	2.1
2	DB	30	PHE	2.1
7	DG	9	GLN	2.1
13	AM	49	SER	2.1
13	DM	63	PHE	2.1
33	BI	71	LYS	2.1
56	B5	85	GLU	2.1
52	B1	28	THR	2.1
32	BH	47	PHE	2.1
2	DB	187	VAL	2.1
31	BG	159	LYS	2.1
36	CL	85	VAL	2.1
25	BA	2166	U	2.1
15	DO	31	LEU	2.1
2	DB	74	ARG	2.1
25	CA	2121	G	2.1
30	BF	177	ARG	2.1
16	AP	20	VAL	2.1
17	DQ	83	VAL	2.1
4	DD	144	SER	2.1
7	AG	57	SER	2.1
9	AI	54	LEU	2.1
25	BA	2402	U	2.1
32	BH	79	THR	2.1
33	CI	3	LYS	2.1
30	CF	66	ILE	2.1
2	DB	33	GLY	2.1
36	CL	92	LEU	2.1
19	DS	69	HIS	2.1
56	B5	87	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
32	CH	131	SER	2.1
27	CC	91	ALA	2.1
44	CT	84	TYR	2.1
25	BA	2139	U	2.1
2	AB	60	ILE	2.1
52	B1	10	LEU	2.1
9	AI	39	PHE	2.1
30	BF	175	PRO	2.1
33	BI	76	ALA	2.1
22	AV	38	LEU	2.1
52	C1	8	ILE	2.1
25	CA	2151	U	2.1
52	C1	11	VAL	2.1
11	AK	42	LEU	2.1
9	AI	32	GLN	2.0
33	CI	135	MET	2.1
31	CG	48	THR	2.0
13	DM	30	SER	2.0
25	CA	2126	A	2.0
30	BF	79	ARG	2.0
37	CM	20	LEU	2.0
32	BH	8	LYS	2.0
18	AR	74	HIS	2.0
16	AP	22	ALA	2.0
19	AS	49	ILE	2.0
52	B1	24	LYS	2.0
13	AM	59	GLU	2.0
30	CF	73	VAL	2.0
31	CG	26	LYS	2.0
24	AX	74	C	2.0
33	CI	18	ASN	2.0
30	CF	41	GLU	2.0
4	AD	150	LYS	2.0
7	AG	92	ARG	2.0
17	AQ	11	ARG	2.0
24	AX	1	G	2.0
33	CI	79	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	AA	1646	1/1	0.41	0.46	99,99,99,99	0
57	MG	CA	3084	1/1	0.57	0.20	193,193,193,193	0
57	MG	DA	1650	1/1	0.58	0.17	81,81,81,81	0
57	MG	CA	3015	1/1	0.59	0.11	126,126,126,126	0
58	PAR	CA	3169	42/42	0.64	0.44	21,68,103,144	42
57	MG	CA	3055	1/1	0.72	0.12	114,114,114,114	0
57	MG	AA	1604	1/1	0.72	0.09	173,173,173,173	0
57	MG	AA	1658	1/1	0.73	0.71	97,97,97,97	0
58	PAR	CA	3168	42/42	0.73	0.61	10,10,10,10	0
57	MG	BA	3109	1/1	0.75	0.37	189,189,189,189	0
57	MG	BA	3021	1/1	0.77	0.39	276,276,276,276	0
57	MG	DA	1608	1/1	0.77	0.16	218,218,218,218	0
57	MG	BA	3179	1/1	0.79	0.39	88,88,88,88	0
57	MG	CA	3095	1/1	0.79	0.77	270,270,270,270	0
57	MG	DA	1634	1/1	0.79	0.06	128,128,128,128	0
57	MG	CA	3013	1/1	0.79	0.85	362,362,362,362	0
57	MG	DA	1606	1/1	0.79	0.08	144,144,144,144	0
57	MG	CA	3049	1/1	0.82	0.12	76,76,76,76	0
57	MG	BA	3095	1/1	0.82	0.16	187,187,187,187	0
57	MG	CA	3110	1/1	0.82	0.09	61,61,61,61	0
57	MG	CA	3053	1/1	0.82	0.16	46,46,46,46	0
57	MG	AA	1648	1/1	0.83	0.23	77,77,77,77	0
58	PAR	DA	1655	42/42	0.83	0.51	10,10,10,10	0
58	PAR	CA	3166	42/42	0.83	0.32	38,86,109,128	42
57	MG	CA	3030	1/1	0.83	0.17	154,154,154,154	0
57	MG	BA	3178	1/1	0.84	0.28	63,63,63,63	0
57	MG	BA	3173	1/1	0.84	0.38	59,59,59,59	0
57	MG	CA	3141	1/1	0.85	0.51	68,68,68,68	0
57	MG	CA	3119	1/1	0.85	0.18	215,215,215,215	0
57	MG	AA	1608	1/1	0.85	0.15	159,159,159,159	0
57	MG	AA	1621	1/1	0.85	0.08	157,157,157,157	0
57	MG	AA	1667	1/1	0.85	0.27	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	1614	1/1	0.85	0.07	96,96,96,96	0
58	PAR	BA	3005	42/42	0.85	0.28	41,100,141,152	42
57	MG	CA	3103	1/1	0.86	0.04	116,116,116,116	0
57	MG	BA	3102	1/1	0.86	1.00	293,293,293,293	0
57	MG	BA	3019	1/1	0.86	0.25	169,169,169,169	0
57	MG	AA	1636	1/1	0.86	1.03	313,313,313,313	0
57	MG	BQ	201	1/1	0.86	1.38	108,108,108,108	0
57	MG	BA	3092	1/1	0.86	0.16	173,173,173,173	0
57	MG	CA	3092	1/1	0.87	0.20	134,134,134,134	0
57	MG	BA	3162	1/1	0.88	0.29	44,44,44,44	0
57	MG	BA	3138	1/1	0.88	0.44	227,227,227,227	0
57	MG	DA	1622	1/1	0.88	0.87	331,331,331,331	0
57	MG	AA	1628	1/1	0.88	0.14	106,106,106,106	0
57	MG	BA	3181	1/1	0.88	0.25	106,106,106,106	0
57	MG	AA	1645	1/1	0.89	0.33	75,75,75,75	0
57	MG	DA	1604	1/1	0.89	0.38	166,166,166,166	0
57	MG	BA	3010	1/1	0.89	0.11	56,56,56,56	0
57	MG	AA	1651	1/1	0.89	0.27	60,60,60,60	0
57	MG	AA	1656	1/1	0.89	0.17	73,73,73,73	0
57	MG	AA	1611	1/1	0.89	0.08	125,125,125,125	0
57	MG	AA	1644	1/1	0.89	0.26	86,86,86,86	0
57	MG	BA	3060	1/1	0.89	0.15	146,146,146,146	0
57	MG	AA	1637	1/1	0.89	0.23	138,138,138,138	0
57	MG	AA	1609	1/1	0.89	0.18	227,227,227,227	0
57	MG	DA	1619	1/1	0.89	0.04	155,155,155,155	0
57	MG	CA	3131	1/1	0.89	0.14	75,75,75,75	0
57	MG	CA	3078	1/1	0.89	0.05	113,113,113,113	0
57	MG	AA	1665	1/1	0.89	0.70	106,106,106,106	0
58	PAR	CA	3167	42/42	0.89	0.36	10,10,10,10	0
57	MG	BA	3190	1/1	0.89	0.23	68,68,68,68	0
57	MG	CA	3061	1/1	0.89	0.26	102,102,102,102	0
58	PAR	BA	3003	42/42	0.89	0.39	10,10,10,10	0
57	MG	BA	3009	1/1	0.89	0.14	63,63,63,63	0
57	MG	BA	3074	1/1	0.89	0.20	105,105,105,105	0
57	MG	BA	3159	1/1	0.89	0.40	38,38,38,38	0
57	MG	BA	3119	1/1	0.90	0.24	262,262,262,262	0
57	MG	CA	3160	1/1	0.90	0.21	79,79,79,79	0
57	MG	BA	3160	1/1	0.90	0.35	74,74,74,74	0
57	MG	AA	1616	1/1	0.90	0.10	118,118,118,118	0
57	MG	CA	3147	1/1	0.90	0.38	77,77,77,77	0
57	MG	DA	1636	1/1	0.90	0.09	82,82,82,82	0
57	MG	BA	3012	1/1	0.90	0.07	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	1618	1/1	0.90	0.20	43,43,43,43	0
57	MG	AA	1652	1/1	0.90	0.10	50,50,50,50	0
57	MG	CA	3162	1/1	0.91	0.29	71,71,71,71	0
57	MG	AA	1642	1/1	0.91	0.30	60,60,60,60	0
57	MG	CA	3074	1/1	0.91	0.15	53,53,53,53	0
57	MG	CA	3083	1/1	0.91	0.14	79,79,79,79	0
57	MG	DA	1645	1/1	0.91	0.23	57,57,57,57	0
57	MG	CA	3054	1/1	0.91	0.12	41,41,41,41	0
57	MG	BA	3044	1/1	0.91	0.25	62,62,62,62	0
58	PAR	CA	3170	42/42	0.91	0.35	10,10,10,10	0
57	MG	DN	201	1/1	0.91	0.48	317,317,317,317	0
57	MG	AA	1643	1/1	0.91	0.70	162,162,162,162	0
57	MG	AA	1627	1/1	0.91	0.21	111,111,111,111	0
57	MG	CA	3086	1/1	0.91	0.23	83,83,83,83	0
57	MG	AA	1619	1/1	0.91	0.19	70,70,70,70	0
57	MG	CA	3087	1/1	0.91	0.20	75,75,75,75	0
57	MG	AA	1671	1/1	0.91	0.25	47,47,47,47	0
57	MG	DA	1638	1/1	0.91	0.30	93,93,93,93	0
57	MG	CA	3065	1/1	0.92	0.09	76,76,76,76	0
57	MG	CA	3071	1/1	0.92	0.51	218,218,218,218	0
57	MG	BA	3182	1/1	0.92	0.28	59,59,59,59	0
57	MG	CA	3068	1/1	0.92	0.19	58,58,58,58	0
57	MG	BA	3172	1/1	0.92	0.27	57,57,57,57	0
57	MG	BA	3075	1/1	0.92	0.17	88,88,88,88	0
57	MG	DA	1641	1/1	0.92	0.21	69,69,69,69	0
57	MG	CD	301	1/1	0.92	0.54	234,234,234,234	0
57	MG	CA	3153	1/1	0.92	0.32	47,47,47,47	0
57	MG	CA	3165	1/1	0.92	0.38	83,83,83,83	0
57	MG	CA	3048	1/1	0.92	0.19	157,157,157,157	0
57	MG	DA	1616	1/1	0.92	0.12	98,98,98,98	0
57	MG	AA	1630	1/1	0.92	0.10	113,113,113,113	0
57	MG	CA	3080	1/1	0.92	0.13	102,102,102,102	0
57	MG	CA	3126	1/1	0.92	0.15	146,146,146,146	0
57	MG	CA	3011	1/1	0.92	0.07	54,54,54,54	0
57	MG	AA	1663	1/1	0.92	0.32	52,52,52,52	0
57	MG	BA	3091	1/1	0.93	0.12	94,94,94,94	0
57	MG	BA	3017	1/1	0.93	0.12	56,56,56,56	0
57	MG	CA	3042	1/1	0.93	0.10	67,67,67,67	0
57	MG	CA	3014	1/1	0.93	0.12	82,82,82,82	0
57	MG	DA	1632	1/1	0.93	0.14	71,71,71,71	0
58	PAR	DA	1654	42/42	0.93	0.31	10,10,10,10	0
57	MG	BB	3201	1/1	0.93	0.10	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	1661	1/1	0.93	0.14	53,53,53,53	0
57	MG	BA	3167	1/1	0.93	0.35	53,53,53,53	0
57	MG	BA	3093	1/1	0.93	0.11	72,72,72,72	0
57	MG	CA	3109	1/1	0.93	0.20	74,74,74,74	0
57	MG	CA	3085	1/1	0.93	0.33	260,260,260,260	0
58	PAR	BA	3001	42/42	0.93	0.30	10,10,10,10	0
57	MG	CA	3123	1/1	0.93	0.25	177,177,177,177	0
58	PAR	BA	3004	42/42	0.93	0.27	10,10,10,10	0
57	MG	CA	3151	1/1	0.93	0.30	44,44,44,44	0
57	MG	CA	3038	1/1	0.93	0.10	71,71,71,71	0
57	MG	CA	3097	1/1	0.93	0.07	63,63,63,63	0
57	MG	DA	1647	1/1	0.94	0.14	59,59,59,59	0
57	MG	BA	3194	1/1	0.94	0.25	46,46,46,46	0
57	MG	BA	3137	1/1	0.94	0.10	95,95,95,95	0
57	MG	BA	3168	1/1	0.94	0.32	39,39,39,39	0
57	MG	AA	1668	1/1	0.94	0.39	70,70,70,70	0
57	MG	BA	3183	1/1	0.94	0.17	37,37,37,37	0
57	MG	CA	3102	1/1	0.94	0.11	123,123,123,123	0
57	MG	CA	3008	1/1	0.94	0.17	74,74,74,74	0
57	MG	BL	202	1/1	0.94	0.43	259,259,259,259	0
57	MG	CB	3201	1/1	0.94	0.11	216,216,216,216	0
57	MG	BA	3165	1/1	0.94	0.26	60,60,60,60	0
57	MG	BA	3170	1/1	0.94	0.10	51,51,51,51	0
57	MG	DA	1617	1/1	0.94	0.24	65,65,65,65	0
57	MG	BA	3056	1/1	0.94	0.11	59,59,59,59	0
57	MG	CA	3047	1/1	0.94	0.20	211,211,211,211	0
57	MG	CA	3135	1/1	0.94	0.14	121,121,121,121	0
57	MG	BA	3145	1/1	0.94	1.48	164,164,164,164	0
57	MG	BA	3164	1/1	0.94	0.31	54,54,54,54	0
57	MG	BA	3083	1/1	0.94	0.14	84,84,84,84	0
57	MG	CA	3156	1/1	0.94	0.17	45,45,45,45	0
57	MG	AA	1607	1/1	0.94	0.74	327,327,327,327	0
57	MG	BA	3082	1/1	0.94	0.24	139,139,139,139	0
57	MG	CA	3138	1/1	0.94	0.36	39,39,39,39	0
57	MG	CA	3006	1/1	0.94	0.06	83,83,83,83	0
57	MG	CA	3043	1/1	0.94	0.07	57,57,57,57	0
57	MG	CA	3146	1/1	0.94	0.14	52,52,52,52	0
57	MG	CA	3125	1/1	0.94	0.08	38,38,38,38	0
57	MG	BA	3154	1/1	0.94	0.76	56,56,56,56	0
58	PAR	AA	1672	42/42	0.94	0.24	10,10,10,10	0
57	MG	CA	3064	1/1	0.94	0.24	118,118,118,118	0
57	MG	BA	3080	1/1	0.95	0.19	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	3136	1/1	0.95	0.05	107,107,107,107	0
57	MG	CA	3091	1/1	0.95	0.07	93,93,93,93	0
57	MG	CA	3124	1/1	0.95	0.15	125,125,125,125	0
57	MG	CA	3019	1/1	0.95	0.98	252,252,252,252	0
57	MG	AA	1664	1/1	0.95	0.07	67,67,67,67	0
57	MG	CA	3034	1/1	0.95	0.29	157,157,157,157	0
57	MG	BA	3023	1/1	0.95	0.25	38,38,38,38	0
57	MG	DA	1633	1/1	0.95	0.85	264,264,264,264	0
57	MG	CA	3026	1/1	0.95	0.14	202,202,202,202	0
57	MG	BA	3061	1/1	0.95	0.04	70,70,70,70	0
57	MG	AA	1655	1/1	0.95	0.47	77,77,77,77	0
57	MG	DA	1648	1/1	0.95	0.50	41,41,41,41	0
57	MG	BA	3055	1/1	0.95	0.09	34,34,34,34	0
57	MG	BA	3034	1/1	0.95	0.15	41,41,41,41	0
57	MG	AA	1602	1/1	0.95	0.07	107,107,107,107	0
57	MG	BA	3110	1/1	0.95	0.44	89,89,89,89	0
57	MG	DA	1602	1/1	0.95	0.12	83,83,83,83	0
57	MG	BA	3064	1/1	0.95	0.17	80,80,80,80	0
57	MG	BA	3013	1/1	0.95	0.10	40,40,40,40	0
58	PAR	BA	3002	42/42	0.95	0.23	10,10,10,10	0
57	MG	DA	1620	1/1	0.95	0.11	78,78,78,78	0
57	MG	CA	3157	1/1	0.95	0.16	54,54,54,54	0
57	MG	CA	3164	1/1	0.95	0.33	44,44,44,44	0
57	MG	BA	3123	1/1	0.95	0.06	115,115,115,115	0
57	MG	BA	3029	1/1	0.95	0.48	240,240,240,240	0
57	MG	AA	1659	1/1	0.95	0.09	84,84,84,84	0
57	MG	AA	1660	1/1	0.95	0.09	67,67,67,67	0
57	MG	DA	1609	1/1	0.95	0.08	97,97,97,97	0
57	MG	AA	1662	1/1	0.95	0.18	69,69,69,69	0
57	MG	CA	3094	1/1	0.95	0.20	94,94,94,94	0
57	MG	BA	3018	1/1	0.95	0.13	59,59,59,59	0
57	MG	BA	3025	1/1	0.95	0.30	134,134,134,134	0
57	MG	AA	1632	1/1	0.95	0.18	149,149,149,149	0
57	MG	BA	3054	1/1	0.95	0.07	46,46,46,46	0
57	MG	AA	1633	1/1	0.95	0.10	86,86,86,86	0
57	MG	AA	1654	1/1	0.96	0.15	82,82,82,82	0
57	MG	CA	3132	1/1	0.96	0.09	67,67,67,67	0
57	MG	DA	1651	1/1	0.96	0.21	51,51,51,51	0
57	MG	BA	3106	1/1	0.96	0.08	71,71,71,71	0
57	MG	BA	3039	1/1	0.96	0.18	48,48,48,48	0
57	MG	BA	3059	1/1	0.96	0.10	60,60,60,60	0
57	MG	DA	1640	1/1	0.96	0.30	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	3099	1/1	0.96	0.16	58,58,58,58	0
57	MG	BA	3180	1/1	0.96	0.32	48,48,48,48	0
57	MG	CA	3117	1/1	0.96	0.08	45,45,45,45	0
57	MG	BA	3105	1/1	0.96	0.26	80,80,80,80	0
57	MG	BA	3031	1/1	0.96	0.08	60,60,60,60	0
57	MG	AA	1669	1/1	0.96	0.43	58,58,58,58	0
57	MG	DA	1612	1/1	0.96	0.12	123,123,123,123	0
57	MG	CA	3037	1/1	0.96	0.14	90,90,90,90	0
57	MG	BA	3144	1/1	0.96	0.25	34,34,34,34	0
57	MG	BA	3104	1/1	0.96	0.10	37,37,37,37	0
57	MG	DA	1627	1/1	0.96	0.09	80,80,80,80	0
57	MG	BA	3169	1/1	0.96	0.34	88,88,88,88	0
57	MG	BA	3115	1/1	0.96	0.25	133,133,133,133	0
57	MG	DA	1628	1/1	0.96	0.25	177,177,177,177	0
57	MG	CA	3009	1/1	0.96	0.15	88,88,88,88	0
57	MG	BA	3108	1/1	0.96	0.18	81,81,81,81	0
57	MG	CA	3158	1/1	0.96	0.45	57,57,57,57	0
57	MG	CA	3005	1/1	0.96	0.05	90,90,90,90	0
57	MG	DA	1613	1/1	0.96	0.12	89,89,89,89	0
57	MG	BA	3032	1/1	0.96	0.11	33,33,33,33	0
57	MG	CA	3052	1/1	0.96	0.09	54,54,54,54	0
57	MG	DD	302	1/1	0.96	0.30	53,53,53,53	0
57	MG	BA	3112	1/1	0.96	0.21	29,29,29,29	0
57	MG	BA	3036	1/1	0.96	0.13	38,38,38,38	0
57	MG	BA	3089	1/1	0.96	0.15	44,44,44,44	0
57	MG	CA	3012	1/1	0.96	0.10	30,30,30,30	0
57	MG	BA	3142	1/1	0.96	0.18	63,63,63,63	0
57	MG	BA	3081	1/1	0.96	0.07	57,57,57,57	0
57	MG	AA	1605	1/1	0.96	0.03	122,122,122,122	0
57	MG	DA	1601	1/1	0.96	0.13	47,47,47,47	0
57	MG	CA	3133	1/1	0.96	0.17	182,182,182,182	0
57	MG	CA	3100	1/1	0.96	0.10	155,155,155,155	0
57	MG	CA	3113	1/1	0.96	0.23	85,85,85,85	0
57	MG	BA	3149	1/1	0.96	0.14	33,33,33,33	0
57	MG	CA	3090	1/1	0.96	0.09	69,69,69,69	0
57	MG	CA	3072	1/1	0.96	0.11	99,99,99,99	0
57	MG	BA	3107	1/1	0.96	0.07	60,60,60,60	0
57	MG	BA	3086	1/1	0.96	0.12	74,74,74,74	0
57	MG	BA	3186	1/1	0.96	0.37	37,37,37,37	0
57	MG	AA	1653	1/1	0.96	0.22	82,82,82,82	0
57	MG	BA	3175	1/1	0.96	0.17	44,44,44,44	0
57	MG	BA	3174	1/1	0.96	0.24	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	1639	1/1	0.96	0.24	161,161,161,161	0
57	MG	BA	3045	1/1	0.96	0.40	217,217,217,217	0
57	MG	CA	3145	1/1	0.96	0.26	59,59,59,59	0
57	MG	AA	1666	1/1	0.96	0.24	44,44,44,44	0
57	MG	BA	3014	1/1	0.96	0.20	101,101,101,101	0
57	MG	CA	3161	1/1	0.96	0.36	39,39,39,39	0
57	MG	BA	3087	1/1	0.96	0.06	139,139,139,139	0
57	MG	CA	3134	1/1	0.96	0.14	55,55,55,55	0
57	MG	BA	3052	1/1	0.96	0.16	50,50,50,50	0
57	MG	BA	3090	1/1	0.96	0.21	71,71,71,71	0
57	MG	AA	1620	1/1	0.96	0.13	133,133,133,133	0
57	MG	BA	3103	1/1	0.96	0.08	41,41,41,41	0
57	MG	CA	3045	1/1	0.96	0.17	46,46,46,46	0
57	MG	BA	3122	1/1	0.96	0.06	60,60,60,60	0
57	MG	CA	3149	1/1	0.96	0.24	69,69,69,69	0
57	MG	CB	3202	1/1	0.96	0.08	114,114,114,114	0
57	MG	BA	3015	1/1	0.96	0.10	58,58,58,58	0
57	MG	CB	3203	1/1	0.97	0.07	115,115,115,115	0
57	MG	AA	1670	1/1	0.97	0.55	50,50,50,50	0
57	MG	CA	3163	1/1	0.97	0.26	44,44,44,44	0
57	MG	CA	3137	1/1	0.97	0.31	22,22,22,22	0
57	MG	DA	1653	1/1	0.97	0.20	51,51,51,51	0
57	MG	AA	1657	1/1	0.97	0.21	78,78,78,78	0
57	MG	BA	3114	1/1	0.97	0.15	65,65,65,65	0
57	MG	BA	3128	1/1	0.97	0.21	99,99,99,99	0
57	MG	BA	3079	1/1	0.97	0.13	42,42,42,42	0
57	MG	BA	3135	1/1	0.97	0.07	79,79,79,79	0
57	MG	DA	1611	1/1	0.97	0.05	60,60,60,60	0
57	MG	CA	3063	1/1	0.97	0.09	50,50,50,50	0
57	MG	BA	3037	1/1	0.97	0.17	52,52,52,52	0
57	MG	BA	3027	1/1	0.97	0.16	57,57,57,57	0
57	MG	DA	1642	1/1	0.97	0.29	60,60,60,60	0
57	MG	CA	3028	1/1	0.97	0.41	312,312,312,312	0
57	MG	CA	3024	1/1	0.97	0.14	65,65,65,65	0
57	MG	DA	1618	1/1	0.97	0.14	51,51,51,51	0
57	MG	BA	3094	1/1	0.97	0.14	153,153,153,153	0
57	MG	AN	201	1/1	0.97	0.08	109,109,109,109	0
57	MG	CA	3096	1/1	0.97	0.07	100,100,100,100	0
57	MG	BA	3077	1/1	0.97	0.22	63,63,63,63	0
57	MG	CA	3106	1/1	0.97	0.20	33,33,33,33	0
57	MG	AA	1634	1/1	0.97	0.08	87,87,87,87	0
57	MG	AA	1614	1/1	0.97	0.21	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3065	1/1	0.97	0.16	98,98,98,98	0
57	MG	CA	3056	1/1	0.97	0.23	155,155,155,155	0
57	MG	BA	3088	1/1	0.97	0.09	147,147,147,147	0
57	MG	CA	3101	1/1	0.97	0.15	58,58,58,58	0
57	MG	CA	3077	1/1	0.97	0.15	131,131,131,131	0
57	MG	BA	3152	1/1	0.97	0.15	56,56,56,56	0
57	MG	BA	3068	1/1	0.97	0.09	27,27,27,27	0
57	MG	BA	3117	1/1	0.97	0.19	65,65,65,65	0
57	MG	AA	1631	1/1	0.97	0.23	115,115,115,115	0
57	MG	DA	1629	1/1	0.97	0.09	86,86,86,86	0
57	MG	AA	1641	1/1	0.97	0.11	124,124,124,124	0
57	MG	CA	3143	1/1	0.97	0.24	69,69,69,69	0
57	MG	CA	3115	1/1	0.97	0.12	235,235,235,235	0
57	MG	DA	1635	1/1	0.97	0.24	126,126,126,126	0
57	MG	BA	3067	1/1	0.97	0.30	218,218,218,218	0
57	MG	BA	3153	1/1	0.97	0.35	34,34,34,34	0
57	MG	DA	1626	1/1	0.97	0.07	98,98,98,98	0
57	MG	CA	3059	1/1	0.97	0.10	88,88,88,88	0
57	MG	AA	1623	1/1	0.97	0.16	67,67,67,67	0
57	MG	CA	3089	1/1	0.97	0.17	215,215,215,215	0
57	MG	BA	3040	1/1	0.97	0.09	66,66,66,66	0
57	MG	AA	1601	1/1	0.97	0.15	50,50,50,50	0
57	MG	AA	1624	1/1	0.97	0.07	99,99,99,99	0
57	MG	CA	3108	1/1	0.97	0.18	101,101,101,101	0
57	MG	CA	3154	1/1	0.97	0.28	42,42,42,42	0
57	MG	DA	1646	1/1	0.97	0.29	31,31,31,31	0
57	MG	DA	1643	1/1	0.97	0.16	73,73,73,73	0
57	MG	DA	1623	1/1	0.97	0.07	64,64,64,64	0
57	MG	AA	1617	1/1	0.97	0.10	104,104,104,104	0
57	MG	DD	301	1/1	0.97	0.26	314,314,314,314	0
57	MG	BA	3071	1/1	0.97	0.11	43,43,43,43	0
57	MG	CA	3032	1/1	0.97	0.18	97,97,97,97	0
57	MG	BA	3130	1/1	0.97	0.32	270,270,270,270	0
57	MG	BO	201	1/1	0.97	0.10	67,67,67,67	0
57	MG	CA	3140	1/1	0.97	0.27	29,29,29,29	0
57	MG	BA	3129	1/1	0.97	0.19	78,78,78,78	0
57	MG	CA	3098	1/1	0.97	0.64	242,242,242,242	0
57	MG	CA	3003	1/1	0.97	0.07	95,95,95,95	0
57	MG	DA	1631	1/1	0.97	0.16	196,196,196,196	0
57	MG	CA	3107	1/1	0.97	0.13	95,95,95,95	0
57	MG	CA	3033	1/1	0.97	0.13	56,56,56,56	0
57	MG	CA	3148	1/1	0.97	0.18	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3035	1/1	0.97	0.12	43,43,43,43	0
57	MG	AA	1650	1/1	0.97	0.40	55,55,55,55	0
57	MG	CA	3070	1/1	0.97	0.14	251,251,251,251	0
57	MG	BA	3048	1/1	0.97	0.16	69,69,69,69	0
57	MG	BA	3140	1/1	0.97	0.06	73,73,73,73	0
57	MG	AA	1615	1/1	0.97	0.09	123,123,123,123	0
57	MG	BA	3016	1/1	0.97	0.10	56,56,56,56	0
57	MG	BA	3176	1/1	0.97	0.30	51,51,51,51	0
57	MG	CA	3073	1/1	0.97	0.12	64,64,64,64	0
57	MG	DA	1649	1/1	0.97	0.09	63,63,63,63	0
57	MG	AA	1622	1/1	0.97	0.06	76,76,76,76	0
57	MG	DA	1630	1/1	0.97	0.14	72,72,72,72	0
57	MG	BA	3006	1/1	0.97	0.12	40,40,40,40	0
57	MG	CA	3001	1/1	0.97	0.09	54,54,54,54	0
57	MG	BA	3101	1/1	0.97	0.16	70,70,70,70	0
57	MG	DA	1624	1/1	0.97	0.11	30,30,30,30	0
57	MG	BA	3118	1/1	0.97	0.37	164,164,164,164	0
57	MG	CA	3069	1/1	0.97	0.17	63,63,63,63	0
57	MG	AA	1638	1/1	0.97	0.08	58,58,58,58	0
57	MG	AA	1649	1/1	0.97	0.27	51,51,51,51	0
57	MG	CA	3007	1/1	0.97	0.28	204,204,204,204	0
57	MG	CA	3060	1/1	0.97	0.08	67,67,67,67	0
57	MG	BA	3024	1/1	0.97	0.08	68,68,68,68	0
57	MG	CA	3159	1/1	0.97	0.17	52,52,52,52	0
57	MG	CA	3150	1/1	0.97	0.24	54,54,54,54	0
57	MG	CA	3031	1/1	0.98	0.17	30,30,30,30	0
57	MG	BA	3020	1/1	0.98	0.08	41,41,41,41	0
57	MG	BA	3139	1/1	0.98	0.12	47,47,47,47	0
57	MG	CA	3027	1/1	0.98	0.04	47,47,47,47	0
57	MG	CA	3128	1/1	0.98	0.10	66,66,66,66	0
57	MG	AA	1626	1/1	0.98	0.09	66,66,66,66	0
57	MG	CA	3021	1/1	0.98	0.05	57,57,57,57	0
57	MG	BA	3148	1/1	0.98	0.32	34,34,34,34	0
57	MG	BA	3070	1/1	0.98	0.12	50,50,50,50	0
57	MG	CA	3062	1/1	0.98	0.11	97,97,97,97	0
57	MG	BA	3072	1/1	0.98	0.08	41,41,41,41	0
57	MG	CA	3039	1/1	0.98	0.14	58,58,58,58	0
57	MG	DA	1621	1/1	0.98	0.09	47,47,47,47	0
57	MG	BB	3202	1/1	0.98	0.08	34,34,34,34	0
57	MG	DA	1652	1/1	0.98	0.17	67,67,67,67	0
57	MG	CA	3076	1/1	0.98	0.18	77,77,77,77	0
57	MG	BA	3150	1/1	0.98	0.71	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	3127	1/1	0.98	0.06	47,47,47,47	0
57	MG	BA	3163	1/1	0.98	0.18	27,27,27,27	0
57	MG	BA	3157	1/1	0.98	0.30	44,44,44,44	0
57	MG	BA	3147	1/1	0.98	0.15	54,54,54,54	0
57	MG	BA	3097	1/1	0.98	0.06	91,91,91,91	0
57	MG	BA	3057	1/1	0.98	0.12	26,26,26,26	0
57	MG	CA	3104	1/1	0.98	0.26	57,57,57,57	0
57	MG	CA	3118	1/1	0.98	0.05	53,53,53,53	0
57	MG	BA	3030	1/1	0.98	0.08	43,43,43,43	0
57	MG	CQ	201	1/1	0.98	0.39	32,32,32,32	0
57	MG	DA	1615	1/1	0.98	0.20	213,213,213,213	0
57	MG	AA	1613	1/1	0.98	0.10	97,97,97,97	0
57	MG	CA	3081	1/1	0.98	0.05	48,48,48,48	0
57	MG	CA	3152	1/1	0.98	0.09	44,44,44,44	0
57	MG	DA	1607	1/1	0.98	0.15	63,63,63,63	0
57	MG	CA	3093	1/1	0.98	0.08	127,127,127,127	0
57	MG	BA	3098	1/1	0.98	0.46	157,157,157,157	0
57	MG	BA	3100	1/1	0.98	0.15	66,66,66,66	0
57	MG	BA	3026	1/1	0.98	0.15	47,47,47,47	0
57	MG	DA	1605	1/1	0.98	0.14	96,96,96,96	0
57	MG	BA	3125	1/1	0.98	0.11	36,36,36,36	0
57	MG	DA	1644	1/1	0.98	0.29	62,62,62,62	0
57	MG	BA	3046	1/1	0.98	0.06	58,58,58,58	0
57	MG	CA	3046	1/1	0.98	0.27	130,130,130,130	0
57	MG	BA	3066	1/1	0.98	0.17	77,77,77,77	0
57	MG	BA	3151	1/1	0.98	0.22	44,44,44,44	0
57	MG	CA	3116	1/1	0.98	0.18	94,94,94,94	0
57	MG	BA	3076	1/1	0.98	0.10	32,32,32,32	0
57	MG	BA	3121	1/1	0.98	0.10	34,34,34,34	0
57	MG	AA	1606	1/1	0.98	0.04	102,102,102,102	0
57	MG	CA	3004	1/1	0.98	0.12	130,130,130,130	0
57	MG	BA	3099	1/1	0.98	0.06	96,96,96,96	0
57	MG	BA	3028	1/1	0.98	0.14	35,35,35,35	0
57	MG	AA	1635	1/1	0.98	0.15	234,234,234,234	0
57	MG	CA	3155	1/1	0.98	0.30	39,39,39,39	0
57	MG	CA	3044	1/1	0.98	0.05	53,53,53,53	0
57	MG	BA	3062	1/1	0.98	0.10	73,73,73,73	0
57	MG	BA	3136	1/1	0.98	0.10	61,61,61,61	0
57	MG	DA	1603	1/1	0.98	0.12	37,37,37,37	0
57	MG	CA	3022	1/1	0.98	0.09	59,59,59,59	0
57	MG	CA	3111	1/1	0.98	0.44	164,164,164,164	0
59	ZN	B4	9501	1/1	0.98	0.54	386,386,386,386	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	1629	1/1	0.98	0.06	54,54,54,54	0
57	MG	BA	3063	1/1	0.98	0.24	93,93,93,93	0
57	MG	CA	3035	1/1	0.98	0.11	35,35,35,35	0
57	MG	DA	1625	1/1	0.98	0.11	42,42,42,42	0
57	MG	CA	3122	1/1	0.98	0.20	88,88,88,88	0
57	MG	BA	3184	1/1	0.98	0.22	40,40,40,40	0
57	MG	BA	3111	1/1	0.98	0.14	52,52,52,52	0
57	MG	CA	3016	1/1	0.98	0.06	40,40,40,40	0
57	MG	CA	3029	1/1	0.98	0.37	168,168,168,168	0
57	MG	BA	3078	1/1	0.98	0.11	86,86,86,86	0
57	MG	BA	3143	1/1	0.98	0.35	25,25,25,25	0
57	MG	CA	3066	1/1	0.98	0.06	45,45,45,45	0
57	MG	BA	3051	1/1	0.98	0.10	70,70,70,70	0
57	MG	AA	1603	1/1	0.98	0.16	45,45,45,45	0
57	MG	BA	3126	1/1	0.99	0.17	39,39,39,39	0
57	MG	CA	3082	1/1	0.99	0.12	50,50,50,50	0
57	MG	CA	3088	1/1	0.99	0.07	98,98,98,98	0
57	MG	BA	3189	1/1	0.99	0.15	47,47,47,47	0
57	MG	CA	3017	1/1	0.99	0.10	36,36,36,36	0
57	MG	BA	3008	1/1	0.99	0.09	62,62,62,62	0
57	MG	CA	3036	1/1	0.99	0.12	53,53,53,53	0
57	MG	BA	3156	1/1	0.99	0.41	35,35,35,35	0
57	MG	BA	3191	1/1	0.99	0.13	43,43,43,43	0
57	MG	BA	3069	1/1	0.99	0.09	20,20,20,20	0
57	MG	CA	3129	1/1	0.99	0.09	33,33,33,33	0
57	MG	BA	3155	1/1	0.99	0.26	23,23,23,23	0
57	MG	BA	3127	1/1	0.99	0.11	88,88,88,88	0
57	MG	CA	3144	1/1	0.99	0.07	56,56,56,56	0
57	MG	CA	3105	1/1	0.99	0.13	44,44,44,44	0
57	MG	BA	3022	1/1	0.99	0.09	28,28,28,28	0
57	MG	AA	1639	1/1	0.99	0.18	59,59,59,59	0
57	MG	BA	3042	1/1	0.99	0.14	32,32,32,32	0
57	MG	BA	3132	1/1	0.99	0.18	30,30,30,30	0
57	MG	CA	3023	1/1	0.99	0.10	37,37,37,37	0
57	MG	BA	3085	1/1	0.99	0.11	57,57,57,57	0
57	MG	BA	3049	1/1	0.99	0.10	57,57,57,57	0
57	MG	CA	3057	1/1	0.99	0.08	46,46,46,46	0
57	MG	BA	3047	1/1	0.99	0.08	42,42,42,42	0
57	MG	BA	3158	1/1	0.99	0.39	30,30,30,30	0
57	MG	CA	3121	1/1	0.99	0.06	27,27,27,27	0
57	MG	CA	3020	1/1	0.99	0.14	37,37,37,37	0
57	MG	AA	1640	1/1	0.99	0.17	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3185	1/1	0.99	0.39	32,32,32,32	0
57	MG	BA	3011	1/1	0.99	0.07	34,34,34,34	0
57	MG	BA	3096	1/1	0.99	0.03	66,66,66,66	0
57	MG	BB	3204	1/1	0.99	0.19	24,24,24,24	0
57	MG	BA	3193	1/1	0.99	0.34	28,28,28,28	0
57	MG	BA	3007	1/1	0.99	0.07	61,61,61,61	0
57	MG	BA	3043	1/1	0.99	0.13	66,66,66,66	0
57	MG	BA	3166	1/1	0.99	0.23	34,34,34,34	0
57	MG	CA	3067	1/1	0.99	0.11	64,64,64,64	0
57	MG	CA	3114	1/1	0.99	0.12	169,169,169,169	0
57	MG	CA	3010	1/1	0.99	0.10	34,34,34,34	0
57	MG	BA	3041	1/1	0.99	0.13	32,32,32,32	0
57	MG	CA	3002	1/1	0.99	0.04	49,49,49,49	0
57	MG	CA	3139	1/1	0.99	0.29	52,52,52,52	0
57	MG	CA	3050	1/1	0.99	0.09	42,42,42,42	0
57	MG	AA	1647	1/1	0.99	0.20	44,44,44,44	0
57	MG	DA	1637	1/1	0.99	0.17	158,158,158,158	0
57	MG	CA	3120	1/1	0.99	0.12	62,62,62,62	0
57	MG	CA	3130	1/1	0.99	0.08	44,44,44,44	0
57	MG	BA	3053	1/1	0.99	0.14	29,29,29,29	0
57	MG	BA	3192	1/1	0.99	0.18	46,46,46,46	0
57	MG	BA	3133	1/1	0.99	0.12	39,39,39,39	0
57	MG	BA	3161	1/1	0.99	0.18	45,45,45,45	0
57	MG	CA	3142	1/1	0.99	0.21	33,33,33,33	0
57	MG	AA	1610	1/1	0.99	0.04	66,66,66,66	0
57	MG	CA	3075	1/1	0.99	0.10	107,107,107,107	0
57	MG	BA	3073	1/1	0.99	0.09	141,141,141,141	0
57	MG	AA	1612	1/1	0.99	0.13	94,94,94,94	0
57	MG	CA	3025	1/1	0.99	0.14	121,121,121,121	0
57	MG	BA	3134	1/1	0.99	0.28	143,143,143,143	0
57	MG	BA	3038	1/1	0.99	0.25	73,73,73,73	0
57	MG	CA	3058	1/1	0.99	0.13	55,55,55,55	0
57	MG	BA	3146	1/1	0.99	0.31	48,48,48,48	0
57	MG	BA	3177	1/1	0.99	0.06	86,86,86,86	0
57	MG	BA	3116	1/1	0.99	0.22	133,133,133,133	0
57	MG	BA	3120	1/1	0.99	0.25	91,91,91,91	0
57	MG	BB	3203	1/1	0.99	0.05	52,52,52,52	0
57	MG	BA	3084	1/1	0.99	0.11	36,36,36,36	0
57	MG	BA	3141	1/1	0.99	0.19	31,31,31,31	0
57	MG	CA	3041	1/1	0.99	0.19	36,36,36,36	0
57	MG	DA	1610	1/1	0.99	0.10	67,67,67,67	0
57	MG	BA	3050	1/1	0.99	0.10	27,27,27,27	0

*Continued on next page...*

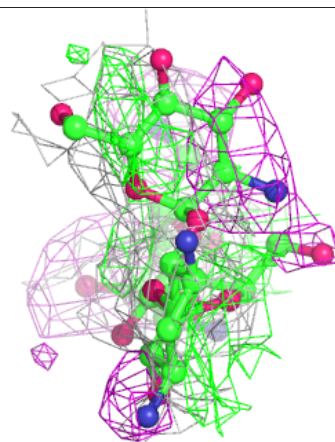
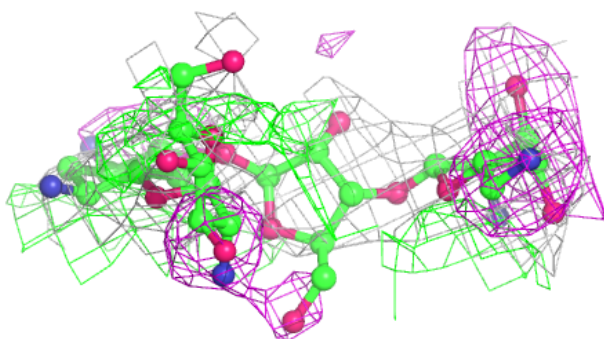
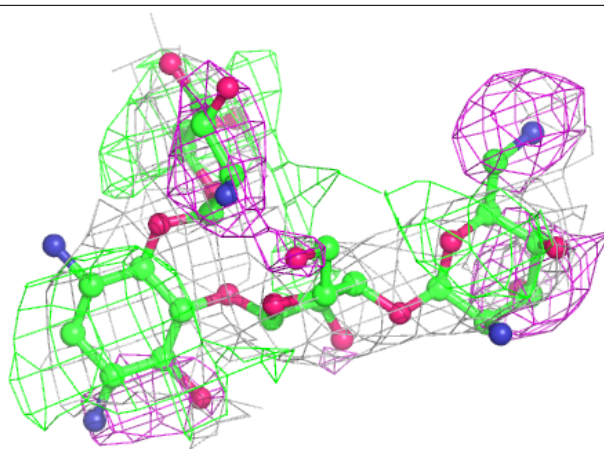
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3187	1/1	0.99	0.23	29,29,29,29	0
57	MG	BA	3058	1/1	0.99	0.12	25,25,25,25	0
57	MG	CA	3112	1/1	0.99	0.20	137,137,137,137	0
57	MG	CA	3018	1/1	0.99	0.05	41,41,41,41	0
57	MG	BA	3188	1/1	0.99	0.15	39,39,39,39	0
57	MG	BA	3124	1/1	0.99	0.13	45,45,45,45	0
57	MG	BA	3131	1/1	0.99	0.08	39,39,39,39	0
59	ZN	C4	9501	1/1	0.99	0.15	109,109,109,109	0
57	MG	CA	3079	1/1	0.99	0.12	195,195,195,195	0
57	MG	BA	3033	1/1	0.99	0.09	48,48,48,48	0
57	MG	BA	3113	1/1	0.99	0.15	96,96,96,96	0
57	MG	BL	201	1/1	0.99	0.12	21,21,21,21	0
57	MG	CA	3051	1/1	1.00	0.07	24,24,24,24	0
57	MG	AA	1625	1/1	1.00	0.13	50,50,50,50	0
57	MG	CA	3040	1/1	1.00	0.14	98,98,98,98	0
57	MG	BA	3171	1/1	1.00	0.19	47,47,47,47	0

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

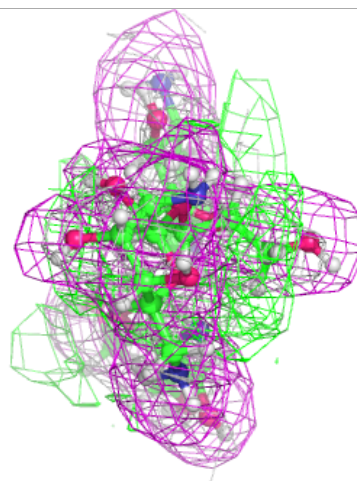
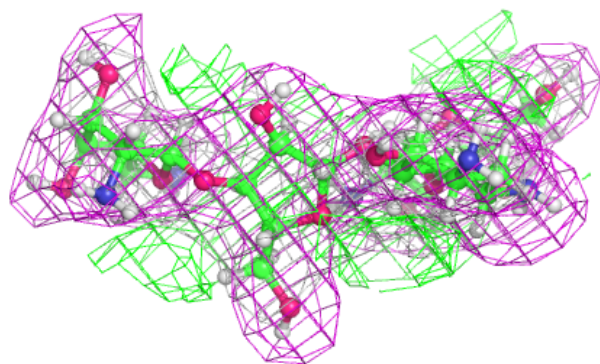
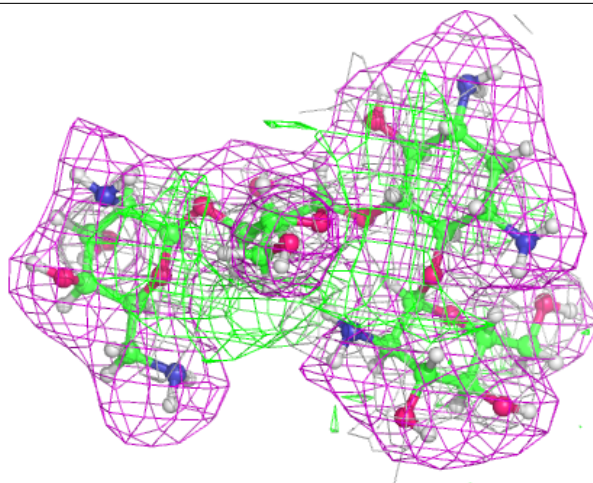
**Electron density around PAR CA 3169:**

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



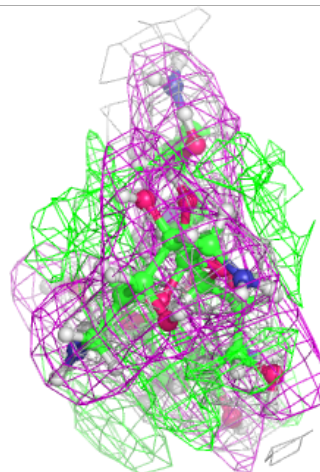
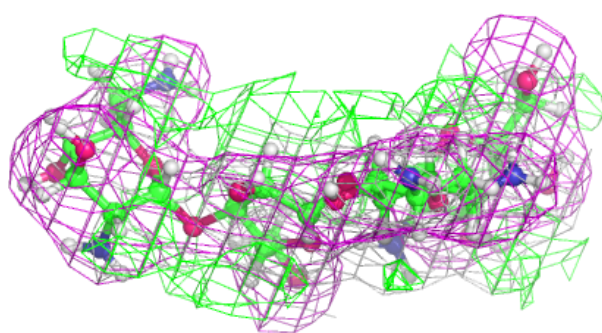
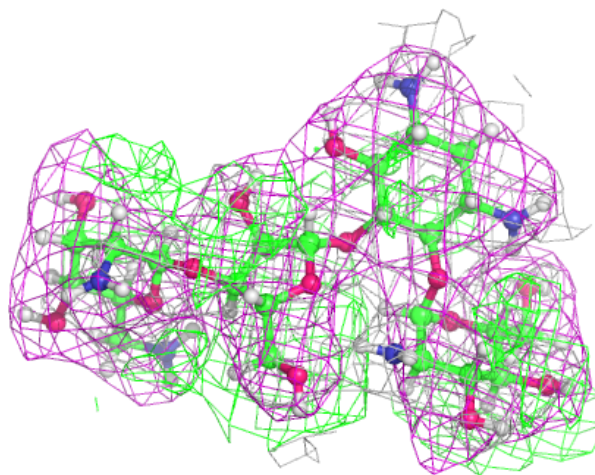
**Electron density around PAR CA 3168:**

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



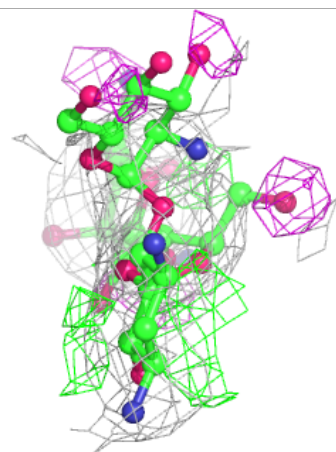
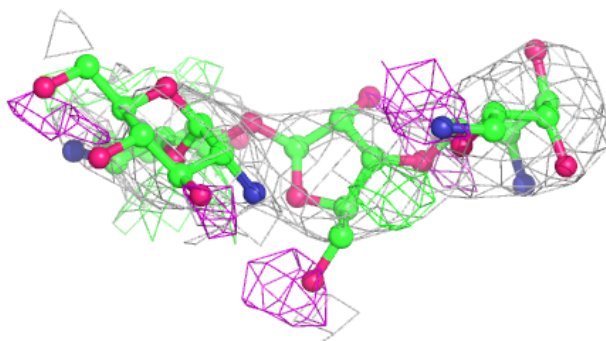
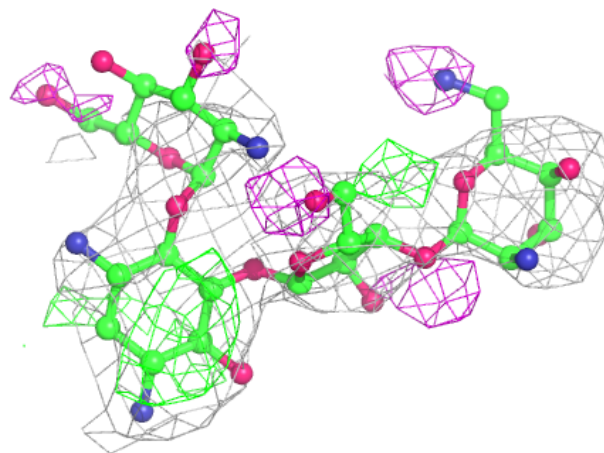
**Electron density around PAR DA 1655:**

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



**Electron density around PAR CA 3166:**

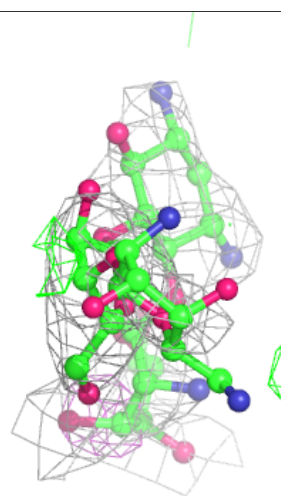
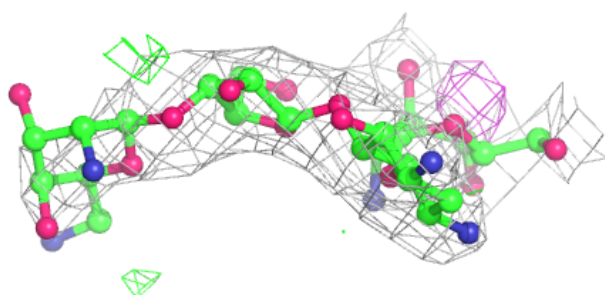
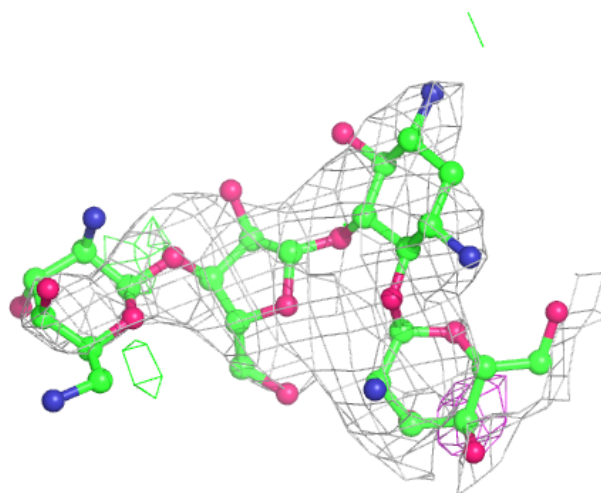
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





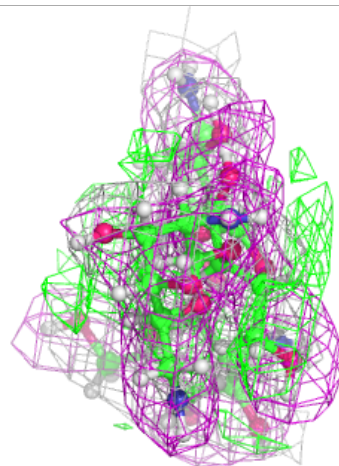
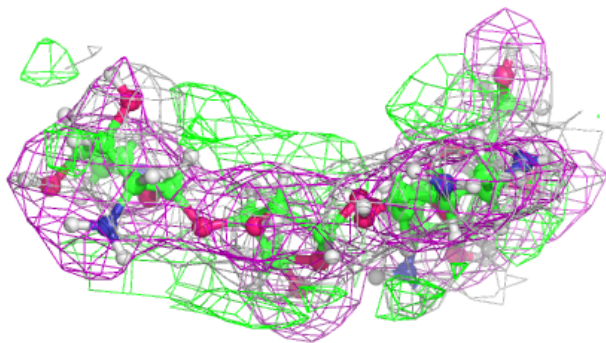
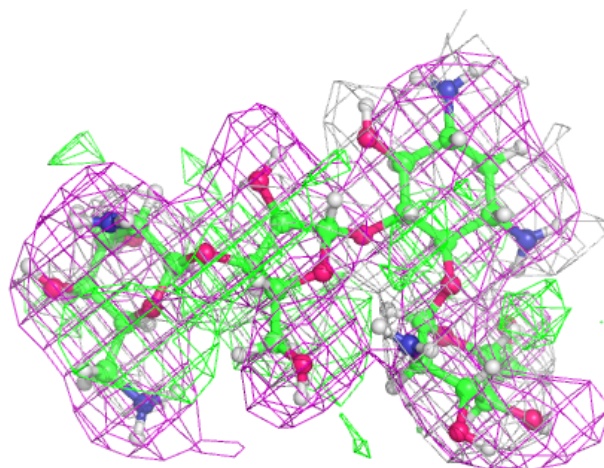
**Electron density around PAR BA 3005:**

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



**Electron density around PAR CA 3167:**

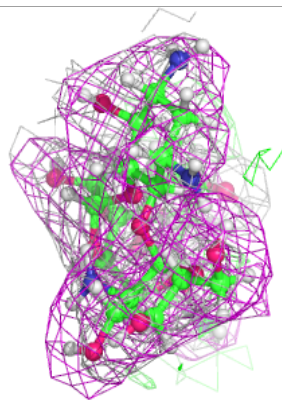
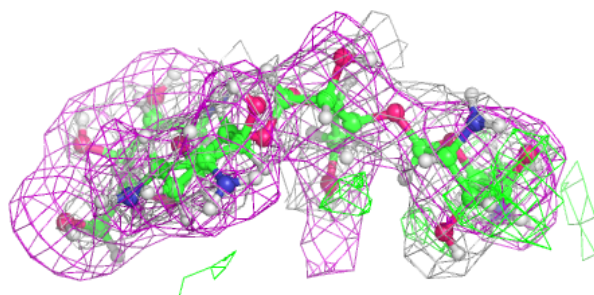
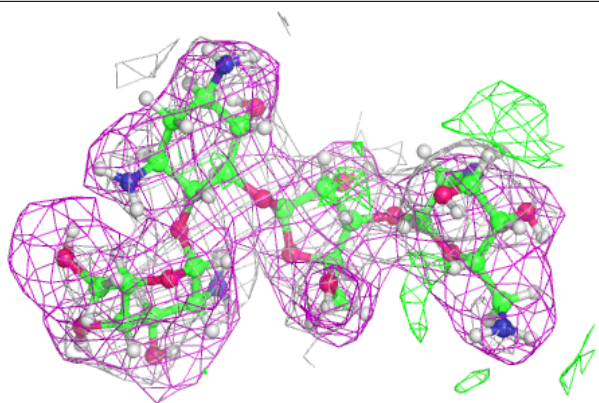
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





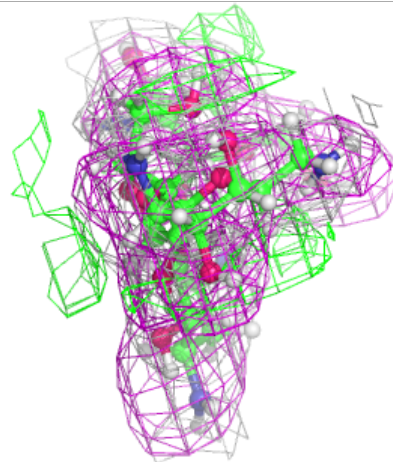
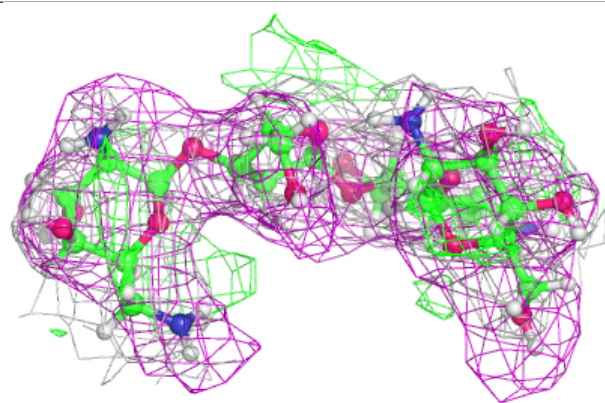
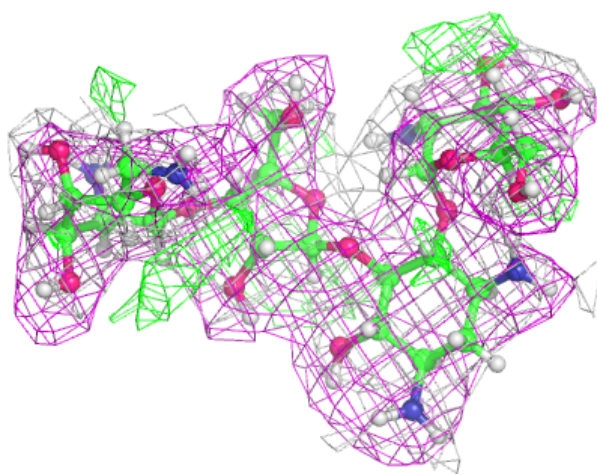
**Electron density around PAR BA 3003:**

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



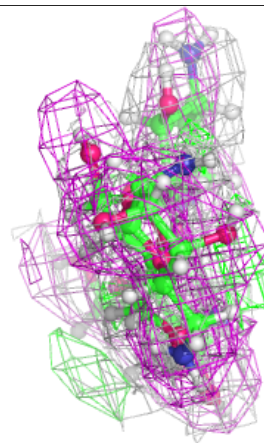
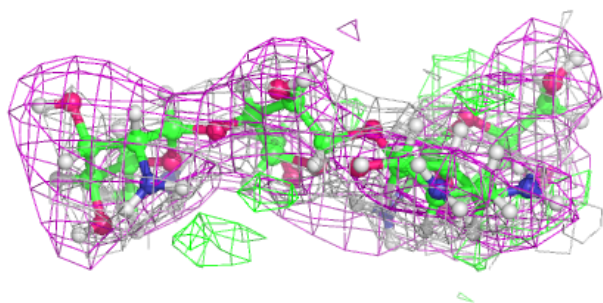
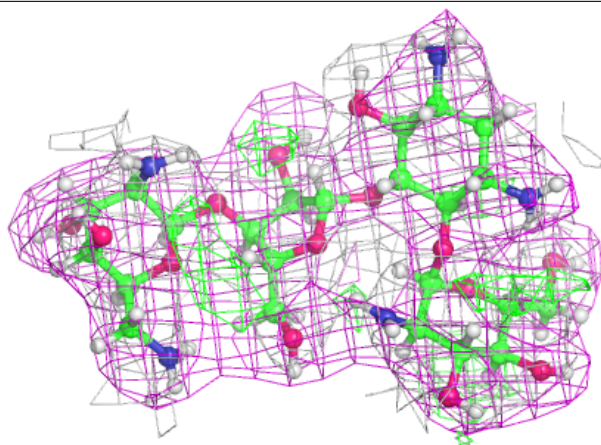
**Electron density around PAR CA 3170:**

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



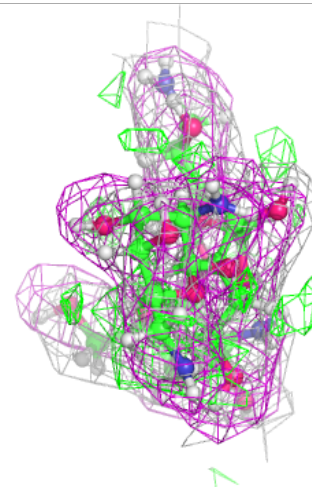
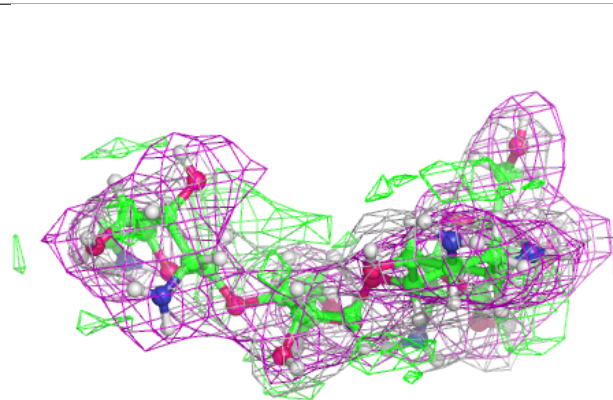
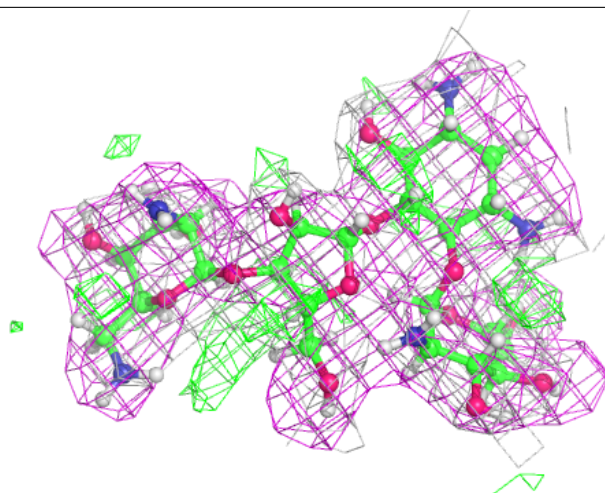
**Electron density around PAR DA 1654:**

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



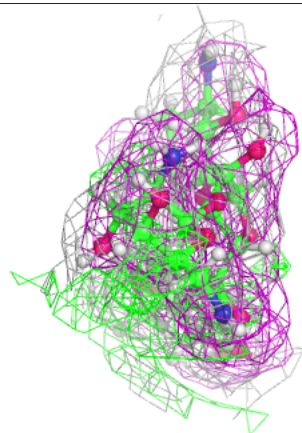
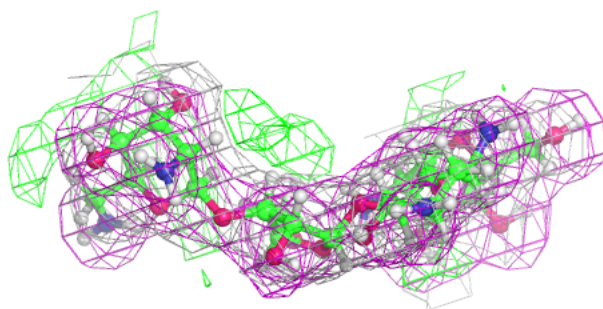
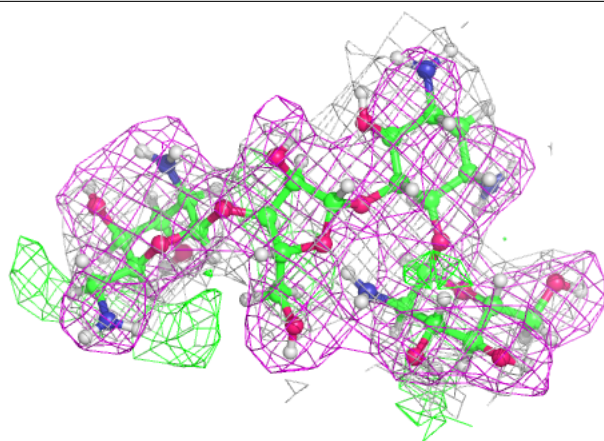
**Electron density around PAR BA 3001:**

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



**Electron density around PAR BA 3004:**

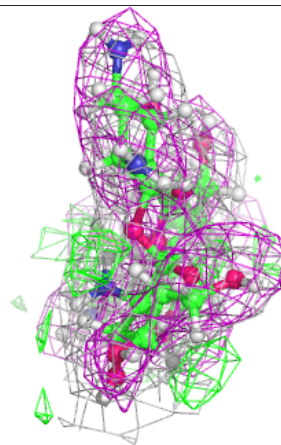
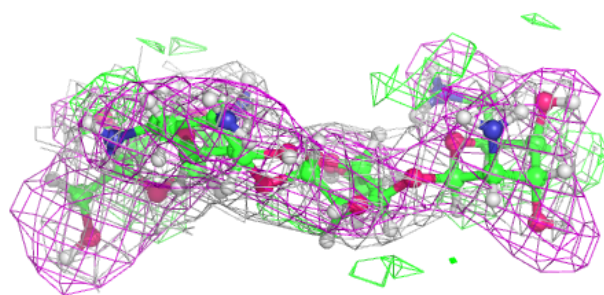
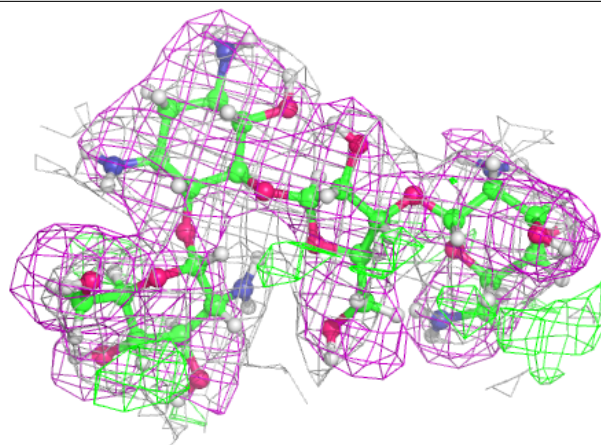
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





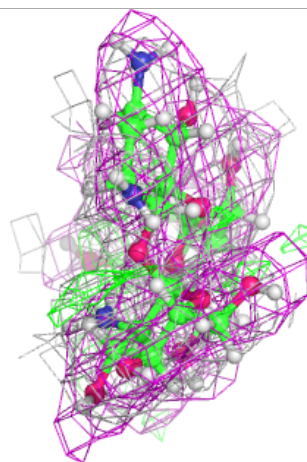
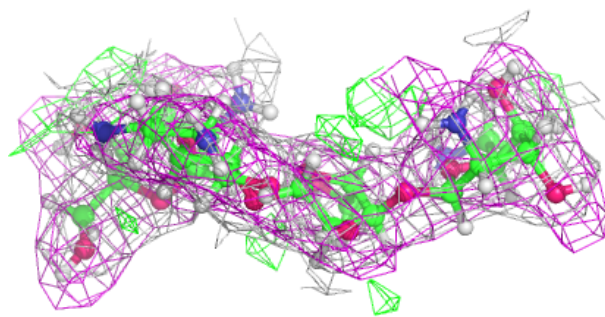
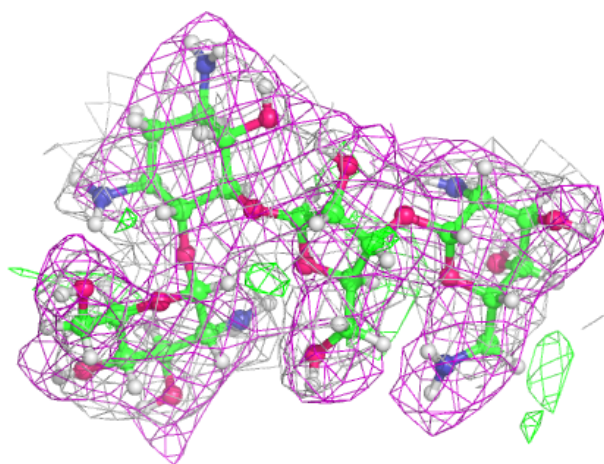
**Electron density around PAR AA 1672:**

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



**Electron density around PAR BA 3002:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.