



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 08:31 AM EDT

PDB ID : 5J88 / pdb_00005j88
Title : Structure of the E coli 70S ribosome with the U1060A mutation in 16S rRNA
Authors : Cocozaki, A.; Ferguson, A.
Deposited on : 2016-04-07
Resolution : 3.32 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

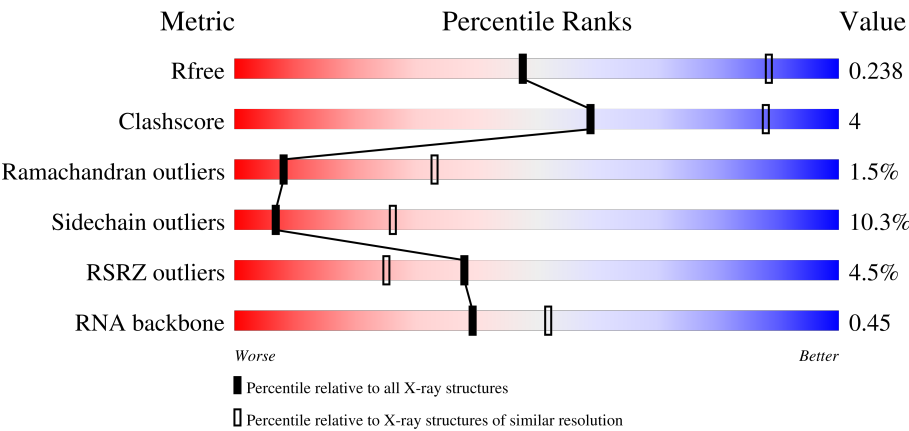
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)
RNA backbone	3983	1067 (3.64-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1534	4% 67% 29%
1	BA	1534	5% 66% 29%
2	AB	224	2% 77% 20%
2	BB	224	% 79% 18%

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	BC	206	
4	AD	205	
4	BD	205	
5	AE	155	
5	BE	155	
6	AF	106	
6	BF	106	
7	AG	151	
7	BG	151	
8	AH	129	
8	BH	129	
9	AI	127	
9	BI	127	
10	AJ	99	
10	BJ	99	
11	AK	129	
11	BK	129	
12	AL	123	
12	BL	123	
13	AM	114	
13	BM	114	
14	AN	100	
14	BN	100	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	BO	88	84% 13% •
16	AP	82	10% 84% 12% •
16	BP	82	10% 84% 12% •
17	AQ	80	74% 24% •
17	BQ	80	5% 75% 20% • •
18	AR	55	2% 78% 18% •
18	BR	55	4% 76% 24%
19	AS	79	10% 66% 29% 5%
19	BS	79	19% 71% 25% • •
20	AT	86	5% 66% 29% 5%
20	BT	86	12% 70% 24% • •
21	AU	56	2% 71% 27% •
21	BU	56	5% 79% 20% •
22	C1	56	21% 68% 29% •
22	D1	56	77% 20% •
23	C2	51	10% 65% 31% • •
23	D2	51	2% 71% 29%
24	C3	46	20% 80% 17% •
24	D3	46	2% 72% 26% •
25	C4	64	42% 84% 16%
25	D4	64	77% 23%
26	C5	38	16% 79% 18% •
26	D5	38	82% 16% •
27	C0	58	10% 76% 19% 5%
27	D0	58	3% 71% 26% •

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Mol	Chain	Length	Quality of chain
28	CB	120	
28	DB	120	
29	CC	272	
29	DC	272	
30	CD	209	
31	CA	2904	
32	DD	209	
33	CE	201	
33	DE	201	
34	CF	178	
34	DF	178	
35	CG	176	
35	DG	176	
36	CH	149	
36	DH	149	
37	CJ	135	
37	DJ	135	
38	CK	142	
38	DK	142	
39	CL	123	
39	DL	123	
40	CM	144	
40	DM	144	
41	CN	136	
41	DN	136	

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Mol	Chain	Length	Quality of chain
42	CO	127	
42	DO	127	
43	CP	117	
43	DP	117	
44	CQ	114	
44	DQ	114	
45	CR	117	
45	DR	117	
46	CS	103	
46	DS	103	
47	CT	110	
47	DT	110	
48	CU	100	
48	DU	100	
49	CV	103	
49	DV	103	
50	CW	94	
50	DW	94	
51	CX	76	
51	DX	76	
52	CY	77	
52	DY	77	
53	CZ	62	
53	DZ	62	
54	DI	135	

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Mol	Chain	Length	Quality of chain
55	DA	2904	% 67% 28% 5%

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
56	MG	CA	3056	-	-	-	X
66	ACY	DA	3196	-	X	-	-
66	ACY	DA	3202	-	-	X	-

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295119 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0	0
			32932	14695	6044	10659	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32910	14685	6039	10653	1533			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1060	A	U	conflict	GB 675819282
BA	1060	A	U	conflict	GB 675819282

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	224	Total	C	N	O	S	0	0	0
			1753	1109	315	321	8			
2	BB	224	Total	C	N	O	S	0	0	0
			1753	1109	315	321	8			

- 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
			1625	1028	305	289	3			
3	BC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	BD	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	155	Total	C	N	O	S	0	0	0
			1144	711	216	211	6			
5	BE	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	106	Total	C	N	O	S	0	0	0
			862	545	156	154	7			
6	BF	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
			1182	735	227	216	4			
7	BG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	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	BH	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	BI	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	99	Total	C	N	O	S	0	0	0
			796	498	152	145	1			
10	BJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	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	BK	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
			957	591	196	165	5			
12	BL	123	Total	C	N	O	S	0	0	0
			957	591	196	165	5			

- 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
			884	546	178	157	3			
13	BM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	100	Total	C	N	O	S	0	0	0
			805	499	164	139	3			
14	BN	100	Total	C	N	O	S	0	0	0
			805	499	164	139	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
			714	439	144	130	1			
15	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	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	BP	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
			649	411	121	114	3			
17	BQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	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
			456	288	86	82			
18	BR	55	Total	C	N	O	0	0	0
			456	288	86	82			

- 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
			638	408	120	108	2			
19	BS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0	0
			670	414	138	115	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BT	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	56	Total	C	N	O	S	0	0	0
			465	290	96	78	1			
21	BU	56	Total	C	N	O	S	0	0	0
			465	290	96	78	1			

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	C1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
22	D1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 23 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	C2	50	Total	C	N	O	0	0	0
			409	263	75	71			
23	D2	51	Total	C	N	O	0	0	0
			414	266	76	72			

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	C3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
24	D3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	C4	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
25	D4	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	C5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
26	D5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	C0	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
27	D0	58	Total	C	N	O	S	0	2	0
			463	290	90	81	2			

- Molecule 28 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
28	DB	120	Total	C	N	O	P	0	0	0
			2569	1144	468	837	120			

- Molecule 29 is a protein called 50S ribosomal protein L2.

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

- Molecule 30 is a protein called 50S ribosomal protein L3.

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

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CA	2898	Total	C	N	O	P	0	0	0
			62229	27768	11448	20115	2898			

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	DD	209	Total	C	N	O	S	0	1	0
			1576	986	290	296	4			

- Molecule 33 is a protein called 50S ribosomal protein L4.

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

- Molecule 34 is a protein called 50S ribosomal protein L5.

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

- Molecule 35 is a protein called 50S ribosomal protein L6.

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

- Molecule 36 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
36	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 37 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CJ	134	Total	C	N	O	S	0	0	0
			979	619	169	185	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	DJ	134	Total	C	N	O	S	0	0	0
			979	619	169	185	6			

- Molecule 38 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	CK	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
38	DK	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 39 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	CL	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
39	DL	123	Total	C	N	O	S	0	0	0
			946	593	181	166	6			

- Molecule 40 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	CM	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
40	DM	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CN	136	Total	C	N	O	S	0	0	0
			1075	686	205	178	6			
41	DN	136	Total	C	N	O	S	0	2	0
			1092	696	211	179	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CN	81	4D4	ARG	conflict	UNP P0ADY7
DN	81	4D4	ARG	conflict	UNP P0ADY7

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CO	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
42	DO	125	Total	C	N	O	S	0	0	0
			993	613	202	173	5			

- Molecule 43 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CP	116	Total	C	N	O		0	0	0
			892	552	178	162				
43	DP	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 44 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	CQ	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
44	DQ	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 45 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	CR	117	Total	C	N	O		0	0	0
			947	604	192	151				
45	DR	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 46 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CS	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
46	DS	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 47 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CT	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	DT	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 48 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	CU	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
48	DU	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 49 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	CV	102	Total	C	N	O	S	0	0	0
			779	492	146	141				
49	DV	102	Total	C	N	O	S	0	0	0
			779	492	146	141				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	CW	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
50	DW	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	CX	75	Total	C	N	O	S	0	0	0
			569	353	113	102	1			
51	DX	76	Total	C	N	O	S	0	1	0
			591	365	121	104	1			

- Molecule 52 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	CY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
52	DY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 53 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	CZ	62	Total	C	N	O	S	0	0	0
			501	308	98	94	1			
53	DZ	62	Total	C	N	O	S	0	0	0
			501	308	98	94	1			

- Molecule 54 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	DI	135	Total	C	N	O	S	0	0	0
			1023	649	179	192	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DI	85	VAL	SER	conflict	UNP P0A7J3
DI	86	THR	MET	conflict	UNP P0A7J3

- Molecule 55 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	DA	2897	Total	C	N	O	P	0	11	0
			62423	27855	11485	20176	2907			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

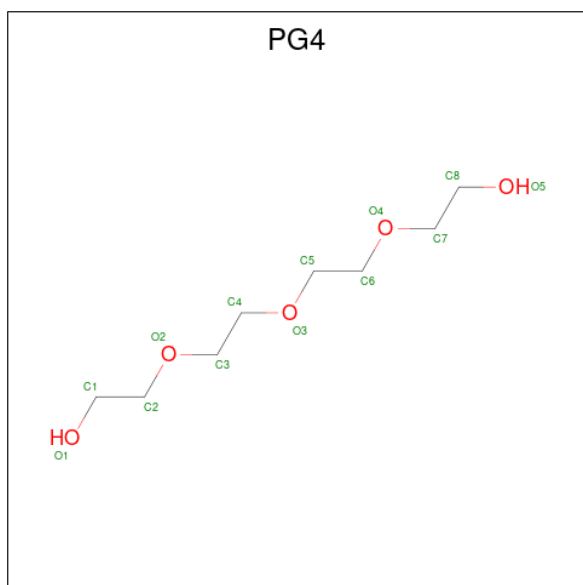
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	70	Total	Mg	0	0
			70	70		
56	BA	41	Total	Mg	0	0
			41	41		
56	CB	3	Total	Mg	0	0
			3	3		
56	CA	156	Total	Mg	0	0
			156	156		
56	DD	1	Total	Mg	0	0
			1	1		
56	DM	1	Total	Mg	0	0
			1	1		
56	DR	1	Total	Mg	0	0
			1	1		

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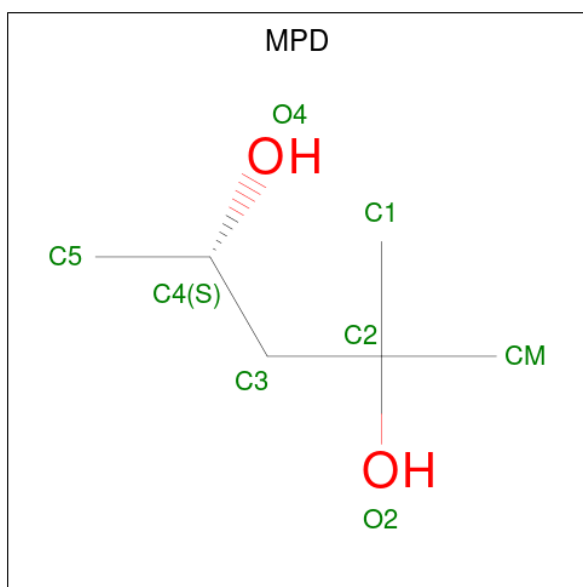
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DB	9	Total	Mg	0	0
			9	9		
56	DA	184	Total	Mg	0	0
			184	184		

- Molecule 57 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



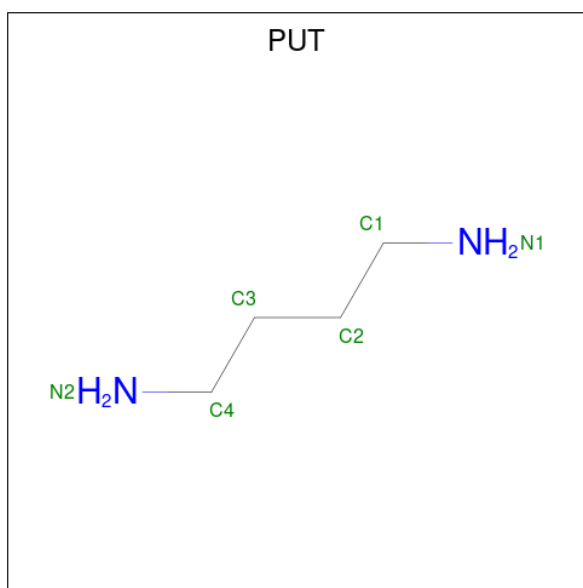
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			13	8	5		
57	BA	1	Total	C	O	0	0
			13	8	5		
57	DQ	1	Total	C	O	0	0
			13	8	5		
57	DR	1	Total	C	O	0	0
			13	8	5		
57	DS	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AA	1	Total	C	O	0	0
			8	6	2		
58	AA	1	Total	C	O	0	0
			8	6	2		
58	DE	1	Total	C	O	0	0
			8	6	2		
58	DE	1	Total	C	O	0	0
			8	6	2		
58	DK	1	Total	C	O	0	0
			8	6	2		
58	DN	1	Total	C	O	0	0
			8	6	2		
58	DS	1	Total	C	O	0	0
			8	6	2		
58	DT	1	Total	C	O	0	0
			8	6	2		
58	DT	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		

- Molecule 59 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	DM	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		

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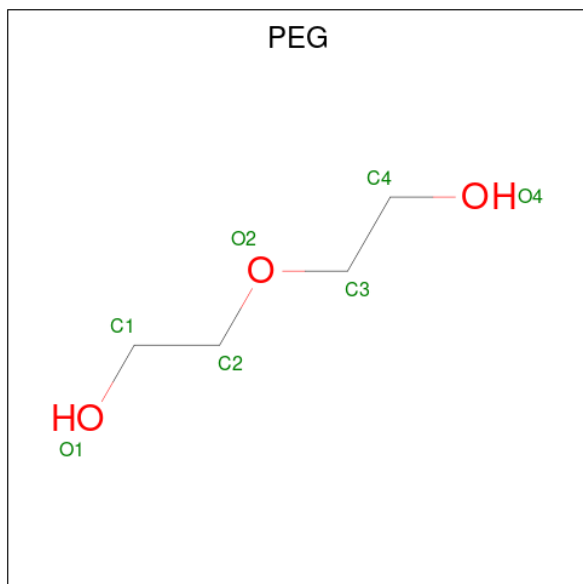
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AB	1	Total	Zn	0	0
			1	1		
60	C5	1	Total	Zn	0	0
			1	1		
60	D5	1	Total	Zn	0	0
			1	1		

- Molecule 61 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



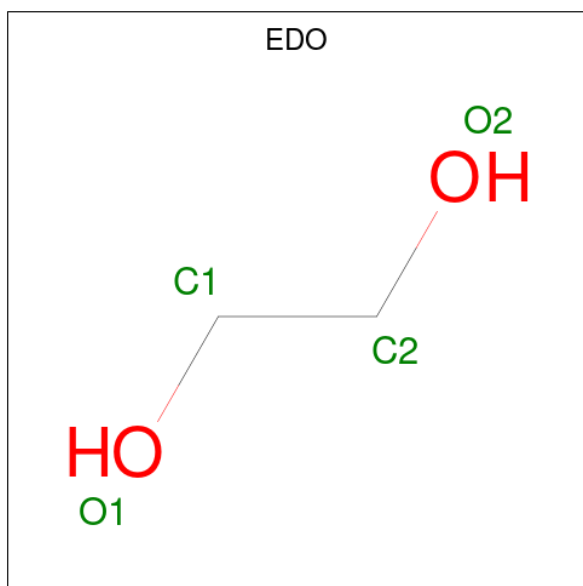
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	D3	1	Total	C	O	0	0
			7	4	3		
61	DL	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	DP	1	Total	C	O	0	0
			7	4	3		
61	DQ	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		

- Molecule 62 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



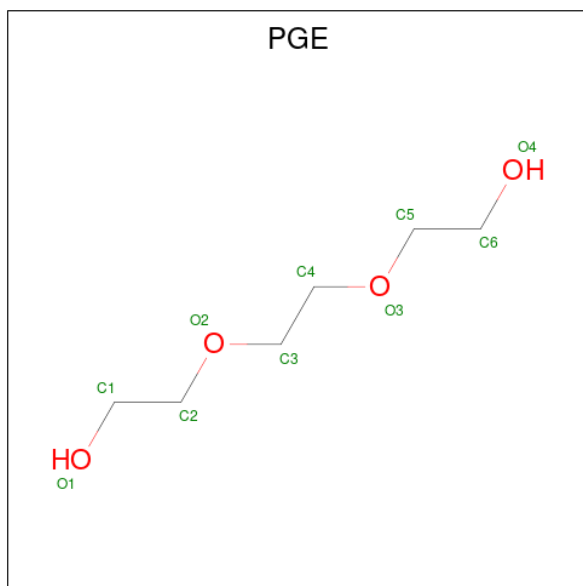
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	D1	1	Total	C	O	0	0
			4	2	2		
62	D0	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 63 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



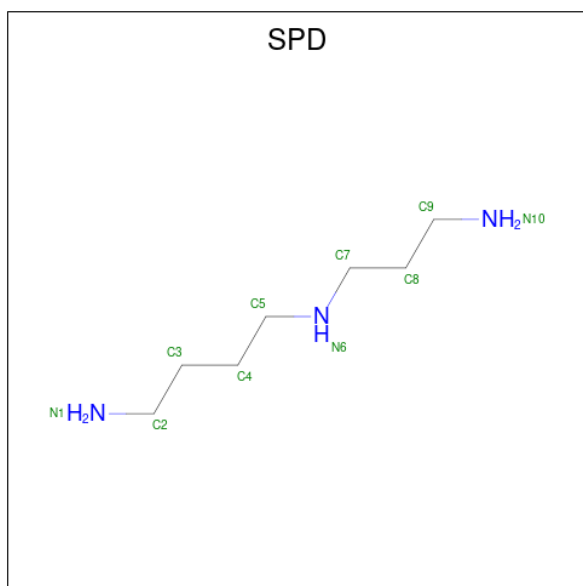
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			10	6	4		
63	D3	1	Total	C	O	0	0
			10	6	4		

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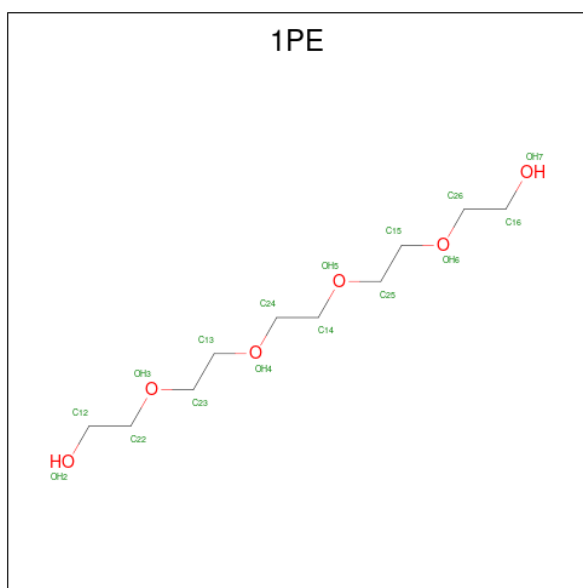
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	DD	1	Total	C	O	0	0
			10	6	4		
63	DS	1	Total	C	O	0	0
			10	6	4		
63	DU	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		

- Molecule 64 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



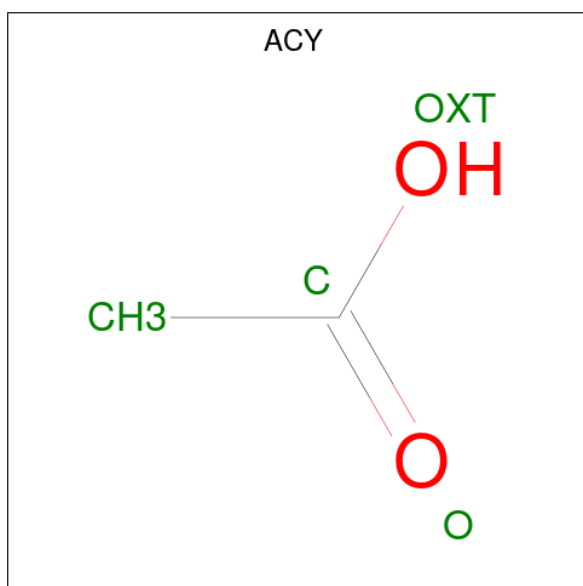
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		

- Molecule 65 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
65	DA	1	Total	C	O	0	0
			16	10	6		
65	DA	1	Total	C	O	0	0
			16	10	6		

- Molecule 66 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



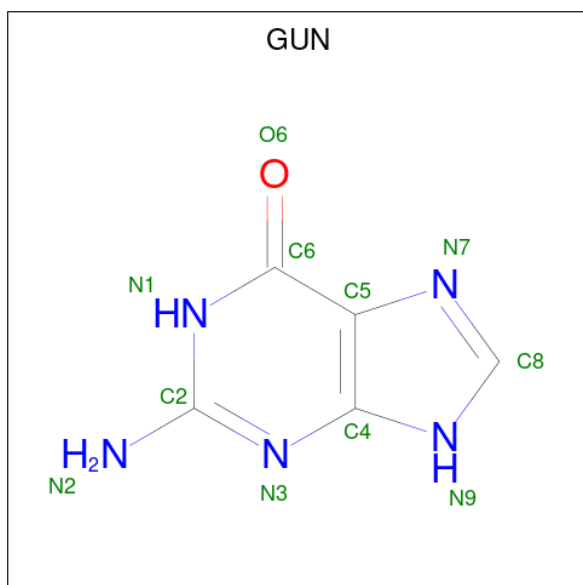
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		

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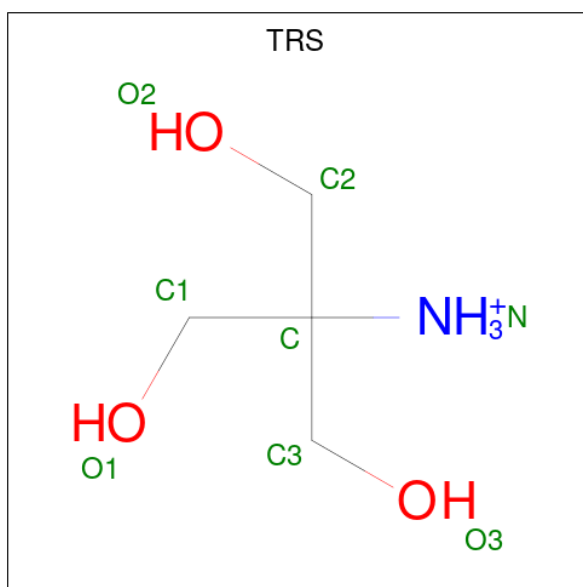
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 67 is GUANINE (CCD ID: GUN) (formula: $C_5H_5N_5O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
67	DA	1	Total	C	N	O	0	0
			11	5	5	1		

- Molecule 68 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
68	DA	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 69 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AA	507	Total	O	0	0
			507	507		
69	AC	4	Total	O	0	0
			4	4		
69	AD	2	Total	O	0	0
			2	2		
69	AE	5	Total	O	0	0
			5	5		
69	AF	1	Total	O	0	0
			1	1		
69	AG	1	Total	O	0	0
			1	1		
69	AJ	3	Total	O	0	0
			3	3		
69	AK	5	Total	O	0	0
			5	5		
69	AL	7	Total	O	0	0
			7	7		
69	AM	4	Total	O	0	0
			4	4		
69	AN	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AO	1	Total 1	O 1	0	0
69	AP	1	Total 1	O 1	0	0
69	AQ	1	Total 1	O 1	0	0
69	AS	1	Total 1	O 1	0	0
69	AT	2	Total 2	O 2	0	0
69	AU	4	Total 4	O 4	0	0
69	C3	3	Total 3	O 3	0	0
69	C4	1	Total 1	O 1	0	0
69	BA	287	Total 287	O 287	0	0
69	BD	12	Total 12	O 12	0	0
69	BE	1	Total 1	O 1	0	0
69	BF	1	Total 1	O 1	0	0
69	BK	3	Total 3	O 3	0	0
69	BL	3	Total 3	O 3	0	0
69	BN	1	Total 1	O 1	0	0
69	BO	1	Total 1	O 1	0	0
69	BP	4	Total 4	O 4	0	0
69	BR	1	Total 1	O 1	0	0
69	BT	5	Total 5	O 5	0	0
69	D1	37	Total 37	O 37	0	0
69	D2	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	D3	30	Total 30	O 30	0	0
69	D4	40	Total 40	O 40	0	0
69	D5	13	Total 13	O 13	0	0
69	D0	24	Total 24	O 24	0	0
69	CB	13	Total 13	O 13	0	0
69	CC	11	Total 11	O 11	0	0
69	CD	4	Total 4	O 4	0	0
69	CA	696	Total 696	O 696	0	0
69	DC	100	Total 100	O 100	0	0
69	DD	97	Total 97	O 97	0	0
69	CE	5	Total 5	O 5	0	0
69	CL	1	Total 1	O 1	0	0
69	CM	3	Total 3	O 3	0	0
69	CO	1	Total 1	O 1	0	0
69	CU	2	Total 2	O 2	0	0
69	CV	1	Total 1	O 1	0	0
69	CW	1	Total 1	O 1	0	0
69	CY	1	Total 1	O 1	0	0
69	DE	54	Total 54	O 54	0	0
69	DF	13	Total 13	O 13	0	0
69	DG	9	Total 9	O 9	0	0

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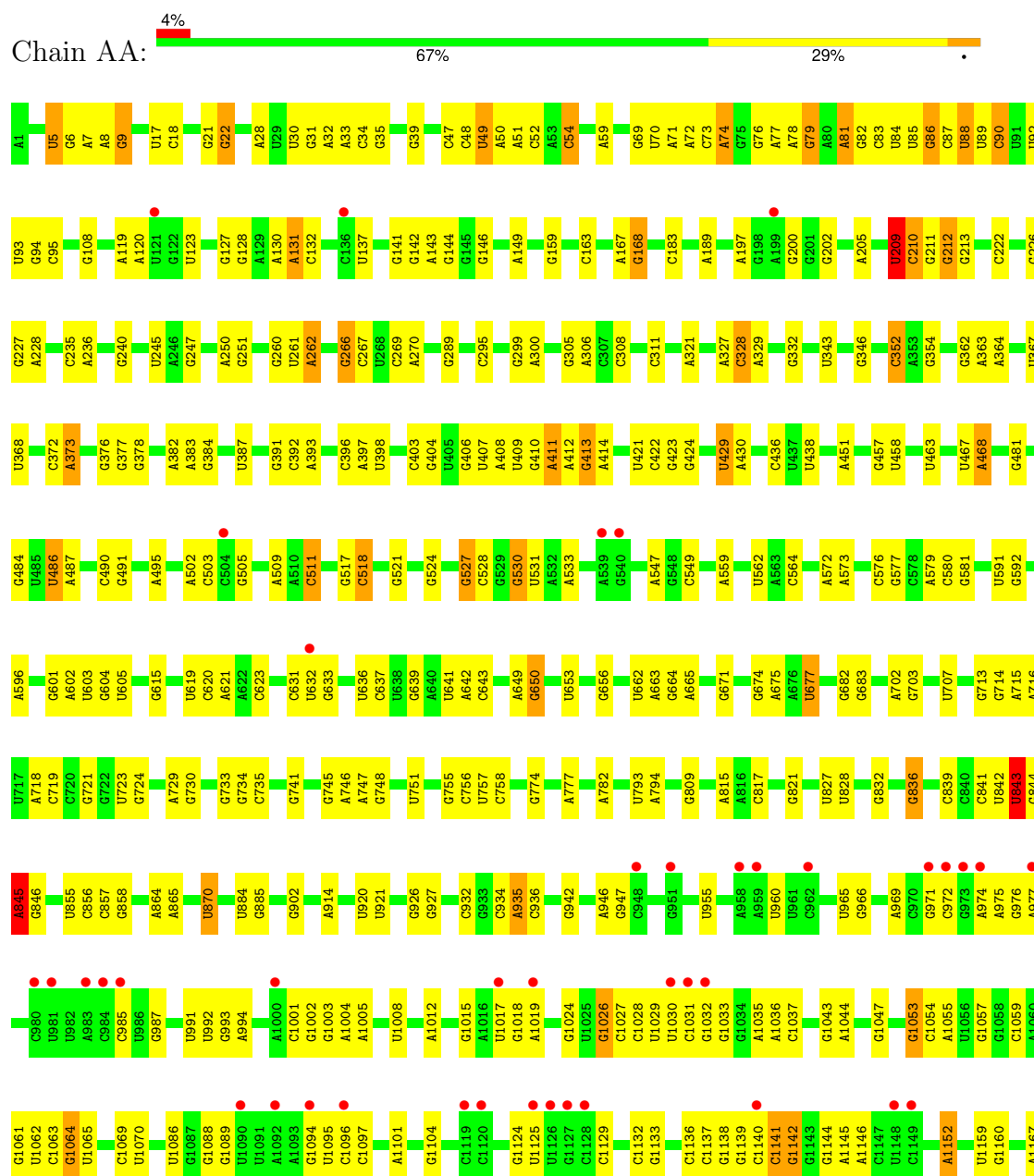
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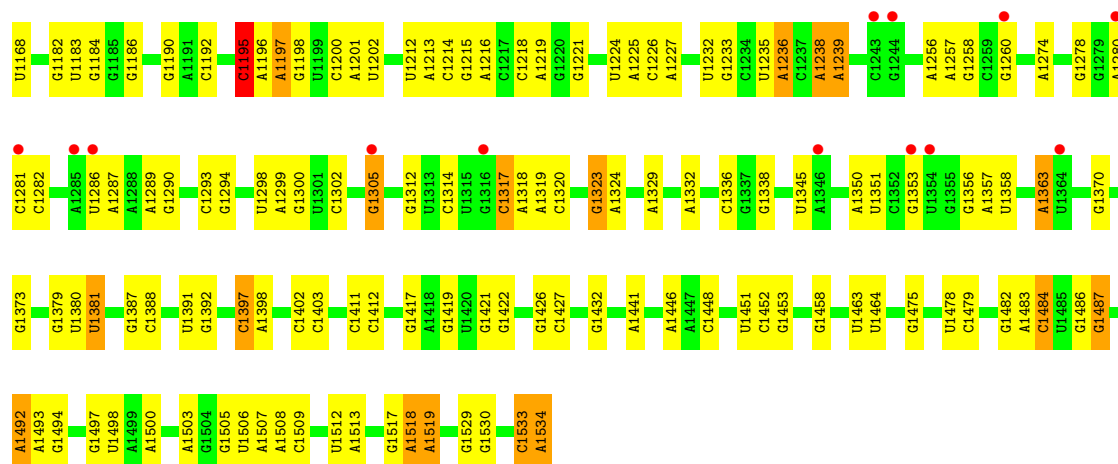
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DH	2	Total	O	0	0
			2	2		
69	DK	61	Total	O	0	0
			61	61		
69	DL	50	Total	O	0	0
			50	50		
69	DM	60	Total	O	0	0
			60	60		
69	DN	81	Total	O	0	0
			81	81		
69	DO	42	Total	O	0	0
			42	42		
69	DP	42	Total	O	0	0
			42	42		
69	DQ	32	Total	O	0	0
			32	32		
69	DR	68	Total	O	0	0
			68	68		
69	DS	52	Total	O	0	0
			52	52		
69	DT	65	Total	O	0	0
			65	65		
69	DU	24	Total	O	0	0
			24	24		
69	DV	19	Total	O	0	0
			19	19		
69	DW	33	Total	O	0	0
			33	33		
69	DX	33	Total	O	0	0
			33	33		
69	DY	11	Total	O	0	0
			11	11		
69	DZ	7	Total	O	0	0
			7	7		
69	DB	203	Total	O	0	0
			203	203		
69	DA	4824	Total	O	0	0
			4824	4824		

3 Residue-property plots [i](#)

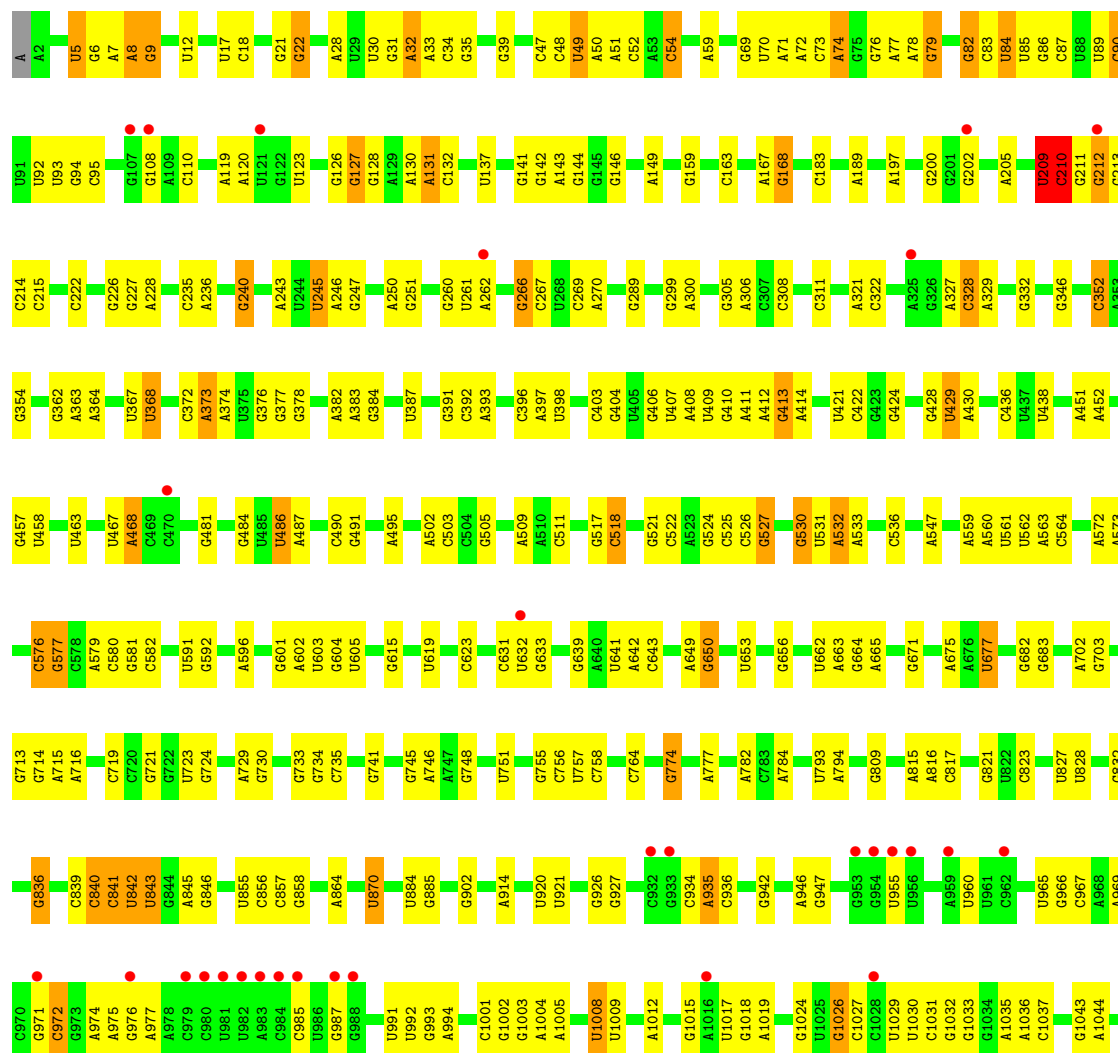
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

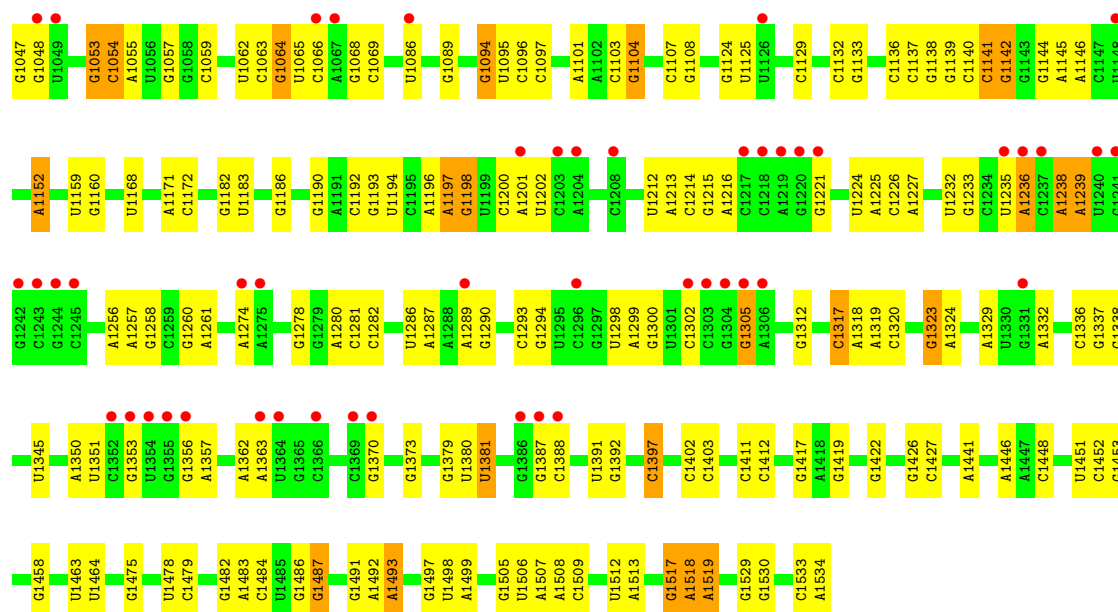
• Molecule 1: 16S rRNA



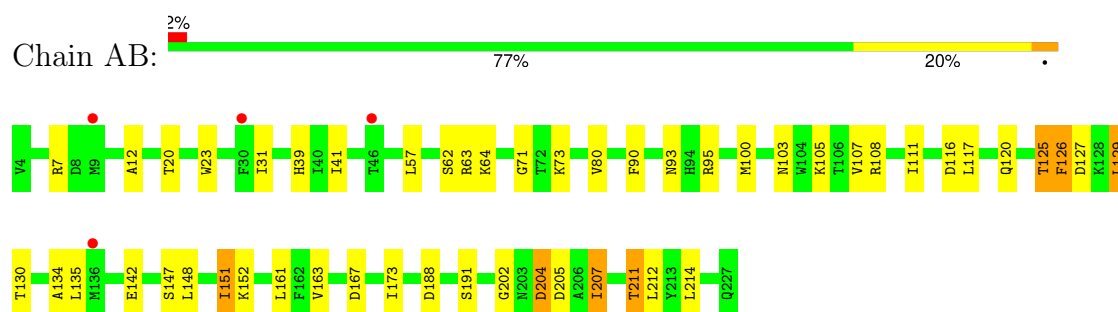


• Molecule 1: 16S rRNA

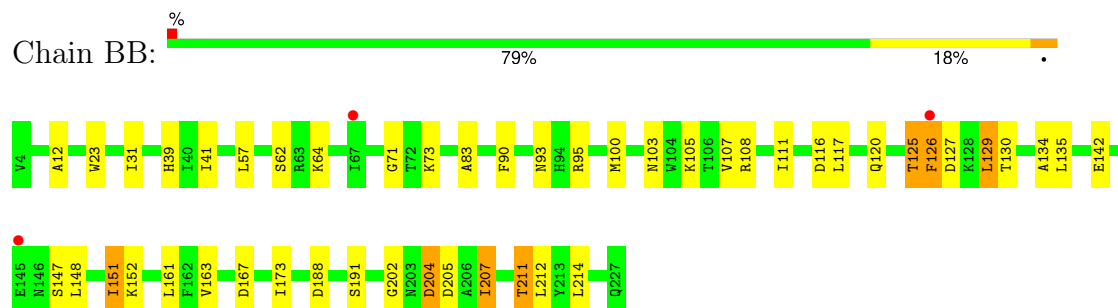




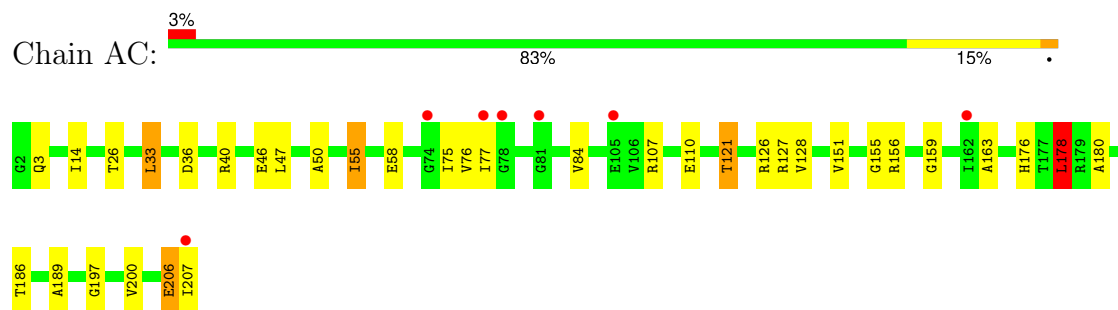
• Molecule 2: 30S ribosomal protein S2



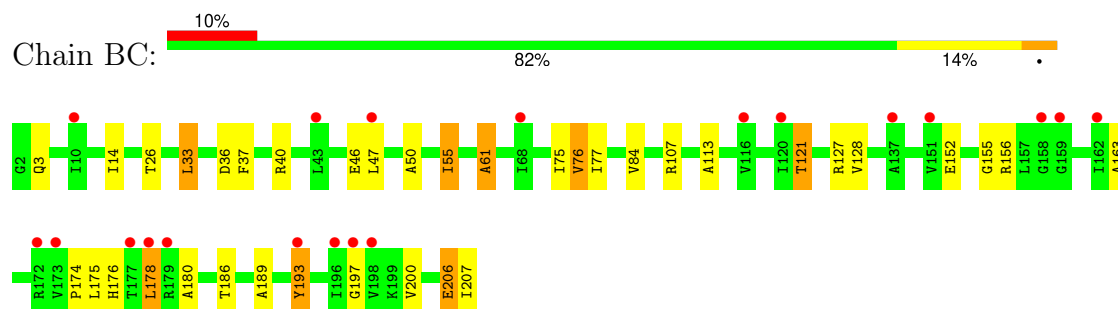
• Molecule 2: 30S ribosomal protein S2



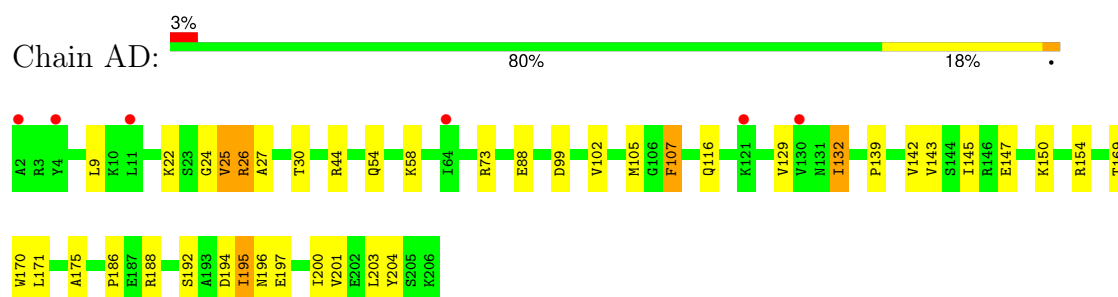
• Molecule 3: 30S ribosomal protein S3



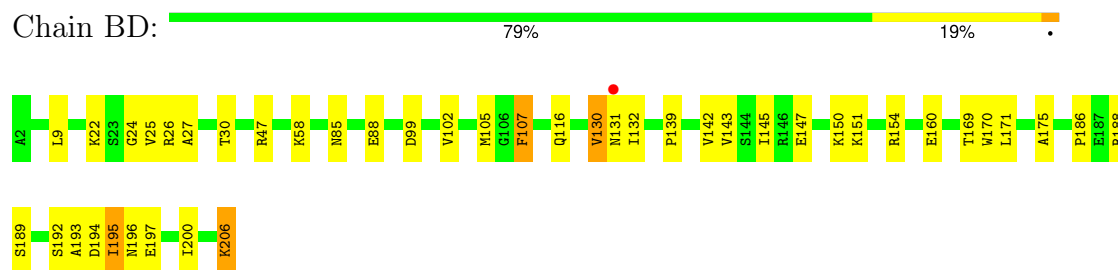
- Molecule 3: 30S ribosomal protein S3



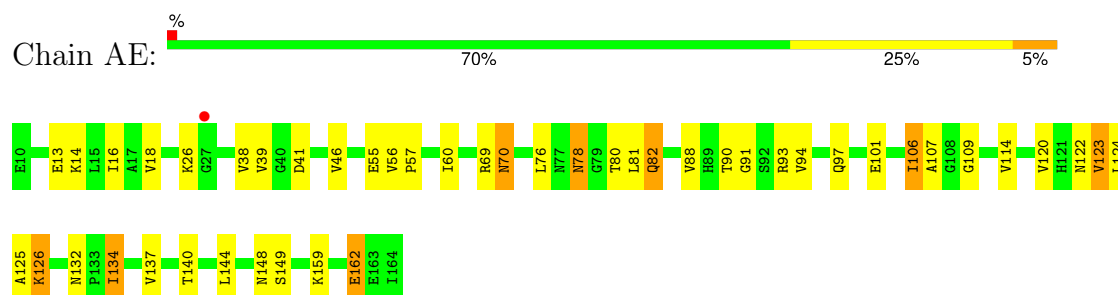
- Molecule 4: 30S ribosomal protein S4



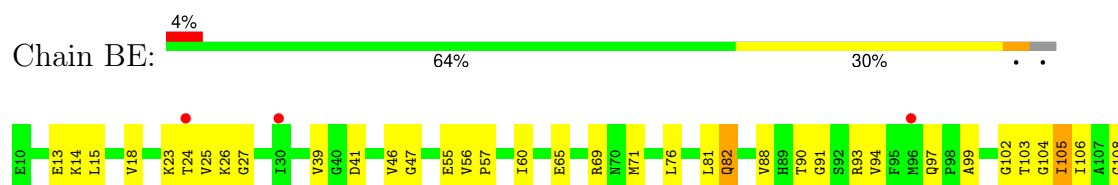
- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S5





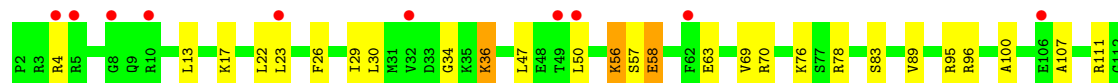
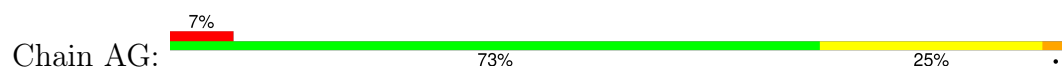
- Molecule 6: 30S ribosomal protein S6



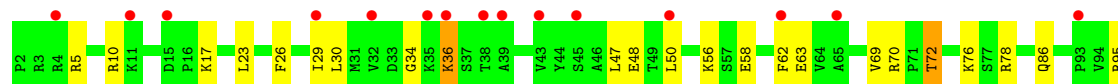
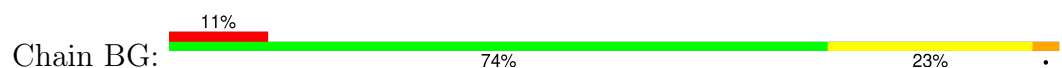
- Molecule 6: 30S ribosomal protein S6



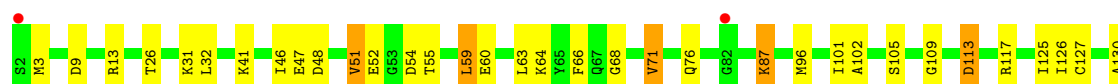
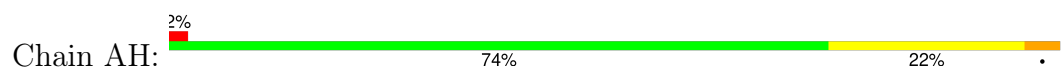
- Molecule 7: 30S ribosomal protein S7



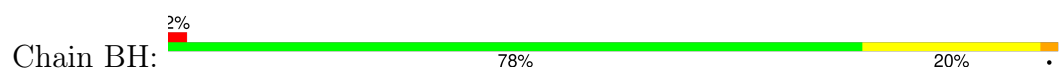
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

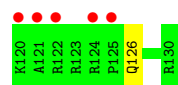
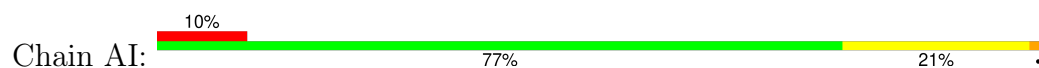


- Molecule 8: 30S ribosomal protein S8

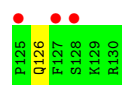
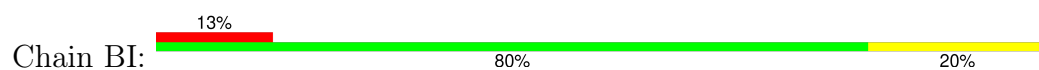




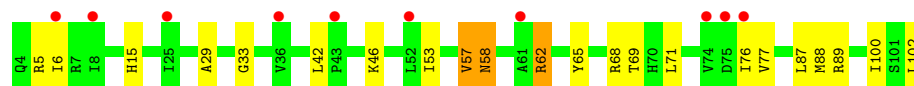
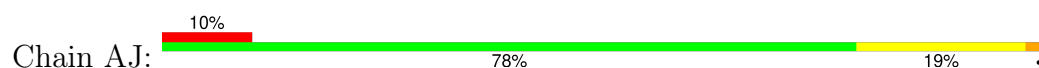
- Molecule 9: 30S ribosomal protein S9



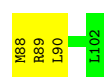
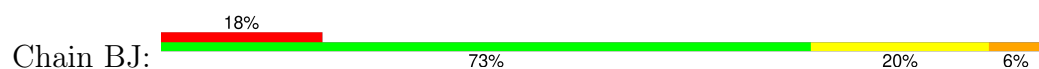
- Molecule 9: 30S ribosomal protein S9



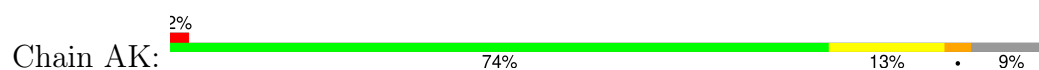
- Molecule 10: 30S ribosomal protein S10



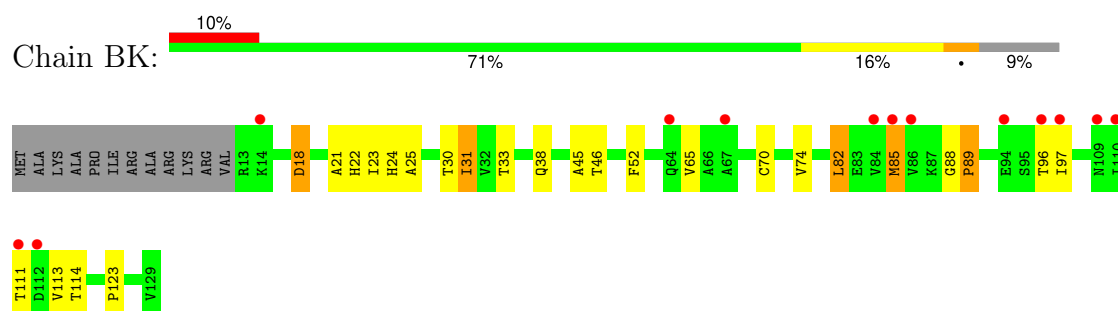
- Molecule 10: 30S ribosomal protein S10



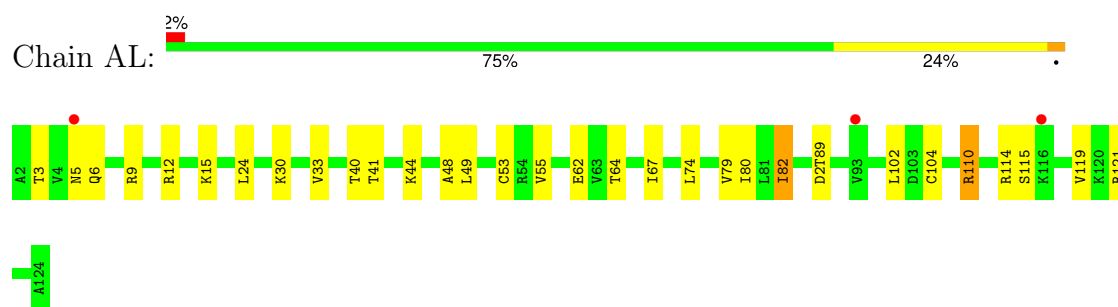
- Molecule 11: 30S ribosomal protein S11



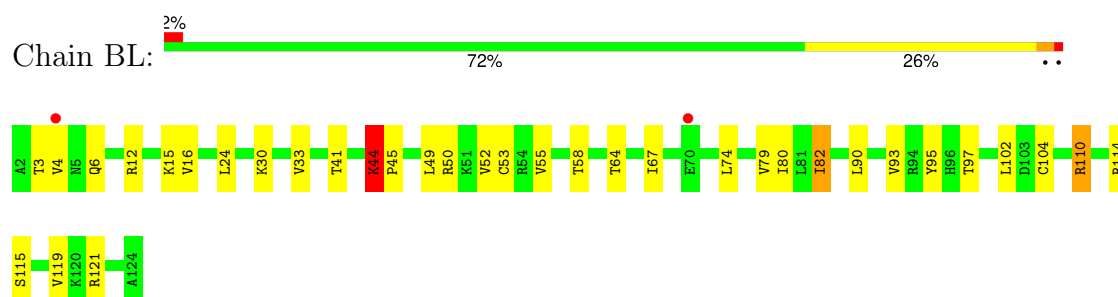
- Molecule 11: 30S ribosomal protein S11



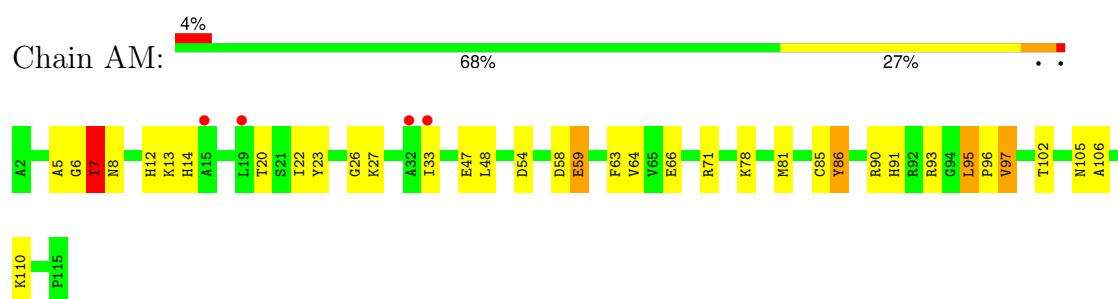
- Molecule 12: 30S ribosomal protein S12



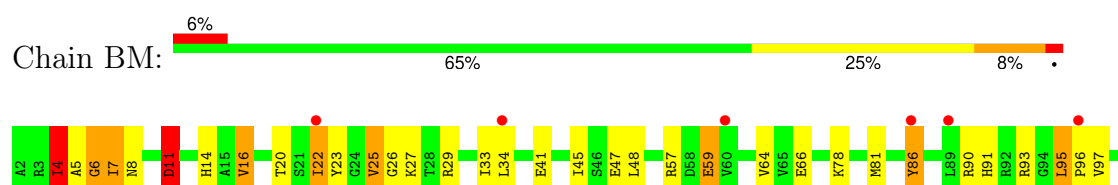
- Molecule 12: 30S ribosomal protein S12

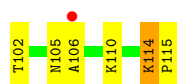


- Molecule 13: 30S ribosomal protein S13

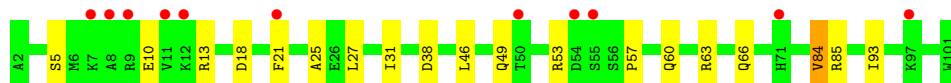
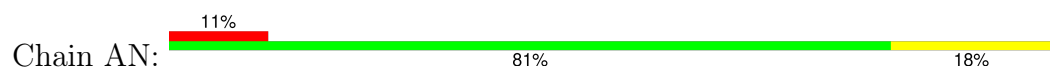


- Molecule 13: 30S ribosomal protein S13

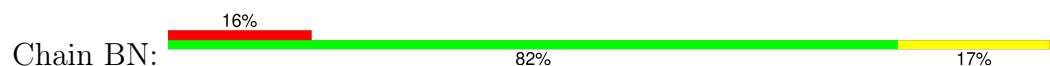




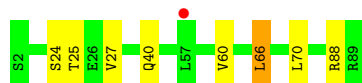
- Molecule 14: 30S ribosomal protein S14



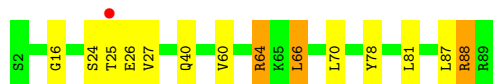
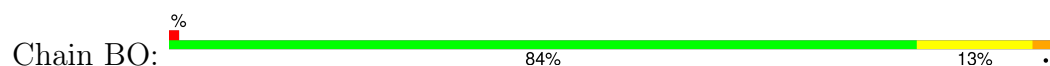
- Molecule 14: 30S ribosomal protein S14



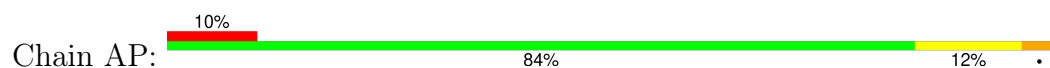
- Molecule 15: 30S ribosomal protein S15



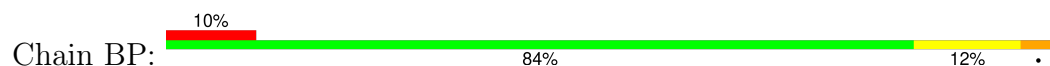
- Molecule 15: 30S ribosomal protein S15



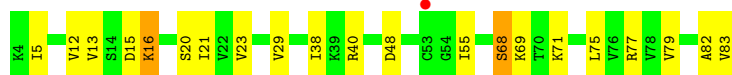
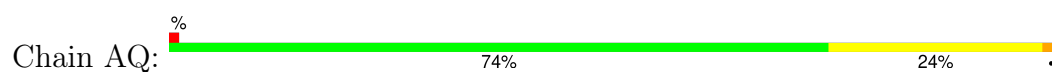
- Molecule 16: 30S ribosomal protein S16



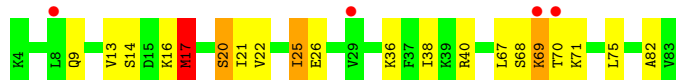
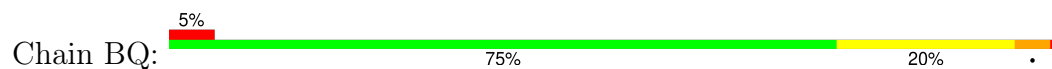
- Molecule 16: 30S ribosomal protein S16



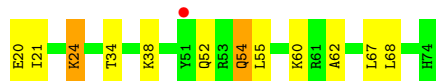
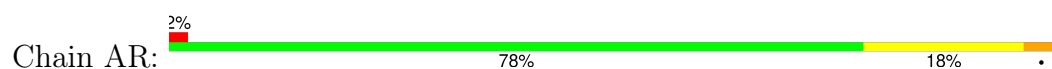
- Molecule 17: 30S ribosomal protein S17



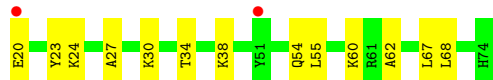
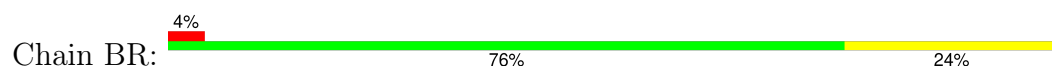
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



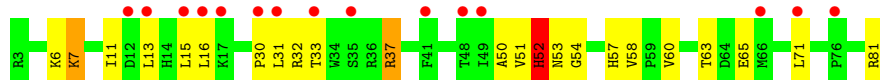
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



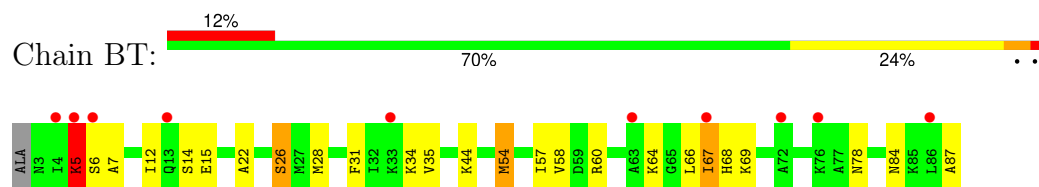
- Molecule 19: 30S ribosomal protein S19



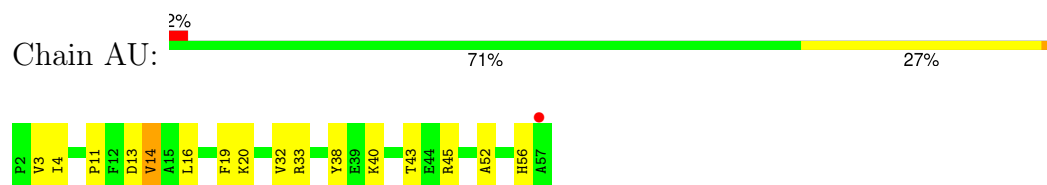
- Molecule 20: 30S ribosomal protein S20



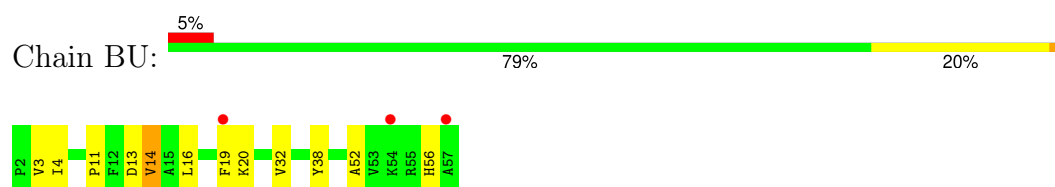
● Molecule 20: 30S ribosomal protein S20



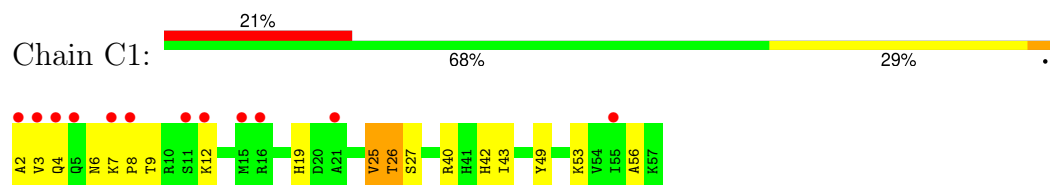
● Molecule 21: 30S ribosomal protein S21



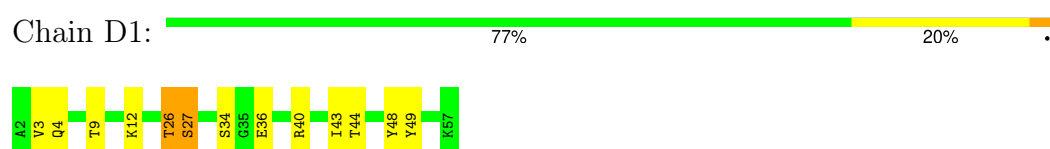
● Molecule 21: 30S ribosomal protein S21



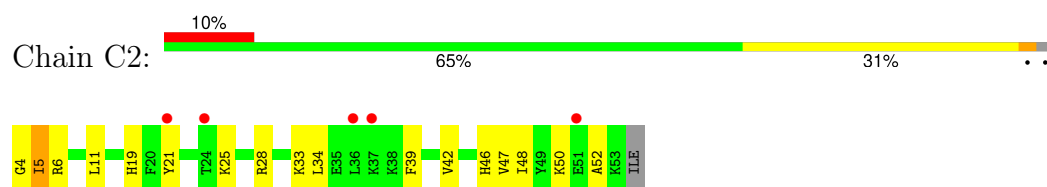
● Molecule 22: 50S ribosomal protein L32



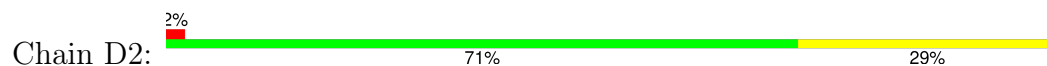
● Molecule 22: 50S ribosomal protein L32



● Molecule 23: 50S ribosomal protein L33

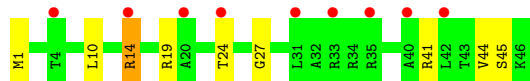
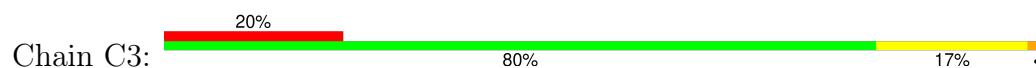


● Molecule 23: 50S ribosomal protein L33

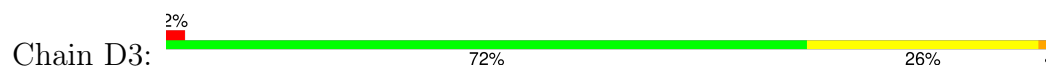




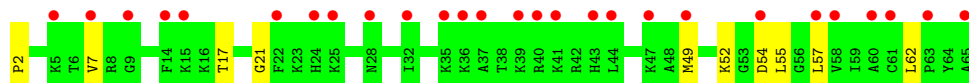
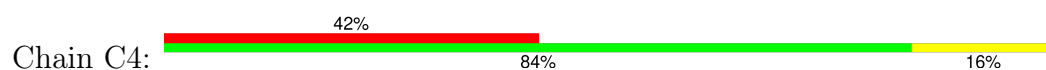
- Molecule 24: 50S ribosomal protein L34



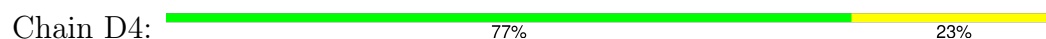
- Molecule 24: 50S ribosomal protein L34



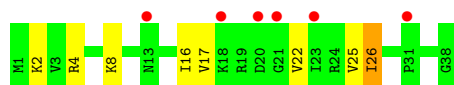
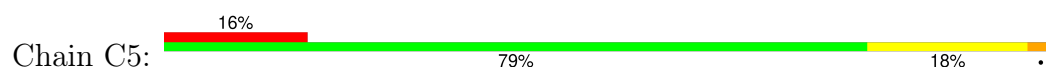
- Molecule 25: 50S ribosomal protein L35



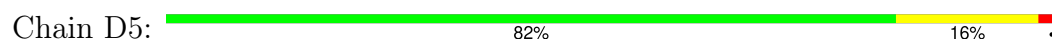
- Molecule 25: 50S ribosomal protein L35



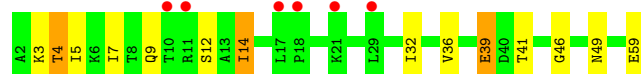
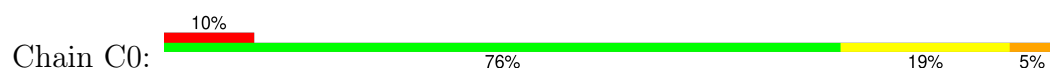
- Molecule 26: 50S ribosomal protein L36



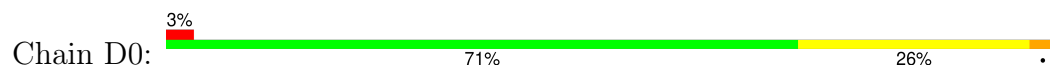
- Molecule 26: 50S ribosomal protein L36



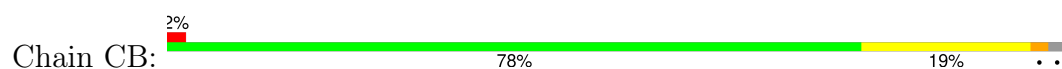
- Molecule 27: 50S ribosomal protein L30



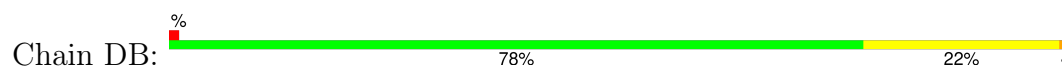
- Molecule 27: 50S ribosomal protein L30



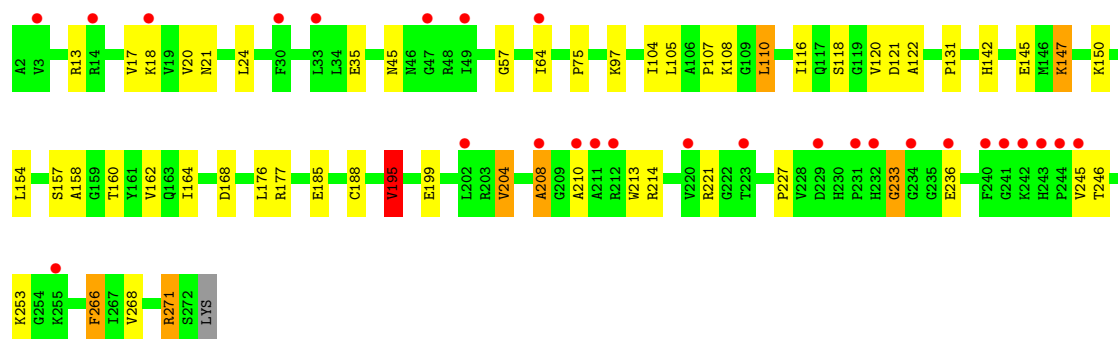
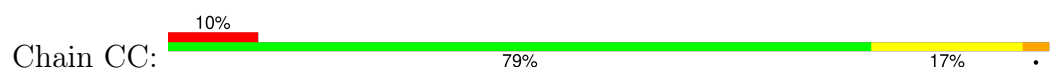
- Molecule 28: 5S rRNA



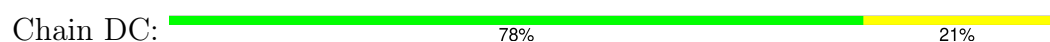
- Molecule 28: 5S rRNA



- Molecule 29: 50S ribosomal protein L2

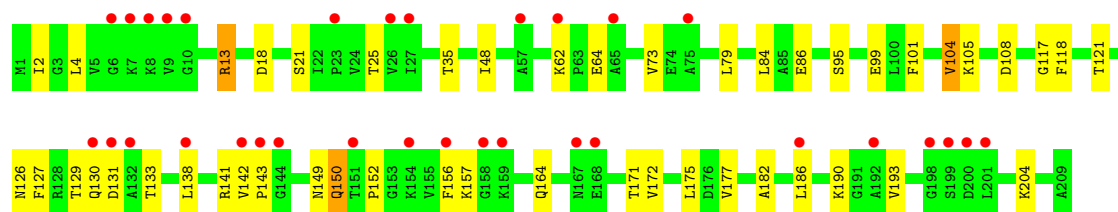
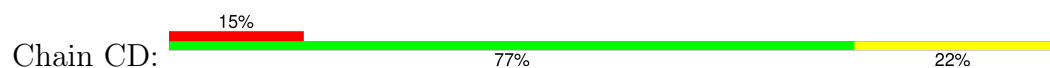


- Molecule 29: 50S ribosomal protein L2

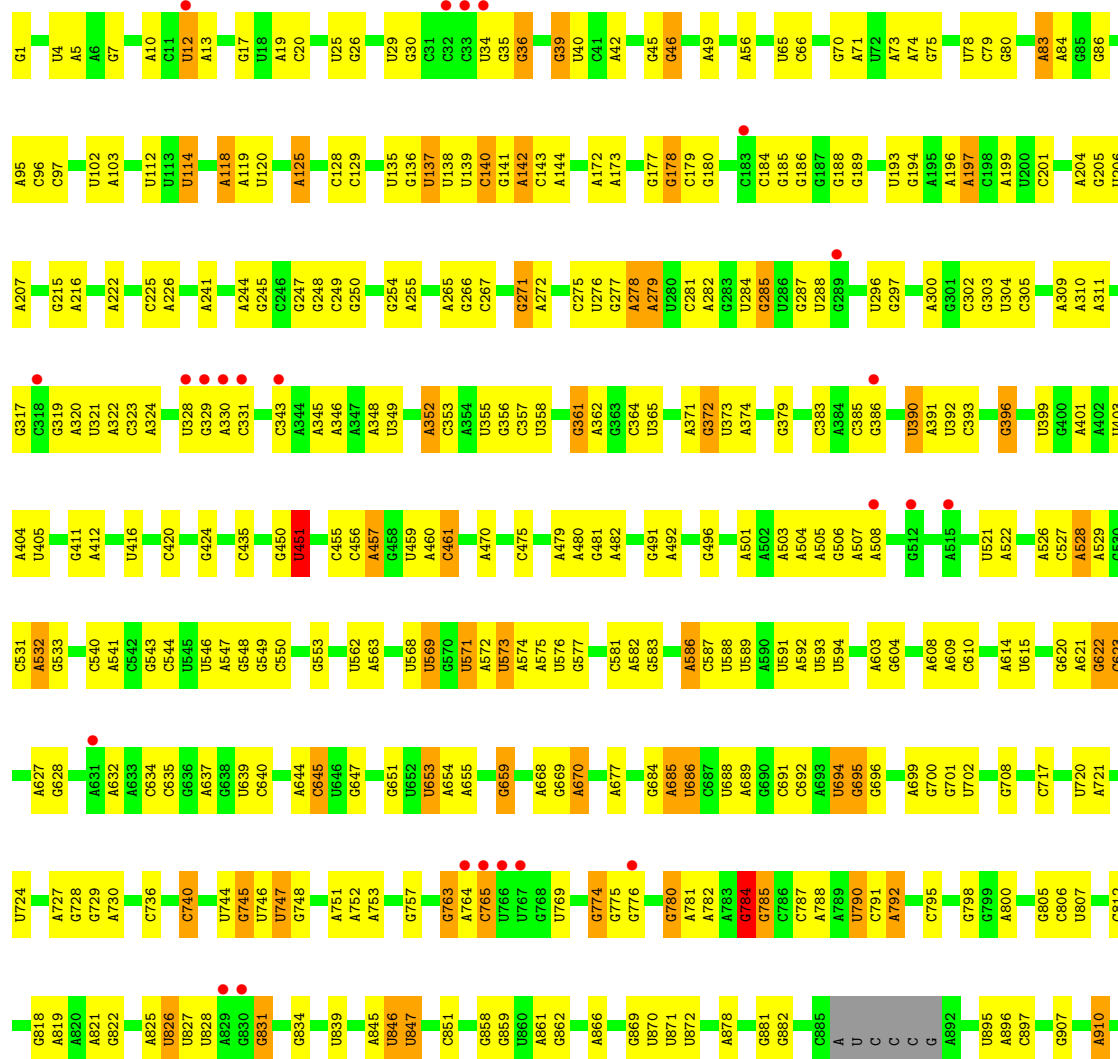




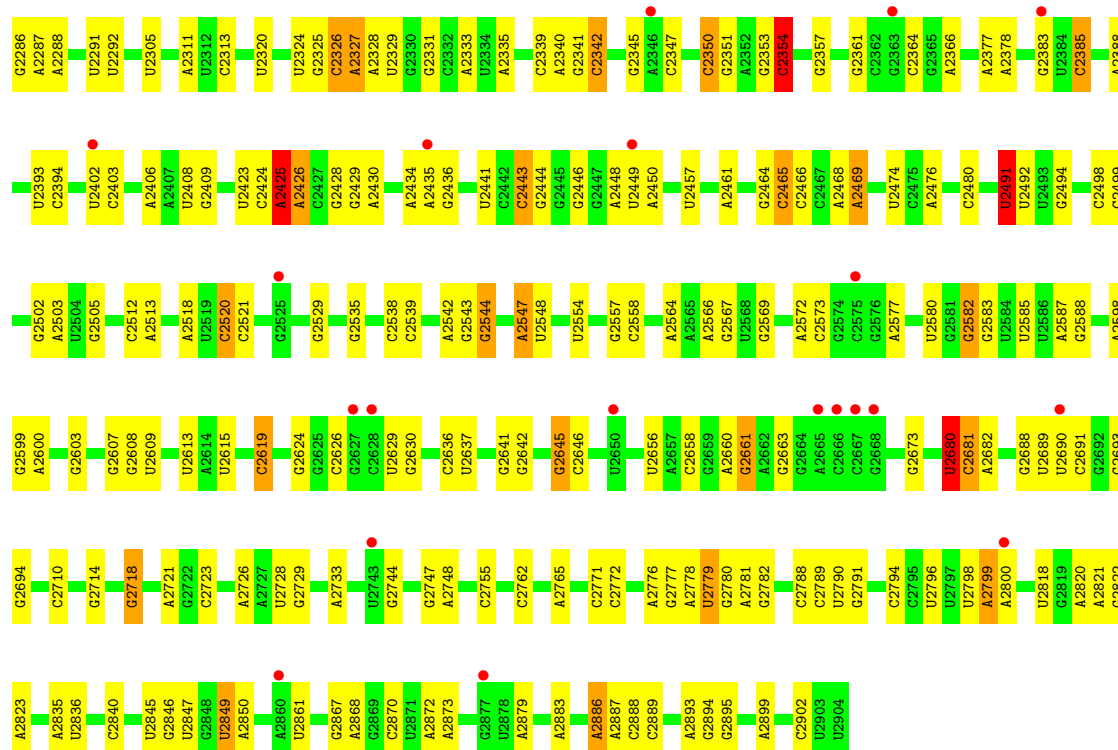
• Molecule 30: 50S ribosomal protein L3



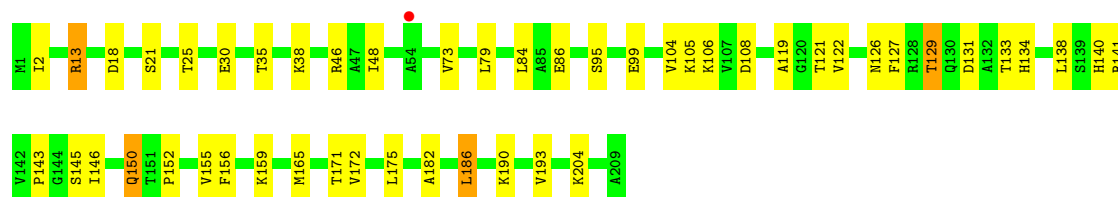
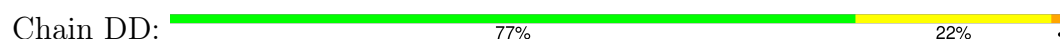
• Molecule 31: 23S rRNA



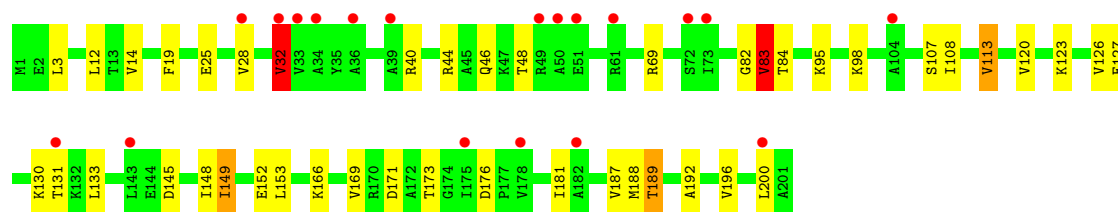
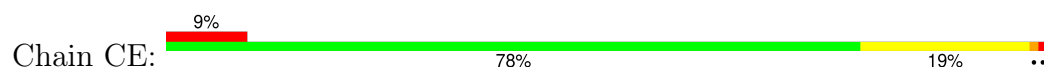
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					U1780	U1683	A1547	G1429	A1321	G1216	A1111	A1020
					U1781	A1664	C1547	G1430	A1321	U1231	G1112	A1021
					U1782	A1664	U1554	G1431	G1324	G1232	U1119	G1022
					A1783	A1664	U1554	A1434	A1328			
					A1784	C1670	G1555					



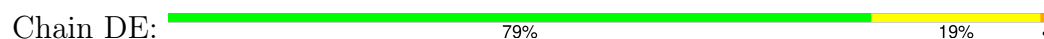
• Molecule 32: 50S ribosomal protein L3



• Molecule 33: 50S ribosomal protein L4

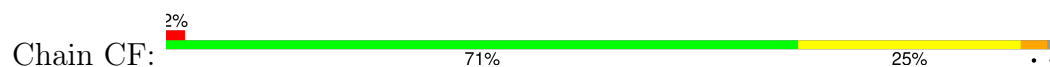


• Molecule 33: 50S ribosomal protein L4

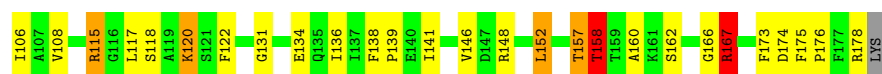




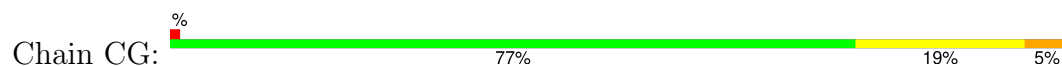
- Molecule 34: 50S ribosomal protein L5



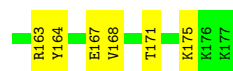
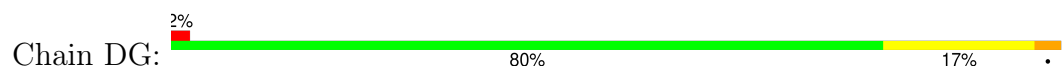
- Molecule 34: 50S ribosomal protein L5



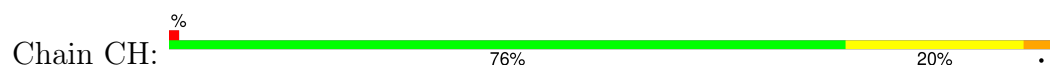
- Molecule 35: 50S ribosomal protein L6

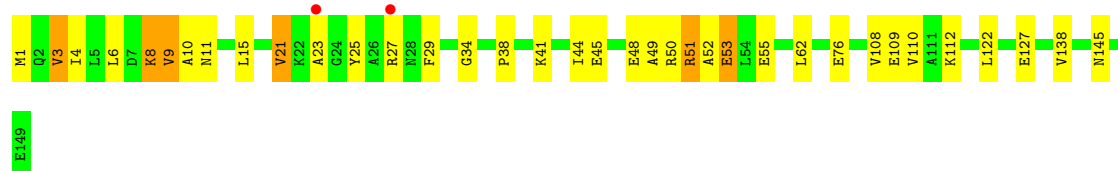


- Molecule 35: 50S ribosomal protein L6

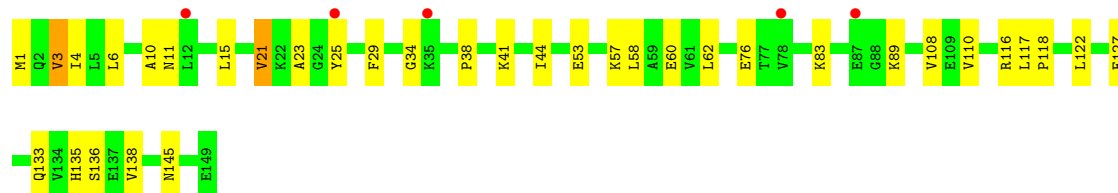


- Molecule 36: 50S ribosomal protein L9

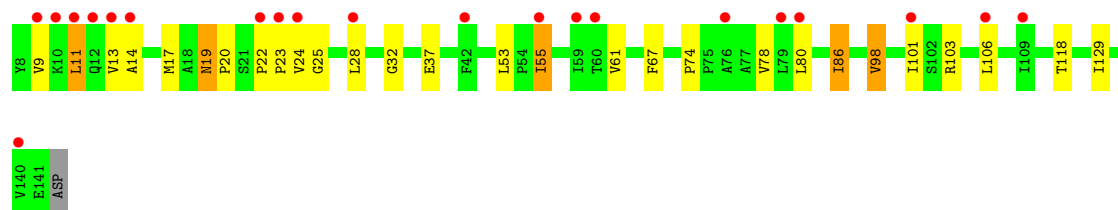
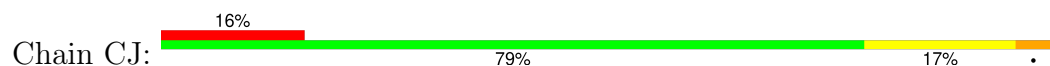




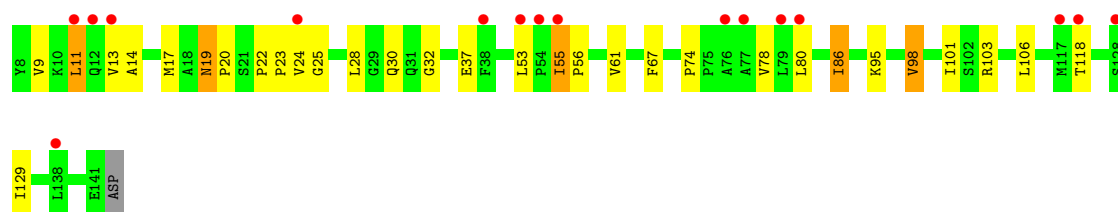
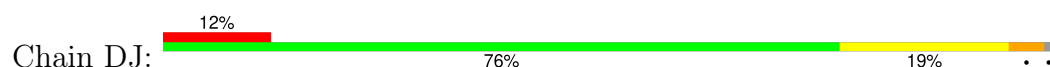
- Molecule 36: 50S ribosomal protein L9



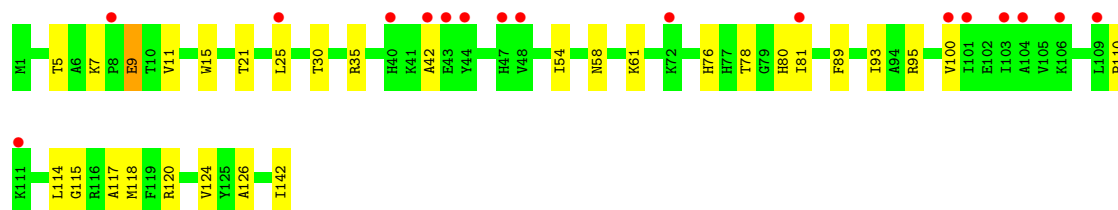
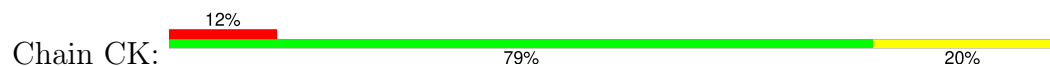
- Molecule 37: 50S ribosomal protein L11



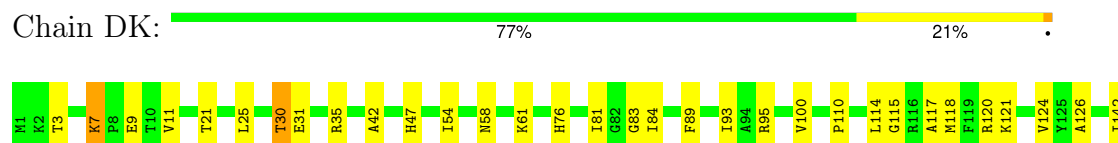
- Molecule 37: 50S ribosomal protein L11



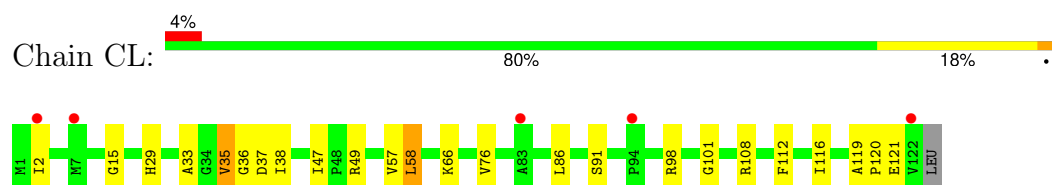
- Molecule 38: 50S ribosomal protein L13



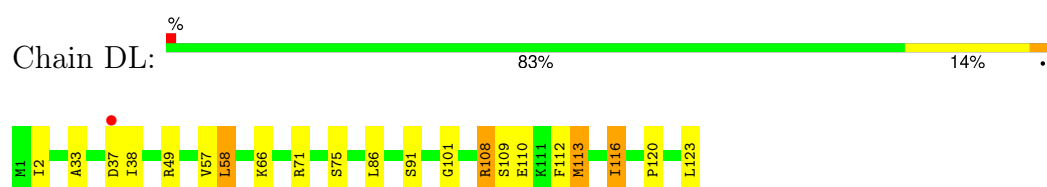
- Molecule 38: 50S ribosomal protein L13



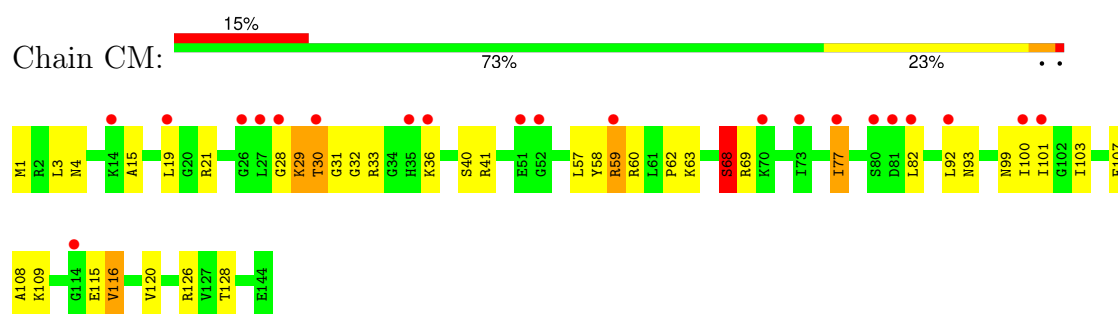
- Molecule 39: 50S ribosomal protein L14



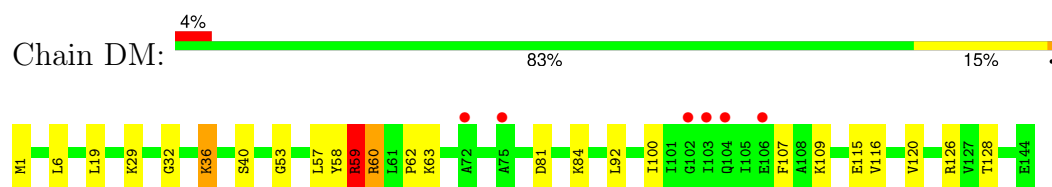
- Molecule 39: 50S ribosomal protein L14



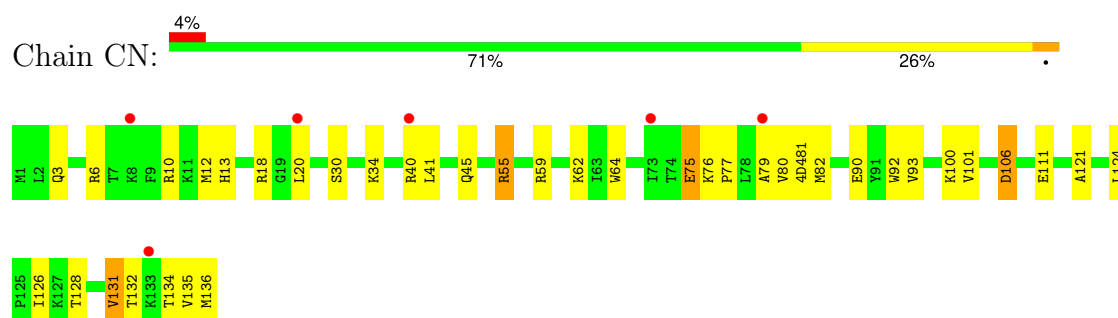
- Molecule 40: 50S ribosomal protein L15



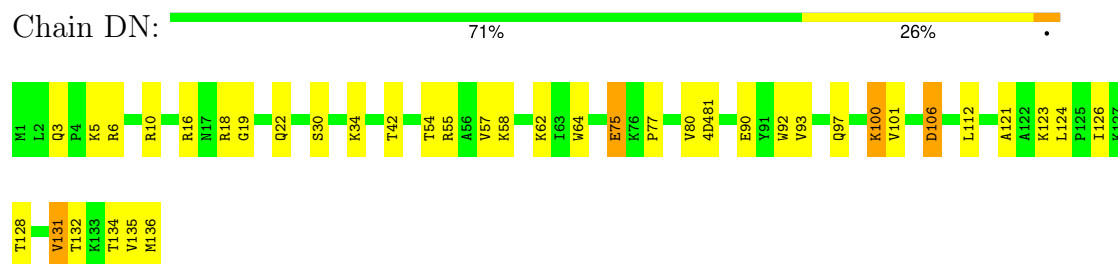
- Molecule 40: 50S ribosomal protein L15



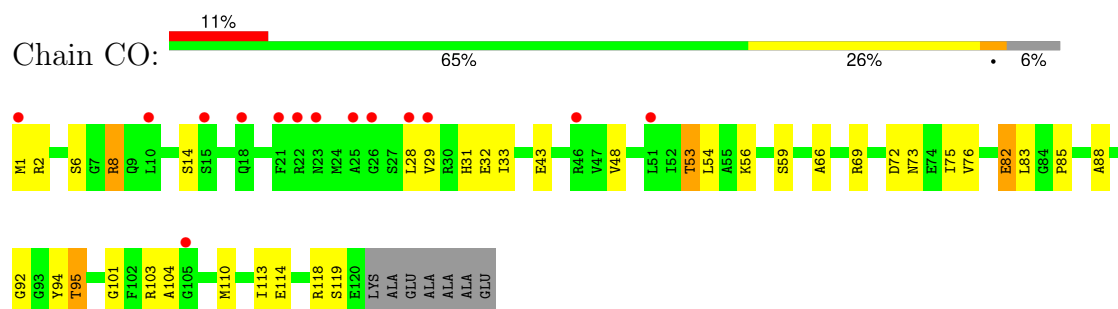
- Molecule 41: 50S ribosomal protein L16



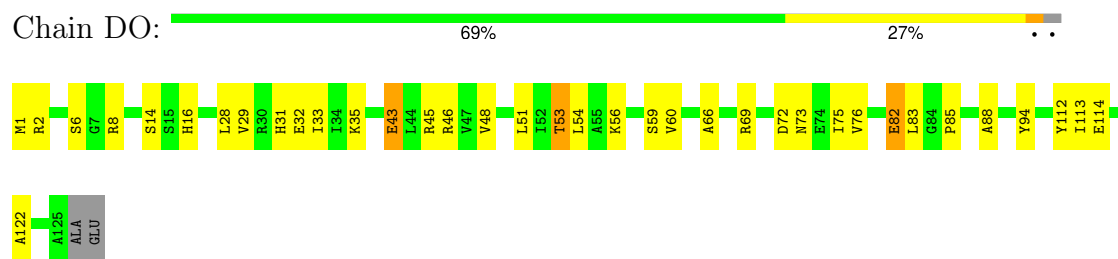
- Molecule 41: 50S ribosomal protein L16



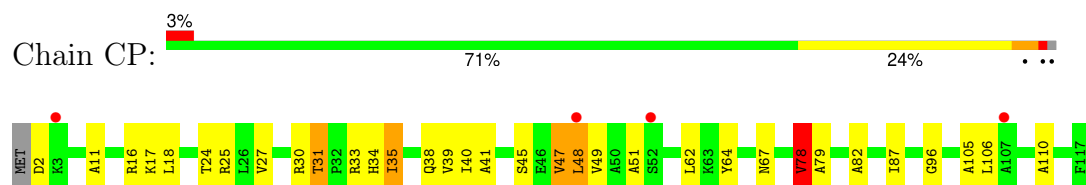
- Molecule 42: 50S ribosomal protein L17



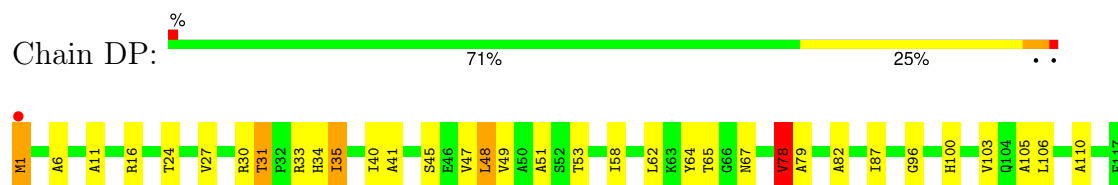
- Molecule 42: 50S ribosomal protein L17



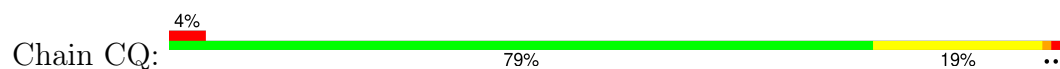
- Molecule 43: 50S ribosomal protein L18

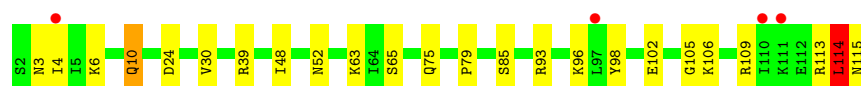


- Molecule 43: 50S ribosomal protein L18

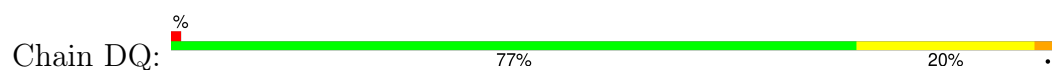


- Molecule 44: 50S ribosomal protein L19

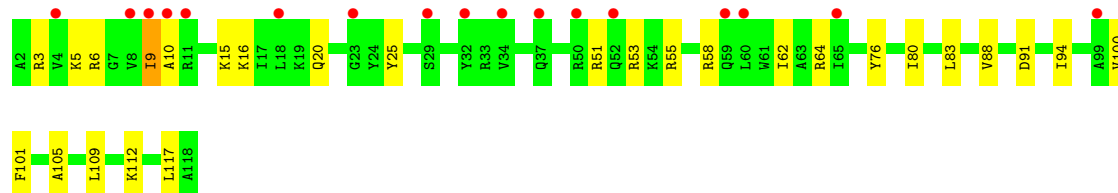
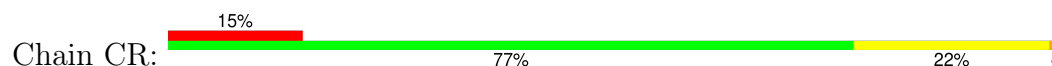




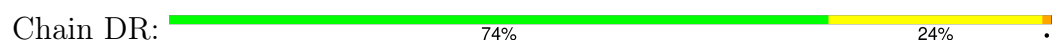
- Molecule 44: 50S ribosomal protein L19



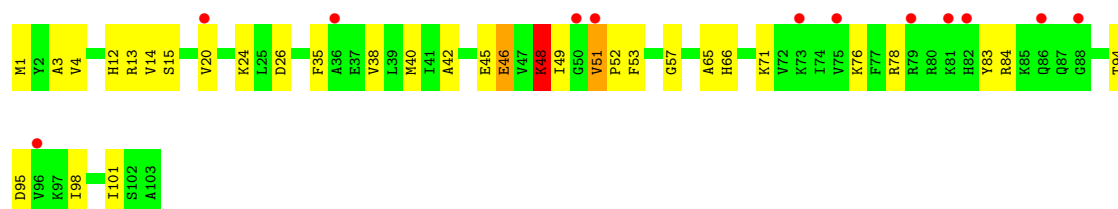
- Molecule 45: 50S ribosomal protein L20



- Molecule 45: 50S ribosomal protein L20



- Molecule 46: 50S ribosomal protein L21

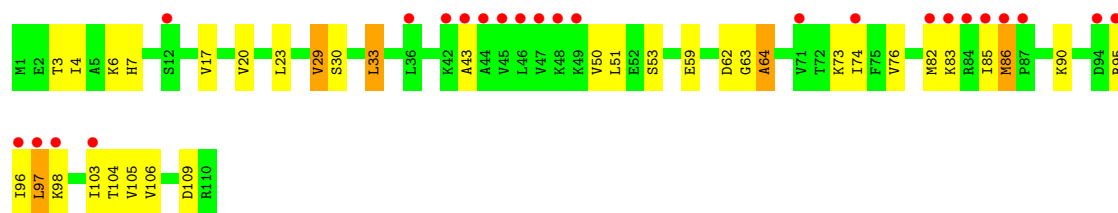


- Molecule 46: 50S ribosomal protein L21

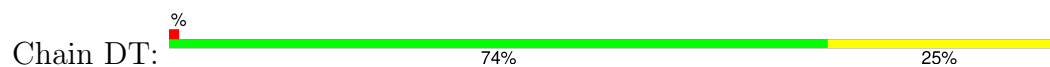


- Molecule 47: 50S ribosomal protein L22

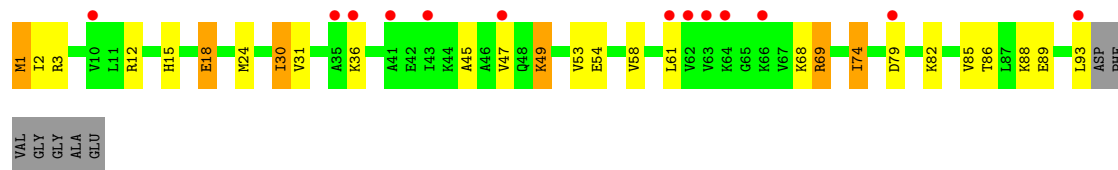




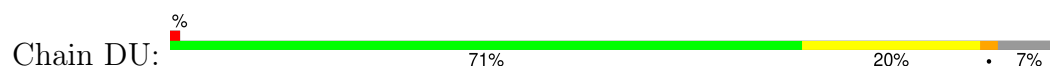
- Molecule 47: 50S ribosomal protein L22



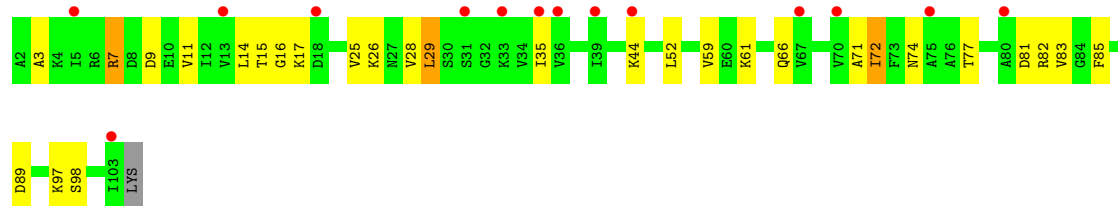
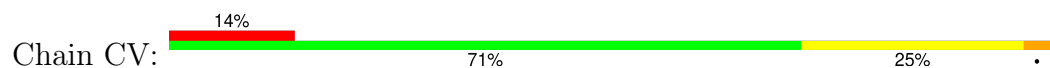
- Molecule 48: 50S ribosomal protein L23



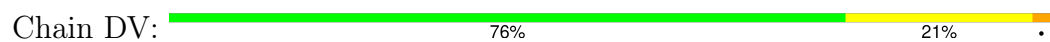
- Molecule 48: 50S ribosomal protein L23



- Molecule 49: 50S ribosomal protein L24



- Molecule 49: 50S ribosomal protein L24



- Molecule 50: 50S ribosomal protein L25

Chain CW:  3% 78% 21%



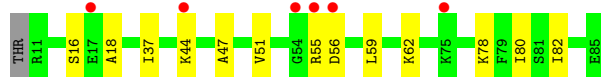
- Molecule 50: 50S ribosomal protein L25

Chain DW:  0% 76% 23%



- Molecule 51: 50S ribosomal protein L27

Chain CX:  8% 82% 17%



- Molecule 51: 50S ribosomal protein L27

Chain DX:  0% 76% 21%



- Molecule 52: 50S ribosomal protein L28

Chain CY:  6% 70% 25% 5%



- Molecule 52: 50S ribosomal protein L28

Chain DY:  0% 75% 22%



- Molecule 53: 50S ribosomal protein L29

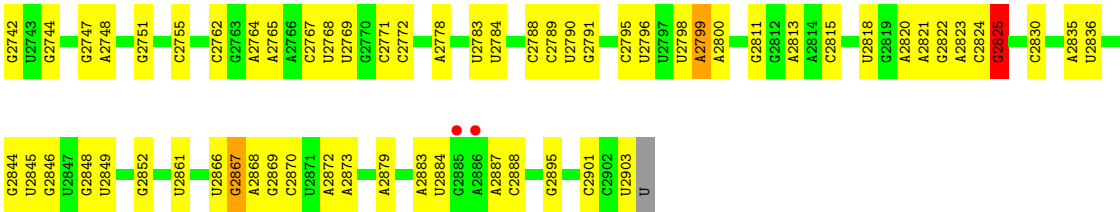
Chain CZ:  2% 82% 16%



Figure 1: A heatmap visualization of the 2022-2023 season. The heatmap is divided into two main sections: 'Top' (top half) and 'Bottom' (bottom half). Each section contains a grid of colored squares representing different categories. The 'Top' section has a grid of 10 rows and 10 columns, with colors ranging from dark green to dark red. The 'Bottom' section has a grid of 10 rows and 10 columns, with colors ranging from light green to light red. The colors indicate the magnitude of the values, with darker colors representing higher values. The 'Top' section shows a clear pattern of high values (dark red) in the top-left and bottom-right corners, and low values (dark green) in the top-right and bottom-left corners. The 'Bottom' section shows a similar pattern but with lower overall values, indicated by lighter colors.

U932	A819	C698	G496	A362	C275	C128	G1
C944	A820	A699	A603	G363	U276	C129	A10
C946	A821	G700	A504	C364	G277	U135	G11
A947	A825	C717	A505	U365	G136	U137	U12
	U826				A278	A14	A13
G953	U827	U710	A508	G372	U280	U138	A15
	U828	A721	C509	C383	A282	U139	G16
G956	G831	G726	C510	G386	C140	G141	A14
C957	U832		U511	G387	U284	G142	C20
	U833	G729	G512	U387	A143	A21	A21
C961	A834	A730	A513	G388	C143	C22	C22
	C835			G389	A144		
U967	C839	G738	U521	U390	U287	A28	A28
	C840	A739	A522	U397	U288	U29	U29
G974		C740	C531	G396	U296	G178	G30
A980	G858	G745	A532	C398	C297	C179	G31
A981	U746	A751	G533	U399		G180	G31
C982	U860		G543	U403	A300	C184	U34
A983	A861	A751	U545	G406	G301	G185	A38
A984			U547		C302	G186	G39
C985	A866		A637		G303	G187	U40
C986		G757	G638	G411	G307	G188	
C987	U878	C758	G548	A412	G308	G189	G45
A988	G879	G759	G549	C413	A190	G46	G46
	G880	G760	C550	C414	A310	A191	
G993	G881	A761		A415	U193	G58	G58
	G882		G553	U416	A311	G194	
A996		A764	U554		G317	U195	U65
G997	C885	C765	U564	C420	C318	A196	C66
C998	A		A563		G319	A197	
U1001	U	C772	G564	G424	A320	C198	A71
C1002	C		C565		U821	A199	A74
	C	G775	U566	C435	A322	U200	G75
C1006	C	G776	U567		C323		
	G	G780	U568	U451	A324	C205	U78
A1010	A892		G570	C452		C79	C79
G1011		A781	G659		G329	G215	G80
C1012	U895	A782	U573	C455	A330	A216	
U1012	A896	A783	A574	C456	C331	A83	A83
C1013	C897	G785	A575	U459	C343	A221	A84
A1014			U576	A466	A344	A222	G85
	G907		G577		A345	C225	G86
G1022		A788	C671	A472	A346	A226	C96
U1023	A910	A789	C672		A347	C97	C97
	A911	U790	G674	U472	A348	G230	
G1026	C912		A675	C475	U349	A101	A101
A1027	U913	C795	U683			G245	U102
A1028	G914		G684	A479	A352	G248	
	C915		A685	A480	C353		A118
U1033	G916	A802	U686	C481	A354	G248	A119
	A917		C687	A482	U355	G266	U120
A1040		G805	U688	G491	G356	G121	G121
A1046	A927	C806	C687	A492	C357	C267	G122
G1047	A928	U807	A693	G493	U358		
	U929		U694			G271	A125
A1061	G930	C812	U593		C361	A272	
	U931		U604				

U2609	A2503	G2286	U2156	C2095	G1873	G1738	G1578	G1450	C1306	U1173	G1062
U2613	U2504	A2287	U2167	A2097	A1885	A1744	A1578	G1451	G1309	U1174	G1068
U2615	G2505	A2288	A2168	U2098	U1886	A1745	A1583	G1452	A1069	A1175	A1068
G2621	U2506	U2292	A2170	G2010	A1900	U1746	U1585	A1453	U1313	G1177	A1070
C2626	C2512	U2305	A2171	A2014	G1906	G1750	A1586	U1460	C1320	G1178	G1071
C2627	A2516	G2308	U2172	A2015	G1907	G1753	G1587	G1478	A1321	U1180	G1072
C2628	U2517	A2311	A2173	G2018	A1913	A1754	U1589	G1482	A1327	U1181	U1083
C2629	U2518	A2312	C2175	A2020	A1914	A1755	A1590	U1484	A1328	G1182	A1088
C2630	G2410	C2313	C2178	A2023	3TD1915	U1758	A1591	U1485	U1329	U1184	A1089
C2636	A2418	U2320	U2180	G2026	C1920	A1759	C1604	U1486	G1332	G1187	A1090
G2643	U2419	G2325	U2181	G2027	C1922	A1764	C1607	A1189	U1352	U1188	A1090
G2644	G2420	A2183	A2182	G2027	A1927	G1773	A1608	A1490	A1353	G1190	U1093
A2660	U2423	G2326	A2184	A2030	G1928	A1774	C1612	G1491	A1354	U1094	U1094
G2661	C2424	A2327	U2185	A2031	G1929	U1775	G1613	G1492	G1355	A1095	A1095
A2662	A2425	A2328	G2186	G2032	G1930	U1776	A1614	C1493	G1356	A1096	A1096
G2663	A2426	U2329	G2188	A2033	A1931	U1778	A1618	A1494	A1359	U1097	U1097
C2667	A2427	G2330	A2198	U2034	A1932	U1781	G1622	U1495	A1365	A1098	A1098
C2668	G2428	G2331	G2204	G2035	G1935	U1782	U1648	U1496	A1366	C1100	C1100
C2669	A2434	A2332	G2205	C2047	A1938	U1783	U1649	U1497	C1376	U1101	U1101
C2670	A2435	U2333	U2131	G2048	U1939	U1784	A1641	A1504	C1377	C1102	C1102
C2673	G2436	G2234	U2132	G2049	U1940	A1783	A1642	A1508	U1379	U1105	U1105
C2681	A2437	G2235	G2133	C2050	C1941	A1786	U1647	A1509	A1383	G1106	G1106
U2689	C2438	A2225	A2134	A2052	A1952	U1796	G1674	G1510	G1386	G1112	G1112
U2690	U2441	U2233	A2135	C2055	G1964	U1797	C1675	G1511	U1231	U1119	U1119
U2695	A2448	G2234	U2132	G2056	U1965	G1797	A1676	A1515	U1396	G1250	G1250
C2703	U2449	G2238	G2133	C2057	C1967	U1798	G1682	A1523	U1397	G1251	G1251
C2704	A2450	G2239	A2134	A2052	G1964	C1800	U1674	G1529	C1398	G1252	G1252
A2705	A2461	U2243	A2135	C2055	C1965	A1801	C1675	A1532	G1401	A1253	A1253
G2714	G2464	G2255	A2142	G2056	A1966	A1808	A1676	A1533	U1402	G1256	G1256
C2715	C2465	G2258	C2145	G2057	C1967	U1812	G1682	A1534	A1403	A1262	A1262
G2719	A2469	C2259	C2146	A2060	A1970	G1813	C1694	A1535	G1416	A1269	A1269
U2720	G2357	C2260	A2147	G2061	G1971	G1816	G1695	A1536	C1417	C1270	C1270
A2721	U2474	C2261	G2148	C2062	G1972	G1826	G1699	A1537	A1420	G1271	G1271
G2722	C2475	U2282	U2149	C2064	G1973	A1829	U1714	A1544	G1424	U1272	U1272
C2723	U2477	A2267	C2150	C2065	G1974	U1715	G1715	C1547	G1425	G1278	G1278
U2724	A2478	A2268	U2151	C2066	U1976	C1832	U1720	U1554	G1426	G1279	G1279
A2725	U2479	A2273	G2152	G2067	U1979	C1833	G1721	A1557	C1428	A1286	A1286
A2726	C2480	A2274	C2153	U2068	G1980	A1847	A1722	C1558	G1436	U1294	U1294
A2727	G2484	A2278	G2157	G2068	A1981	A1853	G1727	U1562	G1441	G1297	G1297
G2729	U2491	G2279	G2158	A2082	C1985	G1869	C1728	U1563	U1442	U1443	U1443
A2733	U2492	G2280	C2160	G2083	U1991	C1870	U1729	A1566	G1446	G1300	G1300
A2740	C2498	A2281	G2162	G2087	G1992	A1871	G1731	A1569	C1447	A1301	A1301
A2741	G2502	G2282	A2163	A2093	U1993	A1872	G1731	A1569	C1447	C1172	C1172



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.55Å 433.65Å 622.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.13 – 3.32 48.13 – 3.32	Depositor EDS
% Data completeness (in resolution range)	83.3 (48.13-3.32) 83.2 (48.13-3.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	40.28 (at 3.33Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, R_{free}	0.176 , 0.219 0.191 , 0.238	Depositor DCC
R_{free} test set	2784 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 146.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	295119	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PGE, UR3, PUT, H2U, TRS, MPD, 3TD, EDO, MEQ, PSU, OMG, 6MZ, MA6, SPD, GUN, 4OC, 7MG, 2MG, PG4, 5MC, 2MA, OMC, 1MG, ZN, OMU, D2T, 4D4, 1PE, PEG, ACY, 5MU

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	0.73	20/36596 (0.1%)	0.68	0/57086
1	BA	0.72	17/36571 (0.0%)	0.68	0/57047
2	AB	0.81	0/1784	1.43	11/2403 (0.5%)
2	BB	0.79	0/1784	1.44	5/2403 (0.2%)
3	AC	0.87	0/1652	1.34	12/2225 (0.5%)
3	BC	0.89	0/1652	1.34	9/2225 (0.4%)
4	AD	0.76	0/1665	1.45	14/2227 (0.6%)
4	BD	0.78	0/1665	1.45	17/2227 (0.8%)
5	AE	0.79	0/1157	1.49	10/1557 (0.6%)
5	BE	0.75	0/1118	1.46	8/1504 (0.5%)
6	AF	0.79	0/881	1.39	7/1189 (0.6%)
6	BF	0.81	0/835	1.46	6/1128 (0.5%)
7	AG	0.89	0/1196	1.37	1/1602 (0.1%)
7	BG	0.88	0/1196	1.37	2/1602 (0.1%)
8	AH	0.74	0/989	1.38	3/1326 (0.2%)
8	BH	0.75	0/989	1.38	3/1326 (0.2%)
9	AI	0.84	0/1034	1.38	6/1375 (0.4%)
9	BI	0.84	0/1034	1.35	1/1375 (0.1%)
10	AJ	0.86	0/806	1.29	2/1089 (0.2%)
10	BJ	0.98	0/797	1.33	2/1077 (0.2%)
11	AK	0.85	1/893 (0.1%)	1.28	0/1205
11	BK	0.82	0/893	1.34	2/1205 (0.2%)
12	AL	0.79	0/960	1.33	1/1286 (0.1%)
12	BL	0.75	0/960	1.29	1/1286 (0.1%)
13	AM	0.94	0/893	1.52	19/1193 (1.6%)
13	BM	0.98	0/893	1.52	18/1193 (1.5%)
14	AN	0.89	0/817	1.35	2/1088 (0.2%)
14	BN	0.87	0/817	1.35	1/1088 (0.1%)
15	AO	0.80	0/722	1.53	3/964 (0.3%)
15	BO	0.76	0/722	1.55	4/964 (0.4%)
16	AP	0.86	0/659	1.38	5/884 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BP	0.84	0/659	1.38	0/884
17	AQ	0.81	0/658	1.27	1/881 (0.1%)
17	BQ	0.84	0/658	1.33	2/881 (0.2%)
18	AR	0.86	0/463	1.52	5/621 (0.8%)
18	BR	0.83	0/463	1.50	7/621 (1.1%)
19	AS	0.95	0/653	1.28	2/877 (0.2%)
19	BS	0.96	0/653	1.26	1/877 (0.1%)
20	AT	0.79	0/676	1.58	3/895 (0.3%)
20	BT	0.90	0/671	1.67	2/888 (0.2%)
21	AU	0.74	0/472	1.41	6/627 (1.0%)
21	BU	0.73	0/472	1.43	2/627 (0.3%)
22	C1	0.86	0/450	1.29	0/599
22	D1	0.98	0/450	1.27	1/599 (0.2%)
23	C2	0.85	0/416	1.36	2/554 (0.4%)
23	D2	0.90	0/421	1.33	1/561 (0.2%)
24	C3	0.77	0/380	1.41	0/498
24	D3	0.87	0/380	1.39	0/498
25	C4	0.78	0/513	1.34	2/676 (0.3%)
25	D4	0.88	0/513	1.39	2/676 (0.3%)
26	C5	0.78	0/303	1.21	0/397
26	D5	1.01	1/303 (0.3%)	1.22	0/397
27	C0	0.95	1/453 (0.2%)	1.40	1/605 (0.2%)
27	D0	0.99	0/467	1.40	2/623 (0.3%)
28	CB	0.71	1/2828 (0.0%)	0.70	1/4410 (0.0%)
28	DB	0.79	2/2872 (0.1%)	0.73	0/4478
29	CC	0.77	0/2121	1.34	15/2852 (0.5%)
29	DC	0.82	0/2121	1.31	12/2852 (0.4%)
30	CD	0.79	0/1586	1.23	7/2134 (0.3%)
31	CA	0.76	77/69165 (0.1%)	0.70	8/107896 (0.0%)
32	DD	0.88	0/1576	1.24	4/2119 (0.2%)
33	CE	0.77	0/1571	1.43	9/2113 (0.4%)
33	DE	0.82	1/1571 (0.1%)	1.43	8/2113 (0.4%)
34	CF	0.78	0/1434	1.39	11/1926 (0.6%)
34	DF	0.82	0/1434	1.42	12/1926 (0.6%)
35	CG	0.75	0/1343	1.36	16/1816 (0.9%)
35	DG	0.77	0/1343	1.31	9/1816 (0.5%)
36	CH	0.85	0/1121	1.43	10/1515 (0.7%)
36	DH	0.86	0/1121	1.39	0/1515
37	CJ	1.03	0/993	1.40	4/1341 (0.3%)
37	DJ	1.02	0/993	1.40	5/1341 (0.4%)
38	CK	0.73	0/1152	1.39	4/1551 (0.3%)
38	DK	0.95	0/1152	1.40	3/1551 (0.2%)
39	CL	0.84	0/947	1.29	3/1268 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DL	0.87	0/955	1.32	3/1279 (0.2%)
40	CM	0.80	1/1062 (0.1%)	1.43	9/1413 (0.6%)
40	DM	0.86	0/1062	1.36	7/1413 (0.5%)
41	CN	0.78	0/1081	1.33	5/1443 (0.3%)
41	DN	0.88	0/1092	1.32	5/1457 (0.3%)
42	CO	0.81	0/973	1.35	2/1301 (0.2%)
42	DO	0.97	0/1006	1.41	6/1345 (0.4%)
43	CP	0.80	0/902	1.46	9/1209 (0.7%)
43	DP	0.87	0/910	1.41	5/1219 (0.4%)
44	CQ	0.74	0/929	1.25	6/1242 (0.5%)
44	DQ	0.84	0/929	1.24	5/1242 (0.4%)
45	CR	0.81	0/960	1.55	10/1278 (0.8%)
45	DR	1.00	0/960	1.53	11/1278 (0.9%)
46	CS	0.78	0/829	1.27	2/1107 (0.2%)
46	DS	0.94	0/829	1.31	2/1107 (0.2%)
47	CT	0.77	0/864	1.48	4/1156 (0.3%)
47	DT	0.97	0/864	1.47	1/1156 (0.1%)
48	CU	0.84	0/744	1.29	0/994
48	DU	0.88	0/744	1.30	0/994
49	CV	0.87	0/787	1.42	4/1051 (0.4%)
49	DV	0.84	0/787	1.43	12/1051 (1.1%)
50	CW	0.76	0/766	1.33	2/1025 (0.2%)
50	DW	0.86	1/766 (0.1%)	1.33	4/1025 (0.4%)
51	CX	0.68	0/576	1.24	1/762 (0.1%)
51	DX	0.83	0/598	1.22	2/790 (0.3%)
52	CY	0.67	0/635	1.39	2/848 (0.2%)
52	DY	0.75	0/635	1.37	2/848 (0.2%)
53	CZ	0.77	0/502	1.60	1/667 (0.1%)
53	DZ	0.85	0/502	1.62	1/667 (0.1%)
54	DI	0.94	1/1037 (0.1%)	1.55	9/1402 (0.6%)
55	DA	0.83	54/69364 (0.1%)	0.76	5/108207 (0.0%)
All	All	0.79	178/309271 (0.1%)	0.94	495/462220 (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
10	BJ	0	1
28	DB	0	1
31	CA	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	DA	0	26
All	All	0	29

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2095	A	O5'-C5'	-10.48	1.26	1.42
55	DA	2585	U	C1'-N1	9.24	1.61	1.47
55	DA	2097	A	O5'-C5'	-8.84	1.29	1.42
26	D5	26	ILE	CG1-CD1	8.54	1.85	1.51
31	CA	2225	A	C3'-O3'	8.50	1.55	1.43
55	DA	790	U	C1'-N1	8.02	1.59	1.47
1	BA	5	U	C1'-N1	7.87	1.60	1.48
55	DA	12	U	C1'-N1	7.84	1.60	1.48
31	CA	769	U	C1'-N1	7.76	1.60	1.48
31	CA	2232	C	C1'-N1	7.62	1.59	1.48
1	AA	632	U	C1'-N1	7.16	1.59	1.48
31	CA	995	C	O5'-C5'	-7.06	1.32	1.42
31	CA	1657	U	C1'-N1	7.02	1.58	1.48
1	AA	1195	C	C1'-N1	7.00	1.58	1.48
31	CA	1825	U	C1'-N1	6.89	1.58	1.48
31	CA	1313	U	C1'-N1	6.85	1.58	1.48
31	CA	12	U	C1'-N1	6.77	1.58	1.48
31	CA	2465	C	C1'-N1	6.74	1.58	1.48
31	CA	790	U	C1'-N1	6.74	1.58	1.48
55	DA	140	C	C1'-N1	6.74	1.57	1.47
31	CA	2215	C	C1'-N1	6.72	1.58	1.48
55	DA	673	C	C3'-O3'	-6.72	1.32	1.42
31	CA	2779	U	C1'-N1	6.72	1.57	1.47
55	DA	2068	U	C3'-O3'	-6.58	1.32	1.42
1	BA	632	U	C1'-N1	6.57	1.58	1.48
1	AA	5	U	C1'-N1	6.53	1.58	1.48
31	CA	461	C	C1'-N1	6.35	1.57	1.48
55	DA	2127	G	C3'-O3'	6.34	1.51	1.42
31	CA	1777	U	C1'-N1	6.28	1.57	1.48
31	CA	2263	C	C1'-N1	6.26	1.57	1.48
31	CA	2320	U	C1'-N1	6.23	1.56	1.47
55	DA	1547	C	C1'-N1	6.22	1.57	1.48
31	CA	1993	U	C1'-N1	6.21	1.57	1.48
1	BA	764	C	C1'-N1	6.19	1.57	1.48
31	CA	140	C	C1'-N1	6.19	1.56	1.47
31	CA	1376	C	C1'-N1	6.14	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2354	C	C1'-N1	6.11	1.57	1.48
31	CA	1584	U	C1'-N1	6.11	1.57	1.48
31	CA	2443	C	C1'-N1	6.08	1.57	1.48
55	DA	1534	U	C1'-N1	6.08	1.57	1.48
55	DA	2502	G	O5'-C5'	-6.07	1.33	1.42
55	DA	784	G	C3'-O3'	5.99	1.51	1.42
55	DA	2491	U	C1'-N1	5.97	1.56	1.47
55	DA	416	U	C1'-N1	5.95	1.57	1.48
31	CA	2006	C	C1'-N1	5.94	1.57	1.48
55	DA	2585	U	C3'-O3'	5.94	1.52	1.43
1	AA	1059	C	C1'-N1	5.90	1.57	1.48
31	CA	653	U	C1'-N1	5.90	1.57	1.48
31	CA	1940	U	C1'-N1	5.85	1.56	1.47
31	CA	20	C	C1'-N1	5.83	1.57	1.48
1	AA	295	C	C1'-N1	5.82	1.57	1.48
1	BA	1008	U	O5'-C5'	-5.82	1.33	1.42
31	CA	1670	C	C3'-O3'	5.78	1.50	1.42
31	CA	1656	C	C1'-N1	5.77	1.57	1.48
55	DA	2586	U	C1'-N1	5.77	1.57	1.48
55	DA	2426	A	C3'-O3'	5.76	1.51	1.43
55	DA	653	U	C1'-N1	5.76	1.57	1.48
31	CA	691	C	C1'-N1	5.75	1.57	1.48
31	CA	2233	U	C1'-N1	5.75	1.57	1.48
31	CA	1352	U	C1'-N1	5.74	1.57	1.48
1	AA	1397	C	C1'-N1	5.74	1.56	1.47
31	CA	961	C	C1'-N1	5.73	1.56	1.47
31	CA	1554	U	C1'-N1	5.72	1.56	1.47
1	AA	932	C	C1'-N1	5.71	1.57	1.48
40	CM	77	ILE	CG1-CD1	-5.71	1.29	1.51
31	CA	1314	C	C1'-N1	5.70	1.57	1.48
55	DA	2220	U	C1'-N1	5.70	1.56	1.48
31	CA	1774	C	C1'-N1	5.69	1.56	1.48
27	C0	14	ILE	CA-C	5.68	1.59	1.52
1	AA	137	U	C1'-N1	5.67	1.56	1.48
1	BA	209	U	C1'-N1	5.67	1.56	1.48
1	BA	843	U	C1'-N1	5.67	1.55	1.47
28	DB	11	C	C1'-N1	5.67	1.56	1.48
55	DA	1584	U	C1'-N1	5.65	1.56	1.48
1	BA	1059	C	C1'-N1	5.64	1.56	1.48
31	CA	2104	C	C1'-N1	5.64	1.56	1.48
1	BA	137	U	C1'-N1	5.62	1.56	1.48
55	DA	2729	G	C3'-O3'	-5.62	1.33	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	222	C	C1'-N1	5.60	1.56	1.48
1	AA	603	U	C1'-N1	5.60	1.56	1.48
31	CA	2790	U	C1'-N1	5.58	1.55	1.47
55	DA	1446	C	C1'-N1	5.57	1.56	1.48
31	CA	1557	C	C1'-N1	5.56	1.56	1.48
55	DA	967	U	C1'-N1	5.56	1.56	1.48
55	DA	2342	C	C1'-N1	5.55	1.56	1.48
55	DA	2506	U	C1'-N1	5.55	1.56	1.48
31	CA	692	C	C1'-N1	5.51	1.56	1.48
55	DA	2354	C	O5'-C5'	-5.49	1.34	1.42
1	AA	222	C	C1'-N1	5.48	1.56	1.48
1	BA	183	C	C1'-N1	5.47	1.55	1.47
31	CA	826	U	C1'-N1	5.46	1.56	1.48
55	DA	2901	C	C1'-N1	5.46	1.56	1.48
55	DA	275	C	C1'-N1	5.46	1.56	1.48
28	DB	91	C	C1'-N1	5.44	1.56	1.48
31	CA	623	C	C1'-N1	5.43	1.56	1.48
31	CA	390	U	C1'-N1	5.42	1.55	1.47
31	CA	1940	U	C3'-O3'	5.40	1.51	1.43
1	AA	549	C	C1'-N1	5.40	1.56	1.48
55	DA	2402	U	C1'-N1	5.39	1.56	1.48
31	CA	1658	C	C1'-N1	5.38	1.56	1.48
31	CA	2619	C	C1'-N1	5.38	1.56	1.48
31	CA	562	U	C1'-N1	5.37	1.56	1.48
1	BA	210	C	C1'-N1	5.37	1.55	1.47
55	DA	694	U	C1'-N1	5.36	1.56	1.48
1	AA	503	C	C1'-N1	5.35	1.56	1.48
55	DA	1180	U	C1'-N1	5.35	1.56	1.48
31	CA	1375	U	C1'-N1	5.34	1.56	1.48
1	AA	845	A	O5'-C5'	5.33	1.50	1.42
31	CA	635	C	C1'-N1	5.33	1.56	1.48
31	CA	114	U	C1'-N1	5.32	1.56	1.48
1	BA	1397	C	C1'-N1	5.30	1.55	1.47
31	CA	784	G	C3'-O3'	5.30	1.50	1.42
31	CA	275	C	C1'-N1	5.30	1.56	1.48
31	CA	2385	C	C1'-N1	5.29	1.56	1.48
31	CA	2680	U	C3'-O3'	5.29	1.50	1.42
31	CA	2656	U	C1'-N1	5.28	1.56	1.48
55	DA	635	C	C1'-N1	5.28	1.56	1.48
31	CA	1994	C	C1'-N1	5.28	1.56	1.48
55	DA	1174	U	C1'-N1	5.28	1.56	1.48
1	BA	823	C	C1'-N1	5.28	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	CB	11	C	C1'-N1	5.28	1.56	1.48
55	DA	29	U	C1'-N1	5.28	1.56	1.48
55	DA	1714	U	C1'-N1	5.25	1.56	1.48
55	DA	2790	U	C1'-N1	5.25	1.55	1.47
31	CA	1629	U	C1'-N1	5.24	1.56	1.48
31	CA	2658	C	C1'-N1	5.24	1.56	1.48
31	CA	2425	A	C3'-O3'	5.24	1.51	1.43
11	AK	31	ILE	CG1-CD1	5.23	1.72	1.51
31	CA	1633	G	C3'-O3'	5.22	1.50	1.42
55	DA	790	U	O5'-C5'	5.22	1.50	1.42
31	CA	2342	C	C1'-N1	5.21	1.56	1.48
1	AA	343	U	C1'-N1	5.19	1.56	1.48
55	DA	1141	U	C1'-N1	5.19	1.55	1.47
55	DA	1727	C	C1'-N1	5.17	1.56	1.48
55	DA	2111	U	C1'-N1	5.17	1.56	1.48
31	CA	1639	C	C1'-N1	5.15	1.56	1.48
31	CA	1353	A	O5'-C5'	5.15	1.50	1.42
1	AA	528	C	C1'-N1	5.15	1.56	1.48
33	DE	78	TRP	CA-C	5.15	1.59	1.52
55	DA	1931	U	C1'-N1	5.14	1.56	1.48
1	AA	183	C	C1'-N1	5.14	1.55	1.47
31	CA	1730	C	C1'-N1	5.14	1.55	1.47
1	BA	603	U	C1'-N1	5.13	1.56	1.48
31	CA	1547	C	C1'-N1	5.12	1.56	1.48
55	DA	1730	C	C1'-N1	5.12	1.55	1.47
55	DA	2795	C	C1'-N1	5.12	1.56	1.48
55	DA	2239	G	C3'-O3'	-5.11	1.34	1.42
31	CA	2847	U	C1'-N1	5.11	1.56	1.48
31	CA	1438	U	C1'-N1	5.11	1.56	1.48
55	DA	1320	C	C3'-O3'	-5.11	1.35	1.43
55	DA	2055	C	C3'-O3'	-5.11	1.34	1.42
1	AA	1498	UR3	O3'-P	5.11	1.61	1.56
1	BA	582	C	C1'-N1	5.10	1.56	1.48
55	DA	982	C	C1'-N1	5.10	1.56	1.48
55	DA	1920	C	C1'-N1	5.09	1.56	1.48
1	AA	209	U	C1'-N1	5.09	1.56	1.48
31	CA	1282	U	C1'-N1	5.08	1.56	1.48
55	DA	998	C	C1'-N1	5.08	1.56	1.48
31	CA	416	U	C1'-N1	5.08	1.56	1.48
31	CA	870	U	C1'-N1	5.07	1.56	1.48
31	CA	1979	U	C1'-N1	5.07	1.56	1.48
54	DI	67	THR	CA-C	5.07	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2491	U	C1'-N1	5.07	1.55	1.47
1	BA	1054	C	C1'-N1	5.07	1.55	1.47
55	DA	188	G	O5'-C5'	-5.06	1.34	1.42
31	CA	451	U	C1'-N1	5.06	1.56	1.48
31	CA	1306	C	C1'-N1	5.06	1.56	1.48
31	CA	2480	C	C1'-N1	5.05	1.56	1.48
55	DA	1170	C	C1'-N1	5.05	1.56	1.48
55	DA	2174	C	C1'-N1	5.04	1.56	1.48
55	DA	2161	C	C1'-N1	5.04	1.56	1.48
31	CA	2691	C	C1'-N1	5.03	1.56	1.48
1	BA	503	C	C1'-N1	5.02	1.55	1.48
1	AA	843	U	C1'-N1	5.01	1.55	1.48
55	DA	2098	U	C1'-N1	5.01	1.55	1.48
50	DW	87	GLN	C-N	5.00	1.39	1.33
1	AA	1028	C	C1'-N1	5.00	1.55	1.48
31	CA	1727	C	C1'-N1	5.00	1.55	1.48

All (495) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DI	132	TYR	CA-C-N	9.75	139.24	121.70
54	DI	132	TYR	C-N-CA	9.75	139.24	121.70
4	AD	99	ASP	CA-CB-CG	8.31	120.91	112.60
4	BD	99	ASP	CA-CB-CG	8.08	120.68	112.60
34	DF	10	ASP	CA-CB-CG	7.93	120.53	112.60
9	AI	58	VAL	N-CA-C	-7.91	105.37	111.62
40	CM	15	ALA	N-CA-C	7.76	119.74	111.28
20	BT	6	SER	N-CA-C	-7.74	103.86	113.38
5	AE	70	ASN	CA-CB-CG	7.65	120.25	112.60
44	CQ	3	ASN	N-CA-C	-7.49	103.76	113.12
54	DI	106	PHE	CA-CB-CG	7.40	121.20	113.80
40	CM	68	SER	CA-C-N	7.38	135.63	121.54
40	CM	68	SER	C-N-CA	7.38	135.63	121.54
29	DC	246	THR	N-CA-C	-7.30	100.84	110.40
36	CH	8	LYS	CA-C-N	7.23	134.98	121.97
36	CH	8	LYS	C-N-CA	7.23	134.98	121.97
5	BE	93	ARG	N-CA-C	-7.18	98.03	109.59
29	CC	246	THR	N-CA-C	-7.09	101.11	110.40
33	DE	32	VAL	N-CA-CB	7.08	118.37	110.51
5	AE	93	ARG	N-CA-C	-7.01	98.30	109.59
30	CD	104	VAL	N-CA-C	6.88	117.00	110.53
35	CG	175	LYS	CA-C-N	6.85	134.62	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	CG	175	LYS	C-N-CA	6.85	134.62	121.54
3	BC	61	ALA	CA-C-N	6.82	132.45	122.63
3	BC	61	ALA	C-N-CA	6.82	132.45	122.63
13	AM	91	HIS	CA-C-N	6.80	129.94	120.29
13	AM	91	HIS	C-N-CA	6.80	129.94	120.29
7	AG	151	PHE	CA-CB-CG	6.80	120.60	113.80
13	BM	91	HIS	CA-C-N	6.76	129.89	120.29
13	BM	91	HIS	C-N-CA	6.76	129.89	120.29
29	DC	199	GLU	CA-C-N	6.75	129.22	120.44
29	DC	199	GLU	C-N-CA	6.75	129.22	120.44
5	AE	55	GLU	CA-C-N	6.75	126.91	120.43
5	AE	55	GLU	C-N-CA	6.75	126.91	120.43
31	CA	2425	A	P-O3'-C3'	6.70	130.24	120.20
44	DQ	3	ASN	N-CA-C	-6.67	103.81	112.68
18	BR	34	THR	CA-C-N	6.67	129.22	120.28
18	BR	34	THR	C-N-CA	6.67	129.22	120.28
2	BB	126	PHE	CA-CB-CG	6.65	120.45	113.80
17	AQ	48	ASP	CA-CB-CG	6.64	119.24	112.60
6	AF	92	THR	CA-C-N	6.60	129.12	120.28
6	AF	92	THR	C-N-CA	6.60	129.12	120.28
40	DM	100	ILE	N-CA-C	-6.60	106.14	111.81
33	CE	32	VAL	N-CA-CB	6.58	117.81	110.51
2	AB	126	PHE	CA-CB-CG	6.55	120.35	113.80
20	AT	78	ASN	CA-CB-CG	6.55	119.15	112.60
13	AM	12	HIS	CA-C-N	6.54	135.37	123.27
13	AM	12	HIS	C-N-CA	6.54	135.37	123.27
34	CF	21	ASN	CA-CB-CG	6.54	119.14	112.60
18	AR	34	THR	CA-C-N	6.51	129.01	120.28
18	AR	34	THR	C-N-CA	6.51	129.01	120.28
5	BE	55	GLU	CA-C-N	6.49	126.66	120.43
5	BE	55	GLU	C-N-CA	6.49	126.66	120.43
35	CG	69	ARG	CA-C-N	6.48	129.26	120.38
35	CG	69	ARG	C-N-CA	6.48	129.26	120.38
20	BT	78	ASN	CA-CB-CG	6.48	119.08	112.60
52	CY	16	ASN	CA-CB-CG	6.44	119.04	112.60
5	BE	69	ARG	N-CA-C	-6.42	101.49	110.35
49	DV	51	ALA	CA-C-N	6.40	133.77	121.54
49	DV	51	ALA	C-N-CA	6.40	133.77	121.54
37	DJ	129	ILE	N-CA-C	-6.40	106.56	112.96
37	CJ	129	ILE	N-CA-C	-6.39	106.57	112.96
45	DR	100	VAL	CA-C-N	6.38	129.11	120.44
45	DR	100	VAL	C-N-CA	6.38	129.11	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AD	107	PHE	CA-C-N	6.37	125.98	121.65
4	AD	107	PHE	C-N-CA	6.37	125.98	121.65
49	CV	3	ALA	CA-C-N	6.36	133.68	121.54
49	CV	3	ALA	C-N-CA	6.36	133.68	121.54
41	DN	101	VAL	N-CA-C	-6.36	101.35	109.30
52	DY	16	ASN	CA-CB-CG	6.35	118.95	112.60
5	AE	69	ARG	N-CA-C	-6.33	101.61	110.35
29	DC	266	PHE	CA-CB-CG	-6.33	107.47	113.80
35	CG	3	ARG	N-CA-C	-6.33	104.25	112.23
43	DP	78	VAL	N-CA-CB	6.30	117.50	110.51
35	DG	3	ARG	N-CA-C	-6.27	104.33	112.23
44	CQ	114	LEU	CD1-CG-CD2	6.25	124.55	110.80
54	DI	90	GLY	CA-C-N	6.24	133.45	121.54
54	DI	90	GLY	C-N-CA	6.24	133.45	121.54
18	AR	67	LEU	N-CA-C	-6.23	105.72	113.38
37	CJ	22	PRO	N-CA-C	6.22	118.29	110.70
6	BF	99	ALA	CA-C-N	6.21	132.88	121.70
6	BF	99	ALA	C-N-CA	6.21	132.88	121.70
43	CP	78	VAL	N-CA-CB	6.20	117.39	110.51
49	DV	3	ALA	CA-C-N	6.20	128.90	120.54
49	DV	3	ALA	C-N-CA	6.20	128.90	120.54
55	DA	271	G	C2'-C3'-O3'	6.19	118.78	109.50
10	AJ	76	ILE	CA-C-N	6.18	128.93	120.46
10	AJ	76	ILE	C-N-CA	6.18	128.93	120.46
32	DD	104	VAL	CA-C-N	6.18	128.47	120.44
32	DD	104	VAL	C-N-CA	6.18	128.47	120.44
32	DD	108	ASP	CA-CB-CG	6.17	118.77	112.60
35	DG	80	THR	CA-C-N	6.16	129.00	120.63
35	DG	80	THR	C-N-CA	6.16	129.00	120.63
37	DJ	22	PRO	N-CA-C	6.15	118.20	110.70
13	AM	14	HIS	CA-C-N	6.14	130.02	120.82
13	AM	14	HIS	C-N-CA	6.14	130.02	120.82
2	BB	204	ASP	CA-CB-CG	6.13	118.73	112.60
29	DC	147	LYS	N-CA-C	-6.12	100.89	110.14
45	CR	91	ASP	CA-CB-CG	6.12	118.72	112.60
4	BD	107	PHE	CA-C-N	6.12	125.81	121.65
4	BD	107	PHE	C-N-CA	6.12	125.81	121.65
45	CR	100	VAL	CA-C-N	6.11	128.76	120.44
45	CR	100	VAL	C-N-CA	6.11	128.76	120.44
47	DT	29	VAL	N-CA-CB	6.11	118.11	110.47
33	CE	113	VAL	CA-C-N	6.09	128.72	120.38
33	CE	113	VAL	C-N-CA	6.09	128.72	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	DY	54	LYS	N-CA-C	-6.09	104.57	111.14
15	AO	88	ARG	N-CA-C	-6.07	100.12	109.76
13	BM	14	HIS	CA-C-N	6.06	129.91	120.82
13	BM	14	HIS	C-N-CA	6.06	129.91	120.82
27	C0	49	ASN	CA-CB-CG	6.06	118.66	112.60
33	DE	113	VAL	CA-C-N	6.04	128.66	120.38
33	DE	113	VAL	C-N-CA	6.04	128.66	120.38
55	DA	1023	U	C4'-C3'-C2'	-6.03	96.58	102.60
54	DI	7	ASP	CA-CB-CG	6.01	118.61	112.60
30	CD	108	ASP	CA-CB-CG	6.00	118.60	112.60
4	AD	201	VAL	CA-C-N	6.00	128.32	120.28
4	AD	201	VAL	C-N-CA	6.00	128.32	120.28
33	CE	82	GLY	CA-C-N	5.98	132.73	121.97
33	CE	82	GLY	C-N-CA	5.98	132.73	121.97
39	CL	121	GLU	CA-C-N	5.97	132.45	121.70
39	CL	121	GLU	C-N-CA	5.97	132.45	121.70
43	CP	17	LYS	CA-C-N	5.97	128.28	120.28
43	CP	17	LYS	C-N-CA	5.97	128.28	120.28
45	CR	91	ASP	CA-C-N	5.96	128.59	120.54
45	CR	91	ASP	C-N-CA	5.96	128.59	120.54
2	AB	204	ASP	CA-CB-CG	5.95	118.55	112.60
34	DF	70	ALA	CA-C-N	5.94	128.52	120.38
34	DF	70	ALA	C-N-CA	5.94	128.52	120.38
29	CC	199	GLU	CA-C-N	5.94	128.16	120.44
29	CC	199	GLU	C-N-CA	5.94	128.16	120.44
34	CF	123	ASP	CA-CB-CG	5.94	118.54	112.60
29	CC	147	LYS	N-CA-C	-5.88	101.25	110.14
13	BM	96	PRO	CA-C-N	5.88	128.08	120.56
13	BM	96	PRO	C-N-CA	5.88	128.08	120.56
49	DV	29	LEU	CA-C-N	5.88	128.43	120.38
49	DV	29	LEU	C-N-CA	5.88	128.43	120.38
25	D4	17	THR	CA-C-N	5.87	126.62	119.99
25	D4	17	THR	C-N-CA	5.87	126.62	119.99
34	DF	158	THR	N-CA-CB	-5.86	101.54	110.45
34	CF	46	ASP	CA-CB-CG	5.85	118.45	112.60
31	CA	271	G	P-O3'-C3'	5.84	128.96	120.20
34	CF	166	GLY	CA-C-N	5.83	128.89	120.79
34	CF	166	GLY	C-N-CA	5.83	128.89	120.79
33	CE	48	THR	N-CA-C	-5.81	103.26	110.41
34	DF	167	ARG	CA-C-N	5.81	128.54	120.29
34	DF	167	ARG	C-N-CA	5.81	128.54	120.29
37	DJ	118	THR	CA-C-N	5.80	125.61	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	DJ	118	THR	C-N-CA	5.80	125.61	120.10
49	CV	29	LEU	CA-C-N	5.80	128.33	120.38
49	CV	29	LEU	C-N-CA	5.80	128.33	120.38
12	AL	64	THR	CB-CA-C	5.79	119.28	109.84
52	CY	54	LYS	N-CA-C	-5.79	104.88	111.14
51	DX	44	LYS	N-CA-C	-5.77	105.08	111.71
47	CT	64	ALA	CA-C-N	5.76	131.63	122.93
47	CT	64	ALA	C-N-CA	5.76	131.63	122.93
31	CA	2095	A	C5'-C4'-C3'	-5.75	107.37	116.00
33	DE	98	LYS	CA-C-N	5.75	127.92	120.44
33	DE	98	LYS	C-N-CA	5.75	127.92	120.44
37	CJ	118	THR	CA-C-N	5.72	125.53	120.10
37	CJ	118	THR	C-N-CA	5.72	125.53	120.10
29	CC	13	ARG	N-CA-C	-5.72	105.97	113.12
34	CF	147	ASP	CA-CB-CG	5.71	118.31	112.60
4	AD	24	GLY	CA-C-N	5.70	127.74	120.56
4	AD	24	GLY	C-N-CA	5.70	127.74	120.56
18	AR	54	GLN	CA-C-N	5.69	128.16	120.65
18	AR	54	GLN	C-N-CA	5.69	128.16	120.65
5	BE	41	ASP	CA-CB-CG	5.68	118.28	112.60
13	BM	6	GLY	CA-C-N	5.68	132.19	121.97
13	BM	6	GLY	C-N-CA	5.68	132.19	121.97
38	DK	81	ILE	N-CA-CB	5.68	117.74	110.13
18	BR	54	GLN	CA-C-N	5.67	128.13	120.65
18	BR	54	GLN	C-N-CA	5.67	128.13	120.65
8	AH	113	ASP	CA-C-N	5.65	128.11	120.65
8	AH	113	ASP	C-N-CA	5.65	128.11	120.65
7	BG	151	PHE	CA-CB-CG	5.64	119.44	113.80
6	BF	98	GLU	CA-C-N	5.63	132.29	121.54
6	BF	98	GLU	C-N-CA	5.63	132.29	121.54
35	CG	80	THR	CA-C-N	5.63	128.29	120.63
35	CG	80	THR	C-N-CA	5.63	128.29	120.63
40	CM	128	THR	CA-C-N	5.63	128.09	120.38
40	CM	128	THR	C-N-CA	5.63	128.09	120.38
3	AC	3	GLN	CA-C-N	5.62	129.77	120.94
3	AC	3	GLN	C-N-CA	5.62	129.77	120.94
14	BN	84	VAL	N-CA-C	-5.62	105.62	111.58
31	CA	2425	A	C4'-C3'-O3'	5.62	117.83	109.40
29	DC	131	PRO	CA-C-N	5.62	128.58	120.38
29	DC	131	PRO	C-N-CA	5.62	128.58	120.38
42	CO	82	GLU	CA-C-N	5.60	128.10	120.54
42	CO	82	GLU	C-N-CA	5.60	128.10	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	DF	146	VAL	N-CA-CB	5.59	117.22	110.95
29	CC	208	ALA	CA-C-N	5.59	126.29	120.03
29	CC	208	ALA	C-N-CA	5.59	126.29	120.03
44	DQ	75	GLN	N-CA-C	-5.59	99.41	108.41
51	CX	44	LYS	N-CA-C	-5.59	105.29	111.71
38	CK	80	HIS	CA-C-N	5.58	132.01	121.97
38	CK	80	HIS	C-N-CA	5.58	132.01	121.97
6	AF	102	MET	CA-C-N	5.58	127.59	120.56
6	AF	102	MET	C-N-CA	5.58	127.59	120.56
8	BH	113	ASP	CA-C-N	5.57	128.01	120.65
8	BH	113	ASP	C-N-CA	5.57	128.01	120.65
29	CC	131	PRO	CA-C-N	5.57	128.52	120.38
29	CC	131	PRO	C-N-CA	5.57	128.52	120.38
34	CF	164	GLU	CA-C-N	5.57	128.77	120.31
34	CF	164	GLU	C-N-CA	5.57	128.77	120.31
45	DR	8	VAL	CA-C-N	5.57	127.66	120.70
45	DR	8	VAL	C-N-CA	5.57	127.66	120.70
12	BL	64	THR	CB-CA-C	5.56	118.90	109.84
5	AE	78	ASN	CA-CB-CG	5.56	118.16	112.60
13	BM	102	THR	CA-C-N	5.56	128.04	120.54
13	BM	102	THR	C-N-CA	5.56	128.04	120.54
45	DR	51	ARG	N-CA-C	-5.56	104.62	111.40
4	BD	24	GLY	CA-C-N	5.55	127.56	120.56
4	BD	24	GLY	C-N-CA	5.55	127.56	120.56
38	CK	9	GLU	CB-CG-CD	5.55	122.04	112.60
43	DP	62	LEU	CA-C-N	5.55	127.99	120.44
43	DP	62	LEU	C-N-CA	5.55	127.99	120.44
6	AF	79	ARG	N-CA-C	-5.55	105.14	111.14
5	AE	144	LEU	CA-C-N	5.54	127.64	120.44
5	AE	144	LEU	C-N-CA	5.54	127.64	120.44
13	AM	96	PRO	CA-C-N	5.54	128.29	120.42
13	AM	96	PRO	C-N-CA	5.54	128.29	120.42
14	AN	84	VAL	N-CA-C	-5.54	105.71	111.58
35	DG	128	GLN	N-CA-C	-5.54	106.48	113.18
54	DI	85	VAL	CA-C-N	5.54	128.16	120.29
54	DI	85	VAL	C-N-CA	5.54	128.16	120.29
54	DI	85	VAL	N-CA-CB	5.54	117.97	111.66
43	CP	2	ASP	CA-C-N	5.53	129.11	120.82
43	CP	2	ASP	C-N-CA	5.53	129.11	120.82
5	BE	23	LYS	CA-C-O	-5.52	115.09	120.89
21	AU	52	ALA	CA-C-N	5.52	128.02	120.46
21	AU	52	ALA	C-N-CA	5.52	128.02	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AM	102	THR	CA-C-N	5.51	127.98	120.54
13	AM	102	THR	C-N-CA	5.51	127.98	120.54
30	CD	186	LEU	N-CA-C	5.51	118.54	109.72
53	DZ	29	ARG	N-CA-C	-5.50	105.19	111.14
8	BH	109	GLY	N-CA-C	5.50	118.73	111.70
55	DA	2825	G	C4'-C3'-C2'	-5.49	97.11	102.60
30	CD	104	VAL	CA-C-N	5.49	132.03	121.54
30	CD	104	VAL	C-N-CA	5.49	132.03	121.54
29	DC	57	GLY	CA-C-N	5.49	129.49	121.31
29	DC	57	GLY	C-N-CA	5.49	129.49	121.31
42	DO	82	GLU	CA-C-N	5.49	127.95	120.54
42	DO	82	GLU	C-N-CA	5.49	127.95	120.54
34	CF	146	VAL	N-CA-CB	5.49	117.09	110.95
44	CQ	75	GLN	N-CA-C	-5.49	99.58	108.41
35	DG	138	LYS	CA-C-N	5.48	127.62	120.28
35	DG	138	LYS	C-N-CA	5.48	127.62	120.28
33	CE	171	ASP	CA-CB-CG	5.48	118.08	112.60
41	CN	45	GLN	CA-C-N	5.47	127.46	120.56
41	CN	45	GLN	C-N-CA	5.47	127.46	120.56
31	CA	271	G	C2'-C3'-O3'	5.47	117.71	109.50
36	CH	9	VAL	CA-C-N	5.47	131.99	121.54
36	CH	9	VAL	C-N-CA	5.47	131.99	121.54
49	DV	56	GLY	N-CA-C	-5.47	105.27	112.82
33	DE	48	THR	N-CA-C	-5.46	103.49	110.53
40	CM	30	THR	N-CA-CB	5.45	119.70	110.49
19	BS	52	HIS	ND1-CE1-NE2	5.45	113.85	108.40
22	D1	26	THR	CB-CA-C	5.45	119.37	110.17
45	DR	91	ASP	CA-CB-CG	5.44	118.04	112.60
34	DF	166	GLY	CA-C-N	5.44	128.98	120.82
34	DF	166	GLY	C-N-CA	5.44	128.98	120.82
34	DF	46	ASP	CA-CB-CG	5.43	118.03	112.60
50	DW	54	ALA	CA-C-N	5.43	128.31	120.38
50	DW	54	ALA	C-N-CA	5.43	128.31	120.38
35	CG	128	GLN	N-CA-C	-5.43	106.61	113.18
4	BD	160	GLU	CB-CG-CD	5.43	121.83	112.60
41	CN	106	ASP	CA-CB-CG	5.42	118.02	112.60
49	DV	53	ASN	N-CA-C	-5.42	107.04	113.38
40	CM	101	ILE	CA-C-N	5.42	125.12	119.92
40	CM	101	ILE	C-N-CA	5.42	125.12	119.92
44	CQ	79	PRO	CA-C-N	5.42	127.59	120.60
44	CQ	79	PRO	C-N-CA	5.42	127.59	120.60
45	DR	91	ASP	CA-C-N	5.41	127.84	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	DR	91	ASP	C-N-CA	5.41	127.84	120.54
17	BQ	69	LYS	CA-C-N	5.41	131.87	121.54
17	BQ	69	LYS	C-N-CA	5.41	131.87	121.54
32	DD	186	LEU	N-CA-C	5.41	118.37	109.72
13	BM	11	ASP	CA-C-N	5.41	129.81	122.19
13	BM	11	ASP	C-N-CA	5.41	129.81	122.19
8	AH	109	GLY	N-CA-C	5.40	118.61	111.70
21	BU	52	ALA	CA-C-N	5.40	127.85	120.46
21	BU	52	ALA	C-N-CA	5.40	127.85	120.46
10	BJ	37	ARG	CA-C-N	5.39	130.33	121.87
10	BJ	37	ARG	C-N-CA	5.39	130.33	121.87
5	AE	123	VAL	N-CA-C	5.38	115.45	108.35
18	BR	67	LEU	N-CA-C	-5.38	106.67	113.18
34	CF	70	ALA	CA-C-N	5.37	127.74	120.38
34	CF	70	ALA	C-N-CA	5.37	127.74	120.38
33	DE	145	ASP	CA-CB-CG	5.37	117.97	112.60
16	AP	44	SER	N-CA-C	-5.35	106.70	113.18
3	BC	26	THR	CA-C-N	5.35	127.39	120.44
3	BC	26	THR	C-N-CA	5.35	127.39	120.44
45	CR	53	ARG	CA-C-N	5.34	127.44	120.28
45	CR	53	ARG	C-N-CA	5.34	127.44	120.28
25	C4	17	THR	CA-C-N	5.34	126.03	119.99
25	C4	17	THR	C-N-CA	5.34	126.03	119.99
11	BK	18	ASP	CA-CB-CG	5.34	117.94	112.60
55	DA	2436	G	C4'-C3'-C2'	-5.34	97.26	102.60
46	CS	35	PHE	CA-C-N	5.33	127.43	120.28
46	CS	35	PHE	C-N-CA	5.33	127.43	120.28
5	BE	144	LEU	CA-C-N	5.33	127.37	120.44
5	BE	144	LEU	C-N-CA	5.33	127.37	120.44
33	DE	78	TRP	N-CA-C	5.32	118.00	110.50
41	DN	54	THR	CA-C-N	5.32	127.42	120.28
41	DN	54	THR	C-N-CA	5.32	127.42	120.28
4	AD	139	PRO	CA-C-N	5.32	130.12	122.35
4	AD	139	PRO	C-N-CA	5.32	130.12	122.35
35	CG	138	LYS	CA-C-N	5.30	127.38	120.28
35	CG	138	LYS	C-N-CA	5.30	127.38	120.28
45	DR	15	LYS	CA-C-N	5.30	127.38	120.28
45	DR	15	LYS	C-N-CA	5.30	127.38	120.28
39	CL	37	ASP	CA-CB-CG	5.29	117.89	112.60
40	DM	128	THR	CA-C-N	5.29	127.63	120.38
40	DM	128	THR	C-N-CA	5.29	127.63	120.38
39	DL	37	ASP	CA-CB-CG	5.29	117.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	DV	7	ARG	CA-C-N	5.29	130.25	122.63
49	DV	7	ARG	C-N-CA	5.29	130.25	122.63
2	BB	103	ASN	CA-CB-CG	5.29	117.89	112.60
40	DM	60	ARG	CA-C-N	5.29	128.00	120.49
40	DM	60	ARG	C-N-CA	5.29	128.00	120.49
4	BD	132	ILE	N-CA-C	5.28	116.36	108.54
16	AP	44	SER	CA-C-N	5.28	131.63	121.54
16	AP	44	SER	C-N-CA	5.28	131.63	121.54
43	CP	105	ALA	CA-C-N	5.28	127.30	120.44
43	CP	105	ALA	C-N-CA	5.28	127.30	120.44
16	AP	47	GLU	CA-C-N	5.28	131.62	121.54
16	AP	47	GLU	C-N-CA	5.28	131.62	121.54
29	CC	195	VAL	CA-C-N	5.28	126.19	120.44
29	CC	195	VAL	C-N-CA	5.28	126.19	120.44
18	BR	23	TYR	CA-C-N	5.27	127.34	120.28
18	BR	23	TYR	C-N-CA	5.27	127.34	120.28
45	CR	15	LYS	CA-C-N	5.26	127.59	120.38
45	CR	15	LYS	C-N-CA	5.26	127.59	120.38
2	BB	142	GLU	CA-C-N	5.26	127.28	120.44
2	BB	142	GLU	C-N-CA	5.26	127.28	120.44
35	DG	159	GLY	CA-C-N	5.26	128.18	120.71
35	DG	159	GLY	C-N-CA	5.26	128.18	120.71
7	BG	62	PHE	CA-CB-CG	5.25	119.05	113.80
9	AI	103	PHE	CA-CB-CG	5.25	119.05	113.80
43	CP	62	LEU	CA-C-N	5.24	127.56	120.44
43	CP	62	LEU	C-N-CA	5.24	127.56	120.44
42	DO	43	GLU	CB-CG-CD	5.24	121.50	112.60
23	C2	50	LYS	CA-C-N	5.23	131.54	121.54
23	C2	50	LYS	C-N-CA	5.23	131.54	121.54
29	CC	57	GLY	CA-C-N	5.23	129.11	121.31
29	CC	57	GLY	C-N-CA	5.23	129.11	121.31
35	CG	174	ALA	CA-C-N	5.23	131.53	121.54
35	CG	174	ALA	C-N-CA	5.23	131.53	121.54
50	CW	54	ALA	CA-C-N	5.22	128.01	120.38
50	CW	54	ALA	C-N-CA	5.22	128.01	120.38
4	BD	154	ARG	CA-C-N	5.22	127.34	120.60
4	BD	154	ARG	C-N-CA	5.22	127.34	120.60
36	CH	50	ARG	CA-C-N	5.22	127.71	120.29
36	CH	50	ARG	C-N-CA	5.22	127.71	120.29
38	CK	93	ILE	N-CA-C	-5.22	105.41	110.42
47	CT	30	SER	CA-C-N	5.21	127.21	120.44
47	CT	30	SER	C-N-CA	5.21	127.21	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	CM	41	ARG	N-CA-C	5.21	117.41	110.53
55	DA	2585	U	P-O3'-C3'	5.21	128.01	120.20
3	AC	26	THR	CA-C-N	5.21	127.21	120.44
3	AC	26	THR	C-N-CA	5.21	127.21	120.44
5	AE	41	ASP	CA-CB-CG	5.20	117.80	112.60
4	AD	154	ARG	CA-C-N	5.20	127.31	120.60
4	AD	154	ARG	C-N-CA	5.20	127.31	120.60
41	DN	22	GLN	N-CA-C	-5.20	100.42	108.90
4	AD	175	ALA	CA-C-N	5.20	125.71	119.94
4	AD	175	ALA	C-N-CA	5.20	125.71	119.94
44	DQ	24	ASP	CA-CB-CG	5.20	117.80	112.60
45	CR	101	PHE	N-CA-C	5.19	116.75	111.14
6	AF	23	GLU	CA-C-N	5.19	127.23	120.28
6	AF	23	GLU	C-N-CA	5.19	127.23	120.28
39	DL	108	ARG	CA-C-N	5.18	131.58	121.63
39	DL	108	ARG	C-N-CA	5.18	131.58	121.63
11	BK	74	VAL	N-CA-C	-5.17	107.78	112.96
33	CE	98	LYS	CA-C-N	5.17	127.17	120.44
33	CE	98	LYS	C-N-CA	5.17	127.17	120.44
29	DC	121	ASP	CA-C-N	5.17	131.42	121.54
29	DC	121	ASP	C-N-CA	5.17	131.42	121.54
42	DO	113	ILE	CB-CA-C	5.17	117.40	110.42
15	BO	16	GLY	CA-C-N	5.17	127.21	120.28
15	BO	16	GLY	C-N-CA	5.17	127.21	120.28
35	CG	118	PRO	CA-C-N	5.17	131.41	121.54
35	CG	118	PRO	C-N-CA	5.17	131.41	121.54
36	CH	52	ALA	CA-C-N	5.17	127.16	120.44
36	CH	52	ALA	C-N-CA	5.17	127.16	120.44
45	DR	31	VAL	N-CA-CB	-5.16	105.11	111.00
13	AM	54	ASP	CA-CB-CG	5.16	117.76	112.60
13	BM	86	TYR	CA-C-N	5.16	127.71	120.28
13	BM	86	TYR	C-N-CA	5.16	127.71	120.28
13	BM	20	THR	CA-C-N	5.16	127.45	120.38
13	BM	20	THR	C-N-CA	5.16	127.45	120.38
3	BC	206	GLU	CA-C-N	5.16	130.98	121.70
3	BC	206	GLU	C-N-CA	5.16	130.98	121.70
3	AC	206	GLU	CA-C-N	5.15	130.97	121.70
3	AC	206	GLU	C-N-CA	5.15	130.97	121.70
9	BI	103	PHE	CA-CB-CG	5.15	118.95	113.80
41	CN	101	VAL	N-CA-C	-5.15	102.86	109.30
53	CZ	29	ARG	N-CA-C	-5.15	105.58	111.14
13	AM	86	TYR	CA-C-N	5.14	127.69	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AM	86	TYR	C-N-CA	5.14	127.69	120.28
3	AC	159	GLY	CA-C-N	5.14	128.38	120.82
3	AC	159	GLY	C-N-CA	5.14	128.38	120.82
3	BC	76	VAL	N-CA-C	-5.14	106.13	111.58
2	AB	103	ASN	CA-CB-CG	5.13	117.73	112.60
13	BM	4	ILE	CA-C-N	5.13	131.35	121.54
13	BM	4	ILE	C-N-CA	5.13	131.35	121.54
19	AS	5	LEU	CA-C-N	5.13	127.87	120.38
19	AS	5	LEU	C-N-CA	5.13	127.87	120.38
29	CC	121	ASP	CA-C-N	5.13	131.34	121.54
29	CC	121	ASP	C-N-CA	5.13	131.34	121.54
15	BO	60	VAL	CA-C-N	5.12	127.14	120.28
15	BO	60	VAL	C-N-CA	5.12	127.14	120.28
51	DX	62	LYS	N-CA-C	-5.11	106.20	112.90
35	DG	60	ASP	CA-CB-CG	5.11	117.71	112.60
38	DK	93	ILE	N-CA-C	-5.11	105.51	110.42
4	BD	130	VAL	CA-C-N	5.11	127.64	120.28
4	BD	130	VAL	C-N-CA	5.11	127.64	120.28
13	AM	97	VAL	CA-C-N	5.11	127.08	120.44
13	AM	97	VAL	C-N-CA	5.11	127.08	120.44
28	CB	15	A	O4'-C1'-N9	5.11	115.86	108.20
3	AC	126	ARG	CA-C-N	5.09	131.27	121.54
3	AC	126	ARG	C-N-CA	5.09	131.27	121.54
44	CQ	24	ASP	CA-CB-CG	5.09	117.69	112.60
2	AB	80	VAL	CA-C-N	5.09	128.45	120.82
2	AB	80	VAL	C-N-CA	5.09	128.45	120.82
4	BD	175	ALA	CA-C-N	5.09	125.59	119.94
4	BD	175	ALA	C-N-CA	5.09	125.59	119.94
41	CN	111	GLU	CB-CG-CD	5.09	121.25	112.60
44	DQ	79	PRO	CA-C-N	5.09	127.16	120.60
44	DQ	79	PRO	C-N-CA	5.09	127.16	120.60
2	AB	63	ARG	CA-C-N	5.08	129.36	122.19
2	AB	63	ARG	C-N-CA	5.08	129.36	122.19
40	DM	59	ARG	CA-C-N	5.08	127.05	120.44
40	DM	59	ARG	C-N-CA	5.08	127.05	120.44
41	DN	106	ASP	CA-CB-CG	5.08	117.68	112.60
3	AC	178	LEU	CA-C-N	5.08	127.09	120.28
3	AC	178	LEU	C-N-CA	5.08	127.09	120.28
9	AI	71	GLY	CA-C-N	5.08	127.43	120.77
9	AI	71	GLY	C-N-CA	5.08	127.43	120.77
31	CA	1786	A	C1'-O4'-C4'	-5.08	104.62	109.70
4	BD	139	PRO	CA-C-N	5.07	129.76	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BD	139	PRO	C-N-CA	5.07	129.76	122.35
20	AT	43	ASP	CA-C-N	5.07	127.08	120.28
20	AT	43	ASP	C-N-CA	5.07	127.08	120.28
38	DK	31	GLU	CB-CG-CD	5.07	121.22	112.60
2	AB	142	GLU	CA-C-N	5.07	127.03	120.44
2	AB	142	GLU	C-N-CA	5.07	127.03	120.44
9	AI	89	GLU	CA-C-N	5.07	127.52	120.63
9	AI	89	GLU	C-N-CA	5.07	127.52	120.63
6	BF	79	ARG	CA-C-N	5.07	127.07	120.28
6	BF	79	ARG	C-N-CA	5.07	127.07	120.28
27	D0	52	SER	CA-C-N	5.07	128.71	120.60
27	D0	52	SER	C-N-CA	5.07	128.71	120.60
13	AM	7	ILE	CA-C-N	5.06	128.04	120.90
13	AM	7	ILE	C-N-CA	5.06	128.04	120.90
50	DW	67	GLY	CA-C-N	5.06	128.04	120.90
50	DW	67	GLY	C-N-CA	5.06	128.04	120.90
49	DV	83	VAL	CA-C-N	5.06	126.27	121.46
49	DV	83	VAL	C-N-CA	5.06	126.27	121.46
13	AM	20	THR	CA-C-N	5.05	127.05	120.28
13	AM	20	THR	C-N-CA	5.05	127.05	120.28
34	DF	157	THR	CA-C-N	5.05	131.93	121.32
34	DF	157	THR	C-N-CA	5.05	131.93	121.32
4	AD	25	VAL	N-CA-C	-5.05	105.57	110.42
3	BC	178	LEU	CA-C-N	5.05	127.05	120.28
3	BC	178	LEU	C-N-CA	5.05	127.05	120.28
23	D2	40	ASP	CA-CB-CG	5.05	117.65	112.60
14	AN	18	ASP	CA-CB-CG	5.05	117.65	112.60
46	DS	35	PHE	CA-C-N	5.04	127.03	120.28
46	DS	35	PHE	C-N-CA	5.04	127.03	120.28
15	AO	60	VAL	CA-C-N	5.04	127.03	120.28
15	AO	60	VAL	C-N-CA	5.04	127.03	120.28
21	AU	45	ARG	CA-C-N	5.04	127.44	120.29
21	AU	45	ARG	C-N-CA	5.04	127.44	120.29
35	CG	159	GLY	CA-C-N	5.04	127.92	120.82
35	CG	159	GLY	C-N-CA	5.04	127.92	120.82
42	DO	122	ALA	CA-C-N	5.04	127.44	120.29
42	DO	122	ALA	C-N-CA	5.04	127.44	120.29
29	DC	121	ASP	CA-CB-CG	5.03	117.63	112.60
37	DJ	95	LYS	N-CA-C	-5.02	107.83	114.31
31	CA	974	G	N9-C1'-C2'	5.01	121.52	114.00
4	BD	47	ARG	CA-C-N	5.01	127.83	120.71
4	BD	47	ARG	C-N-CA	5.01	127.83	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	AU	33	ARG	CA-C-N	5.01	127.25	120.44
21	AU	33	ARG	C-N-CA	5.01	127.25	120.44
30	CD	64	GLU	CA-C-N	5.01	127.31	120.54
30	CD	64	GLU	C-N-CA	5.01	127.31	120.54
43	DP	105	ALA	CA-C-N	5.01	126.95	120.44
43	DP	105	ALA	C-N-CA	5.01	126.95	120.44
31	CA	271	G	C4'-C3'-O3'	5.00	116.91	109.40
2	AB	7	ARG	CA-C-N	5.00	126.98	120.28
2	AB	7	ARG	C-N-CA	5.00	126.98	120.28
36	CH	45	GLU	CA-C-N	5.00	127.48	120.28
36	CH	45	GLU	C-N-CA	5.00	127.48	120.28

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	BJ	37	ARG	Mainchain
31	CA	780	G	Sidechain
55	DA	1047	G	Sidechain
55	DA	1162	G	Sidechain
55	DA	1238	G	Sidechain
55	DA	1682	G	Sidechain
55	DA	1773	A	Sidechain
55	DA	1985	C	Sidechain
55	DA	2010	G	Sidechain
55	DA	2286	G	Sidechain
55	DA	2351	G	Sidechain
55	DA	2512	C	Sidechain
55	DA	2516	A	Sidechain
55	DA	2518	A	Sidechain
55	DA	2582	G	Sidechain
55	DA	2588	G	Sidechain
55	DA	2728	U	Sidechain
55	DA	2825	G	Sidechain
55	DA	329	G	Sidechain
55	DA	452	G	Sidechain
55	DA	512	G	Sidechain
55	DA	577	G	Sidechain
55	DA	700	G	Sidechain
55	DA	726	G	Sidechain
55	DA	953	G	Sidechain
55	DA	956	G	Sidechain

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Mol	Chain	Res	Type	Group
55	DA	980	A	Sidechain
55	DA	983	A	Sidechain
28	DB	13	G	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32932	0	16593	162	0
1	BA	32910	0	16582	179	0
2	AB	1753	0	1780	17	0
2	BB	1753	0	1780	18	0
3	AC	1625	0	1696	13	0
3	BC	1625	0	1696	17	0
4	AD	1643	0	1707	19	0
4	BD	1643	0	1707	19	0
5	AE	1144	0	1185	17	0
5	BE	1105	0	1148	26	0
6	AF	862	0	864	14	0
6	BF	817	0	808	9	0
7	AG	1182	0	1238	17	0
7	BG	1182	0	1238	17	0
8	AH	979	0	1031	10	0
8	BH	979	0	1031	7	0
9	AI	1022	0	1070	11	0
9	BI	1022	0	1070	10	0
10	AJ	796	0	836	8	0
10	BJ	787	0	828	11	0
11	AK	877	0	887	12	0
11	BK	877	0	887	14	0
12	AL	957	0	1017	14	0
12	BL	957	0	1017	16	0
13	AM	884	0	941	12	0
13	BM	884	0	941	15	0
14	AN	805	0	844	10	0
14	BN	805	0	844	10	0
15	AO	714	0	734	3	0
15	BO	714	0	734	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	AP	649	0	666	6	0
16	BP	649	0	666	8	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	5	0
18	AR	456	0	478	6	0
18	BR	456	0	478	5	0
19	AS	638	0	665	13	0
19	BS	638	0	665	11	0
20	AT	670	0	719	12	0
20	BT	665	0	714	9	0
21	AU	465	0	491	6	0
21	BU	465	0	491	5	0
22	C1	444	0	458	17	0
22	D1	444	0	458	10	0
23	C2	409	0	440	6	0
23	D2	414	0	442	5	0
24	C3	377	0	418	3	0
24	D3	377	0	418	7	0
25	C4	504	0	572	4	0
25	D4	504	0	572	8	0
26	C5	302	0	340	5	0
26	D5	302	0	340	4	0
27	C0	449	0	488	4	0
27	D0	463	0	504	7	0
28	CB	2529	0	1281	7	0
28	DB	2569	0	1301	10	0
29	CC	2082	0	2154	24	0
29	DC	2082	0	2154	24	0
30	CD	1565	0	1616	22	0
31	CA	62229	0	31319	399	0
32	DD	1576	0	1627	29	0
33	CE	1552	0	1619	22	0
33	DE	1552	0	1619	21	0
34	CF	1410	0	1444	18	0
34	DF	1410	0	1444	26	0
35	CG	1323	0	1371	17	0
35	DG	1323	0	1371	15	0
36	CH	1110	0	1148	10	0
36	DH	1110	0	1148	11	0
37	CJ	979	0	1028	7	0
37	DJ	979	0	1028	10	0
38	CK	1129	0	1162	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	DK	1129	0	1162	15	0
39	CL	938	0	1012	9	0
39	DL	946	0	1023	8	0
40	CM	1053	0	1129	23	0
40	DM	1053	0	1129	18	0
41	CN	1075	0	1154	16	0
41	DN	1092	0	1177	18	0
42	CO	960	0	1000	17	0
42	DO	993	0	1034	17	0
43	CP	892	0	923	14	0
43	DP	900	0	935	17	0
44	CQ	917	0	962	8	0
44	DQ	917	0	962	14	0
45	CR	947	0	1019	14	0
45	DR	947	0	1019	21	0
46	CS	816	0	839	18	0
46	DS	816	0	839	22	0
47	CT	857	0	922	16	0
47	DT	857	0	922	14	0
48	CU	738	0	807	9	0
48	DU	738	0	807	6	0
49	CV	779	0	831	12	0
49	DV	779	0	831	9	0
50	CW	753	0	780	7	0
50	DW	753	0	780	8	0
51	CX	569	0	581	8	0
51	DX	591	0	606	14	0
52	CY	625	0	652	11	0
52	DY	625	0	652	8	0
53	CZ	501	0	531	5	0
53	DZ	501	0	531	6	0
54	DI	1023	0	1052	26	0
55	DA	62423	0	31411	382	0
56	AA	70	0	0	0	0
56	BA	41	0	0	0	0
56	CA	156	0	0	0	0
56	CB	3	0	0	0	0
56	DA	184	0	0	0	0
56	DB	9	0	0	0	0
56	DD	1	0	0	0	0
56	DM	1	0	0	0	0
56	DR	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AA	13	0	18	0	0
57	BA	13	0	18	1	0
57	DA	26	0	36	0	0
57	DQ	13	0	18	0	0
57	DR	13	0	18	1	0
57	DS	13	0	18	0	0
58	AA	16	0	28	0	0
58	DA	40	0	70	2	0
58	DE	16	0	28	0	0
58	DK	8	0	14	0	0
58	DN	8	0	14	0	0
58	DS	8	0	14	3	0
58	DT	16	0	28	0	0
59	AA	24	0	48	0	0
59	DA	66	0	132	4	0
59	DM	6	0	12	0	0
60	AB	1	0	0	0	0
60	C5	1	0	0	0	0
60	D5	1	0	0	0	0
61	AL	7	0	10	0	0
61	D3	7	0	10	1	0
61	DA	42	0	60	1	0
61	DL	7	0	10	0	0
61	DP	7	0	10	0	0
61	DQ	7	0	10	1	0
62	D0	4	0	6	0	0
62	D1	4	0	6	0	0
62	DA	32	0	48	4	0
62	DB	8	0	12	0	0
63	D1	10	0	14	0	0
63	D3	10	0	14	0	0
63	DA	40	0	56	5	0
63	DD	10	0	14	0	0
63	DS	10	0	14	0	0
63	DU	10	0	14	1	0
64	DA	40	0	76	0	0
65	DA	32	0	44	1	0
66	DA	12	0	9	2	0
67	DA	11	0	5	0	0
68	DA	8	0	12	1	0
69	AA	507	0	0	3	0
69	AC	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	AD	2	0	0	0	0
69	AE	5	0	0	0	0
69	AF	1	0	0	0	0
69	AG	1	0	0	0	0
69	AJ	3	0	0	0	0
69	AK	5	0	0	0	0
69	AL	7	0	0	0	0
69	AM	4	0	0	0	0
69	AN	6	0	0	1	0
69	AO	1	0	0	0	0
69	AP	1	0	0	0	0
69	AQ	1	0	0	0	0
69	AS	1	0	0	0	0
69	AT	2	0	0	0	0
69	AU	4	0	0	0	0
69	BA	287	0	0	2	0
69	BD	12	0	0	0	0
69	BE	1	0	0	0	0
69	BF	1	0	0	0	0
69	BK	3	0	0	0	0
69	BL	3	0	0	0	0
69	BN	1	0	0	0	0
69	BO	1	0	0	0	0
69	BP	4	0	0	0	0
69	BR	1	0	0	0	0
69	BT	5	0	0	0	0
69	C3	3	0	0	0	0
69	C4	1	0	0	0	0
69	CA	696	0	0	3	0
69	CB	13	0	0	0	0
69	CC	11	0	0	0	0
69	CD	4	0	0	0	0
69	CE	5	0	0	0	0
69	CL	1	0	0	0	0
69	CM	3	0	0	0	0
69	CO	1	0	0	0	0
69	CU	2	0	0	0	0
69	CV	1	0	0	0	0
69	CW	1	0	0	0	0
69	CY	1	0	0	0	0
69	D0	24	0	0	2	0
69	D1	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	D2	5	0	0	0	0
69	D3	30	0	0	0	0
69	D4	40	0	0	1	0
69	D5	13	0	0	1	0
69	DA	4824	0	0	39	0
69	DB	203	0	0	3	0
69	DC	100	0	0	1	0
69	DD	97	0	0	5	0
69	DE	54	0	0	2	0
69	DF	13	0	0	1	0
69	DG	9	0	0	0	0
69	DH	2	0	0	0	0
69	DK	61	0	0	0	0
69	DL	50	0	0	0	0
69	DM	60	0	0	0	0
69	DN	81	0	0	1	0
69	DO	42	0	0	1	0
69	DP	42	0	0	2	0
69	DQ	32	0	0	1	0
69	DR	68	0	0	3	0
69	DS	52	0	0	5	0
69	DT	65	0	0	1	0
69	DU	24	0	0	0	0
69	DV	19	0	0	1	0
69	DW	33	0	0	1	0
69	DX	33	0	0	2	0
69	DY	11	0	0	1	0
69	DZ	7	0	0	0	0
All	All	295119	0	194415	2104	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (2104) 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)
26:D5:26:ILE:CD1	26:D5:26:ILE:CG1	1.85	1.50
46:CS:14:VAL:HG21	46:CS:98:ILE:HG13	1.26	1.16
31:CA:1005:C:O2'	38:CK:30:THR:HG21	1.62	0.99
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.44	0.95
31:CA:1311:G:H21	31:CA:1603:A:H62	1.16	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DI:67:THR:HG22	54:DI:68:PRO:HA	1.52	0.91
31:CA:1936:A:H2	31:CA:1943:U:H3	1.15	0.91
51:DX:41[A]:ARG:HH12	55:DA:2262:U:H5''	1.39	0.88
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.56	0.87
13:BM:6:GLY:HA3	13:BM:66:GLU:HG3	1.56	0.87
55:DA:1975:G:H21	63:DA:3225:PGE:H22	1.39	0.86
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.57	0.86
11:BK:89:PRO:HG3	21:BU:32:VAL:HG11	1.57	0.86
40:DM:60:ARG:HH21	55:DA:2428:G:N2	1.72	0.86
2:AB:31:ILE:HG21	2:AB:39:HIS:HD2	1.42	0.85
46:CS:14:VAL:HG21	46:CS:98:ILE:CG1	2.07	0.84
1:AA:1492:A:H5''	12:AL:44:LYS:HG2	1.60	0.84
30:CD:133:THR:HG22	31:CA:1993:U:H4'	1.60	0.83
32:DD:140:HIS:HB3	69:DD:485:HOH:O	1.76	0.83
49:DV:52:LEU:HB3	49:DV:54:GLN:HB2	1.59	0.83
2:BB:31:ILE:HG21	2:BB:39:HIS:HD2	1.43	0.82
33:DE:33:VAL:HG22	58:DA:3192:MPD:H12	1.62	0.82
31:CA:2796:U:H3	31:CA:2799:A:H61	1.23	0.82
55:DA:1927:A:H2'	55:DA:1928:A:C8	2.15	0.82
1:AA:1063:C:H2'	1:AA:1064:G:C8	2.15	0.82
55:DA:2796:U:H3	55:DA:2799:A:H61	1.24	0.82
29:CC:17:VAL:HB	29:CC:204:VAL:CG1	2.10	0.81
40:CM:77:ILE:HD11	40:CM:108:ALA:HB1	1.62	0.80
31:CA:694:U:OP1	31:CA:1569:A:H1'	1.83	0.79
31:CA:206:U:H2'	31:CA:207:A:H8	1.46	0.79
47:DT:90:LYS:HA	55:DA:751:A:H5'	1.62	0.79
46:CS:14:VAL:CG2	46:CS:98:ILE:HG13	2.09	0.78
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.63	0.78
31:CA:2428:G:N2	40:CM:60:ARG:HH21	1.79	0.78
1:AA:81:A:H61	1:AA:86:G:H1	1.29	0.78
11:BK:24:HIS:HB3	11:BK:31:ILE:HG23	1.66	0.78
31:CA:751:A:H5'	47:CT:90:LYS:HA	1.66	0.78
1:BA:841:C:H3'	1:BA:842:U:H5''	1.66	0.78
31:CA:193:U:H2'	31:CA:194:G:H8	1.49	0.77
31:CA:450:G:H2'	31:CA:451:U:H5''	1.65	0.76
34:DF:158:THR:HG23	34:DF:160:ALA:H	1.50	0.76
47:DT:73:LYS:HB2	47:DT:106:VAL:HB	1.67	0.76
33:DE:21:ARG:HD2	69:DE:432:HOH:O	1.85	0.76
5:AE:107:ALA:HB2	5:AE:125:ALA:HB3	1.68	0.76
55:DA:758:C:O2	55:DA:1981:A:H2	1.69	0.75
29:DC:41:GLY:O	29:DC:43:ARG:HD2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:DM:60:ARG:HH21	55:DA:2428:G:H21	1.33	0.75
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.69	0.75
36:CH:27:ARG:HH11	52:CY:60:ASP:HA	1.52	0.75
47:CT:73:LYS:HB2	47:CT:106:VAL:HB	1.68	0.74
25:D4:21:GLY:HA3	25:D4:49:MET:HE1	1.70	0.74
33:DE:130:LYS:HB2	33:DE:133:LEU:HD12	1.69	0.74
43:DP:103:VAL:HG23	69:DP:313:HOH:O	1.87	0.74
1:BA:9:G:H5'	5:BE:108:GLY:HA3	1.68	0.74
49:DV:37:GLU:HB3	69:DV:206:HOH:O	1.88	0.74
31:CA:2641:G:H5''	38:CK:78:THR:HB	1.69	0.73
5:AE:106:ILE:HD11	5:AE:124:LEU:HD23	1.69	0.73
29:CC:266:PHE:N	29:CC:266:PHE:CD1	2.57	0.73
29:CC:266:PHE:H	29:CC:266:PHE:HD1	1.33	0.73
31:CA:1203:U:H5'	40:CM:3:LEU:HD12	1.70	0.73
25:C4:21:GLY:HA3	25:C4:49:MET:HE1	1.71	0.72
42:DO:33:ILE:HD12	42:DO:114:GLU:HB3	1.70	0.72
1:BA:82:G:H1	1:BA:84:U:H5	1.37	0.72
1:BA:1107:C:OP1	3:BC:174:PRO:HB3	1.90	0.71
55:DA:568:U:H1'	55:DA:2030:6MZ:H9C1	1.71	0.71
1:BA:518:C:H2'	1:BA:530:G:C8	2.25	0.71
45:DR:20:GLN:HG2	57:DR:201:PG4:H42	1.73	0.71
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.72	0.71
39:CL:38:ILE:HD11	39:CL:112:PHE:HZ	1.54	0.71
1:BA:664:G:H22	1:BA:741:G:H1	1.39	0.71
7:BG:113:ASP:HB2	7:BG:119:ARG:HG3	1.72	0.71
31:CA:118:A:N3	31:CA:178:G:H1'	2.06	0.71
11:BK:88:GLY:H	11:BK:114:THR:HG22	1.57	0.70
31:CA:1936:A:N6	31:CA:1963:U:H3	1.90	0.70
1:AA:518:C:H2'	1:AA:530:G:C8	2.27	0.70
29:DC:258:ARG:HD2	55:DA:1799:G:OP1	1.92	0.70
55:DA:671:C:O2'	55:DA:672:C:H5'	1.92	0.70
29:CC:107:PRO:HD2	29:CC:110:LEU:HD22	1.74	0.70
55:DA:1137:G:H5''	59:DA:3213:PUT:H12	1.73	0.69
42:CO:33:ILE:HD12	42:CO:114:GLU:HB3	1.73	0.69
1:AA:403:C:H5'	4:AD:132:ILE:HG23	1.74	0.69
35:DG:95:ARG:HG2	35:DG:128:GLN:HB3	1.75	0.69
34:DF:80:ARG:HB3	34:DF:83:TYR:CZ	2.28	0.69
33:CE:130:LYS:HB2	33:CE:133:LEU:HD12	1.73	0.69
9:AI:116:VAL:HG21	10:AJ:62:ARG:HB2	1.75	0.68
1:AA:664:G:H22	1:AA:741:G:H1	1.39	0.68
31:CA:784:G:H5'	31:CA:785:G:OP1	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:CG:95:ARG:HG2	35:CG:128:GLN:HB3	1.76	0.68
31:CA:532:A:N1	31:CA:2020:A:H1'	2.08	0.68
31:CA:1394:U:H4'	31:CA:1603:A:H4'	1.76	0.68
31:CA:1936:A:H2	31:CA:1943:U:N3	1.90	0.68
31:CA:2428:G:H21	40:CM:60:ARG:HH21	1.40	0.68
45:DR:28:ARG:HD3	69:DR:310:HOH:O	1.94	0.68
12:AL:114:ARG:HB3	12:AL:119:VAL:HB	1.76	0.68
29:CC:17:VAL:HB	29:CC:204:VAL:HG13	1.75	0.68
39:DL:38:ILE:HD11	39:DL:112:PHE:HZ	1.58	0.68
55:DA:414:C:H2'	55:DA:415:A:C8	2.29	0.68
39:DL:2:ILE:HB	39:DL:33:ALA:HB3	1.76	0.67
1:BA:841:C:H3'	1:BA:842:U:C5'	2.24	0.67
33:CE:126:VAL:CG2	33:CE:133:LEU:HB3	2.24	0.67
29:DC:107:PRO:HD2	29:DC:110:LEU:HD22	1.76	0.67
54:DI:85:VAL:HG11	54:DI:91:ALA:HB3	1.75	0.67
6:AF:16:GLU:HG2	4:BD:193:ALA:HB2	1.77	0.67
41:DN:19:GLY:HA2	69:DB:338:HOH:O	1.92	0.67
35:CG:80:THR:HG23	35:CG:81:GLU:H	1.58	0.67
42:DO:53:THR:HA	42:DO:56:LYS:HD2	1.77	0.67
1:BA:715:A:H2'	1:BA:716:A:C8	2.30	0.67
55:DA:1028:A:N6	55:DA:1125:G:H2'	2.09	0.67
1:AA:715:A:H2'	1:AA:716:A:C8	2.29	0.67
1:BA:774:G:H21	57:BA:1642:PG4:H62	1.60	0.67
31:CA:910:A:H62	41:CN:12:MET:HA	1.57	0.67
49:CV:7:ARG:O	49:CV:25:VAL:HB	1.94	0.67
1:BA:1305:G:H21	1:BA:1332:A:H2	1.44	0.66
43:CP:18:LEU:HD23	43:CP:25:ARG:HD3	1.76	0.66
31:CA:2189:U:H2'	31:CA:2190:G:H8	1.60	0.66
31:CA:2394:C:H5''	40:CM:63:LYS:HE2	1.76	0.66
31:CA:1779:U:H5	31:CA:1784:A:N7	1.93	0.66
55:DA:1026:G:H2'	55:DA:1027:A:C8	2.31	0.66
39:CL:2:ILE:HB	39:CL:33:ALA:HB3	1.76	0.66
55:DA:2751:G:H2'	69:DA:4887:HOH:O	1.94	0.66
4:BD:85:ASN:HA	5:BE:102:GLY:CA	2.26	0.66
49:CV:82:ARG:HB2	49:CV:97:LYS:HG3	1.78	0.66
54:DI:132:TYR:H	54:DI:133:GLU:HB2	1.60	0.66
1:AA:1197:A:H3'	1:AA:1197:A:OP2	1.96	0.66
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.78	0.66
55:DA:74:A:N3	55:DA:74:A:H5''	2.11	0.66
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.77	0.66
43:DP:64:TYR:HB3	43:DP:67:ASN:HD22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:CP:64:TYR:HB3	43:CP:67:ASN:HD22	1.62	0.65
40:DM:63:LYS:HE2	55:DA:2394:C:H5''	1.78	0.65
55:DA:1002:G:H5'	61:DA:3201:PEG:H32	1.78	0.65
43:DP:51:ALA:HB3	43:DP:78:VAL:HG13	1.77	0.65
45:DR:94:ILE:HG21	46:DS:4:VAL:HG11	1.79	0.65
8:BH:87:LYS:HB2	8:BH:125:ILE:HD11	1.77	0.65
31:CA:2326:C:O2'	31:CA:2327:A:H8	1.80	0.65
48:CU:18:GLU:H	48:CU:18:GLU:CD	2.03	0.65
55:DA:1026:G:H2'	55:DA:1027:A:H8	1.62	0.65
4:BD:107:PHE:HB3	4:BD:145:ILE:HD11	1.79	0.65
31:CA:2366:A:H4'	51:CX:62:LYS:HE3	1.79	0.65
9:BI:116:VAL:HG21	10:BJ:62:ARG:HB2	1.77	0.65
55:DA:2255:G:H21	68:DA:3220:TRS:H12	1.62	0.65
47:CT:29:VAL:HG22	47:CT:51:LEU:HD11	1.79	0.64
2:AB:31:ILE:HG21	2:AB:39:HIS:CD2	2.30	0.64
32:DD:122:VAL:HG23	69:DD:411:HOH:O	1.97	0.64
42:CO:53:THR:HA	42:CO:56:LYS:HD2	1.78	0.64
43:CP:51:ALA:HB3	43:CP:78:VAL:HG13	1.80	0.64
55:DA:2127:G:H4'	55:DA:2128:G:OP1	1.96	0.64
12:BL:114:ARG:HB3	12:BL:119:VAL:HB	1.78	0.64
55:DA:2052:A:H3'	69:DA:3584:HOH:O	1.96	0.64
45:CR:94:ILE:HG21	46:CS:4:VAL:HG11	1.79	0.64
54:DI:64:VAL:HG22	54:DI:69:PHE:HB2	1.79	0.64
1:AA:1144:G:H21	1:AA:1146:A:H62	1.46	0.64
8:AH:87:LYS:HB2	8:AH:125:ILE:HD11	1.80	0.64
33:DE:3:LEU:HD12	33:DE:14:VAL:HG11	1.80	0.63
4:AD:107:PHE:HB3	4:AD:145:ILE:HD11	1.79	0.63
32:DD:186:LEU:HD21	44:DQ:4:ILE:HG21	1.81	0.63
44:DQ:31:TRP:CE2	44:DQ:40:LEU:HD21	2.34	0.63
55:DA:1778:U:H2'	55:DA:1784:A:N6	2.13	0.63
1:AA:1305:G:H21	1:AA:1332:A:H2	1.44	0.63
38:CK:117:ALA:HA	38:CK:120:ARG:HD2	1.81	0.63
36:CH:4:ILE:HD11	36:CH:44:ILE:HG22	1.80	0.63
1:AA:677:U:H3	1:AA:713:G:H22	1.45	0.63
7:BG:86:GLN:HG3	7:BG:144:MET:HE2	1.81	0.63
31:CA:1709:U:H2'	31:CA:1710:G:C8	2.34	0.63
40:DM:36:LYS:HE2	55:DA:807:U:OP1	1.98	0.63
1:BA:677:U:H3	1:BA:713:G:H22	1.43	0.63
1:BA:1063:C:H42	1:BA:1193:G:H1	1.47	0.63
29:DC:38:SER:HA	69:DA:5917:HOH:O	1.98	0.63
34:CF:36:LEU:HD21	34:CF:91:LEU:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:1975:G:H21	63:DA:3225:PGE:C2	2.07	0.63
3:BC:77:ILE:HA	3:BC:84:VAL:HG23	1.81	0.62
43:CP:31:THR:HG22	43:CP:34:HIS:H	1.62	0.62
43:DP:31:THR:HG22	43:DP:34:HIS:H	1.64	0.62
27:D0:39:GLU:HB2	27:D0:41:THR:HG23	1.80	0.62
55:DA:1965:C:OP1	55:DA:1966:A:H2'	1.99	0.62
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.34	0.62
24:C3:19:ARG:HD3	31:CA:125:A:OP2	1.99	0.62
27:C0:39:GLU:HB2	27:C0:41:THR:HG23	1.81	0.62
29:CC:17:VAL:HB	29:CC:204:VAL:HG12	1.78	0.62
29:CC:45:ASN:ND2	31:CA:1812:U:H1'	2.14	0.62
53:DZ:2:LYS:HB3	53:DZ:6:LEU:HD12	1.80	0.62
1:BA:1144:G:H21	1:BA:1146:A:H62	1.47	0.62
1:BA:1323:G:H2'	1:BA:1324:A:C8	2.34	0.62
31:CA:1827:U:H2'	31:CA:1828:G:O4'	2.00	0.62
18:AR:62:ALA:HB3	18:AR:68:LEU:HD12	1.82	0.62
31:CA:528:A:C8	31:CA:528:A:H3'	2.35	0.62
33:CE:3:LEU:HD12	33:CE:14:VAL:HG11	1.82	0.62
55:DA:588:U:H2'	55:DA:589:U:C6	2.34	0.62
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.82	0.62
22:D1:34:SER:OG	22:D1:36:GLU:HB2	2.00	0.62
54:DI:50:VAL:HG11	54:DI:92:ALA:HB2	1.80	0.62
31:CA:197:A:H2	31:CA:2434:A:H62	1.48	0.62
31:CA:571:U:H4'	31:CA:573:U:H5	1.64	0.62
1:BA:663:A:H5'	1:BA:836:G:OP1	1.98	0.62
55:DA:2162:G:H5''	55:DA:2171:A:H2'	1.82	0.62
1:AA:663:A:H5'	1:AA:836:G:OP1	1.99	0.61
31:CA:1707:G:H1	31:CA:1751:U:H3	1.47	0.61
31:CA:1931:U:H2'	31:CA:1932:A:H8	1.64	0.61
31:CA:2291:U:H2'	31:CA:2292:U:C6	2.35	0.61
1:BA:209:U:H4'	1:BA:210:C:OP2	2.00	0.61
11:BK:88:GLY:N	11:BK:114:THR:HG22	2.15	0.61
17:BQ:14:SER:HB3	17:BQ:22:VAL:HG12	1.81	0.61
18:BR:62:ALA:HB3	18:BR:68:LEU:HD12	1.82	0.61
31:CA:320:A:H4'	31:CA:322:A:N7	2.15	0.61
38:DK:117:ALA:HA	38:DK:120:ARG:HD2	1.81	0.61
41:DN:62:LYS:HD3	41:DN:64:TRP:CZ2	2.36	0.61
31:CA:1760:C:H2'	31:CA:1761:C:O4'	2.00	0.61
1:BA:1063:C:N4	1:BA:1193:G:H1	1.97	0.61
39:DL:113:MET:HE1	39:DL:116:ILE:HD11	1.81	0.61
45:DR:78:LYS:HA	69:DA:6376:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:209:U:H4'	1:AA:210:C:OP2	1.99	0.61
6:AF:102:MET:HE1	18:AR:24:LYS:HB3	1.80	0.61
31:CA:806:C:H2'	31:CA:807:U:C6	2.36	0.61
14:AN:66:GLN:HB2	69:AN:202:HOH:O	2.01	0.61
22:C1:43:ILE:HG22	22:C1:49:TYR:HB2	1.83	0.61
38:CK:110:PRO:O	38:CK:115:GLY:HA3	2.01	0.61
55:DA:1141:U:H4'	55:DA:1142:A:O4'	2.01	0.61
1:AA:1314:C:H41	19:AS:4:SER:HA	1.66	0.60
31:CA:1155:A:H5''	45:CR:55:ARG:HD3	1.81	0.60
42:DO:60:VAL:HB	69:DO:217:HOH:O	2.00	0.60
31:CA:588:U:H2'	31:CA:589:U:C6	2.36	0.60
50:DW:63:ILE:HD12	50:DW:72:VAL:HG21	1.83	0.60
54:DI:5:LEU:HA	54:DI:8:LYS:HB2	1.83	0.60
1:BA:562:U:H1'	12:BL:12:ARG:HD2	1.84	0.60
1:AA:707:U:H5''	11:AK:22:HIS:CD2	2.37	0.60
55:DA:1913:A:OP1	55:DA:1913:A:H4'	2.01	0.60
1:AA:1421:G:H3'	69:AA:1814:HOH:O	2.02	0.60
2:BB:163:VAL:HG11	2:BB:173:ILE:HD11	1.82	0.60
31:CA:1006:C:O4'	38:CK:30:THR:HG23	2.01	0.60
31:CA:2443:C:H2'	31:CA:2444:G:O4'	2.01	0.60
29:DC:45:ASN:ND2	55:DA:1812:U:H1'	2.15	0.60
37:CJ:19:ASN:H	37:CJ:20:PRO:HD2	1.67	0.60
1:BA:1289:A:H3'	1:BA:1290:G:H8	1.67	0.60
4:BD:58:LYS:HA	4:BD:200:ILE:HG12	1.84	0.60
31:CA:1709:U:H2'	31:CA:1710:G:H8	1.66	0.60
31:CA:2326:C:O2'	31:CA:2327:A:C8	2.55	0.60
54:DI:94:ARG:HG2	54:DI:127:ALA:HA	1.83	0.60
55:DA:2402:U:O2	55:DA:2402:U:H2'	2.01	0.60
26:D5:1:MET:HG2	69:D5:202:HOH:O	2.01	0.60
22:D1:9:THR:CG2	55:DA:2020:A:H5'	2.32	0.60
42:CO:73:ASN:HA	42:CO:76:VAL:HG22	1.84	0.60
41:DN:18[B]:ARG:HG3	28:DB:90:C:H5'	1.83	0.60
3:AC:151:VAL:HG12	3:AC:200:VAL:HG22	1.84	0.59
48:CU:69:ARG:HB2	48:CU:74:ILE:HG22	1.84	0.59
33:DE:189:THR:HG22	33:DE:192:ALA:H	1.66	0.59
32:DD:150[B]:MEQ:HG3	55:DA:2032:G:N3	2.17	0.59
43:CP:49:VAL:HG21	43:CP:82:ALA:HA	1.84	0.59
51:DX:56:ASP:OD1	55:DA:2364:C:H4'	2.02	0.59
31:CA:1974:C:H3'	69:CA:3320:HOH:O	2.03	0.59
45:DR:50:ARG:O	45:DR:54:LYS:HD2	2.02	0.59
2:AB:163:VAL:HG11	2:AB:173:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:42:LEU:HB2	10:AJ:71:LEU:HB3	1.83	0.59
4:AD:58:LYS:HA	4:AD:200:ILE:HG12	1.84	0.59
1:BA:33:A:H2'	1:BA:34:C:C6	2.37	0.59
45:CR:58:ARG:NH1	45:CR:62:ILE:HD11	2.17	0.59
1:AA:1289:A:H3'	1:AA:1290:G:H8	1.67	0.59
32:DD:30:GLU:HB3	69:DD:457:HOH:O	2.03	0.59
55:DA:1424:G:H21	63:DA:3214:PGE:H32	1.67	0.59
1:BA:967:5MC:HN42	1:BA:1197:A:H61	1.48	0.59
55:DA:2783:U:H2'	55:DA:2784:U:H6	1.67	0.59
2:BB:31:ILE:HG21	2:BB:39:HIS:CD2	2.31	0.59
29:CC:160:THR:HG22	29:CC:177:ARG:HG2	1.84	0.59
31:CA:135:U:H3	31:CA:144:A:H61	1.51	0.59
37:DJ:19:ASN:H	37:DJ:20:PRO:HD2	1.67	0.59
1:AA:562:U:H1'	12:AL:12:ARG:HD2	1.83	0.59
50:CW:63:ILE:HD12	50:CW:72:VAL:HG21	1.85	0.59
3:BC:113:ALA:O	3:BC:200:VAL:HG11	2.03	0.59
54:DI:67:THR:CG2	54:DI:68:PRO:HA	2.29	0.59
6:AF:92:THR:HG22	6:AF:93:LYS:HE2	1.85	0.58
31:CA:320:A:H2'	33:CE:131:THR:HG21	1.83	0.58
33:CE:189:THR:HG22	33:CE:192:ALA:H	1.67	0.58
55:DA:45:G:H5''	55:DA:46:G:H5'	1.85	0.58
55:DA:1105:U:H2'	55:DA:1106:G:H8	1.68	0.58
14:AN:10:GLU:HG3	14:AN:63:ARG:HD2	1.86	0.58
31:CA:1770:G:H4'	31:CA:1938:A:OP1	2.03	0.58
36:DH:4:ILE:HD11	36:DH:44:ILE:HG22	1.84	0.58
55:DA:2771:C:H2'	55:DA:2772:C:H6	1.68	0.58
31:CA:29:U:H2'	31:CA:30:G:C8	2.37	0.58
31:CA:729:G:H2'	31:CA:1775:U:H1'	1.85	0.58
55:DA:1853:A:N1	55:DA:2087:G:H1'	2.19	0.58
31:CA:2728:U:HO2'	31:CA:2729:G:H8	1.49	0.58
29:DC:227:PRO:HA	29:DC:233:GLY:HA2	1.85	0.58
51:DX:21:LEU:HD11	51:DX:41[A]:ARG:HE	1.68	0.58
31:CA:142:A:H1'	48:CU:1:MET:HB3	1.85	0.58
13:BM:114:LYS:HB3	13:BM:115:PRO:HD3	1.85	0.58
33:CE:28:VAL:O	33:CE:32:VAL:HG23	2.04	0.58
41:CN:62:LYS:HD3	41:CN:64:TRP:CZ2	2.37	0.58
53:DZ:41:HIS:CD2	55:DA:96:C:H4'	2.38	0.58
1:AA:54:C:H2'	1:AA:352:C:H41	1.69	0.58
1:AA:73:C:HO2'	1:AA:74:A:H8	1.51	0.58
3:AC:40:ARG:HG2	3:AC:55:ILE:HG21	1.85	0.58
1:BA:54:C:H2'	1:BA:352:C:H41	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:D3:29:GLN:HG2	61:D3:102:PEG:H21	1.86	0.58
29:CC:227:PRO:HA	29:CC:233:GLY:HA2	1.85	0.58
31:CA:45:G:H5''	31:CA:46:G:H5'	1.85	0.58
31:CA:2469:A:H4'	41:CN:55:ARG:HD3	1.86	0.58
32:DD:152:PRO:HG3	32:DD:156:PHE:CZ	2.39	0.58
40:DM:32:GLY:HA2	55:DA:1190:G:H5''	1.84	0.58
42:DO:73:ASN:HA	42:DO:76:VAL:HG22	1.85	0.58
55:DA:2557:G:H2'	55:DA:2558:C:C6	2.39	0.58
12:BL:80:ILE:HD12	12:BL:97:THR:HG22	1.86	0.58
31:CA:586:A:H5'	33:CE:84:THR:HG21	1.84	0.58
31:CA:846:U:H1'	31:CA:847:U:H5	1.68	0.58
31:CA:1105:U:H2'	31:CA:1106:G:H8	1.68	0.58
31:CA:1796:U:H2'	31:CA:1797:G:C8	2.39	0.58
31:CA:1812:U:H2'	31:CA:1813:G:C8	2.38	0.58
31:CA:1936:A:H61	31:CA:1963:U:H3	1.50	0.58
33:CE:108:ILE:HG22	40:CM:1:MET:SD	2.43	0.57
31:CA:2106:U:H2'	31:CA:2107:G:H8	1.70	0.57
41:CN:30:SER:H	41:CN:106:ASP:HB3	1.68	0.57
47:DT:75:PHE:CZ	65:DA:3185:1PE:H142	2.39	0.57
55:DA:1417:C:H5'	55:DA:1588:G:H1'	1.86	0.57
11:BK:85:MET:HE3	11:BK:113:VAL:HG11	1.85	0.57
17:BQ:68:SER:OG	17:BQ:71:LYS:HB3	2.03	0.57
1:BA:73:C:HO2'	1:BA:74:A:H8	1.50	0.57
31:CA:582:A:H2'	31:CA:583:G:C8	2.39	0.57
31:CA:1311:G:H21	31:CA:1603:A:N6	1.95	0.57
41:DN:30:SER:H	41:DN:106:ASP:HB3	1.69	0.57
43:DP:49:VAL:HG21	43:DP:82:ALA:HA	1.86	0.57
55:DA:944:C:H2'	69:DA:6066:HOH:O	2.04	0.57
1:AA:79:G:H22	1:AA:90:C:H42	1.52	0.57
37:CJ:14:ALA:HB3	37:CJ:17:MET:HB2	1.87	0.57
51:DX:40:GLN:HG3	51:DX:42:GLY:O	2.05	0.57
55:DA:2063:C:O2	55:DA:2450:A:N1	2.37	0.57
22:C1:7:LYS:HD2	31:CA:1262:A:C2	2.39	0.57
19:BS:15:LEU:HD13	19:BS:33:THR:HG21	1.85	0.57
50:CW:20:LEU:HD21	50:CW:41:GLU:HB2	1.85	0.57
37:DJ:14:ALA:HB3	37:DJ:17:MET:HB2	1.86	0.57
1:AA:1063:C:H2'	1:AA:1064:G:H8	1.64	0.57
14:AN:21:PHE:HA	14:AN:25:ALA:HB3	1.86	0.57
22:C1:9:THR:CG2	31:CA:2020:A:H5'	2.34	0.57
50:DW:20:LEU:HD21	50:DW:41:GLU:HB2	1.85	0.57
5:BE:104:GLY:HA3	5:BE:122:ASN:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:35:G:H2'	31:CA:36:G:O4'	2.04	0.57
31:CA:96:C:H4'	53:CZ:41:HIS:CD2	2.40	0.57
34:CF:36:LEU:HD21	34:CF:91:LEU:CD1	2.35	0.57
38:DK:110:PRO:O	38:DK:115:GLY:HA3	2.04	0.57
43:DP:48:LEU:HD12	43:DP:87:ILE:HD11	1.87	0.57
55:DA:2728:U:HO2'	55:DA:2729:G:H8	1.51	0.57
55:DA:2783:U:H2'	55:DA:2784:U:C6	2.39	0.57
14:BN:10:GLU:HG3	14:BN:63:ARG:HD2	1.87	0.57
19:AS:15:LEU:HD13	19:AS:33:THR:HG21	1.86	0.57
30:CD:152:PRO:HG3	30:CD:156:PHE:CZ	2.39	0.57
31:CA:528:A:C2	31:CA:2043:C:H4'	2.40	0.57
31:CA:1203:U:H1'	40:CM:4:ASN:HB3	1.87	0.57
55:DA:1885:A:H2'	55:DA:1886:U:O4'	2.04	0.57
10:BJ:42:LEU:HB2	10:BJ:71:LEU:HB3	1.86	0.56
45:DR:31:VAL:HG13	55:DA:580:U:O3'	2.05	0.56
1:AA:33:A:H2'	1:AA:34:C:C6	2.39	0.56
22:D1:4:GLN:HA	55:DA:2615:U:C2	2.41	0.56
14:AN:13:ARG:HB3	14:AN:60:GLN:HG2	1.87	0.56
31:CA:2491:U:HO2'	31:CA:2492:U:H5	1.54	0.56
29:DC:158:ALA:HB1	29:DC:197:ASN:O	2.04	0.56
34:CF:24:SER:H	34:CF:27:GLN:NE2	2.03	0.56
45:DR:16:LYS:O	45:DR:20:GLN:HG3	2.05	0.56
45:DR:22:LYS:HE3	55:DA:20:C:OP1	2.06	0.56
47:DT:17:VAL:HG11	47:DT:103:ILE:HG12	1.88	0.56
54:DI:69:PHE:HB3	54:DI:72:LEU:HD12	1.86	0.56
55:DA:135:U:H3	55:DA:144:A:H61	1.51	0.56
55:DA:1327:A:H2'	55:DA:1328:A:O4'	2.06	0.56
28:CB:114:C:H1'	43:CP:47:VAL:HG11	1.86	0.56
39:CL:38:ILE:HD11	39:CL:112:PHE:CZ	2.38	0.56
47:CT:17:VAL:HG11	47:CT:103:ILE:HG12	1.86	0.56
3:BC:40:ARG:HG2	3:BC:55:ILE:HG21	1.87	0.56
29:CC:105:LEU:HD12	29:CC:105:LEU:H	1.70	0.56
31:CA:677:A:O2'	31:CA:2071:A:H5'	2.05	0.56
55:DA:320:A:H4'	55:DA:322:A:N7	2.20	0.56
1:BA:576:C:H3'	1:BA:577:G:H5''	1.86	0.56
1:BA:840:C:H2'	1:BA:841:C:O4'	2.06	0.56
35:DG:86:LYS:HG2	35:DG:132:VAL:HG22	1.87	0.56
43:DP:16:ARG:HD3	69:DP:310:HOH:O	2.06	0.56
5:AE:97:GLN:HE21	5:AE:124:LEU:HD13	1.71	0.56
31:CA:2636:C:H2'	31:CA:2637:U:C6	2.41	0.56
32:DD:48:ILE:HG23	32:DD:84:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:CE:46:GLN:HB3	33:CE:83:VAL:HG21	1.87	0.56
35:CG:90:VAL:HG21	35:CG:163:ARG:HE	1.71	0.56
35:DG:90:VAL:HG21	35:DG:163:ARG:HE	1.70	0.56
1:BA:79:G:H22	1:BA:90:C:H42	1.54	0.56
14:BN:13:ARG:HB3	14:BN:60:GLN:HG2	1.88	0.56
31:CA:459:U:H2'	31:CA:460:A:H8	1.69	0.56
31:CA:2114:A:N6	31:CA:2119:A:H62	2.03	0.56
31:CA:2728:U:O2'	31:CA:2729:G:H5''	2.05	0.56
34:DF:138:PHE:HE2	34:DF:152:LEU:HD21	1.71	0.56
35:DG:26:ILE:HG22	35:DG:79:VAL:HG21	1.88	0.56
16:BP:20:VAL:CG1	16:BP:32:PHE:HB2	2.36	0.56
24:D3:7:PRO:HG2	55:DA:1309:G:H4'	1.87	0.56
52:CY:37:ARG:HG2	52:CY:48:THR:HG22	1.87	0.56
1:AA:1350:A:H2	7:AG:34:GLY:HA3	1.70	0.55
2:AB:188:ASP:HB2	2:AB:204:ASP:OD2	2.06	0.55
10:BJ:5:ARG:HG2	10:BJ:79:PRO:HG3	1.87	0.55
32:DD:121:THR:HB	32:DD:127:PHE:CD2	2.42	0.55
55:DA:683:U:H2'	55:DA:684:G:H5''	1.88	0.55
55:DA:760:G:H2'	55:DA:761:A:O4'	2.06	0.55
2:AB:129:LEU:HD13	2:AB:134:ALA:HB2	1.87	0.55
2:BB:188:ASP:HB2	2:BB:204:ASP:OD2	2.07	0.55
31:CA:659:G:H4'	33:CE:95:LYS:HD3	1.89	0.55
31:CA:744:U:H4'	31:CA:1658:C:H4'	1.88	0.55
31:CA:822:G:O6	31:CA:943:A:H2	1.89	0.55
36:CH:27:ARG:HH12	36:CH:38:PRO:HG3	1.71	0.55
55:DA:2636:C:H2'	55:DA:2637:U:C6	2.41	0.55
1:AA:674:G:H3'	69:AA:1714:HOH:O	2.05	0.55
31:CA:540:C:H2'	31:CA:541:A:C8	2.41	0.55
35:DG:67:THR:HG23	55:DA:2747:G:O2'	2.06	0.55
1:AA:1012:A:H61	1:AA:1017:U:H3	1.55	0.55
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	1.88	0.55
11:BK:25:ALA:HA	11:BK:30:THR:HG22	1.89	0.55
31:CA:528:A:H3'	31:CA:528:A:H8	1.71	0.55
29:DC:17:VAL:HB	29:DC:204:VAL:HB	1.88	0.55
50:DW:39:ALA:HB3	69:DW:105:HOH:O	2.06	0.55
55:DA:912:C:O2'	55:DA:913:U:H5'	2.07	0.55
2:BB:129:LEU:HD13	2:BB:134:ALA:HB2	1.86	0.55
4:BD:197:GLU:HA	4:BD:200:ILE:HD12	1.89	0.55
31:CA:792:A:H1'	31:CA:2072:C:O2'	2.06	0.55
55:DA:2771:C:H2'	55:DA:2772:C:C6	2.41	0.55
12:AL:3:THR:HB	12:AL:6:GLN:HB2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1350:A:H2	7:BG:34:GLY:HA3	1.70	0.55
34:DF:60:ILE:HG12	34:DF:138:PHE:CD2	2.42	0.55
40:DM:60:ARG:NH2	55:DA:2428:G:N2	2.51	0.55
55:DA:1952:A:H4'	69:DA:5281:HOH:O	2.07	0.55
1:BA:1001:C:H2'	1:BA:1002:G:H8	1.72	0.55
16:BP:2:VAL:CG2	16:BP:33:ILE:HD11	2.36	0.55
31:CA:321:U:H5''	33:CE:131:THR:HG23	1.89	0.55
31:CA:373:U:H2'	31:CA:374:A:H8	1.71	0.55
37:DJ:30:GLN:HE22	55:DA:1095:A:H61	1.54	0.55
39:DL:38:ILE:HD11	39:DL:112:PHE:CZ	2.42	0.55
55:DA:1532:A:H5''	55:DA:1532:A:H8	1.72	0.55
4:BD:27:ALA:HB3	4:BD:30:THR:HG23	1.88	0.55
39:DL:113:MET:CE	39:DL:116:ILE:HD11	2.37	0.55
41:DN:75:GLU:HB2	41:DN:90:GLU:HG3	1.89	0.55
49:DV:52:LEU:HD13	49:DV:54:GLN:HE21	1.72	0.55
5:AE:57:PRO:O	5:AE:60:ILE:HG13	2.07	0.54
31:CA:373:U:H2'	31:CA:374:A:C8	2.41	0.54
31:CA:1509:A:O2'	31:CA:1510:G:H8	1.90	0.54
31:CA:2557:G:H2'	31:CA:2558:C:C6	2.42	0.54
33:CE:149:ILE:HG12	33:CE:188:MET:HE3	1.89	0.54
1:AA:76:G:H1	1:AA:93:U:H3	1.55	0.54
1:AA:269:C:H2'	1:AA:270:A:C8	2.42	0.54
31:CA:2064:C:H2'	31:CA:2065:C:C6	2.43	0.54
33:CE:149:ILE:HG23	33:CE:188:MET:HG2	1.90	0.54
34:CF:24:SER:H	34:CF:27:GLN:HE21	1.56	0.54
40:CM:77:ILE:CD1	40:CM:108:ALA:HB1	2.36	0.54
55:DA:20:C:H2'	55:DA:21:A:H8	1.72	0.54
55:DA:784:G:H5'	55:DA:785:G:OP1	2.08	0.54
1:BA:751:U:H4'	15:BO:24:SER:HA	1.89	0.54
14:BN:21:PHE:HA	14:BN:25:ALA:HB3	1.87	0.54
31:CA:2425:A:H4'	31:CA:2426:A:O5'	2.07	0.54
35:DG:24:ILE:HG21	35:DG:72:LEU:HD21	1.88	0.54
55:DA:1509:A:O2'	55:DA:1510:G:H8	1.89	0.54
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.73	0.54
2:AB:111:ILE:HD12	2:AB:152:LYS:HA	1.89	0.54
12:BL:79:VAL:HG12	12:BL:102:LEU:HD23	1.90	0.54
31:CA:2105:U:H2'	31:CA:2106:U:C6	2.42	0.54
31:CA:2267:A:H5''	31:CA:2268:A:H5'	1.90	0.54
32:DD:99:GLU:HG2	32:DD:182:ALA:HB2	1.87	0.54
52:CY:4:VAL:HG13	52:CY:11:ARG:HG3	1.89	0.54
55:DA:414:C:H2'	55:DA:415:A:H8	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:121:THR:HA	3:AC:189:ALA:HB2	1.88	0.54
45:CR:16:LYS:O	45:CR:20:GLN:HG3	2.08	0.54
34:DF:65:PRO:HA	34:DF:89:VAL:HG23	1.89	0.54
30:CD:99:GLU:HG2	30:CD:182:ALA:HB2	1.89	0.54
55:DA:2887[B]:A:H2'	55:DA:2887[B]:A:N3	2.22	0.54
1:BA:209:U:H2'	1:BA:209:U:O2	2.08	0.54
1:BA:1012:A:H61	1:BA:1017:U:H3	1.54	0.54
1:BA:76:G:H1	1:BA:93:U:H3	1.54	0.54
42:CO:28:LEU:HD23	42:CO:48:VAL:HG11	1.90	0.54
34:DF:8:TYR:HB2	34:DF:173:PHE:HZ	1.73	0.54
42:DO:28:LEU:HD23	42:DO:48:VAL:HG11	1.88	0.54
1:BA:591:U:H2'	1:BA:592:G:C8	2.42	0.54
3:BC:121:THR:HA	3:BC:189:ALA:HB2	1.89	0.54
31:CA:1936:A:N6	31:CA:1963:U:N3	2.54	0.54
35:CG:86:LYS:HG2	35:CG:132:VAL:HG22	1.89	0.54
46:CS:49:ILE:HD12	46:CS:52:PRO:HA	1.90	0.54
6:AF:42:TRP:HB2	6:AF:59:TYR:HB2	1.90	0.54
11:AK:25:ALA:HA	11:AK:30:THR:HG22	1.89	0.54
31:CA:1796:U:H2'	31:CA:1797:G:H8	1.73	0.54
39:CL:58:LEU:HD11	39:CL:86:LEU:HD13	1.89	0.54
46:DS:20:VAL:HG22	69:DS:339:HOH:O	2.07	0.54
55:DA:2767:C:H2'	55:DA:2768:U:H6	1.73	0.54
4:AD:197:GLU:HA	4:AD:200:ILE:HD12	1.89	0.53
13:BM:33:ILE:HG23	13:BM:59:GLU:HB3	1.90	0.53
27:D0:3[B]:LYS:O	27:D0:40:ASP:HB2	2.08	0.53
31:CA:241:A:N1	31:CA:255:A:H5''	2.23	0.53
44:DQ:94:LYS:CE	55:DA:1754:A:C8	2.92	0.53
53:DZ:39:GLN:HB3	53:DZ:41:HIS:CE1	2.44	0.53
1:AA:1411:C:H2'	1:AA:1412:C:C6	2.44	0.53
5:BE:57:PRO:O	5:BE:60:ILE:HG13	2.08	0.53
31:CA:685:A:H5''	31:CA:774:G:O6	2.08	0.53
31:CA:699:A:H2'	31:CA:700:G:O4'	2.09	0.53
33:DE:84:THR:HG21	55:DA:586:A:H5'	1.90	0.53
13:AM:90:ARG:HD3	13:AM:97:VAL:HA	1.91	0.53
1:BA:1411:C:H2'	1:BA:1412:C:C6	2.43	0.53
23:D2:9:ILE:HD13	23:D2:51:GLU:HG3	1.88	0.53
55:DA:1812:U:H2'	55:DA:1813:G:C8	2.44	0.53
30:CD:121:THR:HB	30:CD:127:PHE:CD2	2.43	0.53
34:CF:8:TYR:HB2	34:CF:173:PHE:HZ	1.73	0.53
44:CQ:4:ILE:HD12	44:CQ:4:ILE:H	1.73	0.53
55:DA:985:C:H2'	55:DA:986:C:H6	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:260:G:H2'	1:AA:261:U:C6	2.44	0.53
1:AA:591:U:H2'	1:AA:592:G:C8	2.43	0.53
1:BA:490:C:H2'	1:BA:491:G:H8	1.74	0.53
31:CA:2598:A:H2'	31:CA:2599:G:O4'	2.09	0.53
33:CE:149:ILE:HG12	33:CE:188:MET:HG2	1.91	0.53
55:DA:2233:U:H2'	55:DA:2234:G:C8	2.44	0.53
31:CA:1532:A:H5''	31:CA:1532:A:H8	1.73	0.53
46:CS:46:GLU:H	46:CS:46:GLU:CD	2.16	0.53
47:CT:4:ILE:HG12	47:CT:106:VAL:HG22	1.91	0.53
47:DT:93:ALA:HB2	55:DA:1614:A:C2	2.44	0.53
1:AA:1373:G:H5'	7:AG:36:LYS:HB2	1.91	0.53
22:D1:43:ILE:HG22	22:D1:49:TYR:HB2	1.91	0.53
31:CA:1564:C:H2'	31:CA:1565:C:C6	2.44	0.53
43:DP:79:ALA:HB2	43:DP:110:ALA:HA	1.91	0.53
55:DA:693:A:H2'	55:DA:694:U:O4'	2.08	0.53
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.73	0.53
1:BA:269:C:H2'	1:BA:270:A:C8	2.43	0.53
31:CA:1308:A:H2'	31:CA:1309:G:O4'	2.09	0.53
31:CA:2106:U:H2'	31:CA:2107:G:C8	2.44	0.53
55:DA:2105:U:O4	55:DA:2184:A:H2	1.92	0.53
1:BA:260:G:H2'	1:BA:261:U:C6	2.44	0.53
22:D1:40:ARG:NH2	55:DA:2884[B]:U:H2'	2.24	0.53
22:D1:44:THR:HG23	22:D1:48:TYR:O	2.09	0.53
31:CA:2747:G:O2'	35:CG:67:THR:HG23	2.09	0.53
39:DL:58:LEU:HD11	39:DL:86:LEU:HD13	1.91	0.53
43:DP:27:VAL:HG21	43:DP:40:ILE:HD12	1.91	0.53
55:DA:623:C:H2'	55:DA:624:C:C6	2.44	0.53
55:DA:2128:G:H1	55:DA:2160:C:H42	1.57	0.53
55:DA:2800:A:C2	55:DA:2895:G:H1'	2.43	0.53
1:AA:751:U:H4'	15:AO:24:SER:HA	1.90	0.53
12:AL:79:VAL:HG12	12:AL:102:LEU:HD23	1.90	0.53
31:CA:457:A:N1	31:CA:470:A:H5''	2.24	0.53
31:CA:780:G:O5'	31:CA:780:G:H8	1.90	0.53
31:CA:2189:U:H2'	31:CA:2190:G:C8	2.43	0.53
31:CA:2261:C:C2	31:CA:2280:G:N2	2.77	0.53
55:DA:1166:G:N2	55:DA:1184:U:H1'	2.24	0.53
13:BM:90:ARG:HH21	13:BM:95:LEU:HB3	1.74	0.52
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	1.92	0.52
55:DA:1722:A:N6	55:DA:1738:G:H1'	2.24	0.52
55:DA:1753:G:N2	55:DA:1755:A:H3'	2.25	0.52
26:C5:4:ARG:HB2	31:CA:2466:C:OP1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DC:43:ARG:HG3	29:DC:49:ILE:HA	1.91	0.52
35:CG:24:ILE:HG21	35:CG:72:LEU:HD21	1.90	0.52
52:CY:10:LYS:HE3	52:CY:54:LYS:HG2	1.90	0.52
40:DM:60:ARG:HD3	55:DA:2428:G:H21	1.74	0.52
50:DW:72:VAL:HG12	50:DW:93:ARG:HA	1.91	0.52
55:DA:795:C:H1'	69:DA:4280:HOH:O	2.08	0.52
31:CA:2064:C:H1'	31:CA:2450:A:C6	2.45	0.52
32:DD:134:HIS:HE1	69:DA:5373:HOH:O	1.92	0.52
41:CN:75:GLU:HB2	41:CN:90:GLU:HG3	1.91	0.52
44:DQ:4:ILE:H	44:DQ:4:ILE:HD12	1.74	0.52
55:DA:14:A:H5''	55:DA:15:G:OP2	2.09	0.52
55:DA:612:G:H4'	55:DA:613:A:C2	2.43	0.52
31:CA:1105:U:H2'	31:CA:1106:G:C8	2.44	0.52
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.45	0.52
1:AA:1381:U:H1'	7:AG:78:ARG:HE	1.75	0.52
4:AD:27:ALA:HB3	4:AD:30:THR:HG23	1.90	0.52
6:BF:42:TRP:HB2	6:BF:59:TYR:HB2	1.92	0.52
30:CD:129:THR:HG22	30:CD:141:ARG:HA	1.91	0.52
31:CA:581:C:H2'	31:CA:582:A:C8	2.44	0.52
53:CZ:39:GLN:HB3	53:CZ:41:HIS:CE1	2.44	0.52
55:DA:2183:A:H2'	55:DA:2184:A:C8	2.44	0.52
55:DA:2408:U:H2'	55:DA:2409:G:C8	2.45	0.52
11:AK:85:MET:HE3	11:AK:113:VAL:HG11	1.91	0.52
1:BA:1001:C:H2'	1:BA:1002:G:C8	2.45	0.52
19:BS:52:HIS:HD2	19:BS:54:GLY:H	1.58	0.52
31:CA:587:C:O2'	40:CM:19:LEU:HD13	2.09	0.52
31:CA:861:A:H2'	31:CA:862:G:O4'	2.09	0.52
43:CP:79:ALA:HB2	43:CP:110:ALA:HA	1.90	0.52
55:DA:2037:A:H2'	55:DA:2038:G:C8	2.44	0.52
55:DA:2703:C:H2'	55:DA:2704:C:H6	1.74	0.52
13:BM:90:ARG:HD3	13:BM:97:VAL:HA	1.91	0.52
31:CA:568:U:C1'	31:CA:2030:6MZ:H9C1	2.31	0.52
37:CJ:11:LEU:HD22	37:CJ:24:VAL:HG23	1.92	0.52
44:DQ:101:ARG:HD2	69:DQ:322:HOH:O	2.10	0.52
44:DQ:106:LYS:HA	44:DQ:109:ARG:HD3	1.92	0.52
1:BA:1373:G:H5'	7:BG:36:LYS:HB2	1.92	0.52
31:CA:2888:C:H2'	31:CA:2889:C:C6	2.45	0.52
40:DM:57:LEU:HA	40:DM:60:ARG:HE	1.75	0.52
1:AA:718:A:C8	11:AK:118:HIS:HB3	2.45	0.52
16:AP:2:VAL:CG2	16:AP:33:ILE:HD11	2.40	0.52
13:BM:11:ASP:HA	13:BM:45:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:CD:121:THR:HG21	30:CD:143:PRO:HB3	1.92	0.52
31:CA:568:U:H1'	31:CA:2030:6MZ:C9	2.29	0.52
31:CA:1248:G:O2'	45:CR:3:ARG:HA	2.10	0.52
43:DP:11:ALA:HB2	43:DP:96:GLY:N	2.25	0.52
55:DA:1105:U:H2'	55:DA:1106:G:C8	2.45	0.52
13:AM:33:ILE:HG23	13:AM:59:GLU:HB3	1.91	0.52
33:DE:46:GLN:HB3	33:DE:83:VAL:HG21	1.92	0.52
38:DK:21:THR:HG23	38:DK:61:LYS:HB3	1.92	0.52
55:DA:2097:A:H5''	55:DA:2097:A:H8	1.76	0.52
55:DA:2402:U:H2'	55:DA:2403:C:H5'	1.91	0.52
27:C0:9:GLN:HB3	27:C0:32:ILE:HA	1.91	0.51
1:BA:403:C:H2'	1:BA:404:G:O4'	2.10	0.51
31:CA:1722:A:N6	31:CA:1738:G:H1'	2.24	0.51
31:CA:2262:U:OP2	51:CX:16:SER:HB2	2.10	0.51
35:DG:175:LYS:HG3	55:DA:2529:G:H4'	1.92	0.51
47:DT:4:ILE:HG12	47:DT:106:VAL:HG22	1.92	0.51
1:BA:212:G:H2'	1:BA:213:G:C8	2.44	0.51
1:BA:967:5MC:N4	1:BA:1197:A:H61	2.08	0.51
40:CM:19:LEU:HD23	40:CM:31:GLY:O	2.11	0.51
40:CM:57:LEU:HA	40:CM:60:ARG:HE	1.75	0.51
42:CO:103:ARG:HD3	42:CO:110:MET:SD	2.50	0.51
55:DA:20:C:H2'	55:DA:21:A:C8	2.44	0.51
1:AA:412:A:H3'	1:AA:413:G:H5'	1.92	0.51
6:AF:70:VAL:HA	6:AF:73:GLU:HG2	1.92	0.51
1:BA:1458:G:H5''	20:BT:26:SER:HB3	1.93	0.51
37:DJ:11:LEU:HD22	37:DJ:24:VAL:HG23	1.92	0.51
42:DO:82:GLU:O	42:DO:85:PRO:HD2	2.10	0.51
55:DA:582:A:H2'	55:DA:583:G:C8	2.46	0.51
55:DA:2563:U:H1'	55:DA:2566:A:N6	2.25	0.51
1:AA:1001:C:H2'	1:AA:1002:G:C8	2.45	0.51
1:BA:12:U:H4'	1:BA:526:C:H4'	1.93	0.51
32:DD:150[A]:MEQ:HE3	55:DA:2032:G:C8	2.45	0.51
35:CG:26:ILE:HG22	35:CG:79:VAL:HG21	1.91	0.51
38:CK:21:THR:HG23	38:CK:61:LYS:HB3	1.93	0.51
25:D4:57:LEU:HD11	55:DA:834:G:H5'	1.93	0.51
42:CO:82:GLU:O	42:CO:85:PRO:HD2	2.10	0.51
39:DL:101:GLY:O	39:DL:120:PRO:HD2	2.11	0.51
1:AA:619:U:C2	4:AD:132:ILE:HD11	2.46	0.51
6:AF:17:GLN:HG3	4:BD:189:SER:HB2	1.92	0.51
1:BA:429:U:H5''	4:BD:9:LEU:HD12	1.92	0.51
4:BD:170:TRP:CD2	4:BD:186:PRO:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:DS:65:ALA:HB3	46:DS:95:ASP:HB2	1.92	0.51
52:DY:10:LYS:HE3	52:DY:54:LYS:HG2	1.92	0.51
8:AH:51:VAL:HG13	8:AH:59:LEU:HD12	1.93	0.51
23:D2:11:LEU:HD21	23:D2:34:LEU:HD23	1.92	0.51
46:CS:65:ALA:HB3	46:CS:95:ASP:HB2	1.93	0.51
38:DK:42:ALA:O	45:DR:64:ARG:HD3	2.10	0.51
40:DM:57:LEU:HB2	40:DM:60:ARG:HH11	1.75	0.51
1:AA:77:A:H2'	1:AA:78:A:C8	2.46	0.51
1:AA:1317:C:OP1	14:AN:57:PRO:HD2	2.11	0.51
5:AE:82:GLN:HG2	5:AE:149:SER:HA	1.93	0.51
16:BP:2:VAL:HG21	16:BP:33:ILE:HD11	1.93	0.51
45:CR:9:ILE:HG13	45:CR:10:ALA:N	2.26	0.51
33:DE:32:VAL:HG21	40:DM:6:LEU:HD13	1.93	0.51
35:DG:42:GLU:HA	35:DG:55:ARG:HH21	1.75	0.51
45:DR:64:ARG:HD2	69:DR:323:HOH:O	2.09	0.51
46:DS:24:LYS:HE3	69:DS:312:HOH:O	2.10	0.51
10:AJ:53:ILE:HG13	14:AN:85:ARG:HD2	1.92	0.51
31:CA:1353:A:H2'	31:CA:1354:A:C8	2.46	0.51
31:CA:1380:G:H2'	31:CA:1381:G:H8	1.75	0.51
31:CA:2408:U:H2'	31:CA:2409:G:C8	2.46	0.51
35:CG:42:GLU:HA	35:CG:55:ARG:HH21	1.75	0.51
36:DH:3:VAL:HG12	36:DH:38:PRO:HA	1.93	0.51
54:DI:27:VAL:HG22	54:DI:82:ILE:HG22	1.93	0.51
54:DI:132:TYR:N	54:DI:133:GLU:HB2	2.24	0.51
55:DA:296:U:H2'	55:DA:297:G:C8	2.46	0.51
55:DA:1720:U:H2'	55:DA:1721:G:O4'	2.11	0.51
11:AK:23:ILE:HG21	11:AK:96:THR:HG21	1.93	0.51
1:BA:579:A:H2'	1:BA:580:C:C6	2.46	0.51
1:BA:643:C:H5'	8:BH:32:LEU:HD13	1.93	0.51
23:D2:19:HIS:HE1	23:D2:21:TYR:CE1	2.29	0.51
30:CD:48:ILE:HG23	30:CD:84:LEU:HD11	1.91	0.51
31:CA:1991:U:H6	31:CA:1991:U:H5''	1.76	0.51
32:DD:35:THR:HG22	32:DD:73:VAL:HG21	1.93	0.51
33:CE:148:ILE:HB	33:CE:169:VAL:HG22	1.93	0.51
44:CQ:106:LYS:HA	44:CQ:109:ARG:HD3	1.93	0.51
54:DI:26:VAL:HB	54:DI:83:ALA:HB3	1.93	0.51
55:DA:2788:C:H2'	55:DA:2789:C:C6	2.46	0.51
4:AD:192:SER:HB3	4:AD:195:ILE:HD12	1.93	0.50
5:AE:107:ALA:CB	5:AE:125:ALA:HB3	2.40	0.50
8:AH:102:ALA:HB3	8:AH:113:ASP:HB3	1.93	0.50
22:C1:3:VAL:HG21	31:CA:2016:U:H1'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C1:7:LYS:HD2	31:CA:1262:A:H2	1.76	0.50
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.76	0.50
34:CF:65:PRO:HA	34:CF:89:VAL:HG23	1.91	0.50
41:DN:3:GLN:HG3	41:DN:92:TRP:CD1	2.46	0.50
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.93	0.50
22:C1:25:VAL:HG13	22:C1:26:THR:H	1.76	0.50
23:C2:11:LEU:HD21	23:C2:34:LEU:HD23	1.92	0.50
1:BA:17:U:H2'	1:BA:18:C:C6	2.47	0.50
1:BA:1197:A:H3'	1:BA:1198:G:C5'	2.42	0.50
9:BI:84:THR:HG21	9:BI:103:PHE:HB2	1.93	0.50
31:CA:1170:C:H42	31:CA:1178:C:H41	1.58	0.50
32:DD:121:THR:HG21	32:DD:143:PRO:HB3	1.92	0.50
35:CG:90:VAL:HG21	35:CG:163:ARG:NE	2.27	0.50
36:CH:3:VAL:HG12	36:CH:38:PRO:HA	1.91	0.50
35:DG:90:VAL:HG21	35:DG:163:ARG:NE	2.26	0.50
55:DA:118:A:N3	55:DA:178:G:H1'	2.25	0.50
55:DA:2126:A:H61	55:DA:2163:A:H5'	1.75	0.50
4:AD:170:TRP:CD2	4:AD:186:PRO:HB3	2.47	0.50
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.77	0.50
22:C1:19:HIS:HE1	31:CA:2624:G:H1'	1.75	0.50
10:BJ:53:ILE:HG13	14:BN:85:ARG:HD2	1.93	0.50
31:CA:296:U:H2'	31:CA:297:G:C8	2.46	0.50
31:CA:526:A:N6	31:CA:2626:C:H4'	2.26	0.50
31:CA:2339:C:H2'	31:CA:2340:A:C8	2.47	0.50
35:CG:80:THR:HG23	35:CG:81:GLU:N	2.24	0.50
55:DA:284:U:H2'	55:DA:285:G:H8	1.75	0.50
55:DA:2339:C:H2'	55:DA:2340:A:C8	2.46	0.50
19:AS:52:HIS:HD2	19:AS:54:GLY:H	1.59	0.50
11:BK:23:ILE:HG21	11:BK:96:THR:HG21	1.94	0.50
14:BN:53:ARG:HH21	19:BS:37:ARG:HH22	1.60	0.50
31:CA:806:C:H2'	31:CA:807:U:H6	1.76	0.50
29:DC:154:LEU:HD13	29:DC:176:LEU:HD21	1.94	0.50
32:DD:99:GLU:CG	32:DD:182:ALA:HB2	2.41	0.50
50:CW:64:VAL:HG22	50:CW:69:GLU:HG2	1.94	0.50
28:DB:1:U:H2'	28:DB:2:G:C8	2.46	0.50
28:DB:111:U:H2'	28:DB:112:G:C8	2.45	0.50
55:DA:31:C:O3'	55:DA:1238:G:H5''	2.12	0.50
55:DA:2133:G:H2'	55:DA:2157:G:H1	1.76	0.50
1:AA:1061:G:H1	1:AA:1195:C:H41	1.59	0.50
1:BA:407:U:H2'	1:BA:408:A:C8	2.47	0.50
1:BA:1194:U:H5'	5:BE:27:GLY:CA	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BS:52:HIS:CD2	19:BS:54:GLY:H	2.30	0.50
31:CA:644:A:H2'	31:CA:645:C:O4'	2.12	0.50
31:CA:1720:U:H2'	31:CA:1721:G:O4'	2.11	0.50
52:CY:12:PRO:HB3	52:CY:30:LEU:HD23	1.93	0.50
34:DF:103:LEU:HG	34:DF:108:VAL:HG23	1.94	0.50
43:DP:33:ARG:HD2	69:DB:319:HOH:O	2.10	0.50
52:DY:27:ARG:HD3	69:DY:101:HOH:O	2.10	0.50
55:DA:610:C:H5'	69:DA:3623:HOH:O	2.10	0.50
23:C2:33:LYS:HA	23:C2:52:ALA:HB3	1.92	0.50
39:CL:101:GLY:O	39:CL:120:PRO:HD2	2.11	0.50
47:CT:59:GLU:HA	47:CT:64:ALA:HA	1.93	0.50
41:DN:100:LYS:HD3	69:DN:320:HOH:O	2.10	0.50
55:DA:581:C:H2'	55:DA:582:A:C8	2.46	0.50
55:DA:825:A:OP1	59:DA:3223:PUT:H12	2.12	0.50
1:AA:212:G:H2'	1:AA:213:G:C8	2.46	0.50
1:AA:490:C:H2'	1:AA:491:G:H8	1.75	0.50
7:AG:111:ARG:HB3	7:AG:119:ARG:HG2	1.94	0.50
20:AT:57:ILE:HD12	20:AT:60:ARG:HE	1.76	0.50
5:BE:82:GLN:HG2	5:BE:149:SER:HA	1.93	0.50
12:BL:30:LYS:O	12:BL:82:ILE:HG22	2.11	0.50
20:BT:57:ILE:HD12	20:BT:60:ARG:HE	1.77	0.50
31:CA:2845:U:H2'	31:CA:2846:G:O4'	2.12	0.50
53:CZ:39:GLN:HB3	53:CZ:41:HIS:HE1	1.77	0.50
49:DV:52:LEU:C	49:DV:54:GLN:H	2.18	0.50
55:DA:1181:U:H2'	55:DA:1182:G:C8	2.46	0.50
55:DA:2547:A:H2'	55:DA:2548:U:C6	2.47	0.50
23:C2:19:HIS:HE1	23:C2:21:TYR:CE1	2.29	0.50
25:C4:54:ASP:HB3	40:CM:57:LEU:HD22	1.93	0.50
1:BA:1381:U:H1'	7:BG:78:ARG:HE	1.76	0.50
8:BH:102:ALA:HB3	8:BH:113:ASP:HB3	1.93	0.50
50:CW:72:VAL:HG12	50:CW:93:ARG:HA	1.92	0.50
40:DM:53:GLY:HA3	55:DA:826:U:O2'	2.12	0.50
53:DZ:39:GLN:HB3	53:DZ:41:HIS:HE1	1.77	0.50
55:DA:1975:G:N2	63:DA:3225:PGE:H22	2.19	0.50
1:AA:1232:U:H5''	9:AI:126:GLN:HB3	1.94	0.50
1:AA:1458:G:H5''	20:AT:26:SER:HB3	1.93	0.50
2:AB:41:ILE:HD13	2:AB:202:GLY:HA2	1.93	0.50
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.94	0.50
69:D0:216:HOH:O	55:DA:927:A:H1'	2.11	0.50
31:CA:284:U:H2'	31:CA:285:G:H8	1.77	0.50
31:CA:1181:U:H2'	31:CA:1182:G:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2095:A:H5''	31:CA:2095:A:H8	1.77	0.50
34:DF:106:ILE:HD12	34:DF:139:PRO:HG2	1.94	0.50
54:DI:111:ALA:O	54:DI:118:ILE:HB	2.11	0.50
1:AA:429:U:H5''	4:AD:9:LEU:HD12	1.94	0.49
26:C5:8:LYS:HE3	31:CA:1031:G:H5''	1.93	0.49
1:BA:1317:C:OP1	14:BN:57:PRO:HD2	2.12	0.49
29:CC:162:VAL:HG22	29:CC:176:LEU:HA	1.94	0.49
31:CA:1783:A:N1	31:CA:2587:A:H2'	2.26	0.49
46:DS:73:LYS:NZ	58:DS:203:MPD:H53	2.26	0.49
55:DA:881:G:H1	55:DA:895:U:H3	1.60	0.49
55:DA:2133:G:H21	55:DA:2158:A:N6	2.09	0.49
1:BA:21:G:H2'	1:BA:22:G:C8	2.47	0.49
6:BF:3:HIS:HA	6:BF:65:GLU:HA	1.94	0.49
7:BG:70:ARG:HG2	7:BG:96:ARG:HG2	1.94	0.49
7:BG:111:ARG:HB3	7:BG:119:ARG:HG2	1.93	0.49
29:CC:160:THR:O	29:CC:195:VAL:HG13	2.12	0.49
30:CD:99:GLU:CG	30:CD:182:ALA:HB2	2.42	0.49
31:CA:396:G:H1'	52:CY:29:PHE:CD2	2.47	0.49
32:DD:13:ARG:HD3	32:DD:21:SER:OG	2.12	0.49
34:CF:8:TYR:HA	34:CF:12:VAL:HB	1.94	0.49
46:DS:58:VAL:HG12	46:DS:102:SER:HB2	1.94	0.49
1:AA:403:C:H2'	1:AA:404:G:O4'	2.12	0.49
1:BA:745:G:H2'	1:BA:746:A:C8	2.47	0.49
2:BB:100:MET:HA	2:BB:107:VAL:HG21	1.93	0.49
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	1.95	0.49
28:CB:111:U:H2'	28:CB:112:G:C8	2.47	0.49
31:CA:17:G:H4'	45:CR:25:TYR:HE2	1.76	0.49
31:CA:281:C:H2'	31:CA:282:A:C8	2.47	0.49
45:CR:112:LYS:HD3	46:CS:48:LYS:HE2	1.94	0.49
49:DV:17:LYS:HE3	49:DV:40:ASN:HA	1.94	0.49
55:DA:839:U:H2'	55:DA:840:C:C6	2.48	0.49
55:DA:1425:G:H2'	55:DA:1426:G:C8	2.47	0.49
2:AB:100:MET:HA	2:AB:107:VAL:HG21	1.93	0.49
3:AC:14:ILE:HG21	3:AC:178:LEU:HB3	1.93	0.49
29:CC:210:ALA:HA	29:CC:213:TRP:NE1	2.26	0.49
31:CA:2788:C:H2'	31:CA:2789:C:C6	2.46	0.49
29:DC:162:VAL:HG22	29:DC:176:LEU:HA	1.94	0.49
33:DE:148:ILE:HB	33:DE:169:VAL:HG22	1.93	0.49
50:DW:64:VAL:HG22	50:DW:69:GLU:HG2	1.94	0.49
55:DA:137:U:H3	55:DA:142:A:H61	1.60	0.49
55:DA:648:G:H5''	69:DA:6963:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2577:A:H5''	55:DA:2578:G:H5'	1.93	0.49
1:AA:745:G:H2'	1:AA:746:A:C8	2.48	0.49
12:AL:30:LYS:O	12:AL:82:ILE:HG22	2.11	0.49
30:CD:35:THR:HG22	30:CD:73:VAL:HG21	1.94	0.49
31:CA:83:A:H2	31:CA:103:A:N7	2.09	0.49
31:CA:695:G:H4'	31:CA:1380:G:H5'	1.94	0.49
29:DC:75:PRO:HG2	29:DC:97:LYS:HD3	1.95	0.49
36:CH:49:ALA:O	36:CH:53:GLU:HB2	2.13	0.49
38:CK:42:ALA:O	45:CR:64:ARG:HD3	2.12	0.49
43:CP:11:ALA:HB2	43:CP:96:GLY:N	2.27	0.49
55:DA:1436:G:N2	55:DA:1557:C:C2	2.81	0.49
1:AA:86:G:H21	1:AA:87:C:H41	1.61	0.49
7:AG:70:ARG:HG2	7:AG:96:ARG:HG2	1.94	0.49
13:BM:22:ILE:HB	13:BM:25:VAL:CG1	2.43	0.49
17:BQ:17:MET:HB3	17:BQ:20:SER:HB3	1.93	0.49
37:DJ:103:ARG:HA	37:DJ:106:LEU:HD12	1.95	0.49
45:DR:84:LYS:HG3	62:DA:3002:EDO:H22	1.94	0.49
55:DA:2258:C:H4'	55:DA:2259:U:OP2	2.12	0.49
1:AA:643:C:H5'	8:AH:32:LEU:HD13	1.95	0.49
1:BA:1096:C:H2'	1:BA:1097:C:C6	2.48	0.49
6:BF:70:VAL:HA	6:BF:73:GLU:HG2	1.92	0.49
9:BI:31:ASN:HD21	9:BI:67:VAL:H	1.61	0.49
40:CM:57:LEU:HB2	40:CM:60:ARG:HH11	1.77	0.49
1:AA:17:U:H2'	1:AA:18:C:C6	2.48	0.49
1:AA:202:G:O2'	1:AA:468:A:H8	1.96	0.49
1:AA:1358:U:H3	1:AA:1363:A:H62	1.59	0.49
5:AE:132:ASN:OD1	5:AE:134:ILE:HG22	2.13	0.49
1:BA:77:A:H2'	1:BA:78:A:C8	2.47	0.49
1:BA:202:G:O2'	1:BA:468:A:H8	1.96	0.49
7:BG:130:ASN:HA	7:BG:135:VAL:HG11	1.95	0.49
25:D4:8:ARG:HD2	55:DA:245:G:O6	2.13	0.49
29:CC:154:LEU:HD13	29:CC:176:LEU:HD21	1.95	0.49
31:CA:1299:G:H2'	31:CA:1639:C:N4	2.27	0.49
31:CA:1380:G:H1'	31:CA:1569:A:N6	2.28	0.49
34:DF:8:TYR:HA	34:DF:12:VAL:HB	1.94	0.49
55:DA:388:G:N7	55:DA:390:U:H2'	2.27	0.49
55:DA:821:A:H1'	69:DA:3397:HOH:O	2.13	0.49
1:AA:719:C:O2'	18:AR:38:LYS:HB3	2.13	0.49
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.42	0.49
7:AG:130:ASN:HA	7:AG:135:VAL:HG11	1.95	0.49
26:C5:17:VAL:CG1	26:C5:26:ILE:HD12	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:41:ILE:HD13	2:BB:202:GLY:HA2	1.94	0.49
5:BE:97:GLN:HE21	5:BE:124:LEU:HD13	1.76	0.49
31:CA:247:G:N7	31:CA:249:C:C2	2.81	0.49
34:DF:158:THR:HG23	34:DF:160:ALA:N	2.25	0.49
46:DS:1:MET:HA	46:DS:42:ALA:O	2.13	0.49
52:DY:18:ARG:NH2	52:DY:24:ALA:HB2	2.27	0.49
55:DA:740:C:H5''	55:DA:1784:A:OP1	2.12	0.49
16:BP:4:ILE:HG12	16:BP:21:VAL:HG22	1.94	0.49
26:D5:16:ILE:CD1	26:D5:25:VAL:HG22	2.43	0.49
32:DD:146:ILE:HD12	32:DD:155:VAL:HG21	1.95	0.49
35:CG:80:THR:CG2	35:CG:81:GLU:H	2.24	0.49
41:CN:3:GLN:HG3	41:CN:92:TRP:CD1	2.47	0.49
38:DK:47:HIS:HE1	69:DA:4185:HOH:O	1.96	0.49
1:AA:1096:C:H2'	1:AA:1097:C:C6	2.47	0.48
1:AA:1239:A:H62	1:AA:1299:A:H62	1.61	0.48
31:CA:1324:G:H1'	31:CA:1616:A:N6	2.28	0.48
55:DA:118:A:C8	55:DA:119:A:C8	3.01	0.48
55:DA:284:U:H2'	55:DA:285:G:C8	2.48	0.48
55:DA:1014:A:H1'	69:DA:5823:HOH:O	2.12	0.48
55:DA:2343:U:H2'	55:DA:2344:U:C6	2.48	0.48
55:DA:2427:C:H5''	55:DA:2428:G:OP1	2.12	0.48
9:AI:84:THR:HG21	9:AI:103:PHE:HB2	1.94	0.48
22:C1:42:HIS:CD2	42:CO:101:GLY:H	2.31	0.48
1:BA:1216:A:H5''	14:BN:5:SER:HB3	1.96	0.48
4:BD:147:GLU:HA	4:BD:150:LYS:HD2	1.95	0.48
31:CA:881:G:H1	31:CA:895:U:H3	1.60	0.48
31:CA:1783:A:H5'	31:CA:2608:G:H4'	1.95	0.48
29:DC:162:VAL:CG1	29:DC:174:LEU:HD22	2.43	0.48
34:CF:103:LEU:HG	34:CF:108:VAL:HG23	1.95	0.48
52:DY:12:PRO:HB3	52:DY:30:LEU:HD23	1.94	0.48
55:DA:195:A:H61	55:DA:198:C:H3'	1.77	0.48
6:AF:74:LEU:O	6:AF:77:THR:HG22	2.13	0.48
16:AP:2:VAL:HG21	16:AP:33:ILE:HD11	1.95	0.48
19:AS:52:HIS:CD2	19:AS:54:GLY:H	2.31	0.48
1:BA:429:U:H1'	1:BA:430:A:H5''	1.95	0.48
1:BA:1391:U:H2'	1:BA:1392:G:C8	2.49	0.48
31:CA:2800:A:C2	31:CA:2895:G:H1'	2.48	0.48
44:DQ:6:LYS:O	44:DQ:10:GLN:HG2	2.14	0.48
14:AN:53:ARG:HH21	19:AS:37:ARG:HH22	1.61	0.48
1:BA:392:C:H2'	1:BA:393:A:C8	2.49	0.48
1:BA:1152:A:H5'	10:BJ:15:HIS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:279:A:H61	31:CA:361:G:H1'	1.79	0.48
31:CA:1056:G:H4'	31:CA:1086:A:C8	2.48	0.48
31:CA:1636:U:H2'	31:CA:1637:A:C8	2.47	0.48
31:CA:2350:C:H2'	31:CA:2351:G:O4'	2.13	0.48
31:CA:2393:U:H5''	40:CM:62:PRO:HB3	1.95	0.48
34:CF:33:LYS:HG3	34:CF:157:THR:HB	1.95	0.48
37:CJ:86:ILE:HG21	37:CJ:98:VAL:HB	1.96	0.48
43:CP:27:VAL:HG21	43:CP:40:ILE:HD12	1.94	0.48
41:DN:123:LYS:HB3	55:DA:2484:G:H1'	1.95	0.48
28:DB:81:G:H1'	69:DB:339:HOH:O	2.13	0.48
26:C5:16:ILE:CD1	26:C5:25:VAL:HG22	2.43	0.48
19:BS:32:ARG:HE	19:BS:57:HIS:CD2	2.31	0.48
31:CA:1093:G:H1'	31:CA:1099:G:N2	2.27	0.48
31:CA:2030:6MZ:N3	31:CA:2499:C:H5''	2.28	0.48
1:AA:407:U:H2'	1:AA:408:A:C8	2.49	0.48
1:AA:601:G:H2'	1:AA:602:A:C8	2.49	0.48
1:AA:1216:A:H5''	14:AN:5:SER:HB3	1.95	0.48
1:BA:719:C:O2'	18:BR:38:LYS:HB3	2.13	0.48
1:BA:972:C:H4'	10:BJ:59:LYS:HG2	1.96	0.48
7:BG:72:THR:HG22	7:BG:96:ARG:HH12	1.77	0.48
31:CA:785:G:O2'	31:CA:1779:U:H5''	2.13	0.48
31:CA:818:G:H5'	31:CA:839:U:OP1	2.14	0.48
33:CE:126:VAL:HG21	33:CE:133:LEU:HB3	1.95	0.48
44:DQ:29:LYS:HB3	44:DQ:40:LEU:HD12	1.96	0.48
55:DA:1622:G:H1'	69:DA:6193:HOH:O	2.14	0.48
55:DA:1935:G:H1'	55:DA:1964:G:N2	2.28	0.48
55:DA:2018:G:H2'	55:DA:2019:A:C8	2.49	0.48
1:AA:429:U:H1'	1:AA:430:A:H5''	1.95	0.48
1:AA:1152:A:H5'	10:AJ:15:HIS:HB2	1.96	0.48
1:AA:1239:A:H62	1:AA:1299:A:N6	2.12	0.48
1:AA:1298:U:H3	7:AG:114:LYS:HA	1.79	0.48
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.49	0.48
4:AD:73:ARG:HG3	4:AD:204:TYR:CE1	2.48	0.48
1:BA:1232:U:H5''	9:BI:126:GLN:HB3	1.96	0.48
31:CA:1310:G:H1'	31:CA:1611:C:H5''	1.96	0.48
31:CA:2271:G:OP1	51:CX:18:ALA:HB1	2.13	0.48
42:DO:85:PRO:HA	42:DO:88:ALA:HB2	1.95	0.48
55:DA:281:C:H2'	55:DA:282:A:C8	2.48	0.48
9:AI:31:ASN:HD21	9:AI:67:VAL:H	1.61	0.48
1:BA:601:G:H2'	1:BA:602:A:C8	2.49	0.48
5:BE:18:VAL:HG11	5:BE:56:VAL:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:763:G:H2'	31:CA:765:C:OP2	2.12	0.48
31:CA:2680:U:H2'	31:CA:2681:C:C6	2.48	0.48
33:CE:181:ILE:HG12	40:CM:1:MET:HE3	1.95	0.48
38:DK:30:THR:HG22	55:DA:1006:C:O4'	2.14	0.48
43:DP:1:MET:HB3	43:DP:6:ALA:HB2	1.95	0.48
54:DI:58:THR:HB	55:DA:1046:A:H4'	1.95	0.48
55:DA:2887[A]:A:H2'	55:DA:2888[A]:C:C6	2.49	0.48
1:AA:412:A:H3'	1:AA:413:G:C5'	2.43	0.48
1:AA:662:U:H2'	1:AA:663:A:C8	2.49	0.48
12:AL:53:CYS:HB3	12:AL:67:ILE:HD11	1.96	0.48
31:CA:364:C:H2'	31:CA:365:U:C6	2.48	0.48
31:CA:1141:U:H4'	31:CA:1142:A:O4'	2.14	0.48
31:CA:1405:U:H2'	31:CA:1406:U:C6	2.48	0.48
31:CA:2364:C:H4'	51:CX:56:ASP:OD1	2.14	0.48
31:CA:2849:U:H4'	31:CA:2868:A:C2	2.48	0.48
37:CJ:103:ARG:HA	37:CJ:106:LEU:HD12	1.95	0.48
55:DA:296:U:H2'	55:DA:297:G:H8	1.79	0.48
55:DA:1101:U:H2'	55:DA:1102:C:C6	2.49	0.48
1:AA:1057:G:O3'	3:AC:197:GLY:HA3	2.14	0.48
13:BM:106:ALA:HB3	13:BM:110:LYS:HE3	1.96	0.48
31:CA:137:U:H3	31:CA:142:A:H61	1.62	0.48
34:CF:106:ILE:HD12	34:CF:139:PRO:HG2	1.95	0.48
37:DJ:86:ILE:HG21	37:DJ:98:VAL:HB	1.95	0.48
55:DA:1428:C:C5	55:DA:1569:A:H5''	2.49	0.48
55:DA:1441:G:H2'	55:DA:1442:U:C6	2.49	0.48
24:D3:2:LYS:HE2	55:DA:687:C:H5''	1.96	0.47
27:D0:12:SER:HB3	55:DA:988:A:P	2.54	0.47
31:CA:831:G:H8	31:CA:831:G:O5'	1.96	0.47
31:CA:1776:G:N2	31:CA:1789:A:H1'	2.29	0.47
35:CG:138:LYS:HA	35:CG:141:ILE:HG22	1.96	0.47
38:DK:58:ASN:HA	38:DK:126:ALA:O	2.14	0.47
45:DR:104:VAL:HG11	46:DS:45:GLU:HA	1.96	0.47
55:DA:142:A:H2'	55:DA:143:C:C6	2.49	0.47
55:DA:622:G:H5''	55:DA:622:G:H8	1.79	0.47
1:BA:649:A:H2'	1:BA:650:G:O4'	2.14	0.47
1:BA:662:U:H2'	1:BA:663:A:C8	2.49	0.47
1:BA:714:G:H2'	1:BA:715:A:C8	2.49	0.47
1:BA:1239:A:H62	1:BA:1299:A:N6	2.13	0.47
13:BM:86:TYR:CZ	13:BM:90:ARG:HD2	2.49	0.47
31:CA:528:A:C8	31:CA:528:A:C3'	2.97	0.47
31:CA:942:G:H4'	31:CA:1190:G:H5'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1101:U:H2'	31:CA:1102:C:C6	2.49	0.47
31:CA:1999:C:H5''	31:CA:2723:C:O2'	2.15	0.47
49:CV:82:ARG:CB	49:CV:97:LYS:HG3	2.43	0.47
51:CX:37:ILE:HG21	51:CX:80:ILE:HG21	1.96	0.47
55:DA:21:A:H2'	55:DA:22:C:O4'	2.14	0.47
55:DA:364:C:H2'	55:DA:365:U:C6	2.49	0.47
1:AA:620:C:C2	4:AD:132:ILE:HG21	2.50	0.47
19:AS:51:VAL:HG21	19:AS:71:LEU:HB3	1.97	0.47
3:BC:14:ILE:HG21	3:BC:178:LEU:HB3	1.96	0.47
5:BE:13:GLU:HB3	5:BE:39:VAL:HG12	1.96	0.47
5:BE:90:THR:HG22	5:BE:91:GLY:H	1.79	0.47
31:CA:1028:A:N6	31:CA:1125:G:H2'	2.29	0.47
46:CS:78:ARG:HB2	46:CS:83:TYR:HD1	1.79	0.47
44:DQ:95:ALA:HB3	69:DA:4560:HOH:O	2.13	0.47
55:DA:1746:A:H2'	55:DA:1747:U:C6	2.50	0.47
55:DA:2543:G:H2'	55:DA:2544:G:C8	2.49	0.47
6:AF:6:ILE:HG13	6:AF:89:VAL:HG23	1.95	0.47
4:BD:192:SER:HB3	4:BD:195:ILE:HD12	1.96	0.47
5:BE:157:ARG:HG2	5:BE:158:GLY:N	2.29	0.47
19:BS:30:PRO:HB2	19:BS:50:ALA:HB2	1.97	0.47
31:CA:980:A:C4	31:CA:1136:G:O4'	2.68	0.47
29:DC:21:ASN:HB3	29:DC:24:LEU:HG	1.97	0.47
38:CK:58:ASN:HA	38:CK:126:ALA:O	2.15	0.47
49:CV:74:ASN:HD22	49:CV:77:THR:H	1.61	0.47
55:DA:1796:U:H2'	55:DA:1797:G:H8	1.78	0.47
1:AA:714:G:H2'	1:AA:715:A:C8	2.49	0.47
1:BA:1053:G:N7	1:BA:1200:C:H5''	2.30	0.47
1:BA:1239:A:H62	1:BA:1299:A:H62	1.61	0.47
9:BI:12:ARG:HG3	9:BI:107:ASP:HB3	1.96	0.47
31:CA:1998:A:H2'	31:CA:1999:C:O4'	2.14	0.47
48:DU:58:VAL:HG22	48:DU:85:VAL:HG22	1.96	0.47
28:DB:18:G:H1	28:DB:65:U:H3	1.62	0.47
31:CA:688:U:H2'	31:CA:689:A:H8	1.80	0.47
31:CA:1441:G:H2'	31:CA:1442:U:C6	2.50	0.47
44:DQ:31:TRP:CD2	44:DQ:40:LEU:HD21	2.49	0.47
1:AA:392:C:H2'	1:AA:393:A:C8	2.49	0.47
13:AM:86:TYR:CZ	13:AM:90:ARG:HD2	2.50	0.47
17:AQ:68:SER:OG	17:AQ:71:LYS:HB2	2.14	0.47
1:BA:429:U:C5'	4:BD:9:LEU:HD12	2.45	0.47
29:CC:147:LYS:HB2	29:CC:150:LYS:HD2	1.96	0.47
30:CD:150:GLN:NE2	31:CA:2032:G:H1'	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:142:A:H2'	31:CA:143:C:C6	2.50	0.47
31:CA:460:A:H2'	31:CA:461:C:O4'	2.15	0.47
31:CA:736:C:O5'	31:CA:736:C:H6	1.98	0.47
31:CA:747:5MU:O2	31:CA:2014:A:H1'	2.15	0.47
31:CA:787:C:H5''	31:CA:788:A:H5'	1.97	0.47
31:CA:987:C:H2'	31:CA:988:A:O4'	2.14	0.47
31:CA:1775:U:H2'	31:CA:1776:G:O4'	2.14	0.47
31:CA:2189:U:O2'	31:CA:2190:G:H5'	2.15	0.47
31:CA:2190:G:H2'	31:CA:2191:A:H8	1.78	0.47
31:CA:2520:C:H2'	31:CA:2521:C:H6	1.79	0.47
38:DK:9:GLU:HG3	69:DA:5367:HOH:O	2.15	0.47
40:DM:62:PRO:HB3	55:DA:2393:U:H5''	1.96	0.47
42:DO:56:LYS:HE3	42:DO:94:TYR:OH	2.14	0.47
54:DI:93:ALA:O	54:DI:97:LYS:HG3	2.14	0.47
55:DA:553:G:H2'	55:DA:554:U:O4'	2.14	0.47
55:DA:1069:A:H5'	55:DA:1070:A:H8	1.80	0.47
55:DA:1590:A:H2'	55:DA:1591:A:C8	2.50	0.47
55:DA:2869:G:H2'	55:DA:2870:C:O4'	2.15	0.47
1:AA:649:A:H2'	1:AA:650:G:O4'	2.14	0.47
1:AA:1061:G:H1	1:AA:1195:C:N4	2.13	0.47
4:AD:147:GLU:HA	4:AD:150:LYS:HD2	1.96	0.47
5:AE:13:GLU:HB3	5:AE:39:VAL:HG12	1.96	0.47
5:AE:90:THR:HG22	5:AE:91:GLY:H	1.80	0.47
1:BA:1069:C:O2'	1:BA:1192:C:H1'	2.15	0.47
1:BA:1463:U:H2'	1:BA:1464:U:C6	2.50	0.47
31:CA:25:U:H2'	31:CA:26:G:O4'	2.15	0.47
31:CA:296:U:H2'	31:CA:297:G:H8	1.80	0.47
31:CA:1428:C:C5	31:CA:1569:A:H5''	2.49	0.47
32:DD:150[A]:MEQ:OE1	55:DA:2032:G:H1'	2.15	0.47
35:CG:24:ILE:HD12	35:CG:72:LEU:HD11	1.97	0.47
44:DQ:6:LYS:HG3	61:DQ:201:PEG:H41	1.97	0.47
55:DA:2723:C:H2'	55:DA:2724:U:O4'	2.15	0.47
1:BA:1512:U:H2'	1:BA:1513:A:C8	2.50	0.47
7:BG:47:LEU:HD22	7:BG:58:GLU:HG2	1.96	0.47
31:CA:279:A:N6	31:CA:361:G:H1'	2.29	0.47
31:CA:1343:G:H2'	31:CA:1344:U:C6	2.49	0.47
31:CA:2271:G:H2'	31:CA:2272:U:C6	2.50	0.47
43:DP:100:HIS:CD2	28:DB:48:U:H4'	2.50	0.47
55:DA:1180:U:H6	55:DA:1180:U:H5''	1.80	0.47
55:DA:1182:G:H2'	55:DA:1183:U:O4'	2.15	0.47
55:DA:1278:C:H2'	55:DA:1279:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:1641:A:H2'	55:DA:1642:G:O4'	2.15	0.47
1:AA:392:C:H2'	1:AA:393:A:H8	1.80	0.47
1:AA:1053:G:N7	1:AA:1200:C:H5''	2.30	0.47
13:AM:85:CYS:HB3	19:AS:74:PHE:CE1	2.49	0.47
1:BA:784:A:H4'	31:CA:1837:C:OP1	2.14	0.47
30:CD:25:THR:HG21	30:CD:193:VAL:HG22	1.97	0.47
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.50	0.47
40:DM:81:ASP:HA	40:DM:84:LYS:HD2	1.97	0.47
46:DS:73:LYS:HZ2	58:DS:203:MPD:H53	1.80	0.47
55:DA:279:A:N6	55:DA:361:G:H1'	2.30	0.47
1:AA:620:C:H2'	1:AA:621:A:O4'	2.15	0.46
5:BE:106:ILE:HG13	5:BE:123:VAL:O	2.15	0.46
31:CA:571:U:H1'	31:CA:573:U:C6	2.50	0.46
31:CA:2313:C:H5''	34:CF:88:LYS:HD3	1.98	0.46
34:CF:36:LEU:HB2	34:CF:57:LEU:HD21	1.97	0.46
42:CO:54:LEU:HD23	42:CO:66:ALA:HB2	1.97	0.46
42:CO:72:ASP:OD2	42:CO:75:ILE:HG12	2.15	0.46
45:CR:58:ARG:HH11	45:CR:62:ILE:HD11	1.78	0.46
51:DX:37:ILE:HG21	51:DX:80:ILE:HG21	1.96	0.46
55:DA:2026:U:H2'	55:DA:2027:G:O4'	2.15	0.46
1:BA:532:A:H61	3:BC:193:TYR:HD2	1.62	0.46
5:BE:105:ILE:HA	5:BE:123:VAL:HG23	1.97	0.46
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.97	0.46
31:CA:284:U:H2'	31:CA:285:G:C8	2.50	0.46
31:CA:372:G:H5''	52:CY:61:LYS:HD3	1.97	0.46
31:CA:1641:A:H2'	31:CA:1642:G:O4'	2.16	0.46
31:CA:1813:G:H2'	31:CA:1814:G:O4'	2.15	0.46
29:DC:147:LYS:HB2	29:DC:150:LYS:HD2	1.97	0.46
42:DO:72:ASP:OD2	42:DO:75:ILE:HG12	2.15	0.46
43:DP:41:ALA:HB2	43:DP:48:LEU:HD23	1.97	0.46
49:DV:14:LEU:HD11	49:DV:71:ALA:HB2	1.97	0.46
55:DA:697:G:H2'	55:DA:698:C:C6	2.50	0.46
55:DA:1682:G:H3'	69:DA:4329:HOH:O	2.15	0.46
55:DA:2377:A:H2'	55:DA:2378:A:C8	2.50	0.46
1:BA:735:C:H5'	18:BR:60:LYS:HD3	1.97	0.46
1:BA:1057:G:O3'	3:BC:197:GLY:HA3	2.15	0.46
11:BK:111:THR:HG23	21:BU:3:VAL:HG22	1.96	0.46
31:CA:392:U:H2'	31:CA:393:C:H6	1.79	0.46
31:CA:1809:A:H2'	31:CA:1810:A:C8	2.50	0.46
38:DK:35:ARG:HB3	38:DK:54:ILE:HD11	1.97	0.46
46:DS:37:GLU:HB3	46:DS:53:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:857:C:H2'	1:AA:858:G:O4'	2.15	0.46
1:AA:1463:U:H2'	1:AA:1464:U:C6	2.51	0.46
7:AG:47:LEU:HD22	7:AG:58:GLU:HG2	1.98	0.46
10:AJ:5:ARG:HE	10:AJ:77:VAL:HG22	1.81	0.46
24:C3:24:THR:HG23	24:C3:27:GLY:HA3	1.97	0.46
1:BA:59:A:H5''	1:BA:387:U:H5''	1.97	0.46
1:BA:1026:G:H1	1:BA:1035:A:H2	1.62	0.46
1:BA:1298:U:H3	7:BG:114:LYS:HA	1.79	0.46
31:CA:569:U:H5''	31:CA:821:A:C2	2.50	0.46
31:CA:1754:A:H8	31:CA:1754:A:O5'	1.98	0.46
47:DT:17:VAL:HA	47:DT:43:ALA:HB1	1.96	0.46
55:DA:136:G:H1	55:DA:143:C:H42	1.62	0.46
55:DA:352:A:H5''	55:DA:352:A:H8	1.80	0.46
55:DA:747:5MU:O2	55:DA:2014:A:H1'	2.16	0.46
55:DA:1424:G:H2'	55:DA:1425:G:O4'	2.15	0.46
55:DA:2402:U:C2'	55:DA:2403:C:H5'	2.45	0.46
1:AA:34:C:H2'	1:AA:35:G:C8	2.50	0.46
1:AA:1141:C:O2'	1:AA:1142:G:H8	1.99	0.46
16:AP:54:LEU:HA	16:AP:57:ILE:HD12	1.97	0.46
19:AS:30:PRO:HB2	19:AS:50:ALA:HB2	1.98	0.46
1:BA:1194:U:C5'	5:BE:27:GLY:HA2	2.45	0.46
6:BF:16:GLU:O	6:BF:19:PRO:HD2	2.15	0.46
16:BP:4:ILE:HD13	16:BP:57:ILE:HG23	1.97	0.46
19:BS:51:VAL:HG21	19:BS:71:LEU:HB3	1.98	0.46
31:CA:1430:G:H2'	31:CA:1431:A:O4'	2.16	0.46
31:CA:2233:U:H2'	31:CA:2234:G:C8	2.50	0.46
46:CS:49:ILE:HB	46:CS:51:VAL:O	2.15	0.46
42:DO:35:LYS:HB2	42:DO:112:TYR:CE1	2.51	0.46
46:DS:22:LEU:HA	69:DS:311:HOH:O	2.15	0.46
54:DI:57:ASN:HB3	54:DI:76:PHE:HB3	1.96	0.46
1:AA:735:C:H5'	18:AR:60:LYS:HD3	1.98	0.46
6:AF:16:GLU:O	6:AF:19:PRO:HD2	2.16	0.46
17:AQ:15:ASP:HA	17:AQ:21:ILE:HG22	1.96	0.46
20:AT:48:GLN:HE21	20:AT:52:ASN:ND2	2.13	0.46
31:CA:355:U:H2'	31:CA:356:G:C8	2.51	0.46
41:DN:16:ARG:HB3	28:DB:90:C:OP1	2.16	0.46
55:DA:570:G:H2'	55:DA:2030:6MZ:N7	2.31	0.46
1:BA:490:C:H2'	1:BA:491:G:C8	2.50	0.46
1:BA:1356:G:H2'	1:BA:1357:A:C8	2.50	0.46
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.43	0.46
20:BT:44:LYS:HB3	20:BT:87:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:639:U:H2'	31:CA:640:C:C6	2.51	0.46
31:CA:1510:G:H2'	31:CA:1511:G:O4'	2.16	0.46
31:CA:1974:C:H2'	31:CA:1975:G:H8	1.81	0.46
31:CA:2718:G:OP1	44:CQ:98:TYR:HD2	1.99	0.46
34:CF:44:ILE:HG21	34:CF:79:ILE:HG22	1.97	0.46
44:CQ:6:LYS:O	44:CQ:10:GLN:HG2	2.16	0.46
52:CY:18:ARG:NH2	52:CY:24:ALA:HB2	2.31	0.46
34:DF:44:ILE:HG21	34:DF:79:ILE:HG22	1.98	0.46
42:DO:31:HIS:C	42:DO:33:ILE:H	2.24	0.46
55:DA:639:U:H2'	55:DA:640:C:C6	2.51	0.46
55:DA:2328:A:H2'	55:DA:2329:U:C6	2.51	0.46
55:DA:2626:C:H2'	55:DA:2627:G:O4'	2.16	0.46
55:DA:2849:U:H4'	55:DA:2868:A:C2	2.50	0.46
1:AA:373:A:H61	1:AA:391:G:H1'	1.81	0.46
4:AD:54:GLN:HB3	4:AD:203:LEU:HD13	1.97	0.46
13:AM:93:ARG:HH12	19:AS:81:ARG:HH21	1.63	0.46
1:BA:392:C:H2'	1:BA:393:A:H8	1.79	0.46
28:CB:18:G:H1	28:CB:65:U:H3	1.62	0.46
29:CC:75:PRO:HG2	29:CC:97:LYS:HD3	1.97	0.46
41:CN:34:LYS:HE3	41:CN:131:VAL:HG11	1.98	0.46
43:DP:31:THR:HG22	43:DP:33:ARG:H	1.81	0.46
54:DI:126:LEU:HA	54:DI:129:LEU:HD12	1.96	0.46
55:DA:225:C:H2'	55:DA:226:A:O4'	2.16	0.46
55:DA:279:A:H61	55:DA:361:G:H1'	1.79	0.46
55:DA:2461:A:H1'	55:DA:2492:U:C2	2.51	0.46
55:DA:2830:C:H5'	69:DA:4054:HOH:O	2.16	0.46
6:AF:42:TRP:CH2	6:AF:102:MET:HE3	2.50	0.46
1:BA:73:C:O2'	1:BA:74:A:H8	1.99	0.46
7:BG:69:VAL:HG23	7:BG:100:ALA:HB1	1.97	0.46
16:BP:54:LEU:HA	16:BP:57:ILE:HD12	1.98	0.46
31:CA:1783:A:C2	31:CA:2588:G:O4'	2.69	0.46
31:CA:2328:A:H2'	31:CA:2329:U:C6	2.51	0.46
31:CA:2547:A:H2'	31:CA:2548:U:C6	2.51	0.46
31:CA:2688:G:H1'	31:CA:2721:A:N6	2.31	0.46
40:CM:28:GLY:O	40:CM:29:LYS:C	2.58	0.46
42:CO:85:PRO:HA	42:CO:88:ALA:HB2	1.97	0.46
34:DF:33:LYS:HG3	34:DF:157:THR:HB	1.96	0.46
55:DA:2609:U:C5	62:DA:3194:EDO:H12	2.51	0.46
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.51	0.46
13:AM:106:ALA:HB3	13:AM:110:LYS:HE3	1.98	0.46
1:BA:34:C:H2'	1:BA:35:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BP:20:VAL:HG13	16:BP:32:PHE:HB2	1.98	0.46
25:D4:45:ARG:HD3	55:DA:2418:A:OP1	2.16	0.46
31:CA:352:A:H5''	31:CA:352:A:H8	1.81	0.46
31:CA:2544:G:H5'	31:CA:2645:G:N2	2.31	0.46
32:DD:129:THR:HG22	32:DD:141:ARG:HA	1.98	0.46
51:DX:38:VAL:HG12	51:DX:59:LEU:HB2	1.98	0.46
55:DA:2065:C:H2'	55:DA:2066:C:O4'	2.16	0.46
55:DA:2097:A:H5''	55:DA:2097:A:C8	2.50	0.46
55:DA:2267:A:H5''	55:DA:2268:A:H5'	1.98	0.46
55:DA:2558:C:H2'	55:DA:2559:C:O4'	2.16	0.46
55:DA:2643:G:H2'	55:DA:2644:G:O4'	2.16	0.46
1:AA:73:C:O2'	1:AA:74:A:H8	1.98	0.45
1:AA:429:U:C5'	4:AD:9:LEU:HD12	2.47	0.45
1:AA:579:A:H2'	1:AA:580:C:C6	2.51	0.45
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.96	0.45
11:AK:21:ALA:HB2	11:AK:82:LEU:HD13	1.98	0.45
1:BA:1069:C:H4'	1:BA:1192:C:O2	2.16	0.45
1:BA:1103:C:H2'	1:BA:1104:G:O4'	2.16	0.45
4:BD:105:MET:HE3	4:BD:171:LEU:HD22	1.98	0.45
12:BL:110:ARG:HB2	12:BL:119:VAL:HG21	1.97	0.45
31:CA:2461:A:H1'	31:CA:2492:U:C2	2.51	0.45
31:CA:2886:A:C2	31:CA:2887:A:H1'	2.51	0.45
29:DC:8:PRO:O	55:DA:1695:G:H1'	2.16	0.45
38:CK:35:ARG:HB3	38:CK:54:ILE:HD11	1.98	0.45
33:DE:33:VAL:HG22	58:DA:3192:MPD:C1	2.39	0.45
47:DT:93:ALA:HB2	55:DA:1614:A:N1	2.31	0.45
55:DA:355:U:H2'	55:DA:356:G:C8	2.51	0.45
55:DA:455:C:N3	55:DA:472:A:H2'	2.31	0.45
55:DA:634:C:O5'	55:DA:634:C:H6	1.99	0.45
55:DA:1532:A:H5''	55:DA:1532:A:C8	2.51	0.45
55:DA:2141:G:H2'	55:DA:2142:A:C8	2.52	0.45
66:DA:3202:ACY:H2	69:DA:5043:HOH:O	2.15	0.45
1:AA:1003:G:H21	1:AA:1005:A:H5'	1.81	0.45
69:AA:1745:HOH:O	12:AL:115:SER:HB3	2.16	0.45
16:AP:4:ILE:HD13	16:AP:57:ILE:HG23	1.98	0.45
20:AT:39:ILE:HG23	20:AT:86:LEU:HD11	1.98	0.45
1:BA:857:C:H2'	1:BA:858:G:O4'	2.16	0.45
31:CA:2377:A:H2'	31:CA:2378:A:C8	2.50	0.45
31:CA:2845:U:H5''	44:CQ:52:ASN:O	2.15	0.45
43:CP:41:ALA:HB2	43:CP:48:LEU:HD23	1.97	0.45
35:DG:24:ILE:HD12	35:DG:72:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DR:76:TYR:CZ	45:DR:80:ILE:HG13	2.50	0.45
1:AA:328:C:O2	1:AA:328:C:H2'	2.17	0.45
1:AA:623:C:H6	1:AA:623:C:O5'	2.00	0.45
1:AA:1026:G:H1	1:AA:1035:A:H2	1.63	0.45
6:AF:3:HIS:HA	6:AF:65:GLU:HA	1.98	0.45
1:BA:502:A:OP1	12:BL:115:SER:HB2	2.17	0.45
1:BA:920:U:H2'	1:BA:921:U:C6	2.51	0.45
31:CA:2822:G:H2'	31:CA:2823:A:H5''	1.98	0.45
29:DC:50:THR:OG1	55:DA:1813:G:H1'	2.17	0.45
46:CS:1:MET:HA	46:CS:42:ALA:O	2.16	0.45
49:CV:72:ILE:HG12	49:CV:83:VAL:HG23	1.99	0.45
33:DE:58:LYS:HD2	55:DA:675:A:OP1	2.17	0.45
44:DQ:52:ASN:O	55:DA:2845:U:H5''	2.14	0.45
48:DU:33:LYS:HE2	63:DU:201:PGE:H32	1.98	0.45
55:DA:1426:G:H8	55:DA:1426:G:O5'	1.98	0.45
1:AA:920:U:H2'	1:AA:921:U:C6	2.51	0.45
1:AA:1069:C:H4'	1:AA:1192:C:O2	2.16	0.45
5:AE:38:VAL:HG11	5:AE:114:VAL:HG22	1.99	0.45
23:C2:25:LYS:HD2	23:C2:52:ALA:HB1	1.97	0.45
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	1.99	0.45
1:BA:1141:C:O2'	1:BA:1142:G:H8	1.99	0.45
21:BU:11:PRO:HG2	21:BU:14:VAL:HB	1.98	0.45
31:CA:2182:U:H2'	31:CA:2183:A:C8	2.51	0.45
32:DD:25:THR:HG21	32:DD:193:VAL:HG22	1.98	0.45
41:CN:40:ARG:HD3	41:CN:93:VAL:HG21	1.99	0.45
44:CQ:114:LEU:H	44:CQ:114:LEU:HD22	1.82	0.45
34:DF:88:LYS:HD3	55:DA:2313:C:H5''	1.99	0.45
34:DF:122:PHE:CE2	34:DF:167:ARG:HD3	2.52	0.45
46:DS:72:VAL:HG13	69:DS:346:HOH:O	2.16	0.45
55:DA:191:A:H2'	55:DA:192:C:C6	2.51	0.45
55:DA:1796:U:H2'	55:DA:1797:G:C8	2.52	0.45
5:BE:99:ALA:HB3	5:BE:122:ASN:HB3	1.97	0.45
7:BG:26:PHE:HA	7:BG:29:ILE:HD12	1.97	0.45
23:D2:8:LYS:HE2	55:DA:2420:C:H5''	1.97	0.45
41:CN:121:ALA:HA	41:CN:124:LEU:HD12	1.98	0.45
41:DN:77:PRO:HG2	41:DN:80:VAL:HG21	1.97	0.45
45:DR:78:LYS:HG2	69:DA:6376:HOH:O	2.17	0.45
55:DA:1237:A:H4'	55:DA:1238:G:OP1	2.16	0.45
55:DA:2557:G:H2'	55:DA:2558:C:H6	1.82	0.45
1:AA:167:A:H2'	1:AA:168:G:O4'	2.17	0.45
9:AI:12:ARG:HG3	9:AI:107:ASP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C1:4:GLN:HA	31:CA:2615:U:C2	2.51	0.45
1:BA:212:G:H2'	1:BA:213:G:H8	1.80	0.45
1:BA:1402:4OC:H2'	1:BA:1403:C:O4'	2.16	0.45
24:D3:24:THR:HG23	24:D3:27:GLY:HA3	1.98	0.45
31:CA:197:A:H2	31:CA:2434:A:N6	2.14	0.45
31:CA:2101:A:H2'	31:CA:2102:G:H8	1.81	0.45
31:CA:2728:U:O2'	31:CA:2729:G:H8	1.99	0.45
42:DO:45:ARG:HD2	69:DA:5551:HOH:O	2.16	0.45
55:DA:2014:A:H2'	55:DA:2015:A:C8	2.51	0.45
55:DA:2047:C:C5	66:DA:3202:ACY:H3	2.51	0.45
1:AA:1190:G:H5'	3:AC:176:HIS:CE1	2.51	0.45
5:BE:90:THR:HG22	5:BE:91:GLY:N	2.32	0.45
5:BE:105:ILE:H	5:BE:123:VAL:H	1.65	0.45
31:CA:1380:G:H1'	31:CA:1569:A:H61	1.81	0.45
31:CA:1590:A:H2'	31:CA:1591:A:C8	2.52	0.45
31:CA:2353:G:H2'	31:CA:2354:C:O4'	2.16	0.45
45:CR:76:TYR:CZ	45:CR:80:ILE:HG13	2.52	0.45
42:DO:54:LEU:HD23	42:DO:66:ALA:HB2	1.98	0.45
2:AB:207:ILE:H	2:AB:207:ILE:HG13	1.60	0.45
1:BA:123:U:H5''	1:BA:311:C:O2'	2.17	0.45
1:BA:729:A:H2'	1:BA:730:G:O4'	2.16	0.45
4:BD:88:GLU:HG2	4:BD:188:ARG:HD3	1.97	0.45
15:BO:64:ARG:HH12	15:BO:88:ARG:NH1	2.15	0.45
30:CD:13:ARG:HD3	30:CD:21:SER:OG	2.17	0.45
31:CA:136:G:H1	31:CA:143:C:H42	1.64	0.45
32:DD:159:LYS:HE2	69:DA:4766:HOH:O	2.16	0.45
41:DN:19:GLY:O	41:DN:97:GLN:HB3	2.17	0.45
42:DO:29:VAL:HG13	42:DO:83:LEU:HD11	1.98	0.45
51:DX:57:HIS:N	51:DX:57:HIS:CD2	2.85	0.45
55:DA:780:G:H2'	55:DA:782:A:N7	2.32	0.45
55:DA:825:A:H2'	55:DA:826:U:O4'	2.17	0.45
55:DA:1179:G:H2'	55:DA:1180:U:C6	2.51	0.45
1:AA:843:U:H1'	1:AA:845:A:C6	2.52	0.45
1:AA:1484:C:O2'	55:DA:1961:C:H5'	2.16	0.45
5:AE:16:ILE:HD13	5:AE:137:VAL:HG11	1.99	0.45
5:AE:18:VAL:HG11	5:AE:56:VAL:HG13	1.99	0.45
7:AG:26:PHE:HA	7:AG:29:ILE:HD12	1.99	0.45
1:BA:328:C:O2	1:BA:328:C:H2'	2.16	0.45
1:BA:1194:U:H5'	5:BE:27:GLY:HA2	1.97	0.45
9:BI:84:THR:HG21	9:BI:103:PHE:CB	2.47	0.45
22:D1:3:VAL:HG22	22:D1:4:GLN:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:790:U:H3	31:CA:795:C:H5'	1.82	0.45
31:CA:1069:A:H5'	31:CA:1070:A:H8	1.81	0.45
31:CA:1121:C:H2'	31:CA:1122:G:O4'	2.17	0.45
29:DC:226:ASN:O	29:DC:227:PRO:C	2.59	0.45
34:DF:61:SER:HB2	34:DF:91:LEU:HD21	1.99	0.45
38:DK:7:LYS:O	38:DK:11:VAL:HG23	2.17	0.45
46:DS:83:TYR:CE1	55:DA:1187:G:H5''	2.51	0.45
54:DI:53:ARG:HD2	54:DI:55:VAL:HG23	1.97	0.45
4:AD:88:GLU:HG2	4:AD:188:ARG:HD3	1.98	0.45
13:AM:33:ILE:HD11	13:AM:63:PHE:HE1	1.81	0.45
1:BA:82:G:N1	1:BA:84:U:H5	2.10	0.45
1:BA:1108:G:H5''	3:BC:176:HIS:CE1	2.52	0.45
1:BA:1197:A:H3'	1:BA:1198:G:H5''	1.99	0.45
1:BA:1329:A:H5''	13:BM:26:GLY:H	1.82	0.45
1:BA:1493:A:H1'	31:CA:1913:A:H61	1.82	0.45
13:BM:16:VAL:HG13	13:BM:34:LEU:HD12	1.98	0.45
31:CA:206:U:H2'	31:CA:207:A:C8	2.37	0.45
31:CA:2364:C:OP1	51:CX:55:ARG:HD3	2.17	0.45
55:DA:2182:U:H2'	55:DA:2183:A:C8	2.52	0.45
55:DA:2345:G:N3	55:DA:2381:A:H2'	2.32	0.45
55:DA:2903:U:H3'	69:DA:6757:HOH:O	2.17	0.45
1:AA:235:C:H2'	1:AA:236:A:C8	2.52	0.44
1:AA:1494:G:C8	55:DA:1913:A:C2	3.05	0.44
1:AA:1512:U:H2'	1:AA:1513:A:C8	2.52	0.44
19:AS:53:ASN:HD22	19:AS:58:VAL:HG23	1.82	0.44
22:C1:42:HIS:HD2	42:CO:101:GLY:H	1.63	0.44
1:BA:32:A:H2'	1:BA:33:A:C8	2.52	0.44
1:BA:49:U:O2	1:BA:362:G:H1'	2.17	0.44
1:BA:373:A:H61	1:BA:391:G:H1'	1.82	0.44
12:BL:53:CYS:HB3	12:BL:67:ILE:HD11	1.99	0.44
19:BS:53:ASN:HD22	19:BS:58:VAL:HG23	1.81	0.44
27:D0:19:LYS:O	27:D0:22:ALA:HB3	2.17	0.44
31:CA:309:A:H4'	49:CV:16:GLY:HA2	1.99	0.44
31:CA:1494:A:H2'	31:CA:1495:A:C8	2.52	0.44
31:CA:1532:A:H5''	31:CA:1532:A:C8	2.51	0.44
31:CA:2141:G:H2'	31:CA:2142:A:C8	2.53	0.44
36:DH:29:PHE:HB2	55:DA:2198:A:C2	2.52	0.44
55:DA:466:A:O4'	55:DA:683:U:H4'	2.16	0.44
55:DA:1401:G:H2'	55:DA:1402:U:C6	2.52	0.44
55:DA:2767:C:H2'	55:DA:2768:U:C6	2.52	0.44
1:AA:864:A:H4'	5:AE:90:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:6:TYR:HB2	9:AI:21:ILE:HB	1.99	0.44
1:BA:591:U:H2'	1:BA:592:G:H8	1.83	0.44
1:BA:1063:C:H2'	1:BA:1064:G:C8	2.52	0.44
2:BB:207:ILE:H	2:BB:207:ILE:HG13	1.61	0.44
5:BE:13:GLU:CB	5:BE:39:VAL:HG12	2.47	0.44
7:BG:138:ARG:HE	7:BG:138:ARG:HB3	1.62	0.44
28:CB:29:A:H2'	28:CB:30:C:C6	2.53	0.44
31:CA:225:C:H2'	31:CA:226:A:O4'	2.17	0.44
31:CA:593:U:H2'	31:CA:594:U:C6	2.53	0.44
31:CA:686:U:H2'	31:CA:788:A:N1	2.32	0.44
31:CA:2261:C:H1'	31:CA:2388:A:N3	2.32	0.44
33:DE:181:ILE:HG12	40:DM:1:MET:HE3	1.98	0.44
55:DA:739:A:H2'	69:DA:7494:HOH:O	2.18	0.44
55:DA:1171:G:H1'	55:DA:1179:G:N2	2.32	0.44
55:DA:1510:G:H2'	55:DA:1511:G:O4'	2.16	0.44
55:DA:1979:U:OP1	59:DA:3212:PUT:H32	2.17	0.44
1:AA:1329:A:H5''	13:AM:26:GLY:H	1.82	0.44
6:AF:16:GLU:HB3	4:BD:189:SER:HA	1.98	0.44
1:BA:1238:A:H5'	1:BA:1336:C:H41	1.82	0.44
13:BM:93:ARG:HH12	19:BS:81:ARG:HH21	1.66	0.44
20:BT:5:LYS:HB3	20:BT:7:ALA:H	1.83	0.44
25:D4:4:ILE:HD11	55:DA:592:A:N3	2.33	0.44
29:CC:107:PRO:HB3	29:CC:142:HIS:NE2	2.32	0.44
29:CC:271:ARG:HD3	31:CA:1819:A:H2	1.83	0.44
31:CA:2428:G:H21	40:CM:60:ARG:HD3	1.83	0.44
42:CO:8:ARG:HE	42:CO:43:GLU:HG2	1.83	0.44
47:CT:86:MET:HB2	47:CT:96:ILE:HD11	2.00	0.44
36:DH:41:LYS:HA	36:DH:44:ILE:HG12	1.99	0.44
55:DA:278:A:H2'	55:DA:278:A:N3	2.33	0.44
55:DA:2184:A:O5'	55:DA:2184:A:H8	2.01	0.44
55:DA:2578:G:OP2	55:DA:2578:G:H4'	2.17	0.44
11:AK:111:THR:HG23	21:AU:3:VAL:HG22	2.00	0.44
17:AQ:77:ARG:NH2	17:AQ:79:VAL:HG22	2.33	0.44
1:BA:623:C:O5'	1:BA:623:C:H6	2.01	0.44
11:BK:21:ALA:HB2	11:BK:82:LEU:HD13	1.99	0.44
31:CA:392:U:H2'	31:CA:393:C:C6	2.53	0.44
42:CO:95:THR:HG21	42:CO:113:ILE:HD11	1.99	0.44
43:CP:16:ARG:HA	43:CP:16:ARG:HD2	1.81	0.44
34:DF:36:LEU:HB2	34:DF:57:LEU:HD21	1.99	0.44
46:DS:76:LYS:O	46:DS:84:ARG:HA	2.17	0.44
51:DX:39:ARG:HD3	69:DX:117:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:78:U:H2'	55:DA:79:C:C6	2.53	0.44
55:DA:96:C:H2'	55:DA:97:C:H6	1.83	0.44
55:DA:128:C:H2'	55:DA:129:C:C6	2.53	0.44
55:DA:757:G:H5''	69:DA:3996:HOH:O	2.18	0.44
1:AA:123:U:H5''	1:AA:311:C:O2'	2.18	0.44
1:AA:212:G:H2'	1:AA:213:G:H8	1.81	0.44
1:AA:946:A:H2'	1:AA:947:G:C8	2.53	0.44
1:AA:1402:4OC:H2'	1:AA:1403:C:O4'	2.17	0.44
18:AR:52:GLN:HA	18:AR:55:LEU:HD12	1.98	0.44
1:BA:243:A:C2	1:BA:245:U:C2	3.05	0.44
31:CA:128:C:H2'	31:CA:129:C:C6	2.52	0.44
31:CA:1344:U:O2'	31:CA:1384:A:H2'	2.17	0.44
31:CA:1447:C:H2'	31:CA:1448:G:C8	2.52	0.44
31:CA:2014:A:H2'	31:CA:2015:A:C8	2.52	0.44
37:CJ:55:ILE:HD12	37:CJ:74:PRO:HD3	1.99	0.44
40:CM:82:LEU:HD11	40:CM:116:VAL:HG23	1.99	0.44
41:CN:77:PRO:HG2	41:CN:80:VAL:HG21	2.00	0.44
42:CO:31:HIS:C	42:CO:33:ILE:H	2.25	0.44
45:DR:40:ILE:HG12	58:DS:203:MPD:H31	2.00	0.44
46:DS:44:GLY:C	46:DS:46:GLU:H	2.25	0.44
49:DV:25:VAL:HA	49:DV:36:VAL:HG22	1.98	0.44
5:AE:90:THR:HG22	5:AE:91:GLY:N	2.33	0.44
25:D4:19:LYS:HB2	55:DA:651:G:OP1	2.18	0.44
29:CC:145:GLU:HB2	29:CC:188:CYS:HB3	1.99	0.44
31:CA:96:C:H2'	31:CA:97:C:H6	1.82	0.44
31:CA:2641:G:H2'	31:CA:2642:G:H8	1.83	0.44
36:CH:1:MET:HE3	36:CH:23:ALA:HA	1.99	0.44
50:CW:77:VAL:HG23	50:CW:89:ILE:HG12	2.00	0.44
35:DG:17:VAL:HG11	35:DG:50:LEU:HD21	2.00	0.44
40:DM:19:LEU:HD12	55:DA:587:C:O2'	2.18	0.44
55:DA:1278:C:H2'	55:DA:1279:G:C8	2.53	0.44
1:AA:411:A:P	4:AD:26:ARG:HH12	2.40	0.44
7:AG:50:LEU:HD22	7:AG:124:LEU:HD13	1.99	0.44
1:BA:522:C:H41	12:BL:50:ARG:NH2	2.15	0.44
1:BA:532:A:N1	3:BC:193:TYR:HB3	2.33	0.44
1:BA:935:A:H2'	1:BA:936:C:C6	2.53	0.44
30:CD:104:VAL:HG23	30:CD:177:VAL:HG21	2.00	0.44
31:CA:78:U:H2'	31:CA:79:C:C6	2.53	0.44
31:CA:278:A:N3	31:CA:278:A:H2'	2.33	0.44
31:CA:576:U:H2'	31:CA:577:G:C8	2.52	0.44
47:DT:6:LYS:HA	47:DT:103:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:DU:15:HIS:HB3	48:DU:31:VAL:HG12	2.00	0.44
55:DA:1442:U:H2'	55:DA:1443:U:C6	2.52	0.44
55:DA:1965:C:OP1	55:DA:1966:A:C2'	2.66	0.44
55:DA:2607:G:H2'	55:DA:2608:G:O4'	2.17	0.44
55:DA:2681:C:C2	55:DA:2724:U:O4	2.71	0.44
1:AA:1238:A:H5'	1:AA:1336:C:H41	1.83	0.44
22:C1:2:ALA:N	31:CA:2577:A:H2	2.16	0.44
1:BA:407:U:H2'	1:BA:408:A:H8	1.83	0.44
1:BA:1003:G:H21	1:BA:1005:A:H5'	1.81	0.44
18:BR:20:GLU:HA	18:BR:55:LEU:HD23	2.00	0.44
28:CB:89:U:C6	31:CA:958:U:H2'	2.53	0.44
31:CA:1401:G:H2'	31:CA:1402:U:C6	2.53	0.44
43:CP:31:THR:HG22	43:CP:33:ARG:H	1.83	0.44
48:CU:15:HIS:HB3	48:CU:31:VAL:HG12	1.99	0.44
48:CU:58:VAL:HG22	48:CU:85:VAL:HG22	1.98	0.44
33:DE:23:PHE:HE2	33:DE:25:GLU:HG3	1.82	0.44
41:DN:34:LYS:HE3	41:DN:131:VAL:HG11	1.98	0.44
51:DX:47:ALA:HB1	51:DX:51:VAL:O	2.17	0.44
51:DX:59:LEU:HD12	51:DX:80:ILE:HD12	1.99	0.44
54:DI:50:VAL:CG1	54:DI:92:ALA:HB2	2.48	0.44
1:AA:1486:G:H2'	1:AA:1487:G:O4'	2.18	0.44
4:AD:105:MET:HE3	4:AD:171:LEU:HD22	1.99	0.44
6:AF:93:LYS:HE2	6:AF:93:LYS:H	1.82	0.44
10:AJ:46:LYS:HG2	10:AJ:68:ARG:HG2	1.99	0.44
12:AL:5:ASN:O	12:AL:9:ARG:HD2	2.18	0.44
23:C2:39:PHE:HB2	23:C2:46:HIS:CE1	2.53	0.44
1:BA:1517:G:H1'	31:CA:1919:A:O3'	2.17	0.44
9:BI:19:VAL:HG22	9:BI:65:ILE:HG22	2.00	0.44
17:BQ:9:GLN:O	17:BQ:25:ILE:HG23	2.18	0.44
31:CA:571:U:H1'	31:CA:573:U:H6	1.82	0.44
36:CH:21:VAL:HG21	36:CH:25:TYR:HD2	1.82	0.44
37:DJ:19:ASN:N	37:DJ:20:PRO:HD2	2.33	0.44
37:DJ:55:ILE:HD12	37:DJ:74:PRO:HD3	1.99	0.44
40:DM:57:LEU:C	40:DM:59:ARG:H	2.26	0.44
42:DO:8:ARG:HE	42:DO:43:GLU:HG2	1.83	0.44
54:DI:120:ALA:HA	54:DI:123:ILE:HD11	2.00	0.44
55:DA:577:G:H1'	69:DA:3571:HOH:O	2.17	0.44
55:DA:2849:U:N3	55:DA:2867:G:O4'	2.50	0.44
1:BA:235:C:H2'	1:BA:236:A:C8	2.53	0.43
1:BA:946:A:H2'	1:BA:947:G:C8	2.53	0.43
6:BF:38:ARG:HH12	6:BF:99:ALA:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BG:116:MET:HA	7:BG:119:ARG:HB2	2.00	0.43
10:BJ:46:LYS:HG2	10:BJ:68:ARG:HG2	1.99	0.43
30:CD:118:PHE:HZ	31:CA:2048:G:H21	1.66	0.43
31:CA:12:U:O2	31:CA:12:U:H2'	2.17	0.43
31:CA:1024:G:H3'	31:CA:1025:G:H2'	1.99	0.43
31:CA:1791:A:N6	31:CA:1828:G:O2'	2.51	0.43
47:CT:6:LYS:HG2	47:CT:104:THR:HG23	2.00	0.43
34:DF:14:LYS:O	34:DF:18:THR:HG22	2.18	0.43
44:DQ:113:ARG:HG2	44:DQ:115:ASN:HD21	1.83	0.43
55:DA:320:A:H4'	55:DA:322:A:C8	2.53	0.43
55:DA:492:A:H2'	55:DA:493:G:O4'	2.18	0.43
55:DA:729:G:H2'	55:DA:1775:U:H1'	2.00	0.43
55:DA:739:A:H1'	55:DA:740:C:H5	1.83	0.43
1:AA:490:C:H2'	1:AA:491:G:C8	2.52	0.43
5:AE:13:GLU:CB	5:AE:39:VAL:HG12	2.47	0.43
21:AU:11:PRO:HG2	21:AU:14:VAL:HB	1.99	0.43
27:C0:46:GLY:HA3	31:CA:851:C:O2'	2.19	0.43
1:BA:363:A:H2'	1:BA:364:A:O4'	2.18	0.43
1:BA:604:G:H2'	1:BA:605:U:O4'	2.18	0.43
12:BL:90:LEU:HD23	12:BL:93:VAL:HG21	2.00	0.43
31:CA:727:A:H2'	31:CA:728:G:C8	2.53	0.43
31:CA:2006:C:H2'	31:CA:2007:U:C6	2.53	0.43
31:CA:2582:G:C2	31:CA:2583:G:C8	3.06	0.43
33:DE:145:ASP:HA	33:DE:166:LYS:HB3	2.01	0.43
50:DW:77:VAL:HG23	50:DW:89:ILE:HG12	2.01	0.43
55:DA:521:U:H2'	55:DA:522:A:C8	2.53	0.43
1:AA:756:C:H2'	1:AA:757:U:O4'	2.19	0.43
9:AI:84:THR:HG21	9:AI:103:PHE:CB	2.47	0.43
1:BA:994:A:N1	1:BA:1047:G:H4'	2.33	0.43
20:BT:22:ALA:O	20:BT:26:SER:HB2	2.18	0.43
27:D0:24:LEU:HD11	27:D0:54:MET:CE	2.48	0.43
31:CA:197:A:C2	31:CA:2434:A:N6	2.84	0.43
31:CA:1280:G:H1	31:CA:1290:C:H42	1.67	0.43
31:CA:2771:C:H2'	31:CA:2772:C:H6	1.83	0.43
32:DD:119:ALA:HB3	32:DD:165:MET:HB2	1.99	0.43
33:CE:108:ILE:HG21	33:CE:181:ILE:HD11	1.99	0.43
42:CO:29:VAL:HG13	42:CO:83:LEU:HD11	2.00	0.43
44:CQ:113:ARG:HG2	44:CQ:115:ASN:HD21	1.82	0.43
49:CV:72:ILE:H	49:CV:72:ILE:HG13	1.64	0.43
36:DH:116:ARG:HH21	36:DH:133:GLN:HB2	1.83	0.43
55:DA:1354:A:H2'	55:DA:1355:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:1485:U:H2'	55:DA:1486:U:C6	2.53	0.43
55:DA:2123:G:H2'	55:DA:2124:G:H8	1.82	0.43
1:AA:729:A:H2'	1:AA:730:G:O4'	2.17	0.43
1:AA:855:U:H2'	1:AA:856:C:C6	2.53	0.43
9:AI:19:VAL:HG22	9:AI:65:ILE:HG22	2.00	0.43
22:C1:19:HIS:CE1	31:CA:2624:G:H1'	2.53	0.43
1:BA:167:A:H2'	1:BA:168:G:O4'	2.18	0.43
1:BA:619:U:H3	4:BD:131:ASN:HB3	1.82	0.43
1:BA:1478:U:H2'	1:BA:1479:C:C6	2.54	0.43
29:CC:208:ALA:HB2	31:CA:1790:C:O2'	2.19	0.43
31:CA:492:A:H2	47:CT:7:HIS:NE2	2.16	0.43
31:CA:609:A:H2'	31:CA:610:C:O4'	2.19	0.43
31:CA:1826:G:C6	31:CA:1827:U:C4	3.06	0.43
31:CA:2840:C:H5''	42:CO:53:THR:HG21	1.99	0.43
34:CF:61:SER:HB2	34:CF:91:LEU:HD21	2.00	0.43
36:CH:41:LYS:HA	36:CH:44:ILE:HG12	2.00	0.43
38:CK:7:LYS:O	38:CK:11:VAL:HG23	2.19	0.43
35:DG:155:GLU:HG2	35:DG:157:TYR:H	1.84	0.43
39:DL:71:ARG:HH22	39:DL:123:LEU:C	2.27	0.43
41:DN:136:MET:HE3	50:DW:57:TYR:HB3	2.01	0.43
43:DP:30:ARG:HG3	43:DP:35:ILE:HD12	2.00	0.43
47:DT:6:LYS:HG2	47:DT:104:THR:HG23	2.00	0.43
55:DA:2101:A:H2'	55:DA:2102:G:H8	1.83	0.43
1:AA:682:G:H2'	1:AA:683:G:H8	1.83	0.43
1:AA:1478:U:H2'	1:AA:1479:C:C6	2.53	0.43
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	2.01	0.43
3:AC:180:ALA:HA	3:AC:206:GLU:HA	2.01	0.43
8:AH:64:LYS:HB3	8:AH:71:VAL:HG21	2.01	0.43
12:AL:33:VAL:HG22	12:AL:79:VAL:HG22	2.00	0.43
23:C2:4:GLY:C	23:C2:6:ARG:H	2.27	0.43
1:BA:1417:G:C6	1:BA:1482:G:C6	3.07	0.43
13:BM:23:TYR:HB3	13:BM:66:GLU:HA	2.00	0.43
31:CA:56:A:H61	31:CA:114:U:H3	1.66	0.43
31:CA:521:U:H2'	31:CA:522:A:C8	2.53	0.43
31:CA:1274:A:N3	31:CA:1297:C:H1'	2.33	0.43
31:CA:1447:C:H2'	31:CA:1448:G:H8	1.84	0.43
35:CG:17:VAL:HG11	35:CG:50:LEU:HD21	1.99	0.43
41:CN:41:LEU:HD21	41:CN:124:LEU:HD22	2.01	0.43
47:CT:17:VAL:HA	47:CT:43:ALA:HB1	2.00	0.43
47:CT:62:ASP:HB3	47:CT:63:GLY:H	1.73	0.43
47:CT:95:ARG:CZ	47:CT:97:LEU:HD21	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DF:40:VAL:HG23	34:DF:86:GLY:HA2	2.00	0.43
55:DA:861:A:C2	55:DA:917:A:C4	3.06	0.43
1:AA:1500:A:H5''	1:AA:1508:A:H5''	2.01	0.43
4:AD:102:VAL:HG13	4:AD:107:PHE:HB2	2.00	0.43
8:AH:76:GLN:O	8:AH:127:CYS:HB2	2.19	0.43
8:AH:105:SER:HB2	8:AH:126:ILE:HD11	2.01	0.43
12:AL:80:ILE:HG22	12:AL:104:CYS:HB2	2.00	0.43
12:AL:110:ARG:HB2	12:AL:119:VAL:HG21	1.99	0.43
24:C3:10:LEU:O	24:C3:14:ARG:HB2	2.18	0.43
1:BA:9:G:OP2	5:BE:126:LYS:HE2	2.19	0.43
5:BE:106:ILE:HD11	5:BE:124:LEU:HD23	1.99	0.43
6:BF:3:HIS:CD2	6:BF:92:THR:HG23	2.53	0.43
22:D1:40:ARG:HH22	55:DA:2884[B]:U:H2'	1.84	0.43
30:CD:172:VAL:HG12	30:CD:175:LEU:HD21	2.01	0.43
31:CA:685:A:H1'	31:CA:688:U:O4	2.18	0.43
31:CA:1791:A:N6	31:CA:1828:G:HO2'	2.16	0.43
31:CA:2027:G:C6	31:CA:2028:U:C4	3.07	0.43
31:CA:2781:A:H5''	31:CA:2782:G:H5'	2.01	0.43
32:DD:105:LYS:HD3	32:DD:106:LYS:HG3	1.99	0.43
47:CT:6:LYS:HA	47:CT:103:ILE:O	2.18	0.43
38:DK:114:LEU:HG	38:DK:118:MET:HE3	2.00	0.43
52:DY:10:LYS:HD3	55:DA:397:U:OP2	2.19	0.43
55:DA:738:G:C6	55:DA:739:A:C6	3.07	0.43
1:AA:994:A:N1	1:AA:1047:G:H4'	2.34	0.43
1:AA:1373:G:C5'	7:AG:36:LYS:HB2	2.48	0.43
20:AT:31:PHE:HA	20:AT:34:LYS:HD2	2.00	0.43
25:C4:2:PRO:N	31:CA:591:U:H1'	2.34	0.43
1:BA:601:G:H2'	1:BA:602:A:H8	1.84	0.43
1:BA:1486:G:H2'	1:BA:1487:G:O4'	2.17	0.43
2:BB:167:ASP:CG	2:BB:191:SER:HA	2.44	0.43
9:BI:6:TYR:HB2	9:BI:21:ILE:HB	1.99	0.43
15:BO:64:ARG:HH22	15:BO:88:ARG:NH2	2.17	0.43
29:CC:21:ASN:HB3	29:CC:24:LEU:HG	2.00	0.43
31:CA:184:C:H2'	31:CA:185:G:C8	2.54	0.43
31:CA:357:C:H2'	31:CA:358:U:C6	2.54	0.43
31:CA:1484:U:H2'	31:CA:1485:U:C6	2.54	0.43
31:CA:1485:U:H2'	31:CA:1486:U:C6	2.53	0.43
31:CA:2179:C:H2'	31:CA:2180:U:C6	2.53	0.43
31:CA:2607:G:H2'	31:CA:2608:G:O4'	2.18	0.43
31:CA:2636:C:H2'	31:CA:2637:U:H6	1.82	0.43
46:DS:53:PHE:HB3	69:DS:301:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:307:G:N2	55:DA:309:A:H3'	2.33	0.43
55:DA:831:G:C6	55:DA:832:U:C4	3.07	0.43
55:DA:1759:A:H4'	55:DA:2715:C:O4'	2.18	0.43
1:AA:363:A:H2'	1:AA:364:A:O4'	2.18	0.43
1:AA:409:U:H2'	1:AA:410:G:O4'	2.19	0.43
1:AA:502:A:OP1	12:AL:115:SER:HB2	2.19	0.43
1:AA:601:G:H2'	1:AA:602:A:H8	1.84	0.43
1:AA:865:A:H8	1:AA:865:A:O5'	2.02	0.43
1:AA:1387:G:H2'	1:AA:1388:C:C6	2.53	0.43
3:AC:47:LEU:HD22	3:AC:76:VAL:HG22	2.01	0.43
1:BA:855:U:H2'	1:BA:856:C:C6	2.54	0.43
1:BA:864:A:H4'	5:BE:90:THR:HG23	2.00	0.43
31:CA:1170:C:H42	31:CA:1178:C:N4	2.16	0.43
31:CA:1231:U:H2'	31:CA:1232:G:H8	1.83	0.43
31:CA:1442:U:H2'	31:CA:1443:U:C6	2.53	0.43
31:CA:1939:5MU:H3'	69:CA:3666:HOH:O	2.17	0.43
31:CA:2024:G:C4	31:CA:2040:G:N2	2.87	0.43
38:CK:89:PHE:CE2	38:CK:100:VAL:HG11	2.54	0.43
43:CP:30:ARG:HG3	43:CP:35:ILE:HD12	2.00	0.43
45:CR:105:ALA:HB1	46:CS:40:MET:HE1	2.01	0.43
33:DE:72:SER:HB2	69:DE:449:HOH:O	2.19	0.43
36:DH:1:MET:HE3	36:DH:23:ALA:HA	2.01	0.43
36:DH:57:LYS:HA	36:DH:60:GLU:HG2	2.00	0.43
40:DM:109:LYS:HA	40:DM:126:ARG:O	2.18	0.43
45:DR:51:ARG:HH22	55:DA:993:G:P	2.42	0.43
46:DS:45:GLU:HG3	46:DS:46:GLU:OE2	2.18	0.43
55:DA:357:C:H2'	55:DA:358:U:C6	2.54	0.43
1:AA:59:A:H5''	1:AA:387:U:H5''	2.00	0.43
1:AA:81:A:H2	1:AA:88:U:H3	1.66	0.43
1:AA:591:U:H2'	1:AA:592:G:H8	1.84	0.43
2:AB:62:SER:C	2:AB:64:LYS:H	2.27	0.43
1:BA:409:U:H2'	1:BA:410:G:O4'	2.19	0.43
9:BI:51:PRO:HB3	9:BI:84:THR:HG23	2.00	0.43
30:CD:157:LYS:CG	31:CA:2619:C:H5''	2.48	0.43
31:CA:825:A:H2'	31:CA:826:U:O4'	2.19	0.43
31:CA:2185:U:H2'	31:CA:2186:G:C8	2.53	0.43
29:DC:233:GLY:HA3	69:DC:347:HOH:O	2.19	0.43
33:CE:145:ASP:HA	33:CE:166:LYS:HB3	2.01	0.43
40:CM:21:ARG:HA	40:CM:21:ARG:HD3	1.77	0.43
53:CZ:21:LEU:HB3	53:CZ:50:VAL:HG22	2.01	0.43
55:DA:834:G:H2'	55:DA:835:C:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:1484:U:H2'	55:DA:1485:U:C6	2.54	0.43
55:DA:2243:U:O2	55:DA:2434:A:C2	2.72	0.43
1:AA:49:U:O2	1:AA:362:G:H1'	2.19	0.43
1:AA:935:A:H2'	1:AA:936:C:C6	2.54	0.43
20:AT:36:TYR:CE2	20:AT:79:LEU:HD21	2.54	0.43
1:BA:214:C:H2'	1:BA:215:C:H6	1.83	0.43
1:BA:299:G:H2'	1:BA:300:A:C8	2.54	0.43
8:BH:22:LYS:O	8:BH:63:LEU:HD12	2.19	0.43
15:BO:26:GLU:HG3	15:BO:81:LEU:HD22	2.01	0.43
15:BO:78:TYR:HE1	15:BO:88:ARG:HH21	1.67	0.43
20:BT:67:ILE:O	20:BT:68:HIS:HB2	2.19	0.43
29:CC:18:LYS:HE3	31:CA:1565:C:H5'	2.01	0.43
31:CA:2123:G:O5'	31:CA:2123:G:H8	2.02	0.43
31:CA:2747:G:O6	31:CA:2755:C:H5''	2.18	0.43
34:CF:40:VAL:HG23	34:CF:86:GLY:HA2	1.99	0.43
40:CM:57:LEU:C	40:CM:59:ARG:H	2.27	0.43
41:DN:18[B]:ARG:HG3	28:DB:90:C:C5'	2.49	0.43
42:DO:16:HIS:C	42:DO:16:HIS:CD2	2.97	0.43
53:DZ:18:LEU:HB2	53:DZ:53:VAL:HG11	2.01	0.43
55:DA:1001:A:H8	55:DA:1001:A:O5'	2.01	0.43
55:DA:1093:G:H1'	55:DA:1099:G:N2	2.34	0.43
55:DA:1494:A:H2'	55:DA:1495:A:C8	2.53	0.43
13:AM:23:TYR:HB3	13:AM:66:GLU:HA	2.00	0.42
4:BD:102:VAL:HG13	4:BD:107:PHE:HB2	2.00	0.42
30:CD:104:VAL:CG2	30:CD:177:VAL:HG21	2.48	0.42
29:DC:35:GLU:HG3	29:DC:64:ILE:HD11	2.00	0.42
29:DC:145:GLU:HB2	29:DC:188:CYS:HB3	2.00	0.42
36:CH:48:GLU:HA	36:CH:51:ARG:HB3	2.00	0.42
33:DE:28:VAL:O	33:DE:32:VAL:HG23	2.19	0.42
41:DN:121:ALA:HA	41:DN:124:LEU:HD12	2.01	0.42
55:DA:184:C:H2'	55:DA:185:G:C8	2.54	0.42
1:AA:604:G:H2'	1:AA:605:U:O4'	2.18	0.42
27:C0:12:SER:HB3	31:CA:988:A:P	2.59	0.42
1:BA:8:A:C6	4:BD:206:LYS:HB3	2.54	0.42
3:BC:47:LEU:HD22	3:BC:76:VAL:HG22	2.01	0.42
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	2.01	0.42
21:BU:4:ILE:HG13	21:BU:19:PHE:HA	2.00	0.42
24:D3:10:LEU:O	24:D3:14:ARG:HB2	2.19	0.42
25:D4:39:LYS:HB3	69:D4:133:HOH:O	2.18	0.42
31:CA:95:A:H4'	53:CZ:38:GLN:O	2.19	0.42
31:CA:935:C:H2'	31:CA:936:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DF:118:SER:OG	34:DF:120:LYS:HG3	2.19	0.42
34:DF:131:GLY:HA3	55:DA:2305:U:H5''	2.01	0.42
55:DA:720:U:H2'	55:DA:721:A:C8	2.55	0.42
55:DA:1183:U:H2'	55:DA:1184:U:C6	2.54	0.42
55:DA:1847:A:H8	55:DA:1847:A:O5'	2.01	0.42
55:DA:2609:U:H5	62:DA:3194:EDO:H12	1.84	0.42
55:DA:2747:G:O6	55:DA:2755:C:H5''	2.19	0.42
55:DA:2848:G:H1'	55:DA:2867:G:N2	2.33	0.42
1:AA:1293:C:H2'	1:AA:1294:G:C8	2.54	0.42
19:AS:64:ASP:HB3	34:DF:115:ARG:HH21	1.83	0.42
26:C5:17:VAL:HG11	26:C5:26:ILE:HD12	2.01	0.42
1:BA:1387:G:H2'	1:BA:1388:C:C6	2.54	0.42
30:CD:101:PHE:HA	30:CD:104:VAL:HG13	2.01	0.42
31:CA:459:U:H2'	31:CA:460:A:C8	2.50	0.42
31:CA:540:C:H2'	31:CA:541:A:H8	1.84	0.42
31:CA:622:G:H2'	31:CA:623:C:C6	2.54	0.42
31:CA:720:U:H2'	31:CA:721:A:C8	2.54	0.42
31:CA:1562:U:H2'	31:CA:1563:U:O4'	2.19	0.42
31:CA:1825:U:O5'	31:CA:1825:U:H6	2.02	0.42
52:DY:66:THR:O	52:DY:69:ALA:HB3	2.19	0.42
55:DA:2105:U:O4	55:DA:2184:A:C2	2.71	0.42
55:DA:2133:G:H2'	55:DA:2157:G:H22	1.83	0.42
55:DA:2621:G:H5''	69:DA:4246:HOH:O	2.19	0.42
55:DA:2721:A:H2'	55:DA:2722:G:O4'	2.18	0.42
55:DA:2852:G:H4'	69:DA:5849:HOH:O	2.19	0.42
7:AG:56:LYS:HB3	7:AG:57:SER:H	1.63	0.42
22:C1:8:PRO:HG2	31:CA:1264:A:H5'	2.01	0.42
1:BA:631:C:O5'	1:BA:631:C:H6	2.02	0.42
1:BA:756:C:H2'	1:BA:757:U:O4'	2.19	0.42
1:BA:1293:C:H2'	1:BA:1294:G:C8	2.55	0.42
1:BA:1373:G:C5'	7:BG:36:LYS:HB2	2.49	0.42
28:CB:90:C:H5'	41:CN:18:ARG:HA	2.02	0.42
31:CA:39:G:H2'	31:CA:40:U:C6	2.54	0.42
31:CA:70:G:H5''	31:CA:112:U:O2	2.19	0.42
31:CA:328:U:O3'	49:CV:66:GLN:HG3	2.18	0.42
31:CA:2282:G:OP1	31:CA:2283:C:H1'	2.19	0.42
31:CA:2341:G:H2'	31:CA:2342:C:O4'	2.19	0.42
41:CN:136:MET:HE3	50:CW:57:TYR:HB3	2.01	0.42
46:CS:24:LYS:HA	46:CS:94:THR:OG1	2.20	0.42
52:CY:51:VAL:HG22	52:CY:52:SER:O	2.18	0.42
35:DG:145:ALA:HB1	35:DG:164:TYR:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DK:3:THR:HA	69:DR:307:HOH:O	2.19	0.42
54:DI:65:GLU:HA	54:DI:70:GLU:HG3	2.00	0.42
55:DA:1231:U:H2'	55:DA:1232:G:H8	1.84	0.42
55:DA:1976:U:H1'	63:DA:3225:PGE:H2	2.01	0.42
55:DA:2741:A:H2'	55:DA:2742:G:O4'	2.19	0.42
55:DA:2845:U:H2'	55:DA:2846:G:O4'	2.20	0.42
1:AA:21:G:H2'	1:AA:22:G:C8	2.54	0.42
1:BA:1491:G:H2'	1:BA:1492:A:C8	2.55	0.42
10:BJ:29:ALA:HB2	10:BJ:87:LEU:HD11	2.02	0.42
31:CA:608:A:H2'	31:CA:609:A:C8	2.54	0.42
31:CA:740:C:H5'	31:CA:1784:A:H3'	2.02	0.42
31:CA:1677:A:H5''	31:CA:1677:A:C8	2.55	0.42
31:CA:2494:G:O3'	41:CN:79:ALA:HA	2.18	0.42
32:DD:143:PRO:HA	69:DD:410:HOH:O	2.20	0.42
55:DA:609:A:H2'	55:DA:610:C:O4'	2.20	0.42
55:DA:1446:C:H2'	55:DA:1447:C:C6	2.54	0.42
55:DA:2064:C:H2'	55:DA:2065:C:C6	2.55	0.42
55:DA:2341:G:H2'	55:DA:2342:C:O4'	2.20	0.42
55:DA:2636:C:H2'	55:DA:2637:U:H6	1.82	0.42
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	2.01	0.42
1:BA:682:G:H2'	1:BA:683:G:H8	1.84	0.42
2:BB:100:MET:HE2	2:BB:148:LEU:HD23	2.02	0.42
5:BE:47:GLY:HA3	5:BE:71:MET:HG2	2.01	0.42
31:CA:374:A:C2	31:CA:401:A:C4	3.08	0.42
31:CA:396:G:H1'	52:CY:29:PHE:HD2	1.83	0.42
31:CA:740:C:H42	31:CA:757:G:H1	1.66	0.42
31:CA:998:C:OP2	45:CR:58:ARG:NH2	2.52	0.42
31:CA:2520:C:H2'	31:CA:2521:C:C6	2.55	0.42
31:CA:2569:G:H5''	31:CA:2569:G:C8	2.55	0.42
31:CA:2641:G:H2'	31:CA:2642:G:C8	2.55	0.42
33:CE:126:VAL:HG23	33:CE:133:LEU:HB3	1.98	0.42
37:CJ:37:GLU:HB3	37:CJ:67:PHE:HZ	1.84	0.42
50:CW:31:TYR:O	50:CW:92:VAL:HA	2.20	0.42
51:CX:47:ALA:HB1	51:CX:51:VAL:O	2.19	0.42
40:DM:36:LYS:HB3	69:DA:4844:HOH:O	2.20	0.42
41:DN:42:THR:HG22	41:DN:93:VAL:HG12	2.02	0.42
53:DZ:21:LEU:HB3	53:DZ:50:VAL:HG22	2.01	0.42
55:DA:348:A:H2'	55:DA:349:U:O4'	2.20	0.42
55:DA:1028:A:H61	55:DA:1125:G:H2'	1.81	0.42
55:DA:1604:C:H5'	69:DA:3982:HOH:O	2.18	0.42
1:AA:486:U:H2'	1:AA:487:A:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:116:MET:HA	7:AG:119:ARG:HB2	2.00	0.42
21:AU:4:ILE:HG13	21:AU:19:PHE:HA	2.01	0.42
1:BA:322:C:H41	1:BA:328:C:H6	1.68	0.42
1:BA:1508:A:H2'	1:BA:1509:C:O4'	2.19	0.42
2:BB:62:SER:C	2:BB:64:LYS:H	2.27	0.42
2:BB:211:THR:HA	2:BB:214:LEU:HB2	2.01	0.42
3:BC:180:ALA:HA	3:BC:206:GLU:HA	2.01	0.42
11:BK:31:ILE:HA	11:BK:46:THR:HG22	2.02	0.42
13:BM:78:LYS:HA	13:BM:81:MET:HE3	2.02	0.42
20:BT:28:MET:HE1	20:BT:67:ILE:HG12	2.02	0.42
31:CA:1093:G:H1'	31:CA:1099:G:H22	1.84	0.42
31:CA:1635:A:H2'	31:CA:1636:U:O4'	2.19	0.42
32:DD:145:SER:O	55:DA:2512:C:H1'	2.19	0.42
35:CG:145:ALA:HB1	35:CG:164:TYR:HE1	1.85	0.42
49:CV:14:LEU:HD11	49:CV:71:ALA:HB2	2.01	0.42
55:DA:28:A:H1'	55:DA:513:A:C2	2.55	0.42
55:DA:2824:C:C4	55:DA:2825:G:C5	3.07	0.42
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	2.01	0.42
16:AP:44:SER:C	16:AP:46:LYS:H	2.28	0.42
19:AS:11:ILE:HG12	19:AS:16:LEU:HD13	2.02	0.42
11:BK:123:PRO:HD2	21:BU:38:TYR:HB2	2.01	0.42
20:BT:35:VAL:HG21	20:BT:54:MET:HG2	2.01	0.42
31:CA:19:A:O2'	31:CA:553:G:H4'	2.19	0.42
31:CA:300:A:H1'	31:CA:319:G:H1'	2.02	0.42
31:CA:668:A:H2'	31:CA:670:A:H62	1.85	0.42
31:CA:2207:C:H2'	31:CA:2208:C:C6	2.55	0.42
32:DD:146:ILE:HD12	32:DD:155:VAL:CG2	2.50	0.42
34:CF:29:PRO:HB2	34:CF:169:LEU:HD22	2.02	0.42
48:CU:45:ALA:O	48:CU:49:LYS:HG2	2.19	0.42
28:DB:29:A:H2'	28:DB:30:C:C6	2.54	0.42
55:DA:1313:U:O2	55:DA:1313:U:H2'	2.19	0.42
55:DA:1446:C:O5'	55:DA:1446:C:H6	2.02	0.42
1:AA:299:G:H2'	1:AA:300:A:C8	2.54	0.42
10:AJ:29:ALA:HB2	10:AJ:87:LEU:HD11	2.02	0.42
20:AT:28:MET:HG2	20:AT:32:ILE:HD11	2.02	0.42
1:BA:413:G:H1'	1:BA:428:G:H21	1.84	0.42
1:BA:580:C:H2'	1:BA:581:G:O4'	2.19	0.42
1:BA:1426:G:H2'	1:BA:1427:C:O4'	2.20	0.42
8:BH:105:SER:HB2	8:BH:126:ILE:HD11	2.02	0.42
31:CA:573:U:N3	31:CA:2030:6MZ:H3'	2.34	0.42
31:CA:956:G:H5''	41:CN:76:LYS:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1376:C:H2'	31:CA:1377:G:O4'	2.20	0.42
29:DC:107:PRO:HB3	29:DC:142:HIS:NE2	2.34	0.42
32:DD:133:THR:HG21	55:DA:1676:A:H1'	2.02	0.42
48:CU:54:GLU:HB3	48:CU:88:LYS:HD2	2.02	0.42
36:DH:21:VAL:HG21	36:DH:25:TYR:HD2	1.85	0.42
38:DK:114:LEU:O	38:DK:117:ALA:HB3	2.19	0.42
41:DN:5:LYS:HE2	69:DA:6106:HOH:O	2.20	0.42
46:DS:3:ALA:HB3	46:DS:101:ILE:HD12	2.02	0.42
46:DS:24:LYS:HA	46:DS:94:THR:OG1	2.19	0.42
48:DU:3:ARG:HD3	48:DU:5:GLU:H	1.85	0.42
50:DW:31:TYR:O	50:DW:92:VAL:HA	2.20	0.42
55:DA:593:U:H2'	55:DA:594:U:C6	2.55	0.42
55:DA:686:U:H2'	55:DA:788:A:N1	2.34	0.42
55:DA:2813:A:H2	55:DA:2887[A]:A:N1	2.18	0.42
55:DA:2887[A]:A:H2'	55:DA:2888[A]:C:H6	1.85	0.42
1:AA:227:G:H2'	1:AA:228:A:O4'	2.20	0.42
9:AI:51:PRO:HB3	9:AI:84:THR:HG23	2.00	0.42
13:AM:78:LYS:HA	13:AM:81:MET:HE3	2.02	0.42
22:C1:2:ALA:N	31:CA:2577:A:C2	2.88	0.42
22:C1:6:ASN:ND2	31:CA:2020:A:H62	2.18	0.42
1:BA:131:A:H2'	1:BA:132:C:C6	2.54	0.42
1:BA:382:A:H2'	1:BA:383:A:C8	2.54	0.42
20:BT:31:PHE:HA	20:BT:34:LYS:HD2	2.01	0.42
31:CA:745:1MG:O2'	31:CA:748:G:H1'	2.19	0.42
31:CA:1847:A:H8	31:CA:1847:A:O5'	2.03	0.42
29:DC:146:MET:HE1	55:DA:1800:C:H5''	2.02	0.42
32:DD:172:VAL:HG12	32:DD:175:LEU:HD21	2.01	0.42
38:CK:114:LEU:O	38:CK:117:ALA:HB3	2.20	0.42
45:CR:83:LEU:HB3	45:CR:88:VAL:HB	2.01	0.42
41:DN:57:VAL:HA	41:DN:112:LEU:HD21	2.02	0.42
45:DR:92:ARG:HB2	55:DA:997:G:OP1	2.20	0.42
55:DA:121:G:H2'	55:DA:122:G:H8	1.85	0.42
55:DA:2706:A:H8	55:DA:2706:A:O5'	2.03	0.42
20:AT:22:ALA:O	20:AT:26:SER:HB2	2.20	0.41
20:AT:43:ASP:HB3	20:AT:46:ALA:HB3	2.01	0.41
25:C4:57:LEU:HD11	31:CA:834:G:H5'	2.02	0.41
1:BA:374:A:OP1	1:BA:452:A:N1	2.53	0.41
1:BA:517:G:O2'	1:BA:530:G:H4'	2.20	0.41
1:BA:827:U:H2'	1:BA:870:U:O4	2.19	0.41
6:BF:38:ARG:NH1	6:BF:99:ALA:HB3	2.35	0.41
12:BL:33:VAL:HG22	12:BL:79:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D1:12:LYS:HD2	22:D1:12:LYS:HA	1.72	0.41
23:D2:39:PHE:HB2	23:D2:46:HIS:CE1	2.55	0.41
29:CC:35:GLU:HG3	29:CC:64:ILE:HD11	2.02	0.41
30:CD:141:ARG:HB2	31:CA:1656:C:H5''	2.02	0.41
46:CS:1:MET:HE2	46:CS:1:MET:HB3	1.98	0.41
46:CS:3:ALA:HB3	46:CS:101:ILE:HD12	2.02	0.41
37:DJ:37:GLU:HB3	37:DJ:67:PHE:HZ	1.84	0.41
45:DR:13:ARG:HD2	69:DA:3914:HOH:O	2.19	0.41
55:DA:39:G:H2'	55:DA:40:U:C6	2.55	0.41
55:DA:543:G:H5''	55:DA:543:G:H8	1.85	0.41
55:DA:2243:U:O2	55:DA:2434:A:H2	2.02	0.41
7:AG:116:MET:O	7:AG:120:LEU:HB2	2.19	0.41
22:C1:53:LYS:HE3	22:C1:56:ALA:HA	2.02	0.41
2:BB:90:PHE:HB3	2:BB:151:ILE:HG22	2.02	0.41
5:BE:15:LEU:HD11	5:BE:18:VAL:HG23	2.02	0.41
31:CA:787:C:H3'	31:CA:791:C:H41	1.85	0.41
31:CA:2544:G:H5'	31:CA:2645:G:C2	2.55	0.41
38:CK:114:LEU:HG	38:CK:118:MET:HE3	2.02	0.41
40:CM:109:LYS:HA	40:CM:126:ARG:O	2.20	0.41
33:DE:66:GLY:HA2	55:DA:2060:A:OP2	2.20	0.41
38:DK:118:MET:HA	38:DK:121:LYS:NZ	2.35	0.41
55:DA:612:G:H2'	55:DA:614:A:C8	2.55	0.41
55:DA:2740:A:C6	55:DA:2764:A:C8	3.08	0.41
1:AA:1426:G:H2'	1:AA:1427:C:O4'	2.20	0.41
1:AA:1533:C:H5'	1:AA:1534:A:OP1	2.20	0.41
17:AQ:21:ILE:HD12	17:AQ:23:VAL:CG2	2.50	0.41
3:BC:33:LEU:HD21	14:BN:93:ILE:HG12	2.02	0.41
9:BI:46:MET:HA	9:BI:49:ARG:HD2	2.02	0.41
11:BK:45:ALA:HB3	11:BK:70:CYS:HB2	2.02	0.41
22:D1:27:SER:HA	69:DA:4108:HOH:O	2.20	0.41
30:CD:133:THR:CG2	31:CA:1993:U:H4'	2.39	0.41
31:CA:1190:G:H5''	40:CM:32:GLY:HA2	2.02	0.41
31:CA:1259:G:H2'	31:CA:1260:A:C8	2.55	0.41
31:CA:1638:C:H5''	31:CA:2710:C:O2'	2.19	0.41
31:CA:2198:A:C2	36:CH:29:PHE:HB2	2.55	0.41
31:CA:2428:G:N2	40:CM:60:ARG:NH2	2.58	0.41
52:CY:66:THR:O	52:CY:69:ALA:HB3	2.20	0.41
35:DG:59:ALA:C	35:DG:61:GLY:H	2.28	0.41
54:DI:29:ASP:HB3	54:DI:106:PHE:HB2	2.00	0.41
55:DA:179:C:H2'	55:DA:180:G:O4'	2.21	0.41
55:DA:565:C:H2'	55:DA:566:U:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:1450:G:C6	55:DA:1451:C:N4	2.88	0.41
55:DA:1562:U:H2'	55:DA:1563:U:O4'	2.20	0.41
55:DA:2005:A:H5''	69:DA:4377:HOH:O	2.20	0.41
1:AA:636:U:H2'	1:AA:637:C:C6	2.55	0.41
8:AH:41:LYS:HD2	8:AH:48:ASP:HA	2.02	0.41
1:BA:1062:U:H2'	1:BA:1063:C:C6	2.55	0.41
1:BA:1190:G:H5'	3:BC:176:HIS:CE1	2.55	0.41
31:CA:2849:U:P	44:CQ:93:ARG:HH21	2.43	0.41
32:DD:38:LYS:O	32:DD:46:ARG:HA	2.20	0.41
35:CG:155:GLU:HG2	35:CG:157:TYR:H	1.85	0.41
49:CV:11:VAL:HG12	49:CV:72:ILE:HA	2.01	0.41
45:DR:83:LEU:HB3	45:DR:88:VAL:HB	2.01	0.41
46:DS:1:MET:HB2	46:DS:43:ASN:CG	2.45	0.41
51:DX:39:ARG:HA	69:DX:110:HOH:O	2.19	0.41
51:DX:62:LYS:HE3	55:DA:2366:A:H4'	2.01	0.41
54:DI:91:ALA:O	54:DI:95:LEU:HB2	2.20	0.41
55:DA:198:C:O5'	55:DA:198:C:H6	2.03	0.41
55:DA:300:A:H1'	55:DA:319:G:H1'	2.02	0.41
55:DA:1482:G:H1'	55:DA:1509:A:H61	1.85	0.41
55:DA:1554:U:H1'	59:DA:3219:PUT:H32	2.03	0.41
55:DA:2822:G:H2'	55:DA:2823:A:H5''	2.03	0.41
1:AA:262:A:H5'	20:AT:68:HIS:HB3	2.03	0.41
1:AA:1017:U:H2'	1:AA:1018:G:H8	1.86	0.41
1:AA:1417:G:C6	1:AA:1482:G:C6	3.08	0.41
2:BB:129:LEU:H	2:BB:129:LEU:HG	1.53	0.41
8:BH:38:ASN:O	8:BH:42:GLU:HG3	2.21	0.41
24:D3:19:ARG:HD3	55:DA:125:A:OP2	2.21	0.41
31:CA:1:G:H1	31:CA:2902:C:H42	1.68	0.41
31:CA:708:G:N2	31:CA:724:U:H1'	2.36	0.41
31:CA:984:A:H2'	31:CA:984:A:N3	2.35	0.41
35:CG:59:ALA:C	35:CG:61:GLY:H	2.28	0.41
46:CS:38:VAL:CG2	46:CS:57:GLY:HA3	2.50	0.41
38:DK:89:PHE:CE2	38:DK:100:VAL:HG11	2.55	0.41
52:DY:18:ARG:HH21	52:DY:24:ALA:HB2	1.85	0.41
54:DI:132:TYR:HD2	54:DI:133:GLU:HG2	1.84	0.41
28:DB:1:U:H2'	28:DB:2:G:H8	1.83	0.41
55:DA:189:G:H2'	55:DA:205:G:N2	2.36	0.41
55:DA:622:G:H5''	55:DA:622:G:C8	2.55	0.41
55:DA:1093:G:H1'	55:DA:1099:G:H22	1.85	0.41
55:DA:1195:G:N3	55:DA:1226:A:H2	2.19	0.41
55:DA:1286:A:C6	55:DA:1329:U:C2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:1664:A:C8	55:DA:1664:A:O5'	2.73	0.41
55:DA:2714:G:O2'	55:DA:2715:C:H5'	2.20	0.41
1:AA:827:U:H2'	1:AA:870:U:O4	2.20	0.41
8:AH:96:MET:HE2	8:AH:130:ALA:HB1	2.02	0.41
15:AO:66:LEU:H	15:AO:66:LEU:HG	1.71	0.41
1:BA:562:U:H5	12:BL:15:LYS:HE2	1.85	0.41
26:D5:11:CYS:HB3	26:D5:33:HIS:HE1	1.85	0.41
31:CA:5:A:C2	31:CA:2899:A:C2	3.09	0.41
31:CA:323:C:H6	31:CA:1205:A:N1	2.18	0.41
31:CA:871:U:H2'	31:CA:872:U:C6	2.55	0.41
51:CX:59:LEU:HD12	51:CX:80:ILE:HD12	2.01	0.41
34:DF:104:ILE:HD11	34:DF:175:PHE:HD1	1.85	0.41
42:DO:51:LEU:HD23	42:DO:51:LEU:HA	1.87	0.41
55:DA:1189:A:H2'	55:DA:1190:G:O4'	2.21	0.41
55:DA:2057:G:H5'	69:DA:5229:HOH:O	2.20	0.41
62:DA:3194:EDO:H22	69:DA:7234:HOH:O	2.19	0.41
1:AA:517:G:O2'	1:AA:530:G:H4'	2.21	0.41
2:BB:117:LEU:HA	2:BB:120:GLN:HG2	2.01	0.41
6:BF:64:VAL:HG12	6:BF:65:GLU:N	2.36	0.41
12:BL:3:THR:HB	12:BL:6:GLN:HB2	2.03	0.41
12:BL:80:ILE:HG22	12:BL:104:CYS:HB2	2.01	0.41
16:BP:20:VAL:HG11	16:BP:32:PHE:HB2	2.02	0.41
18:BR:27:ALA:O	18:BR:30:LYS:HG2	2.21	0.41
30:CD:130:GLN:NE2	30:CD:142:VAL:HG23	2.35	0.41
31:CA:348:A:H2'	31:CA:349:U:O4'	2.20	0.41
31:CA:2250:G:N7	41:CN:82:MET:HB2	2.34	0.41
46:CS:3:ALA:HA	46:CS:40:MET:O	2.21	0.41
47:CT:20:VAL:O	47:CT:23:LEU:HB2	2.21	0.41
48:CU:47:VAL:HG11	48:CU:85:VAL:HG11	2.02	0.41
33:DE:163:ASN:HB2	55:DA:322:A:OP2	2.20	0.41
34:DF:162:SER:HB2	69:DF:207:HOH:O	2.20	0.41
47:DT:20:VAL:O	47:DT:23:LEU:HB2	2.20	0.41
48:DU:47:VAL:HG11	48:DU:85:VAL:HG11	2.02	0.41
48:DU:48:GLN:HG2	48:DU:53:VAL:O	2.20	0.41
51:DX:41[A]:ARG:HG3	55:DA:2386:A:C2	2.55	0.41
52:DY:37:ARG:HG3	52:DY:48:THR:HG23	2.03	0.41
54:DI:50:VAL:HG13	54:DI:85:VAL:HG22	2.03	0.41
55:DA:83:A:H2'	55:DA:84:A:C8	2.56	0.41
55:DA:323:C:H6	55:DA:1205:A:N1	2.19	0.41
55:DA:819:A:C4	55:DA:1189:A:C2	3.09	0.41
55:DA:1832:C:N4	55:DA:1833:C:C4	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2438:U:O2'	55:DA:2439:A:H5''	2.21	0.41
55:DA:2695:U:H3'	69:DA:4531:HOH:O	2.21	0.41
1:AA:631:C:O5'	1:AA:631:C:H6	2.04	0.41
1:AA:746:A:H2'	1:AA:747:A:C8	2.55	0.41
2:AB:90:PHE:HB3	2:AB:151:ILE:HG22	2.02	0.41
7:AG:107:ALA:HB1	7:AG:133:THR:HB	2.03	0.41
11:AK:36:ASP:OD2	11:AK:40:ASN:HB2	2.21	0.41
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	2.03	0.41
1:BA:126:G:H2'	1:BA:127:G:O4'	2.21	0.41
1:BA:202:G:H1	1:BA:215:C:H42	1.69	0.41
1:BA:1017:U:H2'	1:BA:1018:G:H8	1.85	0.41
2:BB:12:ALA:HB2	2:BB:212:LEU:HD13	2.01	0.41
29:CC:214:ARG:NH1	31:CA:1566:A:H5'	2.36	0.41
31:CA:287:G:H2'	31:CA:288:U:C6	2.56	0.41
31:CA:2660:A:H2'	31:CA:2661:G:C8	2.56	0.41
33:CE:19:PHE:HB3	33:CE:113:VAL:HG21	2.03	0.41
34:DF:40:VAL:HG21	34:DF:50:LEU:HD12	2.03	0.41
35:DG:109:PHE:CD1	55:DA:2667:C:H1'	2.55	0.41
36:DH:135:HIS:CG	36:DH:136:SER:H	2.39	0.41
45:DR:92:ARG:NH1	55:DA:997:G:H5''	2.36	0.41
55:DA:302:C:H2'	55:DA:303:G:H8	1.86	0.41
55:DA:1585:C:H2'	55:DA:1586:A:O4'	2.21	0.41
55:DA:2019:A:H2	55:DA:2035:G:H22	1.69	0.41
55:DA:2273:A:H2'	55:DA:2274:A:C8	2.55	0.41
55:DA:2519:U:C6	55:DA:2542:A:N6	2.89	0.41
1:AA:131:A:H2'	1:AA:132:C:C6	2.55	0.41
1:AA:382:A:H2'	1:AA:383:A:C8	2.56	0.41
1:AA:580:C:H2'	1:AA:581:G:O4'	2.21	0.41
1:AA:845:A:P	1:AA:845:A:O4'	2.79	0.41
2:AB:12:ALA:HB2	2:AB:212:LEU:HD13	2.02	0.41
2:AB:211:THR:HA	2:AB:214:LEU:HB2	2.01	0.41
9:AI:46:MET:HA	9:AI:49:ARG:HD2	2.02	0.41
11:AK:31:ILE:HA	11:AK:46:THR:HG22	2.02	0.41
1:BA:240:G:H5''	1:BA:240:G:C8	2.56	0.41
1:BA:486:U:H2'	1:BA:487:A:H8	1.85	0.41
1:BA:536:C:OP1	69:BA:1701:HOH:O	2.22	0.41
7:BG:116:MET:O	7:BG:120:LEU:HB2	2.20	0.41
15:BO:24:SER:HB3	15:BO:27:VAL:HG23	2.03	0.41
15:BO:66:LEU:H	15:BO:66:LEU:HG	1.71	0.41
27:D0:18:PRO:HD2	69:D0:206:HOH:O	2.21	0.41
30:CD:117:GLY:HA2	30:CD:164:GLN:HE22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1676:A:H2'	31:CA:1677:A:O4'	2.20	0.41
31:CA:2146:C:H4'	31:CA:2147:A:O5'	2.21	0.41
39:CL:119:ALA:HA	39:CL:120:PRO:HD3	1.91	0.41
47:CT:82:MET:HB2	47:CT:98:LYS:HB2	2.02	0.41
33:DE:45:ALA:HB3	55:DA:38:A:H5'	2.02	0.41
37:DJ:55:ILE:HA	37:DJ:56:PRO:HD3	2.00	0.41
47:DT:20:VAL:HG11	47:DT:44:ALA:HA	2.02	0.41
47:DT:100:THR:HG21	69:DT:346:HOH:O	2.21	0.41
51:DX:41[B]:ARG:HA	51:DX:41[B]:ARG:HH11	1.85	0.41
55:DA:287:G:H2'	55:DA:288:U:C6	2.56	0.41
55:DA:1356:G:C2	55:DA:1376:C:O2	2.74	0.41
55:DA:1782:U:H2'	55:DA:1783:A:H5'	2.03	0.41
55:DA:2082:A:H2'	55:DA:2083:G:O4'	2.20	0.41
55:DA:2660:A:H2'	55:DA:2661:G:C8	2.56	0.41
1:AA:845:A:H2'	1:AA:846:G:O4'	2.21	0.41
1:AA:1088:G:H21	1:AA:1167:A:H62	1.69	0.41
1:AA:1508:A:H2'	1:AA:1509:C:O4'	2.21	0.41
2:AB:167:ASP:CG	2:AB:191:SER:HA	2.45	0.41
17:AQ:12:VAL:HG12	17:AQ:55:ILE:HA	2.03	0.41
1:BA:368:U:O4	36:DH:83:LYS:HB2	2.21	0.41
1:BA:577:G:C1'	1:BA:816:A:H2'	2.51	0.41
1:BA:1048:G:H4'	14:BN:3:LYS:HE2	2.03	0.41
1:BA:1171:A:H2'	1:BA:1172:C:C6	2.55	0.41
1:BA:1411:C:H2'	1:BA:1412:C:H6	1.85	0.41
3:BC:47:LEU:HB3	3:BC:50:ALA:HB3	2.02	0.41
5:BE:57:PRO:HA	5:BE:60:ILE:HG13	2.02	0.41
12:BL:82:ILE:HD11	12:BL:95:TYR:HB2	2.03	0.41
19:BS:11:ILE:HG12	19:BS:16:LEU:HD13	2.02	0.41
31:CA:172:A:H2'	31:CA:173:A:C8	2.56	0.41
31:CA:297:G:H5''	49:CV:85:PHE:HB2	2.02	0.41
31:CA:379:G:O4'	31:CA:2232:C:H5''	2.21	0.41
46:CS:76:LYS:O	46:CS:84:ARG:HA	2.21	0.41
45:DR:105:ALA:HB1	46:DS:40:MET:HE1	2.02	0.41
46:DS:3:ALA:HA	46:DS:40:MET:O	2.21	0.41
47:DT:20:VAL:HA	47:DT:23:LEU:HD12	2.03	0.41
55:DA:665:U:H2'	55:DA:666:A:H8	1.85	0.41
55:DA:1782:U:H3'	69:DA:4190:HOH:O	2.21	0.41
1:AA:9:G:OP2	5:AE:126:LYS:HE2	2.21	0.40
11:AK:52:PHE:CE2	11:AK:65:VAL:HG21	2.56	0.40
14:AN:46:LEU:HA	14:AN:49:GLN:HE21	1.85	0.40
22:C1:12:LYS:HA	22:C1:12:LYS:HD2	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:377:G:H2'	1:BA:378:G:H8	1.86	0.40
1:BA:1068:G:N7	1:BA:1094:G:H2'	2.36	0.40
27:D0:26:GLY:O	55:DA:929:U:H1'	2.21	0.40
28:CB:24:G:H1'	28:CB:27:C:N4	2.36	0.40
31:CA:65:U:H2'	31:CA:66:C:C6	2.56	0.40
31:CA:528:A:N1	31:CA:2042:A:H2'	2.36	0.40
31:CA:2598:A:C8	31:CA:2599:G:H1'	2.56	0.40
42:CO:92:GLY:HA2	42:CO:94:TYR:CZ	2.56	0.40
43:CP:39:VAL:HG11	43:CP:87:ILE:HG21	2.03	0.40
49:DV:15:THR:HG23	55:DA:310:A:H5''	2.03	0.40
54:DI:64:VAL:CG2	54:DI:69:PHE:HB2	2.50	0.40
55:DA:65:U:H2'	55:DA:66:C:C6	2.56	0.40
55:DA:2261:C:H1'	55:DA:2388:A:N3	2.35	0.40
11:AK:123:PRO:HD2	21:AU:38:TYR:HB2	2.03	0.40
20:AT:44:LYS:H	20:AT:44:LYS:HG3	1.48	0.40
21:AU:40:LYS:HB2	21:AU:43:THR:OG1	2.21	0.40
1:BA:562:U:H4'	1:BA:563:A:O5'	2.21	0.40
11:BK:52:PHE:HE2	11:BK:65:VAL:HG21	1.86	0.40
31:CA:189:G:H2'	31:CA:205:G:N2	2.37	0.40
31:CA:244:A:H62	31:CA:254:G:H21	1.70	0.40
31:CA:304:U:H2'	31:CA:305:C:C6	2.56	0.40
31:CA:1940:U:H5''	31:CA:1965:C:C5	2.55	0.40
31:CA:2538:C:H2'	31:CA:2539:C:C6	2.56	0.40
33:CE:196:VAL:HG13	33:CE:200:LEU:HD13	2.03	0.40
39:CL:35:VAL:HB	39:CL:36:GLY:H	1.66	0.40
36:DH:117:LEU:HA	36:DH:118:PRO:HD3	2.00	0.40
55:DA:2042:A:H2	69:DA:7342:HOH:O	2.04	0.40
3:AC:33:LEU:HD21	14:AN:93:ILE:HG12	2.02	0.40
5:AE:80:THR:HB	5:AE:122:ASN:HB2	2.03	0.40
9:AI:98:LEU:HB3	9:AI:104:VAL:HG13	2.02	0.40
20:AT:27:MET:HE3	20:AT:27:MET:HB3	2.00	0.40
2:BB:83:ALA:HB3	2:BB:214:LEU:HD22	2.02	0.40
8:BH:76:GLN:O	8:BH:127:CYS:HB2	2.21	0.40
25:D4:26:HIS:NE2	25:D4:48:ALA:HB2	2.36	0.40
31:CA:302:C:H2'	31:CA:303:G:H8	1.85	0.40
31:CA:2328:A:H8	31:CA:2328:A:O5'	2.04	0.40
31:CA:2464:G:C2	31:CA:2465:C:H1'	2.57	0.40
31:CA:2693:G:H2'	31:CA:2694:G:H8	1.85	0.40
29:DC:53:HIS:NE2	29:DC:219:THR:HG23	2.37	0.40
32:DD:175:LEU:HA	69:DD:435:HOH:O	2.22	0.40
34:CF:8:TYR:HB2	34:CF:173:PHE:CZ	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:CF:40:VAL:HG21	34:CF:50:LEU:HD12	2.04	0.40
39:CL:15:GLY:HA2	39:CL:47:ILE:HG12	2.03	0.40
44:DQ:94:LYS:HE2	55:DA:1754:A:C8	2.56	0.40
55:DA:638:G:H2'	55:DA:639:U:C6	2.57	0.40
1:AA:377:G:H2'	1:AA:378:G:H8	1.87	0.40
1:AA:511:C:H5'	4:AD:44:ARG:CZ	2.52	0.40
1:AA:1235:U:H2'	1:AA:1236:A:O4'	2.22	0.40
2:AB:20:THR:HA	2:AB:39:HIS:CE1	2.56	0.40
2:AB:100:MET:HE2	2:AB:148:LEU:HD23	2.03	0.40
2:AB:117:LEU:HA	2:AB:120:GLN:HG2	2.03	0.40
15:AO:24:SER:HB3	15:AO:27:VAL:HG23	2.04	0.40
1:BA:1235:U:H2'	1:BA:1236:A:O4'	2.22	0.40
10:BJ:59:LYS:H	10:BJ:59:LYS:HG3	1.66	0.40
11:BK:52:PHE:CE2	11:BK:65:VAL:HG21	2.56	0.40
13:BM:4:ILE:HA	13:BM:57:ARG:HG2	2.04	0.40
31:CA:7:G:H4'	38:CK:15:TRP:CZ2	2.56	0.40
31:CA:179:C:H2'	31:CA:180:G:O4'	2.22	0.40
31:CA:1101:U:H2'	31:CA:1102:C:H6	1.86	0.40
31:CA:1313:U:H5'	69:CA:3366:HOH:O	2.21	0.40
31:CA:2547:A:H4'	39:CL:29:HIS:NE2	2.36	0.40
47:CT:29:VAL:O	47:CT:33:LEU:HD12	2.21	0.40
34:DF:138:PHE:HA	34:DF:139:PRO:HD3	1.93	0.40
34:DF:175:PHE:HA	34:DF:176:PRO:HD3	1.95	0.40
43:DP:53:THR:HB	43:DP:65:THR:HG22	2.04	0.40
49:DV:52:LEU:C	49:DV:54:GLN:N	2.79	0.40
55:DA:2498:OMC:HM23	55:DA:2498:OMC:H1'	1.95	0.40
55:DA:2538:C:H2'	55:DA:2539:C:C6	2.57	0.40
1:AA:407:U:H2'	1:AA:408:A:H8	1.86	0.40
1:AA:562:U:H5	12:AL:15:LYS:HE2	1.86	0.40
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.57	0.40
8:AH:87:LYS:HB2	8:AH:125:ILE:CD1	2.50	0.40
1:BA:110:C:H1'	69:BA:1786:HOH:O	2.21	0.40
1:BA:227:G:H2'	1:BA:228:A:O4'	2.20	0.40
1:BA:240:G:OP1	1:BA:240:G:H4'	2.22	0.40
10:BJ:12:ALA:HB3	10:BJ:18:ILE:HB	2.03	0.40
12:BL:44:LYS:HB2	12:BL:45:PRO:HD3	2.03	0.40
24:D3:3:ARG:HB2	55:DA:1612:C:O2'	2.21	0.40
31:CA:4:U:H2'	31:CA:5:A:C8	2.57	0.40
31:CA:963:U:H2'	31:CA:964:C:C6	2.56	0.40
31:CA:2066:C:O2'	31:CA:2067:G:H5'	2.22	0.40
48:CU:30:ILE:HG22	48:CU:85:VAL:HB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:CV:26:LYS:HB2	49:CV:35:ILE:HG22	2.04	0.40
33:DE:19:PHE:HB3	33:DE:113:VAL:HG21	2.03	0.40
33:DE:132:LYS:HD2	55:DA:320:A:OP2	2.21	0.40
55:DA:192:C:O2'	55:DA:802:A:H1'	2.21	0.40
55:DA:2521:C:H2'	55:DA:2522:U:C6	2.57	0.40
55:DA:2844:G:H2'	55:DA:2845:U:O4'	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	203 (91%)	14 (6%)	5 (2%)	5	26
2	BB	222/224 (99%)	203 (91%)	14 (6%)	5 (2%)	5	26
3	AC	204/206 (99%)	193 (95%)	9 (4%)	2 (1%)	12	41
3	BC	204/206 (99%)	193 (95%)	8 (4%)	3 (2%)	8	33
4	AD	203/205 (99%)	191 (94%)	12 (6%)	0	100	100
4	BD	203/205 (99%)	192 (95%)	11 (5%)	0	100	100
5	AE	153/155 (99%)	139 (91%)	12 (8%)	2 (1%)	9	35
5	BE	148/155 (96%)	126 (85%)	17 (12%)	5 (3%)	3	19
6	AF	104/106 (98%)	95 (91%)	8 (8%)	1 (1%)	12	41
6	BF	98/106 (92%)	83 (85%)	12 (12%)	3 (3%)	3	21
7	AG	149/151 (99%)	137 (92%)	10 (7%)	2 (1%)	9	35
7	BG	149/151 (99%)	140 (94%)	7 (5%)	2 (1%)	9	35
8	AH	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	7	32
8	BH	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	16	45
9	AI	125/127 (98%)	109 (87%)	16 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	BI	125/127 (98%)	109 (87%)	16 (13%)	0	100	100
10	AJ	97/99 (98%)	86 (89%)	8 (8%)	3 (3%)	3	21
10	BJ	96/99 (97%)	78 (81%)	14 (15%)	4 (4%)	2	15
11	AK	115/129 (89%)	104 (90%)	10 (9%)	1 (1%)	14	43
11	BK	115/129 (89%)	101 (88%)	13 (11%)	1 (1%)	14	43
12	AL	120/123 (98%)	110 (92%)	8 (7%)	2 (2%)	7	31
12	BL	120/123 (98%)	109 (91%)	9 (8%)	2 (2%)	7	31
13	AM	112/114 (98%)	99 (88%)	9 (8%)	4 (4%)	2	18
13	BM	112/114 (98%)	96 (86%)	10 (9%)	6 (5%)	1	10
14	AN	98/100 (98%)	89 (91%)	8 (8%)	1 (1%)	12	41
14	BN	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	12	41
15	AO	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
15	BO	86/88 (98%)	79 (92%)	6 (7%)	1 (1%)	10	37
16	AP	80/82 (98%)	71 (89%)	7 (9%)	2 (2%)	4	24
16	BP	80/82 (98%)	67 (84%)	10 (12%)	3 (4%)	2	17
17	AQ	78/80 (98%)	70 (90%)	5 (6%)	3 (4%)	2	17
17	BQ	78/80 (98%)	69 (88%)	5 (6%)	4 (5%)	1	12
18	AR	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/79 (98%)	68 (88%)	6 (8%)	3 (4%)	2	16
19	BS	77/79 (98%)	68 (88%)	7 (9%)	2 (3%)	4	24
20	AT	84/86 (98%)	80 (95%)	4 (5%)	0	100	100
20	BT	83/86 (96%)	78 (94%)	4 (5%)	1 (1%)	10	37
21	AU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
21	BU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
22	C1	54/56 (96%)	45 (83%)	6 (11%)	3 (6%)	1	10
22	D1	54/56 (96%)	54 (100%)	0	0	100	100
23	C2	48/51 (94%)	43 (90%)	4 (8%)	1 (2%)	5	27
23	D2	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
24	C3	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	5	26
24	D3	44/46 (96%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	C4	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	7	32
25	D4	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	7	32
26	C5	36/38 (95%)	36 (100%)	0	0	100	100
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	51 (91%)	3 (5%)	2 (4%)	2	18
27	D0	57/58 (98%)	52 (91%)	5 (9%)	0	100	100
29	CC	269/272 (99%)	243 (90%)	21 (8%)	5 (2%)	6	29
29	DC	269/272 (99%)	245 (91%)	19 (7%)	5 (2%)	6	29
30	CD	207/209 (99%)	193 (93%)	11 (5%)	3 (1%)	9	34
32	DD	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
33	CE	199/201 (99%)	184 (92%)	14 (7%)	1 (0%)	24	56
33	DE	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
34	CF	175/178 (98%)	161 (92%)	14 (8%)	0	100	100
34	DF	175/178 (98%)	163 (93%)	12 (7%)	0	100	100
35	CG	174/176 (99%)	158 (91%)	12 (7%)	4 (2%)	5	26
35	DG	174/176 (99%)	160 (92%)	13 (8%)	1 (1%)	21	52
36	CH	147/149 (99%)	129 (88%)	12 (8%)	6 (4%)	2	15
36	DH	147/149 (99%)	131 (89%)	12 (8%)	4 (3%)	4	23
37	CJ	132/135 (98%)	120 (91%)	8 (6%)	4 (3%)	3	21
37	DJ	132/135 (98%)	120 (91%)	8 (6%)	4 (3%)	3	21
38	CK	140/142 (99%)	130 (93%)	7 (5%)	3 (2%)	5	27
38	DK	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	5	27
39	CL	120/123 (98%)	111 (92%)	7 (6%)	2 (2%)	7	31
39	DL	121/123 (98%)	114 (94%)	6 (5%)	1 (1%)	16	45
40	CM	142/144 (99%)	128 (90%)	8 (6%)	6 (4%)	2	15
40	DM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	5	27
41	CN	133/136 (98%)	121 (91%)	12 (9%)	0	100	100
41	DN	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
42	CO	118/127 (93%)	98 (83%)	16 (14%)	4 (3%)	3	19
42	DO	123/127 (97%)	106 (86%)	16 (13%)	1 (1%)	16	45
43	CP	114/117 (97%)	110 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	DP	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
44	CQ	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	14	43
44	DQ	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	14	43
45	CR	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
45	DR	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
46	CS	101/103 (98%)	89 (88%)	10 (10%)	2 (2%)	6	28
46	DS	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	12	41
47	CT	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
47	DT	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	14	43
48	CU	91/100 (91%)	85 (93%)	5 (6%)	1 (1%)	11	40
48	DU	91/100 (91%)	86 (94%)	4 (4%)	1 (1%)	11	40
49	CV	100/103 (97%)	85 (85%)	12 (12%)	3 (3%)	3	21
49	DV	100/103 (97%)	87 (87%)	11 (11%)	2 (2%)	6	28
50	CW	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	11	40
50	DW	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	11	40
51	CX	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
51	DX	75/76 (99%)	71 (95%)	4 (5%)	0	100	100
52	CY	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
52	DY	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
53	CZ	60/62 (97%)	51 (85%)	8 (13%)	1 (2%)	7	31
53	DZ	60/62 (97%)	51 (85%)	8 (13%)	1 (2%)	7	31
54	DI	133/135 (98%)	112 (84%)	17 (13%)	4 (3%)	3	21
All	All	11407/11679 (98%)	10425 (91%)	815 (7%)	167 (2%)	8	33

All (167) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	95	ARG
2	AB	126	PHE
3	AC	156	ARG
13	AM	5	ALA
17	AQ	82	ALA
22	C1	25	VAL
22	C1	27	SER

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Mol	Chain	Res	Type
23	C2	5	ILE
27	C0	4	THR
2	BB	95	ARG
2	BB	126	PHE
3	BC	156	ARG
6	BF	98	GLU
13	BM	7	ILE
17	BQ	82	ALA
20	BT	5	LYS
29	CC	108	LYS
29	CC	158	ALA
33	CE	83	VAL
35	CG	46	ALA
35	CG	119	ALA
35	CG	175	LYS
35	CG	176	LYS
36	CH	10	ALA
37	CJ	19	ASN
38	CK	81	ILE
40	CM	29	LYS
48	CU	89	GLU
35	DG	46	ALA
36	DH	11	ASN
37	DJ	19	ASN
49	DV	52	LEU
54	DI	91	ALA
3	AC	127	ARG
5	AE	162	GLU
8	AH	66	PHE
10	AJ	33	GLY
10	AJ	57	VAL
11	AK	89	PRO
14	AN	38	ASP
16	AP	31	ARG
19	AS	31	LEU
3	BC	61	ALA
3	BC	127	ARG
5	BE	110	ALA
6	BF	99	ALA
8	BH	66	PHE
10	BJ	38	GLY
10	BJ	57	VAL

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Mol	Chain	Res	Type
11	BK	89	PRO
13	BM	5	ALA
14	BN	38	ASP
15	BO	88	ARG
16	BP	31	ARG
17	BQ	16	LYS
17	BQ	70	THR
29	CC	122	ALA
29	DC	122	ALA
29	DC	261	LYS
36	CH	11	ASN
38	CK	95	ARG
39	CL	35	VAL
40	CM	30	THR
40	CM	36	LYS
40	CM	69	ARG
44	CQ	105	GLY
49	CV	89	ASP
38	DK	95	ARG
40	DM	29	LYS
40	DM	36	LYS
44	DQ	105	GLY
46	DS	44	GLY
48	DU	89	GLU
49	DV	89	ASP
54	DI	130	PRO
2	AB	127	ASP
7	AG	56	LYS
10	AJ	58	ASN
12	AL	48	ALA
12	AL	74	LEU
19	AS	8	GLY
22	C1	26	THR
2	BB	127	ASP
5	BE	103	THR
5	BE	109	GLY
7	BG	56	LYS
10	BJ	36	VAL
10	BJ	58	ASN
13	BM	114	LYS
19	BS	7	LYS
19	BS	31	LEU

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Mol	Chain	Res	Type
29	CC	233	GLY
29	CC	253	LYS
30	CD	105	LYS
29	DC	233	GLY
36	CH	9	VAL
36	CH	122	LEU
37	CJ	23	PRO
37	CJ	32	GLY
39	CL	108	ARG
42	CO	119	SER
49	CV	7	ARG
49	CV	17	LYS
36	DH	122	LEU
37	DJ	23	PRO
37	DJ	32	GLY
39	DL	108	ARG
5	AE	109	GLY
6	AF	56	LYS
13	AM	7	ILE
17	AQ	16	LYS
17	AQ	68	SER
24	C3	45	SER
6	BF	56	LYS
12	BL	74	LEU
13	BM	47	GLU
16	BP	44	SER
16	BP	80	LYS
30	CD	86	GLU
37	CJ	25	GLY
53	CZ	41	HIS
37	DJ	25	GLY
50	DW	23	ALA
53	DZ	41	HIS
54	DI	88	HIS
2	AB	125	THR
7	AG	17	LYS
13	AM	47	GLU
13	AM	105	ASN
16	AP	45	GLU
19	AS	7	LYS
2	BB	125	THR
5	BE	24	THR

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Mol	Chain	Res	Type
7	BG	17	LYS
12	BL	44	LYS
13	BM	4	ILE
13	BM	105	ASN
17	BQ	17	MET
30	CD	149	ASN
29	DC	253	LYS
29	DC	262	ARG
36	CH	8	LYS
36	CH	34	GLY
40	CM	58	TYR
42	CO	32	GLU
42	CO	104	ALA
42	CO	118	ARG
46	CS	53	PHE
50	CW	23	ALA
38	DK	25	LEU
40	DM	58	TYR
42	DO	32	GLU
54	DI	108	VAL
8	AH	68	GLY
38	CK	25	LEU
40	CM	68	SER
46	CS	48	LYS
36	DH	10	ALA
36	DH	34	GLY
47	DT	66	ILE
2	AB	71	GLY
2	BB	71	GLY
25	D4	7	VAL
27	C0	14	ILE
25	C4	7	VAL
5	BE	25	VAL
38	DK	83	GLY

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	186/186 (100%)	169 (91%)	17 (9%)	9	32
2	BB	186/186 (100%)	169 (91%)	17 (9%)	9	32
3	AC	170/170 (100%)	157 (92%)	13 (8%)	12	38
3	BC	170/170 (100%)	155 (91%)	15 (9%)	9	33
4	AD	172/172 (100%)	160 (93%)	12 (7%)	14	41
4	BD	172/172 (100%)	159 (92%)	13 (8%)	12	38
5	AE	118/118 (100%)	98 (83%)	20 (17%)	2	10
5	BE	113/118 (96%)	95 (84%)	18 (16%)	2	12
6	AF	92/92 (100%)	79 (86%)	13 (14%)	3	15
6	BF	87/92 (95%)	72 (83%)	15 (17%)	2	10
7	AG	124/124 (100%)	107 (86%)	17 (14%)	3	16
7	BG	124/124 (100%)	107 (86%)	17 (14%)	3	16
8	AH	104/104 (100%)	86 (83%)	18 (17%)	2	9
8	BH	104/104 (100%)	88 (85%)	16 (15%)	2	13
9	AI	105/105 (100%)	95 (90%)	10 (10%)	8	30
9	BI	105/105 (100%)	94 (90%)	11 (10%)	6	25
10	AJ	87/87 (100%)	79 (91%)	8 (9%)	8	31
10	BJ	86/87 (99%)	76 (88%)	10 (12%)	5	21
11	AK	90/99 (91%)	86 (96%)	4 (4%)	25	54
11	BK	90/99 (91%)	82 (91%)	8 (9%)	9	32
12	AL	102/102 (100%)	93 (91%)	9 (9%)	9	33
12	BL	102/102 (100%)	90 (88%)	12 (12%)	5	21
13	AM	92/92 (100%)	81 (88%)	11 (12%)	5	20
13	BM	92/92 (100%)	79 (86%)	13 (14%)	3	15
14	AN	83/83 (100%)	80 (96%)	3 (4%)	31	58
14	BN	83/83 (100%)	80 (96%)	3 (4%)	31	58
15	AO	76/76 (100%)	72 (95%)	4 (5%)	20	49
15	BO	76/76 (100%)	70 (92%)	6 (8%)	11	37
16	AP	65/65 (100%)	61 (94%)	4 (6%)	16	45
16	BP	65/65 (100%)	60 (92%)	5 (8%)	12	38
17	AQ	74/74 (100%)	65 (88%)	9 (12%)	5	20
17	BQ	74/74 (100%)	63 (85%)	11 (15%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	48/48 (100%)	46 (96%)	2 (4%)	26	55
18	BR	48/48 (100%)	47 (98%)	1 (2%)	47	66
19	AS	70/70 (100%)	61 (87%)	9 (13%)	4	18
19	BS	70/70 (100%)	62 (89%)	8 (11%)	5	22
20	AT	65/65 (100%)	53 (82%)	12 (18%)	1	8
20	BT	65/65 (100%)	53 (82%)	12 (18%)	1	8
21	AU	48/48 (100%)	43 (90%)	5 (10%)	7	25
21	BU	48/48 (100%)	43 (90%)	5 (10%)	7	25
22	C1	47/47 (100%)	46 (98%)	1 (2%)	47	66
22	D1	47/47 (100%)	45 (96%)	2 (4%)	26	54
23	C2	45/46 (98%)	40 (89%)	5 (11%)	6	23
23	D2	45/46 (98%)	40 (89%)	5 (11%)	6	23
24	C3	38/38 (100%)	34 (90%)	4 (10%)	6	25
24	D3	38/38 (100%)	33 (87%)	5 (13%)	4	17
25	C4	51/51 (100%)	48 (94%)	3 (6%)	18	46
25	D4	51/51 (100%)	48 (94%)	3 (6%)	18	46
26	C5	34/34 (100%)	31 (91%)	3 (9%)	9	33
26	D5	34/34 (100%)	32 (94%)	2 (6%)	18	46
27	C0	48/48 (100%)	41 (85%)	7 (15%)	3	14
27	D0	49/48 (102%)	41 (84%)	8 (16%)	2	11
29	CC	216/217 (100%)	198 (92%)	18 (8%)	10	35
29	DC	216/217 (100%)	200 (93%)	16 (7%)	13	39
30	CD	164/164 (100%)	150 (92%)	14 (8%)	10	34
32	DD	163/163 (100%)	150 (92%)	13 (8%)	11	37
33	CE	165/165 (100%)	147 (89%)	18 (11%)	6	24
33	DE	165/165 (100%)	151 (92%)	14 (8%)	10	34
34	CF	148/149 (99%)	126 (85%)	22 (15%)	3	14
34	DF	148/149 (99%)	127 (86%)	21 (14%)	3	15
35	CG	137/137 (100%)	126 (92%)	11 (8%)	11	37
35	DG	137/137 (100%)	125 (91%)	12 (9%)	9	33
36	CH	114/114 (100%)	98 (86%)	16 (14%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	DH	114/114 (100%)	100 (88%)	14 (12%)	4	19
37	CJ	104/105 (99%)	92 (88%)	12 (12%)	5	21
37	DJ	104/105 (99%)	92 (88%)	12 (12%)	5	21
38	CK	116/116 (100%)	111 (96%)	5 (4%)	26	54
38	DK	116/116 (100%)	110 (95%)	6 (5%)	21	49
39	CL	103/104 (99%)	95 (92%)	8 (8%)	11	37
39	DL	104/104 (100%)	94 (90%)	10 (10%)	8	29
40	CM	103/103 (100%)	90 (87%)	13 (13%)	4	19
40	DM	103/103 (100%)	96 (93%)	7 (7%)	14	42
41	CN	108/108 (100%)	94 (87%)	14 (13%)	4	17
41	DN	109/108 (101%)	97 (89%)	12 (11%)	6	23
42	CO	100/103 (97%)	91 (91%)	9 (9%)	9	32
42	DO	102/103 (99%)	94 (92%)	8 (8%)	11	37
43	CP	86/87 (99%)	77 (90%)	9 (10%)	6	25
43	DP	87/87 (100%)	77 (88%)	10 (12%)	5	21
44	CQ	99/99 (100%)	89 (90%)	10 (10%)	7	27
44	DQ	99/99 (100%)	89 (90%)	10 (10%)	7	27
45	CR	89/89 (100%)	83 (93%)	6 (7%)	15	43
45	DR	89/89 (100%)	83 (93%)	6 (7%)	15	43
46	CS	84/84 (100%)	73 (87%)	11 (13%)	4	17
46	DS	84/84 (100%)	76 (90%)	8 (10%)	8	30
47	CT	93/93 (100%)	80 (86%)	13 (14%)	3	15
47	DT	93/93 (100%)	80 (86%)	13 (14%)	3	15
48	CU	80/84 (95%)	62 (78%)	18 (22%)	1	5
48	DU	80/84 (95%)	67 (84%)	13 (16%)	2	11
49	CV	83/84 (99%)	72 (87%)	11 (13%)	4	17
49	DV	83/84 (99%)	76 (92%)	7 (8%)	10	35
50	CW	78/78 (100%)	70 (90%)	8 (10%)	7	26
50	DW	78/78 (100%)	71 (91%)	7 (9%)	9	32
51	CX	56/58 (97%)	54 (96%)	2 (4%)	31	58
51	DX	58/58 (100%)	53 (91%)	5 (9%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	CY	67/67 (100%)	59 (88%)	8 (12%)	5	20
52	DY	67/67 (100%)	59 (88%)	8 (12%)	5	20
53	CZ	54/54 (100%)	49 (91%)	5 (9%)	8	31
53	DZ	54/54 (100%)	50 (93%)	4 (7%)	13	39
54	DI	103/103 (100%)	91 (88%)	12 (12%)	5	21
All	All	9461/9514 (99%)	8488 (90%)	973 (10%)	7	26

All (973) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	23	TRP
2	AB	57	LEU
2	AB	73	LYS
2	AB	93	ASN
2	AB	105	LYS
2	AB	108	ARG
2	AB	116	ASP
2	AB	125	THR
2	AB	129	LEU
2	AB	130	THR
2	AB	135	LEU
2	AB	147	SER
2	AB	151	ILE
2	AB	161	LEU
2	AB	205	ASP
2	AB	207	ILE
2	AB	211	THR
3	AC	33	LEU
3	AC	36	ASP
3	AC	46	GLU
3	AC	55	ILE
3	AC	58	GLU
3	AC	75	ILE
3	AC	107	ARG
3	AC	110	GLU
3	AC	121	THR
3	AC	128	VAL
3	AC	178	LEU
3	AC	186	THR
3	AC	207	ILE

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Mol	Chain	Res	Type
4	AD	22	LYS
4	AD	25	VAL
4	AD	26	ARG
4	AD	116	GLN
4	AD	129	VAL
4	AD	132	ILE
4	AD	142	VAL
4	AD	143	VAL
4	AD	169	THR
4	AD	194	ASP
4	AD	195	ILE
4	AD	196	ASN
5	AE	14	LYS
5	AE	26	LYS
5	AE	46	VAL
5	AE	70	ASN
5	AE	76	LEU
5	AE	78	ASN
5	AE	81	LEU
5	AE	82	GLN
5	AE	88	VAL
5	AE	94	VAL
5	AE	101	GLU
5	AE	106	ILE
5	AE	120	VAL
5	AE	123	VAL
5	AE	126	LYS
5	AE	134	ILE
5	AE	140	THR
5	AE	148	ASN
5	AE	159	LYS
5	AE	162	GLU
6	AF	14	GLN
6	AF	17	GLN
6	AF	36	ILE
6	AF	39	LEU
6	AF	62	MET
6	AF	68	GLN
6	AF	69	GLU
6	AF	71	ILE
6	AF	72	ASP
6	AF	79	ARG

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Mol	Chain	Res	Type
6	AF	90	MET
6	AF	92	THR
6	AF	93	LYS
7	AG	4	ARG
7	AG	13	LEU
7	AG	22	LEU
7	AG	23	LEU
7	AG	30	LEU
7	AG	36	LYS
7	AG	58	GLU
7	AG	63	GLU
7	AG	76	LYS
7	AG	83	SER
7	AG	89	VAL
7	AG	95	ARG
7	AG	120	LEU
7	AG	131	LYS
7	AG	138	ARG
7	AG	142	HIS
7	AG	146	GLU
8	AH	3	MET
8	AH	9	ASP
8	AH	13	ARG
8	AH	26	THR
8	AH	31	LYS
8	AH	46	ILE
8	AH	47	GLU
8	AH	51	VAL
8	AH	52	GLU
8	AH	54	ASP
8	AH	55	THR
8	AH	59	LEU
8	AH	60	GLU
8	AH	63	LEU
8	AH	71	VAL
8	AH	87	LYS
8	AH	101	ILE
8	AH	117	ARG
9	AI	9	THR
9	AI	11	ARG
9	AI	30	ILE
9	AI	36	GLU

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Mol	Chain	Res	Type
9	AI	61	LEU
9	AI	63	LEU
9	AI	66	THR
9	AI	87	LEU
9	AI	89	GLU
9	AI	111	VAL
10	AJ	6	ILE
10	AJ	62	ARG
10	AJ	65	TYR
10	AJ	69	THR
10	AJ	88	MET
10	AJ	89	ARG
10	AJ	100	ILE
10	AJ	102	LEU
11	AK	33	THR
11	AK	82	LEU
11	AK	85	MET
11	AK	97	ILE
12	AL	24	LEU
12	AL	40	THR
12	AL	41	THR
12	AL	49	LEU
12	AL	55	VAL
12	AL	62	GLU
12	AL	82	ILE
12	AL	110	ARG
12	AL	121	ARG
13	AM	7	ILE
13	AM	8	ASN
13	AM	13	LYS
13	AM	22	ILE
13	AM	27	LYS
13	AM	48	LEU
13	AM	58	ASP
13	AM	59	GLU
13	AM	64	VAL
13	AM	71	ARG
13	AM	95	LEU
14	AN	27	LEU
14	AN	31	ILE
14	AN	84	VAL
15	AO	25	THR

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Mol	Chain	Res	Type
15	AO	40	GLN
15	AO	66	LEU
15	AO	70	LEU
16	AP	2	VAL
16	AP	20	VAL
16	AP	33	ILE
16	AP	48	GLU
17	AQ	5	ILE
17	AQ	13	VAL
17	AQ	16	LYS
17	AQ	20	SER
17	AQ	29	VAL
17	AQ	38	ILE
17	AQ	40	ARG
17	AQ	75	LEU
17	AQ	83	VAL
18	AR	20	GLU
18	AR	24	LYS
19	AS	5	LEU
19	AS	7	LYS
19	AS	13	LEU
19	AS	27	ASP
19	AS	37	ARG
19	AS	52	HIS
19	AS	60	VAL
19	AS	63	THR
19	AS	65	GLU
20	AT	12	ILE
20	AT	14	SER
20	AT	15	GLU
20	AT	24	ARG
20	AT	26	SER
20	AT	44	LYS
20	AT	54	MET
20	AT	64	LYS
20	AT	66	LEU
20	AT	67	ILE
20	AT	85	LYS
20	AT	86	LEU
21	AU	13	ASP
21	AU	14	VAL
21	AU	16	LEU

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Mol	Chain	Res	Type
21	AU	20	LYS
21	AU	56	HIS
22	C1	40	ARG
23	C2	5	ILE
23	C2	28	ARG
23	C2	42	VAL
23	C2	47	VAL
23	C2	48	ILE
24	C3	1	MET
24	C3	14	ARG
24	C3	41	ARG
24	C3	44	VAL
25	C4	52	LYS
25	C4	55	LEU
25	C4	62	LEU
26	C5	2	LYS
26	C5	22	VAL
26	C5	26	ILE
27	C0	3	LYS
27	C0	4	THR
27	C0	5	ILE
27	C0	7	ILE
27	C0	36	VAL
27	C0	39	GLU
27	C0	59	GLU
2	BB	23	TRP
2	BB	57	LEU
2	BB	73	LYS
2	BB	93	ASN
2	BB	105	LYS
2	BB	108	ARG
2	BB	116	ASP
2	BB	125	THR
2	BB	129	LEU
2	BB	130	THR
2	BB	135	LEU
2	BB	147	SER
2	BB	151	ILE
2	BB	161	LEU
2	BB	205	ASP
2	BB	207	ILE
2	BB	211	THR

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Mol	Chain	Res	Type
3	BC	3	GLN
3	BC	33	LEU
3	BC	36	ASP
3	BC	37	PHE
3	BC	46	GLU
3	BC	55	ILE
3	BC	75	ILE
3	BC	107	ARG
3	BC	121	THR
3	BC	128	VAL
3	BC	152	GLU
3	BC	175	LEU
3	BC	186	THR
3	BC	193	TYR
3	BC	207	ILE
4	BD	22	LYS
4	BD	25	VAL
4	BD	26	ARG
4	BD	116	GLN
4	BD	130	VAL
4	BD	142	VAL
4	BD	143	VAL
4	BD	151	LYS
4	BD	169	THR
4	BD	194	ASP
4	BD	195	ILE
4	BD	196	ASN
4	BD	206	LYS
5	BE	14	LYS
5	BE	26	LYS
5	BE	46	VAL
5	BE	65	GLU
5	BE	76	LEU
5	BE	81	LEU
5	BE	82	GLN
5	BE	88	VAL
5	BE	94	VAL
5	BE	105	ILE
5	BE	115	LEU
5	BE	120	VAL
5	BE	123	VAL
5	BE	126	LYS

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Mol	Chain	Res	Type
5	BE	140	THR
5	BE	148	ASN
5	BE	157	ARG
5	BE	159	LYS
6	BF	9	MET
6	BF	14	GLN
6	BF	16	GLU
6	BF	17	GLN
6	BF	36	ILE
6	BF	39	LEU
6	BF	53	LYS
6	BF	62	MET
6	BF	65	GLU
6	BF	68	GLN
6	BF	69	GLU
6	BF	71	ILE
6	BF	72	ASP
6	BF	89	VAL
6	BF	93	LYS
7	BG	5	ARG
7	BG	10	ARG
7	BG	23	LEU
7	BG	30	LEU
7	BG	36	LYS
7	BG	48	GLU
7	BG	50	LEU
7	BG	63	GLU
7	BG	72	THR
7	BG	76	LYS
7	BG	95	ARG
7	BG	120	LEU
7	BG	131	LYS
7	BG	138	ARG
7	BG	142	HIS
7	BG	144	MET
7	BG	146	GLU
8	BH	3	MET
8	BH	9	ASP
8	BH	13	ARG
8	BH	26	THR
8	BH	46	ILE
8	BH	47	GLU

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Mol	Chain	Res	Type
8	BH	52	GLU
8	BH	60	GLU
8	BH	71	VAL
8	BH	76	GLN
8	BH	77	ARG
8	BH	80	ARG
8	BH	83	LEU
8	BH	87	LYS
8	BH	101	ILE
8	BH	117	ARG
9	BI	9	THR
9	BI	11	ARG
9	BI	30	ILE
9	BI	36	GLU
9	BI	57	MET
9	BI	61	LEU
9	BI	63	LEU
9	BI	66	THR
9	BI	87	LEU
9	BI	89	GLU
9	BI	111	VAL
10	BJ	5	ARG
10	BJ	6	ILE
10	BJ	59	LYS
10	BJ	62	ARG
10	BJ	65	TYR
10	BJ	69	THR
10	BJ	78	GLU
10	BJ	88	MET
10	BJ	89	ARG
10	BJ	90	LEU
11	BK	18	ASP
11	BK	22	HIS
11	BK	31	ILE
11	BK	33	THR
11	BK	38	GLN
11	BK	82	LEU
11	BK	85	MET
11	BK	97	ILE
12	BL	4	VAL
12	BL	16	VAL
12	BL	24	LEU

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Mol	Chain	Res	Type
12	BL	41	THR
12	BL	44	LYS
12	BL	49	LEU
12	BL	52	VAL
12	BL	55	VAL
12	BL	58	THR
12	BL	82	ILE
12	BL	110	ARG
12	BL	121	ARG
13	BM	7	ILE
13	BM	8	ASN
13	BM	11	ASP
13	BM	16	VAL
13	BM	22	ILE
13	BM	25	VAL
13	BM	27	LYS
13	BM	29	ARG
13	BM	41	GLU
13	BM	48	LEU
13	BM	59	GLU
13	BM	64	VAL
13	BM	95	LEU
14	BN	26	GLU
14	BN	27	LEU
14	BN	84	VAL
15	BO	25	THR
15	BO	40	GLN
15	BO	64	ARG
15	BO	66	LEU
15	BO	70	LEU
15	BO	87	LEU
16	BP	2	VAL
16	BP	20	VAL
16	BP	33	ILE
16	BP	48	GLU
16	BP	76	LYS
17	BQ	13	VAL
17	BQ	17	MET
17	BQ	20	SER
17	BQ	21	ILE
17	BQ	25	ILE
17	BQ	26	GLU

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Mol	Chain	Res	Type
17	BQ	36	LYS
17	BQ	38	ILE
17	BQ	40	ARG
17	BQ	67	LEU
17	BQ	75	LEU
18	BR	24	LYS
19	BS	6	LYS
19	BS	7	LYS
19	BS	13	LEU
19	BS	37	ARG
19	BS	52	HIS
19	BS	60	VAL
19	BS	63	THR
19	BS	65	GLU
20	BT	5	LYS
20	BT	12	ILE
20	BT	14	SER
20	BT	15	GLU
20	BT	26	SER
20	BT	54	MET
20	BT	58	VAL
20	BT	64	LYS
20	BT	66	LEU
20	BT	67	ILE
20	BT	69	LYS
20	BT	84	ASN
21	BU	13	ASP
21	BU	14	VAL
21	BU	16	LEU
21	BU	20	LYS
21	BU	56	HIS
22	D1	26	THR
22	D1	27	SER
23	D2	5	ILE
23	D2	12	VAL
23	D2	42	VAL
23	D2	47	VAL
23	D2	48	ILE
24	D3	1	MET
24	D3	11	LYS
24	D3	14	ARG
24	D3	41	ARG

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Mol	Chain	Res	Type
24	D3	44	VAL
25	D4	52	LYS
25	D4	55	LEU
25	D4	62	LEU
26	D5	22	VAL
26	D5	26	ILE
27	D0	3[A]	LYS
27	D0	3[B]	LYS
27	D0	4	THR
27	D0	7	ILE
27	D0	36	VAL
27	D0	39	GLU
27	D0	55	VAL
27	D0	58	GLU
29	CC	20	VAL
29	CC	104	ILE
29	CC	110	LEU
29	CC	116	ILE
29	CC	118	SER
29	CC	120	VAL
29	CC	157	SER
29	CC	164	ILE
29	CC	168	ASP
29	CC	185	GLU
29	CC	195	VAL
29	CC	204	VAL
29	CC	221	ARG
29	CC	236	GLU
29	CC	245	VAL
29	CC	266	PHE
29	CC	268	VAL
29	CC	271	ARG
30	CD	2	ILE
30	CD	4	LEU
30	CD	13	ARG
30	CD	18	ASP
30	CD	62	LYS
30	CD	79	LEU
30	CD	95	SER
30	CD	126	ASN
30	CD	131	ASP
30	CD	138	LEU

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Mol	Chain	Res	Type
30	CD	150	GLN
30	CD	171	THR
30	CD	190	LYS
30	CD	204	LYS
29	DC	20	VAL
29	DC	24	LEU
29	DC	28	LYS
29	DC	70	ASN
29	DC	104	ILE
29	DC	116	ILE
29	DC	118	SER
29	DC	120	VAL
29	DC	164	ILE
29	DC	165	VAL
29	DC	185	GLU
29	DC	236	GLU
29	DC	245	VAL
29	DC	265	LYS
29	DC	268	VAL
29	DC	271	ARG
32	DD	2	ILE
32	DD	13	ARG
32	DD	18	ASP
32	DD	79	LEU
32	DD	86	GLU
32	DD	95	SER
32	DD	126	ASN
32	DD	129	THR
32	DD	131	ASP
32	DD	138	LEU
32	DD	171	THR
32	DD	190	LYS
32	DD	204	LYS
33	CE	12	LEU
33	CE	25	GLU
33	CE	32	VAL
33	CE	40	ARG
33	CE	44	ARG
33	CE	69	ARG
33	CE	83	VAL
33	CE	107	SER
33	CE	120	VAL

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Mol	Chain	Res	Type
33	CE	123	LYS
33	CE	127	GLU
33	CE	149	ILE
33	CE	152	GLU
33	CE	153	LEU
33	CE	173	THR
33	CE	176	ASP
33	CE	187	VAL
33	CE	189	THR
34	CF	31	VAL
34	CF	35	THR
34	CF	36	LEU
34	CF	37	ASN
34	CF	40	VAL
34	CF	42	GLU
34	CF	57	LEU
34	CF	72	LYS
34	CF	80	ARG
34	CF	94	GLU
34	CF	98	GLU
34	CF	115	ARG
34	CF	117	LEU
34	CF	123	ASP
34	CF	134	GLU
34	CF	136	ILE
34	CF	141	ILE
34	CF	147	ASP
34	CF	148	ARG
34	CF	152	LEU
34	CF	167	ARG
34	CF	174	ASP
35	CG	11	VAL
35	CG	18	LYS
35	CG	24	ILE
35	CG	49	THR
35	CG	50	LEU
35	CG	72	LEU
35	CG	127	THR
35	CG	155	GLU
35	CG	167	GLU
35	CG	168	VAL
35	CG	171	THR

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Mol	Chain	Res	Type
36	CH	3	VAL
36	CH	6	LEU
36	CH	15	LEU
36	CH	21	VAL
36	CH	51	ARG
36	CH	53	GLU
36	CH	55	GLU
36	CH	62	LEU
36	CH	76	GLU
36	CH	108	VAL
36	CH	109	GLU
36	CH	110	VAL
36	CH	112	LYS
36	CH	127	GLU
36	CH	138	VAL
36	CH	145	ASN
37	CJ	9	VAL
37	CJ	11	LEU
37	CJ	13	VAL
37	CJ	28	LEU
37	CJ	53	LEU
37	CJ	55	ILE
37	CJ	61	VAL
37	CJ	78	VAL
37	CJ	80	LEU
37	CJ	86	ILE
37	CJ	98	VAL
37	CJ	101	ILE
38	CK	5	THR
38	CK	9	GLU
38	CK	76	HIS
38	CK	124	VAL
38	CK	142	ILE
39	CL	49	ARG
39	CL	57	VAL
39	CL	58	LEU
39	CL	66	LYS
39	CL	76	VAL
39	CL	91	SER
39	CL	98	ARG
39	CL	116	ILE
40	CM	33	ARG

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Mol	Chain	Res	Type
40	CM	40	SER
40	CM	59	ARG
40	CM	68	SER
40	CM	92	LEU
40	CM	93	ASN
40	CM	99	ASN
40	CM	100	ILE
40	CM	103	ILE
40	CM	107	PHE
40	CM	115	GLU
40	CM	116	VAL
40	CM	120	VAL
41	CN	6	ARG
41	CN	10	ARG
41	CN	13	HIS
41	CN	20	LEU
41	CN	55	ARG
41	CN	59	ARG
41	CN	75	GLU
41	CN	100	LYS
41	CN	126	ILE
41	CN	128	THR
41	CN	131	VAL
41	CN	132	THR
41	CN	134	THR
41	CN	135	VAL
42	CO	1	MET
42	CO	2	ARG
42	CO	6	SER
42	CO	8	ARG
42	CO	14	SER
42	CO	53	THR
42	CO	59	SER
42	CO	69	ARG
42	CO	95	THR
43	CP	24	THR
43	CP	31	THR
43	CP	35	ILE
43	CP	38	GLN
43	CP	45	SER
43	CP	47	VAL
43	CP	48	LEU

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Mol	Chain	Res	Type
43	CP	78	VAL
43	CP	106	LEU
44	CQ	10	GLN
44	CQ	30	VAL
44	CQ	39	ARG
44	CQ	48	ILE
44	CQ	63	LYS
44	CQ	65	SER
44	CQ	85	SER
44	CQ	96	LYS
44	CQ	102	GLU
44	CQ	114	LEU
45	CR	5	LYS
45	CR	6	ARG
45	CR	9	ILE
45	CR	51	ARG
45	CR	109	LEU
45	CR	117	LEU
46	CS	12	HIS
46	CS	13	ARG
46	CS	15	SER
46	CS	20	VAL
46	CS	26	ASP
46	CS	45	GLU
46	CS	46	GLU
46	CS	48	LYS
46	CS	51	VAL
46	CS	66	HIS
46	CS	71	LYS
47	CT	3	THR
47	CT	29	VAL
47	CT	33	LEU
47	CT	50	VAL
47	CT	53	SER
47	CT	74	ILE
47	CT	76	VAL
47	CT	83	LYS
47	CT	85	ILE
47	CT	86	MET
47	CT	97	LEU
47	CT	105	VAL
47	CT	109	ASP

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Mol	Chain	Res	Type
48	CU	1	MET
48	CU	2	ILE
48	CU	3	ARG
48	CU	12	ARG
48	CU	18	GLU
48	CU	24	MET
48	CU	30	ILE
48	CU	36	LYS
48	CU	49	LYS
48	CU	53	VAL
48	CU	61	LEU
48	CU	68	LYS
48	CU	69	ARG
48	CU	74	ILE
48	CU	79	ASP
48	CU	82	LYS
48	CU	86	THR
48	CU	93	LEU
49	CV	9	ASP
49	CV	15	THR
49	CV	28	VAL
49	CV	29	LEU
49	CV	44	LYS
49	CV	52	LEU
49	CV	59	VAL
49	CV	61	LYS
49	CV	72	ILE
49	CV	81	ASP
49	CV	98	SER
50	CW	7	GLU
50	CW	10	LYS
50	CW	18	ARG
50	CW	20	LEU
50	CW	29	ILE
50	CW	61	LEU
50	CW	62	THR
50	CW	65	VAL
51	CX	78	LYS
51	CX	82	ILE
52	CY	4	VAL
52	CY	25	THR
52	CY	28	ARG

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Mol	Chain	Res	Type
52	CY	40	VAL
52	CY	44	LYS
52	CY	51	VAL
52	CY	66	THR
52	CY	71	LEU
53	CZ	2	LYS
53	CZ	18	LEU
53	CZ	19	LEU
53	CZ	22	LEU
53	CZ	58	ASN
33	DE	12	LEU
33	DE	32	VAL
33	DE	69	ARG
33	DE	80	SER
33	DE	88	ARG
33	DE	107	SER
33	DE	120	VAL
33	DE	123	LYS
33	DE	127	GLU
33	DE	153	LEU
33	DE	173	THR
33	DE	176	ASP
33	DE	187	VAL
33	DE	189	THR
34	DF	10	ASP
34	DF	35	THR
34	DF	37	ASN
34	DF	40	VAL
34	DF	42	GLU
34	DF	57	LEU
34	DF	72	LYS
34	DF	94	GLU
34	DF	98	GLU
34	DF	115	ARG
34	DF	117	LEU
34	DF	120	LYS
34	DF	134	GLU
34	DF	136	ILE
34	DF	141	ILE
34	DF	148	ARG
34	DF	152	LEU
34	DF	158	THR

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Mol	Chain	Res	Type
34	DF	167	ARG
34	DF	174	ASP
34	DF	178	ARG
35	DG	11	VAL
35	DG	18	LYS
35	DG	24	ILE
35	DG	49	THR
35	DG	50	LEU
35	DG	67	THR
35	DG	72	LEU
35	DG	127	THR
35	DG	155	GLU
35	DG	167	GLU
35	DG	168	VAL
35	DG	171	THR
36	DH	3	VAL
36	DH	6	LEU
36	DH	15	LEU
36	DH	21	VAL
36	DH	53	GLU
36	DH	58	LEU
36	DH	62	LEU
36	DH	76	GLU
36	DH	89	LYS
36	DH	108	VAL
36	DH	110	VAL
36	DH	127	GLU
36	DH	138	VAL
36	DH	145	ASN
37	DJ	9	VAL
37	DJ	11	LEU
37	DJ	13	VAL
37	DJ	28	LEU
37	DJ	53	LEU
37	DJ	55	ILE
37	DJ	61	VAL
37	DJ	78	VAL
37	DJ	80	LEU
37	DJ	86	ILE
37	DJ	98	VAL
37	DJ	101	ILE
38	DK	7	LYS

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Mol	Chain	Res	Type
38	DK	30	THR
38	DK	76	HIS
38	DK	84	ILE
38	DK	124	VAL
38	DK	142	ILE
39	DL	49	ARG
39	DL	57	VAL
39	DL	58	LEU
39	DL	66	LYS
39	DL	75	SER
39	DL	91	SER
39	DL	109	SER
39	DL	110	GLU
39	DL	113	MET
39	DL	116	ILE
40	DM	40	SER
40	DM	59	ARG
40	DM	92	LEU
40	DM	107	PHE
40	DM	115	GLU
40	DM	116	VAL
40	DM	120	VAL
41	DN	6	ARG
41	DN	10	ARG
41	DN	55	ARG
41	DN	58	LYS
41	DN	75	GLU
41	DN	100	LYS
41	DN	126	ILE
41	DN	128	THR
41	DN	131	VAL
41	DN	132	THR
41	DN	134	THR
41	DN	135	VAL
42	DO	1	MET
42	DO	2	ARG
42	DO	6	SER
42	DO	14	SER
42	DO	46	ARG
42	DO	53	THR
42	DO	59	SER
42	DO	69	ARG

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Mol	Chain	Res	Type
43	DP	1	MET
43	DP	24	THR
43	DP	31	THR
43	DP	35	ILE
43	DP	45	SER
43	DP	47	VAL
43	DP	48	LEU
43	DP	58	ILE
43	DP	78	VAL
43	DP	106	LEU
44	DQ	4	ILE
44	DQ	10	GLN
44	DQ	30	VAL
44	DQ	40	LEU
44	DQ	48	ILE
44	DQ	63	LYS
44	DQ	65	SER
44	DQ	85	SER
44	DQ	96	LYS
44	DQ	102	GLU
45	DR	5	LYS
45	DR	6	ARG
45	DR	51	ARG
45	DR	109	LEU
45	DR	112	LYS
45	DR	117	LEU
46	DS	7	SER
46	DS	13	ARG
46	DS	15	SER
46	DS	20	VAL
46	DS	26	ASP
46	DS	38	VAL
46	DS	58	VAL
46	DS	66	HIS
47	DT	3	THR
47	DT	29	VAL
47	DT	33	LEU
47	DT	50	VAL
47	DT	53	SER
47	DT	74	ILE
47	DT	76	VAL
47	DT	85	ILE

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Mol	Chain	Res	Type
47	DT	86	MET
47	DT	92	ARG
47	DT	105	VAL
47	DT	109	ASP
47	DT	110	ARG
48	DU	2	ILE
48	DU	3	ARG
48	DU	18	GLU
48	DU	25	GLU
48	DU	36	LYS
48	DU	53	VAL
48	DU	61	LEU
48	DU	68	LYS
48	DU	69	ARG
48	DU	74	ILE
48	DU	79	ASP
48	DU	82	LYS
48	DU	86	THR
49	DV	26	LYS
49	DV	28	VAL
49	DV	29	LEU
49	DV	44	LYS
49	DV	59	VAL
49	DV	61	LYS
49	DV	81	ASP
50	DW	7	GLU
50	DW	20	LEU
50	DW	29	ILE
50	DW	53	LYS
50	DW	61	LEU
50	DW	62	THR
50	DW	65	VAL
51	DX	11	ARG
51	DX	41[A]	ARG
51	DX	41[B]	ARG
51	DX	78	LYS
51	DX	82	ILE
52	DY	4	VAL
52	DY	25	THR
52	DY	28	ARG
52	DY	40	VAL
52	DY	44	LYS

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Mol	Chain	Res	Type
52	DY	48	THR
52	DY	51	VAL
52	DY	71	LEU
53	DZ	2	LYS
53	DZ	6	LEU
53	DZ	19	LEU
53	DZ	22	LEU
54	DI	23	LEU
54	DI	53	ARG
54	DI	58	THR
54	DI	61	ARG
54	DI	64	VAL
54	DI	67	THR
54	DI	70	GLU
54	DI	74	ASP
54	DI	82	ILE
54	DI	85	VAL
54	DI	95	LEU
54	DI	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (173) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	39	HIS
2	AB	42	ASN
2	AB	58	ASN
2	AB	93	ASN
2	AB	120	GLN
2	AB	177	ASN
3	AC	41	GLN
3	AC	176	HIS
4	AD	136	GLN
4	AD	140	ASN
4	AD	152	GLN
5	AE	89	HIS
5	AE	97	GLN
5	AE	122	ASN
5	AE	146	ASN
6	AF	37	HIS
6	AF	94	HIS
7	AG	9	GLN
7	AG	97	ASN

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Mol	Chain	Res	Type
7	AG	130	ASN
8	AH	4	GLN
8	AH	21	ASN
9	AI	5	GLN
9	AI	31	ASN
9	AI	110	GLN
10	AJ	58	ASN
11	AK	24	HIS
11	AK	40	ASN
11	AK	81	ASN
11	AK	101	ASN
11	AK	118	HIS
12	AL	112	GLN
13	AM	14	HIS
13	AM	52	GLN
14	AN	35	ASN
14	AN	60	GLN
16	AP	63	GLN
19	AS	52	HIS
19	AS	53	ASN
19	AS	56	GLN
19	AS	57	HIS
20	AT	13	GLN
20	AT	48	GLN
20	AT	84	ASN
22	C1	6	ASN
22	C1	42	HIS
23	C2	26	ASN
23	C2	46	HIS
24	C3	29	GLN
25	C4	28	ASN
27	C0	9	GLN
27	C0	49	ASN
2	BB	39	HIS
2	BB	42	ASN
2	BB	58	ASN
2	BB	93	ASN
2	BB	120	GLN
2	BB	146	ASN
2	BB	177	ASN
4	BD	140	ASN
5	BE	82	GLN

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Mol	Chain	Res	Type
5	BE	89	HIS
5	BE	97	GLN
5	BE	121	HIS
5	BE	122	ASN
5	BE	132	ASN
5	BE	146	ASN
6	BF	3	HIS
6	BF	14	GLN
6	BF	37	HIS
7	BG	9	GLN
7	BG	97	ASN
7	BG	130	ASN
7	BG	142	HIS
8	BH	4	GLN
8	BH	21	ASN
9	BI	5	GLN
9	BI	110	GLN
11	BK	40	ASN
11	BK	81	ASN
11	BK	101	ASN
12	BL	112	GLN
13	BM	52	GLN
14	BN	35	ASN
14	BN	60	GLN
15	BO	28	GLN
16	BP	63	GLN
19	BS	52	HIS
19	BS	53	ASN
19	BS	57	HIS
20	BT	13	GLN
20	BT	20	HIS
24	D3	26	ASN
24	D3	29	GLN
25	D4	26	HIS
29	CC	25	HIS
29	CC	45	ASN
29	CC	90	ASN
29	CC	251	GLN
30	CD	130	GLN
30	CD	150	GLN
30	CD	164	GLN
29	DC	25	HIS

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Mol	Chain	Res	Type
29	DC	70	ASN
32	DD	42	ASN
32	DD	58	ASN
33	CE	41	GLN
33	CE	136	GLN
34	CF	27	GLN
34	CF	52	ASN
35	CG	22	GLN
35	CG	38	ASN
36	CH	2	GLN
36	CH	18	GLN
36	CH	20	ASN
36	CH	66	ASN
37	CJ	43	ASN
37	CJ	94	ASN
37	CJ	107	GLN
38	CK	47	HIS
40	CM	38	GLN
40	CM	99	ASN
40	CM	104	GLN
41	CN	60	GLN
42	CO	13	ASN
42	CO	73	ASN
43	CP	116	GLN
44	CQ	115	ASN
45	CR	44	GLN
45	CR	52	GLN
45	CR	56	GLN
46	CS	89	HIS
48	CU	92	ASN
49	CV	74	ASN
50	CW	24	ASN
51	CX	57	HIS
52	CY	36	HIS
53	CZ	36	GLN
33	DE	41	GLN
33	DE	90	GLN
35	DG	22	GLN
35	DG	30	ASN
35	DG	73	ASN
36	DH	2	GLN
36	DH	18	GLN

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Mol	Chain	Res	Type
36	DH	20	ASN
37	DJ	30	GLN
37	DJ	43	ASN
37	DJ	94	ASN
37	DJ	107	GLN
38	DK	47	HIS
38	DK	80	HIS
38	DK	86	GLN
38	DK	138	GLN
39	DL	93	GLN
40	DM	104	GLN
42	DO	9	GLN
42	DO	13	ASN
42	DO	73	ASN
43	DP	29	HIS
43	DP	116	GLN
44	DQ	115	ASN
45	DR	44	GLN
46	DS	18	GLN
46	DS	89	HIS
48	DU	92	ASN
49	DV	40	ASN
49	DV	46	GLN
49	DV	54	GLN
50	DW	24	ASN
52	DY	36	HIS
53	DZ	36	GLN
54	DI	122	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1533/1534 (99%)	305 (19%)	48 (3%)
1	BA	1532/1534 (99%)	307 (20%)	52 (3%)
28	CB	117/120 (97%)	14 (11%)	2 (1%)
28	DB	119/120 (99%)	14 (11%)	1 (0%)
31	CA	2896/2904 (99%)	593 (20%)	110 (3%)
55	DA	2884/2904 (99%)	504 (17%)	73 (2%)
All	All	9081/9116 (99%)	1737 (19%)	286 (3%)

All (1737) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	8	A
1	AA	9	G
1	AA	22	G
1	AA	28	A
1	AA	30	U
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	49	U
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	54	C
1	AA	69	G
1	AA	70	U
1	AA	71	A
1	AA	72	A
1	AA	74	A
1	AA	79	G
1	AA	81	A
1	AA	82	G
1	AA	83	C
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	88	U
1	AA	89	U
1	AA	90	C
1	AA	92	U
1	AA	94	G
1	AA	95	C
1	AA	108	G
1	AA	119	A
1	AA	120	A
1	AA	127	G
1	AA	128	G
1	AA	130	A
1	AA	131	A

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Mol	Chain	Res	Type
1	AA	141	G
1	AA	142	G
1	AA	143	A
1	AA	144	G
1	AA	146	G
1	AA	149	A
1	AA	159	G
1	AA	163	C
1	AA	168	G
1	AA	189	A
1	AA	197	A
1	AA	200	G
1	AA	205	A
1	AA	210	C
1	AA	211	G
1	AA	212	G
1	AA	226	G
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	305	G
1	AA	306	A
1	AA	308	C
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	332	G
1	AA	346	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	368	U
1	AA	372	C
1	AA	373	A
1	AA	376	G
1	AA	384	G
1	AA	396	C

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Mol	Chain	Res	Type
1	AA	397	A
1	AA	398	U
1	AA	406	G
1	AA	411	A
1	AA	413	G
1	AA	414	A
1	AA	421	U
1	AA	422	C
1	AA	423	G
1	AA	424	G
1	AA	429	U
1	AA	436	C
1	AA	451	A
1	AA	457	G
1	AA	458	U
1	AA	463	U
1	AA	467	U
1	AA	468	A
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	505	G
1	AA	509	A
1	AA	511	C
1	AA	521	G
1	AA	524	G
1	AA	527	7MG
1	AA	530	G
1	AA	531	U
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	564	C
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	596	A
1	AA	615	G
1	AA	633	G
1	AA	639	G

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Mol	Chain	Res	Type
1	AA	641	U
1	AA	642	A
1	AA	650	G
1	AA	653	U
1	AA	656	G
1	AA	665	A
1	AA	671	G
1	AA	675	A
1	AA	677	U
1	AA	702	A
1	AA	703	G
1	AA	721	G
1	AA	723	U
1	AA	724	G
1	AA	733	G
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	758	C
1	AA	774	G
1	AA	777	A
1	AA	782	A
1	AA	793	U
1	AA	794	A
1	AA	809	G
1	AA	815	A
1	AA	817	C
1	AA	821	G
1	AA	828	U
1	AA	832	G
1	AA	836	G
1	AA	839	C
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	884	U
1	AA	885	G
1	AA	902	G
1	AA	914	A
1	AA	926	G

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Mol	Chain	Res	Type
1	AA	927	G
1	AA	934	C
1	AA	935	A
1	AA	942	G
1	AA	955	U
1	AA	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	971	G
1	AA	972	C
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	985	C
1	AA	987	G
1	AA	991	U
1	AA	992	U
1	AA	993	G
1	AA	1004	A
1	AA	1008	U
1	AA	1015	G
1	AA	1019	A
1	AA	1024	G
1	AA	1026	G
1	AA	1027	C
1	AA	1029	U
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	G
1	AA	1036	A
1	AA	1037	C
1	AA	1043	G
1	AA	1044	A
1	AA	1053	G
1	AA	1054	C
1	AA	1055	A
1	AA	1064	G
1	AA	1065	U
1	AA	1070	U
1	AA	1086	U
1	AA	1089	G

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Mol	Chain	Res	Type
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1104	G
1	AA	1124	G
1	AA	1125	U
1	AA	1132	C
1	AA	1133	G
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	1142	G
1	AA	1145	A
1	AA	1152	A
1	AA	1159	U
1	AA	1160	G
1	AA	1168	U
1	AA	1182	G
1	AA	1183	U
1	AA	1184	G
1	AA	1186	G
1	AA	1195	C
1	AA	1196	A
1	AA	1197	A
1	AA	1198	G
1	AA	1201	A
1	AA	1202	U
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
1	AA	1221	G
1	AA	1224	U
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1233	G
1	AA	1236	A
1	AA	1238	A

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Mol	Chain	Res	Type
1	AA	1239	A
1	AA	1256	A
1	AA	1257	A
1	AA	1258	G
1	AA	1260	G
1	AA	1274	A
1	AA	1280	A
1	AA	1281	C
1	AA	1282	C
1	AA	1286	U
1	AA	1287	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1312	G
1	AA	1317	C
1	AA	1318	A
1	AA	1319	A
1	AA	1320	C
1	AA	1323	G
1	AA	1338	G
1	AA	1351	U
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1379	G
1	AA	1381	U
1	AA	1398	A
1	AA	1419	G
1	AA	1422	G
1	AA	1441	A
1	AA	1446	A
1	AA	1448	C
1	AA	1451	U
1	AA	1452	C
1	AA	1453	G
1	AA	1475	G
1	AA	1483	A
1	AA	1484	C
1	AA	1487	G
1	AA	1492	A
1	AA	1493	A

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Mol	Chain	Res	Type
1	AA	1497	G
1	AA	1503	A
1	AA	1505	G
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1533	C
1	AA	1534	A
1	BA	5	U
1	BA	6	G
1	BA	7	A
1	BA	8	A
1	BA	9	G
1	BA	22	G
1	BA	28	A
1	BA	31	G
1	BA	32	A
1	BA	39	G
1	BA	47	C
1	BA	48	C
1	BA	49	U
1	BA	50	A
1	BA	51	A
1	BA	52	C
1	BA	54	C
1	BA	69	G
1	BA	70	U
1	BA	71	A
1	BA	72	A
1	BA	74	A
1	BA	79	G
1	BA	82	G
1	BA	83	C
1	BA	84	U
1	BA	85	U
1	BA	86	G
1	BA	87	C
1	BA	89	U
1	BA	90	C
1	BA	92	U

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Mol	Chain	Res	Type
1	BA	94	G
1	BA	95	C
1	BA	108	G
1	BA	119	A
1	BA	120	A
1	BA	127	G
1	BA	128	G
1	BA	130	A
1	BA	131	A
1	BA	141	G
1	BA	142	G
1	BA	143	A
1	BA	144	G
1	BA	146	G
1	BA	149	A
1	BA	159	G
1	BA	163	C
1	BA	168	G
1	BA	189	A
1	BA	197	A
1	BA	200	G
1	BA	205	A
1	BA	210	C
1	BA	211	G
1	BA	212	G
1	BA	226	G
1	BA	240	G
1	BA	245	U
1	BA	247	G
1	BA	251	G
1	BA	262	A
1	BA	266	G
1	BA	267	C
1	BA	289	G
1	BA	305	G
1	BA	306	A
1	BA	308	C
1	BA	321	A
1	BA	328	C
1	BA	329	A
1	BA	332	G
1	BA	346	G

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Mol	Chain	Res	Type
1	BA	352	C
1	BA	354	G
1	BA	367	U
1	BA	368	U
1	BA	372	C
1	BA	373	A
1	BA	376	G
1	BA	384	G
1	BA	396	C
1	BA	397	A
1	BA	398	U
1	BA	406	G
1	BA	411	A
1	BA	412	A
1	BA	413	G
1	BA	414	A
1	BA	421	U
1	BA	422	C
1	BA	424	G
1	BA	429	U
1	BA	436	C
1	BA	451	A
1	BA	457	G
1	BA	458	U
1	BA	463	U
1	BA	467	U
1	BA	468	A
1	BA	481	G
1	BA	484	G
1	BA	486	U
1	BA	495	A
1	BA	505	G
1	BA	509	A
1	BA	511	C
1	BA	521	G
1	BA	524	G
1	BA	525	C
1	BA	527	7MG
1	BA	530	G
1	BA	531	U
1	BA	532	A
1	BA	533	A

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Mol	Chain	Res	Type
1	BA	547	A
1	BA	559	A
1	BA	560	A
1	BA	564	C
1	BA	572	A
1	BA	573	A
1	BA	576	C
1	BA	577	G
1	BA	596	A
1	BA	615	G
1	BA	633	G
1	BA	639	G
1	BA	641	U
1	BA	642	A
1	BA	650	G
1	BA	653	U
1	BA	656	G
1	BA	665	A
1	BA	671	G
1	BA	675	A
1	BA	677	U
1	BA	702	A
1	BA	703	G
1	BA	721	G
1	BA	723	U
1	BA	724	G
1	BA	733	G
1	BA	734	G
1	BA	748	G
1	BA	755	G
1	BA	758	C
1	BA	774	G
1	BA	777	A
1	BA	782	A
1	BA	793	U
1	BA	794	A
1	BA	809	G
1	BA	815	A
1	BA	817	C
1	BA	821	G
1	BA	828	U
1	BA	832	G

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Mol	Chain	Res	Type
1	BA	836	G
1	BA	839	C
1	BA	840	C
1	BA	841	C
1	BA	842	U
1	BA	843	U
1	BA	845	A
1	BA	846	G
1	BA	884	U
1	BA	885	G
1	BA	902	G
1	BA	914	A
1	BA	926	G
1	BA	927	G
1	BA	934	C
1	BA	935	A
1	BA	942	G
1	BA	955	U
1	BA	960	U
1	BA	966	2MG
1	BA	969	A
1	BA	971	G
1	BA	972	C
1	BA	975	A
1	BA	976	G
1	BA	977	A
1	BA	985	C
1	BA	987	G
1	BA	991	U
1	BA	992	U
1	BA	993	G
1	BA	1004	A
1	BA	1008	U
1	BA	1009	U
1	BA	1015	G
1	BA	1019	A
1	BA	1024	G
1	BA	1026	G
1	BA	1027	C
1	BA	1029	U
1	BA	1030	U
1	BA	1031	C

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Mol	Chain	Res	Type
1	BA	1032	G
1	BA	1033	G
1	BA	1036	A
1	BA	1037	C
1	BA	1043	G
1	BA	1044	A
1	BA	1053	G
1	BA	1054	C
1	BA	1055	A
1	BA	1064	G
1	BA	1065	U
1	BA	1066	C
1	BA	1086	U
1	BA	1089	G
1	BA	1094	G
1	BA	1095	U
1	BA	1101	A
1	BA	1104	G
1	BA	1124	G
1	BA	1125	U
1	BA	1132	C
1	BA	1133	G
1	BA	1136	C
1	BA	1137	C
1	BA	1138	G
1	BA	1139	G
1	BA	1140	C
1	BA	1141	C
1	BA	1142	G
1	BA	1145	A
1	BA	1152	A
1	BA	1159	U
1	BA	1160	G
1	BA	1168	U
1	BA	1182	G
1	BA	1183	U
1	BA	1186	G
1	BA	1196	A
1	BA	1197	A
1	BA	1198	G
1	BA	1201	A
1	BA	1202	U

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Mol	Chain	Res	Type
1	BA	1212	U
1	BA	1213	A
1	BA	1214	C
1	BA	1215	G
1	BA	1221	G
1	BA	1224	U
1	BA	1225	A
1	BA	1226	C
1	BA	1227	A
1	BA	1233	G
1	BA	1236	A
1	BA	1238	A
1	BA	1239	A
1	BA	1256	A
1	BA	1257	A
1	BA	1258	G
1	BA	1260	G
1	BA	1261	A
1	BA	1274	A
1	BA	1280	A
1	BA	1281	C
1	BA	1282	C
1	BA	1286	U
1	BA	1287	A
1	BA	1300	G
1	BA	1302	C
1	BA	1305	G
1	BA	1312	G
1	BA	1317	C
1	BA	1318	A
1	BA	1319	A
1	BA	1320	C
1	BA	1323	G
1	BA	1337	G
1	BA	1338	G
1	BA	1351	U
1	BA	1353	G
1	BA	1362	A
1	BA	1363	A
1	BA	1370	G
1	BA	1379	G
1	BA	1381	U

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Mol	Chain	Res	Type
1	BA	1419	G
1	BA	1422	G
1	BA	1441	A
1	BA	1446	A
1	BA	1448	C
1	BA	1451	U
1	BA	1452	C
1	BA	1453	G
1	BA	1475	G
1	BA	1483	A
1	BA	1484	C
1	BA	1487	G
1	BA	1493	A
1	BA	1497	G
1	BA	1499	A
1	BA	1505	G
1	BA	1506	U
1	BA	1507	A
1	BA	1517	G
1	BA	1529	G
1	BA	1530	G
1	BA	1533	C
1	BA	1534	A
28	CB	25	U
28	CB	35	C
28	CB	44	G
28	CB	45	A
28	CB	51	G
28	CB	52	A
28	CB	56	G
28	CB	57	A
28	CB	87	U
28	CB	88	C
28	CB	89	U
28	CB	90	C
28	CB	99	A
28	CB	109	A
31	CA	10	A
31	CA	13	A
31	CA	34	U
31	CA	36	G
31	CA	39	G

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Mol	Chain	Res	Type
31	CA	42	A
31	CA	46	G
31	CA	49	A
31	CA	71	A
31	CA	73	A
31	CA	74	A
31	CA	75	G
31	CA	80	G
31	CA	83	A
31	CA	84	A
31	CA	86	G
31	CA	102	U
31	CA	118	A
31	CA	119	A
31	CA	120	U
31	CA	125	A
31	CA	137	U
31	CA	138	U
31	CA	139	U
31	CA	140	C
31	CA	141	G
31	CA	142	A
31	CA	177	G
31	CA	178	G
31	CA	186	G
31	CA	188	G
31	CA	196	A
31	CA	197	A
31	CA	199	A
31	CA	201	C
31	CA	204	A
31	CA	215	G
31	CA	216	A
31	CA	222	A
31	CA	245	G
31	CA	248	G
31	CA	250	G
31	CA	265	A
31	CA	266	G
31	CA	267	C
31	CA	271	G
31	CA	272	A

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Mol	Chain	Res	Type
31	CA	276	U
31	CA	277	G
31	CA	278	A
31	CA	279	A
31	CA	285	G
31	CA	310	A
31	CA	311	A
31	CA	317	G
31	CA	324	A
31	CA	329	G
31	CA	330	A
31	CA	331	C
31	CA	343	C
31	CA	346	A
31	CA	352	A
31	CA	353	C
31	CA	361	G
31	CA	362	A
31	CA	371	A
31	CA	372	G
31	CA	383	C
31	CA	385	C
31	CA	386	G
31	CA	390	U
31	CA	391	A
31	CA	396	G
31	CA	399	U
31	CA	403	U
31	CA	404	A
31	CA	405	U
31	CA	411	G
31	CA	412	A
31	CA	420	C
31	CA	424	G
31	CA	435	C
31	CA	451	U
31	CA	455	C
31	CA	456	C
31	CA	457	A
31	CA	475	C
31	CA	479	A
31	CA	480	A

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Mol	Chain	Res	Type
31	CA	481	G
31	CA	482	A
31	CA	491	G
31	CA	496	G
31	CA	501	A
31	CA	503	A
31	CA	504	A
31	CA	505	A
31	CA	506	G
31	CA	507	A
31	CA	508	A
31	CA	527	C
31	CA	528	A
31	CA	529	A
31	CA	531	C
31	CA	532	A
31	CA	533	G
31	CA	543	G
31	CA	544	C
31	CA	546	U
31	CA	547	A
31	CA	548	G
31	CA	549	G
31	CA	550	C
31	CA	563	A
31	CA	569	U
31	CA	572	A
31	CA	573	U
31	CA	574	A
31	CA	575	A
31	CA	586	A
31	CA	592	A
31	CA	603	A
31	CA	604	G
31	CA	614	A
31	CA	615	U
31	CA	620	G
31	CA	621	A
31	CA	622	G
31	CA	627	A
31	CA	628	G
31	CA	632	A

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Mol	Chain	Res	Type
31	CA	634	C
31	CA	637	A
31	CA	645	C
31	CA	647	G
31	CA	651	G
31	CA	653	U
31	CA	654	A
31	CA	655	A
31	CA	659	G
31	CA	669	G
31	CA	670	A
31	CA	684	G
31	CA	685	A
31	CA	686	U
31	CA	694	U
31	CA	695	G
31	CA	696	G
31	CA	701	G
31	CA	702	U
31	CA	717	C
31	CA	730	A
31	CA	740	C
31	CA	747	5MU
31	CA	752	A
31	CA	753	A
31	CA	763	G
31	CA	764	A
31	CA	765	C
31	CA	774	G
31	CA	775	G
31	CA	776	G
31	CA	781	A
31	CA	782	A
31	CA	784	G
31	CA	785	G
31	CA	792	A
31	CA	798	G
31	CA	800	A
31	CA	805	G
31	CA	812	C
31	CA	819	A
31	CA	827	U

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Mol	Chain	Res	Type
31	CA	828	U
31	CA	831	G
31	CA	845	A
31	CA	846	U
31	CA	847	U
31	CA	858	G
31	CA	859	G
31	CA	866	A
31	CA	869	G
31	CA	878	A
31	CA	882	G
31	CA	896	A
31	CA	897	C
31	CA	907	G
31	CA	910	A
31	CA	914	G
31	CA	931	U
31	CA	932	U
31	CA	941	A
31	CA	945	A
31	CA	946	C
31	CA	953	G
31	CA	957	C
31	CA	961	C
31	CA	973	A
31	CA	974	G
31	CA	983	A
31	CA	984	A
31	CA	985	C
31	CA	995	C
31	CA	996	A
31	CA	999	U
31	CA	1009	A
31	CA	1012	U
31	CA	1013	C
31	CA	1017	G
31	CA	1020	A
31	CA	1021	A
31	CA	1022	G
31	CA	1024	G
31	CA	1026	G
31	CA	1033	U

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Mol	Chain	Res	Type
31	CA	1040	A
31	CA	1045	C
31	CA	1046	A
31	CA	1047	G
31	CA	1051	G
31	CA	1061	U
31	CA	1062	G
31	CA	1068	G
31	CA	1069	A
31	CA	1070	A
31	CA	1071	G
31	CA	1073	A
31	CA	1083	U
31	CA	1087	G
31	CA	1088	A
31	CA	1090	A
31	CA	1097	U
31	CA	1111	A
31	CA	1112	G
31	CA	1119	U
31	CA	1122	G
31	CA	1128	G
31	CA	1129	A
31	CA	1132	U
31	CA	1133	A
31	CA	1135	C
31	CA	1136	G
31	CA	1141	U
31	CA	1142	A
31	CA	1143	A
31	CA	1151	A
31	CA	1168	G
31	CA	1169	A
31	CA	1172	C
31	CA	1175	A
31	CA	1176	U
31	CA	1177	G
31	CA	1179	G
31	CA	1180	U
31	CA	1186	G
31	CA	1212	G
31	CA	1236	G

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Mol	Chain	Res	Type
31	CA	1238	G
31	CA	1244	A
31	CA	1247	A
31	CA	1248	G
31	CA	1250	G
31	CA	1253	A
31	CA	1256	G
31	CA	1262	A
31	CA	1266	G
31	CA	1271	G
31	CA	1272	A
31	CA	1288	G
31	CA	1289	C
31	CA	1294	U
31	CA	1300	G
31	CA	1301	A
31	CA	1306	C
31	CA	1312	U
31	CA	1313	U
31	CA	1321	A
31	CA	1328	A
31	CA	1329	U
31	CA	1330	C
31	CA	1332	G
31	CA	1344	U
31	CA	1352	U
31	CA	1355	G
31	CA	1359	A
31	CA	1365	A
31	CA	1370	C
31	CA	1376	C
31	CA	1379	U
31	CA	1380	G
31	CA	1383	A
31	CA	1386	C
31	CA	1395	A
31	CA	1398	C
31	CA	1403	A
31	CA	1416	G
31	CA	1417	C
31	CA	1420	A
31	CA	1424	G

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Mol	Chain	Res	Type
31	CA	1427	A
31	CA	1428	C
31	CA	1434	A
31	CA	1437	C
31	CA	1452	G
31	CA	1458	U
31	CA	1460	U
31	CA	1478	G
31	CA	1482	G
31	CA	1490	A
31	CA	1491	G
31	CA	1493	C
31	CA	1494	A
31	CA	1497	U
31	CA	1504	A
31	CA	1509	A
31	CA	1510	G
31	CA	1515	A
31	CA	1522	A
31	CA	1523	U
31	CA	1529	G
31	CA	1532	A
31	CA	1534	U
31	CA	1535	A
31	CA	1536	C
31	CA	1537	G
31	CA	1544	A
31	CA	1555	G
31	CA	1565	C
31	CA	1566	A
31	CA	1569	A
31	CA	1578	U
31	CA	1583	A
31	CA	1585	C
31	CA	1607	C
31	CA	1608	A
31	CA	1611	C
31	CA	1613	G
31	CA	1617	C
31	CA	1634	A
31	CA	1647	U
31	CA	1648	U

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Mol	Chain	Res	Type
31	CA	1649	G
31	CA	1663	G
31	CA	1664	A
31	CA	1674	G
31	CA	1677	A
31	CA	1694	C
31	CA	1697	G
31	CA	1698	A
31	CA	1699	G
31	CA	1703	G
31	CA	1715	G
31	CA	1729	U
31	CA	1730	C
31	CA	1738	G
31	CA	1744	A
31	CA	1750	G
31	CA	1754	A
31	CA	1758	U
31	CA	1764	C
31	CA	1773	A
31	CA	1781	U
31	CA	1782	U
31	CA	1784	A
31	CA	1786	A
31	CA	1787	A
31	CA	1800	C
31	CA	1801	A
31	CA	1808	A
31	CA	1812	U
31	CA	1815	A
31	CA	1816	C
31	CA	1821	A
31	CA	1822	C
31	CA	1823	G
31	CA	1828	G
31	CA	1829	A
31	CA	1833	C
31	CA	1834	U
31	CA	1839	G
31	CA	1869	G
31	CA	1870	C
31	CA	1871	A

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Mol	Chain	Res	Type
31	CA	1872	A
31	CA	1873	G
31	CA	1882	U
31	CA	1900	A
31	CA	1902	C
31	CA	1903	G
31	CA	1906	G
31	CA	1907	G
31	CA	1914	C
31	CA	1928	A
31	CA	1929	G
31	CA	1930	G
31	CA	1931	U
31	CA	1934	C
31	CA	1938	A
31	CA	1940	U
31	CA	1955	U
31	CA	1965	C
31	CA	1966	A
31	CA	1967	C
31	CA	1970	A
31	CA	1972	G
31	CA	1991	U
31	CA	1992	G
31	CA	1993	U
31	CA	1997	C
31	CA	2020	A
31	CA	2022	U
31	CA	2023	C
31	CA	2027	G
31	CA	2030	6MZ
31	CA	2031	A
31	CA	2033	A
31	CA	2035	G
31	CA	2036	C
31	CA	2043	C
31	CA	2046	G
31	CA	2049	G
31	CA	2051	A
31	CA	2055	C
31	CA	2056	G
31	CA	2060	A

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Mol	Chain	Res	Type
31	CA	2061	G
31	CA	2062	A
31	CA	2069	7MG
31	CA	2072	C
31	CA	2092	U
31	CA	2093	G
31	CA	2095	A
31	CA	2096	C
31	CA	2100	G
31	CA	2101	A
31	CA	2108	A
31	CA	2110	G
31	CA	2111	U
31	CA	2112	G
31	CA	2113	U
31	CA	2114	A
31	CA	2115	G
31	CA	2117	A
31	CA	2118	U
31	CA	2119	A
31	CA	2120	G
31	CA	2123	G
31	CA	2124	G
31	CA	2125	G
31	CA	2126	A
31	CA	2127	G
31	CA	2128	G
31	CA	2131	U
31	CA	2132	U
31	CA	2133	G
31	CA	2145	C
31	CA	2146	C
31	CA	2147	A
31	CA	2157	G
31	CA	2158	A
31	CA	2159	G
31	CA	2161	C
31	CA	2162	G
31	CA	2163	A
31	CA	2164	C
31	CA	2165	C
31	CA	2171	A

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Mol	Chain	Res	Type
31	CA	2172	U
31	CA	2173	A
31	CA	2174	C
31	CA	2178	C
31	CA	2190	G
31	CA	2198	A
31	CA	2203	U
31	CA	2204	G
31	CA	2211	A
31	CA	2225	A
31	CA	2226	C
31	CA	2238	G
31	CA	2239	G
31	CA	2243	U
31	CA	2259	U
31	CA	2268	A
31	CA	2278	A
31	CA	2282	G
31	CA	2283	C
31	CA	2286	G
31	CA	2287	A
31	CA	2288	A
31	CA	2305	U
31	CA	2311	A
31	CA	2324	U
31	CA	2325	G
31	CA	2326	C
31	CA	2327	A
31	CA	2331	G
31	CA	2333	A
31	CA	2335	A
31	CA	2345	G
31	CA	2347	C
31	CA	2350	C
31	CA	2354	C
31	CA	2357	G
31	CA	2361	G
31	CA	2383	G
31	CA	2385	C
31	CA	2402	U
31	CA	2403	C
31	CA	2406	A

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Mol	Chain	Res	Type
31	CA	2423	U
31	CA	2424	C
31	CA	2425	A
31	CA	2426	A
31	CA	2429	G
31	CA	2430	A
31	CA	2435	A
31	CA	2436	G
31	CA	2441	U
31	CA	2446	G
31	CA	2448	A
31	CA	2449	U
31	CA	2468	A
31	CA	2469	A
31	CA	2474	U
31	CA	2476	A
31	CA	2491	U
31	CA	2498	OMC
31	CA	2502	G
31	CA	2505	G
31	CA	2512	C
31	CA	2513	A
31	CA	2518	A
31	CA	2520	C
31	CA	2529	G
31	CA	2535	G
31	CA	2543	G
31	CA	2544	G
31	CA	2547	A
31	CA	2554	U
31	CA	2564	A
31	CA	2566	A
31	CA	2567	G
31	CA	2573	C
31	CA	2582	G
31	CA	2585	U
31	CA	2600	A
31	CA	2603	G
31	CA	2609	U
31	CA	2613	U
31	CA	2629	U
31	CA	2630	G

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Mol	Chain	Res	Type
31	CA	2645	G
31	CA	2646	C
31	CA	2661	G
31	CA	2663	G
31	CA	2673	G
31	CA	2681	C
31	CA	2682	A
31	CA	2689	U
31	CA	2690	U
31	CA	2714	G
31	CA	2718	G
31	CA	2726	A
31	CA	2733	A
31	CA	2744	G
31	CA	2748	A
31	CA	2762	C
31	CA	2765	A
31	CA	2776	A
31	CA	2777	G
31	CA	2778	A
31	CA	2779	U
31	CA	2780	G
31	CA	2791	G
31	CA	2794	C
31	CA	2798	U
31	CA	2799	A
31	CA	2818	U
31	CA	2820	A
31	CA	2821	A
31	CA	2835	A
31	CA	2836	U
31	CA	2849	U
31	CA	2850	A
31	CA	2861	U
31	CA	2867	G
31	CA	2870	C
31	CA	2872	A
31	CA	2879	A
31	CA	2883	A
31	CA	2886	A
31	CA	2893	A
31	CA	2894	G

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Mol	Chain	Res	Type
28	DB	25	U
28	DB	35	C
28	DB	37	C
28	DB	44	G
28	DB	45	A
28	DB	51	G
28	DB	52	A
28	DB	56	G
28	DB	57	A
28	DB	87	U
28	DB	88	C
28	DB	89	U
28	DB	90	C
28	DB	109	A
55	DA	10	A
55	DA	12	U
55	DA	13	A
55	DA	14	A
55	DA	15	G
55	DA	34	U
55	DA	46	G
55	DA	58	G
55	DA	71	A
55	DA	74	A
55	DA	75	G
55	DA	80	G
55	DA	84	A
55	DA	86	G
55	DA	101	A
55	DA	102	U
55	DA	118	A
55	DA	119	A
55	DA	120	U
55	DA	125	A
55	DA	137	U
55	DA	138	U
55	DA	139	U
55	DA	140	C
55	DA	141	G
55	DA	142	A
55	DA	177	G
55	DA	178	G

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Mol	Chain	Res	Type
55	DA	186	G
55	DA	188	G
55	DA	193	U
55	DA	196	A
55	DA	197	A
55	DA	198	C
55	DA	199	A
55	DA	200	U
55	DA	215	G
55	DA	216	A
55	DA	221	A
55	DA	222	A
55	DA	230	G
55	DA	248	G
55	DA	265	A
55	DA	266	G
55	DA	267	C
55	DA	272	A
55	DA	276	U
55	DA	277	G
55	DA	278	A
55	DA	279	A
55	DA	285	G
55	DA	302	C
55	DA	311	A
55	DA	317	G
55	DA	324	A
55	DA	329	G
55	DA	330	A
55	DA	331	C
55	DA	343	C
55	DA	346	A
55	DA	352	A
55	DA	353	C
55	DA	361	G
55	DA	362	A
55	DA	372	G
55	DA	383	C
55	DA	386	G
55	DA	396	G
55	DA	399	U
55	DA	403	U

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Mol	Chain	Res	Type
55	DA	406	G
55	DA	411	G
55	DA	412	A
55	DA	420	C
55	DA	424	G
55	DA	435	C
55	DA	451	U
55	DA	455	C
55	DA	456	C
55	DA	459	U
55	DA	475	C
55	DA	479	A
55	DA	480	A
55	DA	481	G
55	DA	482	A
55	DA	491	G
55	DA	496	G
55	DA	503	A
55	DA	504	A
55	DA	505	A
55	DA	508	A
55	DA	510	C
55	DA	513	A
55	DA	531	C
55	DA	532	A
55	DA	533	G
55	DA	543	G
55	DA	544	C
55	DA	546	U
55	DA	547	A
55	DA	548	G
55	DA	549	G
55	DA	550	C
55	DA	563	A
55	DA	573	U
55	DA	575	A
55	DA	586	A
55	DA	603	A
55	DA	604	G
55	DA	613	A
55	DA	614	A
55	DA	615	U

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Mol	Chain	Res	Type
55	DA	620	G
55	DA	621	A
55	DA	622	G
55	DA	627	A
55	DA	637	A
55	DA	645	C
55	DA	647	G
55	DA	651	G
55	DA	653	U
55	DA	654	A
55	DA	655	A
55	DA	659	G
55	DA	684	G
55	DA	685	A
55	DA	686	U
55	DA	717	C
55	DA	730	A
55	DA	738	G
55	DA	747	5MU
55	DA	764	A
55	DA	765	C
55	DA	772	C
55	DA	775	G
55	DA	776	G
55	DA	782	A
55	DA	783	A
55	DA	784	G
55	DA	785	G
55	DA	790	U
55	DA	801	G
55	DA	802	A
55	DA	805	G
55	DA	806	C
55	DA	812	C
55	DA	827	U
55	DA	828	U
55	DA	858	G
55	DA	859	G
55	DA	866	A
55	DA	878	A
55	DA	882	G
55	DA	885	C

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Mol	Chain	Res	Type
55	DA	896	A
55	DA	897	C
55	DA	907	G
55	DA	910	A
55	DA	914	G
55	DA	915	C
55	DA	931	U
55	DA	932	U
55	DA	946	C
55	DA	947	A
55	DA	957	C
55	DA	961	C
55	DA	974	G
55	DA	983	A
55	DA	984	A
55	DA	985	C
55	DA	996	A
55	DA	1010	A
55	DA	1012	U
55	DA	1013	C
55	DA	1022	G
55	DA	1023	U
55	DA	1026	G
55	DA	1033	U
55	DA	1040	A
55	DA	1047	G
55	DA	1061	U
55	DA	1062	G
55	DA	1068	G
55	DA	1069	A
55	DA	1070	A
55	DA	1071	G
55	DA	1073	A
55	DA	1083	U
55	DA	1087	G
55	DA	1088	A
55	DA	1090	A
55	DA	1096	A
55	DA	1097	U
55	DA	1112	G
55	DA	1119	U
55	DA	1128	G

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Mol	Chain	Res	Type
55	DA	1129	A
55	DA	1132	U
55	DA	1133	A
55	DA	1135	C
55	DA	1136	G
55	DA	1141	U
55	DA	1142	A
55	DA	1151	A
55	DA	1168	G
55	DA	1171	G
55	DA	1172	C
55	DA	1174	U
55	DA	1176	U
55	DA	1177	G
55	DA	1180	U
55	DA	1212	G
55	DA	1238	G
55	DA	1244	A
55	DA	1250	G
55	DA	1253	A
55	DA	1256	G
55	DA	1262	A
55	DA	1269	A
55	DA	1271	G
55	DA	1272	A
55	DA	1273	U
55	DA	1294	U
55	DA	1297	C
55	DA	1300	G
55	DA	1301	A
55	DA	1306	C
55	DA	1321	A
55	DA	1328	A
55	DA	1332	G
55	DA	1352	U
55	DA	1355	G
55	DA	1359	A
55	DA	1365	A
55	DA	1379	U
55	DA	1383	A
55	DA	1386	C
55	DA	1398	C

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Mol	Chain	Res	Type
55	DA	1403	A
55	DA	1416	G
55	DA	1417	C
55	DA	1420	A
55	DA	1427	A
55	DA	1428	C
55	DA	1452	G
55	DA	1453	A
55	DA	1460	U
55	DA	1478	G
55	DA	1482	G
55	DA	1490	A
55	DA	1491	G
55	DA	1493	C
55	DA	1494	A
55	DA	1497	U
55	DA	1504	A
55	DA	1508	A
55	DA	1509	A
55	DA	1510	G
55	DA	1515	A
55	DA	1523	U
55	DA	1529	G
55	DA	1532	A
55	DA	1534	U
55	DA	1535	A
55	DA	1537	G
55	DA	1544	A
55	DA	1554	U
55	DA	1566	A
55	DA	1569	A
55	DA	1578	U
55	DA	1583	A
55	DA	1585	C
55	DA	1607	C
55	DA	1608	A
55	DA	1613	G
55	DA	1647	U
55	DA	1648	U
55	DA	1649	G
55	DA	1663	G
55	DA	1674	G

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Mol	Chain	Res	Type
55	DA	1694	C
55	DA	1699	G
55	DA	1715	G
55	DA	1729	U
55	DA	1730	C
55	DA	1738	G
55	DA	1744	A
55	DA	1750	G
55	DA	1758	U
55	DA	1764	C
55	DA	1773	A
55	DA	1781	U
55	DA	1782	U
55	DA	1786	A
55	DA	1800	C
55	DA	1801	A
55	DA	1808	A
55	DA	1812	U
55	DA	1816	C
55	DA	1826	G
55	DA	1829	A
55	DA	1869	G
55	DA	1870	C
55	DA	1871	A
55	DA	1872	A
55	DA	1873	G
55	DA	1900	A
55	DA	1906	G
55	DA	1907	G
55	DA	1913	A
55	DA	1914	C
55	DA	1927	A
55	DA	1929	G
55	DA	1930	G
55	DA	1931	U
55	DA	1932	A
55	DA	1938	A
55	DA	1941	C
55	DA	1955	U
55	DA	1965	C
55	DA	1967	C
55	DA	1970	A

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Mol	Chain	Res	Type
55	DA	1972	G
55	DA	1974	C
55	DA	1991	U
55	DA	1992	G
55	DA	1993	U
55	DA	1997	C
55	DA	2020	A
55	DA	2023	C
55	DA	2031	A
55	DA	2033	A
55	DA	2035	G
55	DA	2036	C
55	DA	2043	C
55	DA	2049	G
55	DA	2055	C
55	DA	2056	G
55	DA	2060	A
55	DA	2061	G
55	DA	2062	A
55	DA	2069	7MG
55	DA	2093	G
55	DA	2095	A
55	DA	2097	A
55	DA	2098	U
55	DA	2100	G
55	DA	2101	A
55	DA	2105	U
55	DA	2108	A
55	DA	2111	U
55	DA	2112	G
55	DA	2113	U
55	DA	2116	G
55	DA	2117	A
55	DA	2118	U
55	DA	2119	A
55	DA	2120	G
55	DA	2121	G
55	DA	2123	G
55	DA	2125	G
55	DA	2126	A
55	DA	2127	G
55	DA	2128	G

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Mol	Chain	Res	Type
55	DA	2131	U
55	DA	2132	U
55	DA	2133	G
55	DA	2134	A
55	DA	2135	A
55	DA	2145	C
55	DA	2146	C
55	DA	2147	A
55	DA	2148	G
55	DA	2157	G
55	DA	2158	A
55	DA	2159	G
55	DA	2160	C
55	DA	2161	C
55	DA	2162	G
55	DA	2163	A
55	DA	2164	C
55	DA	2165	C
55	DA	2167	U
55	DA	2168	G
55	DA	2169	A
55	DA	2170	A
55	DA	2171	A
55	DA	2172	U
55	DA	2173	A
55	DA	2178	C
55	DA	2179	C
55	DA	2181	U
55	DA	2185	U
55	DA	2186	G
55	DA	2198	A
55	DA	2204	G
55	DA	2211	A
55	DA	2225	A
55	DA	2238	G
55	DA	2239	G
55	DA	2268	A
55	DA	2278	A
55	DA	2280	G
55	DA	2282	G
55	DA	2283	C
55	DA	2286	G

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Mol	Chain	Res	Type
55	DA	2287	A
55	DA	2288	A
55	DA	2292	U
55	DA	2305	U
55	DA	2308	G
55	DA	2311	A
55	DA	2312	U
55	DA	2320	U
55	DA	2325	G
55	DA	2327	A
55	DA	2328	A
55	DA	2331	G
55	DA	2333	A
55	DA	2335	A
55	DA	2347	C
55	DA	2350	C
55	DA	2357	G
55	DA	2383	G
55	DA	2385	C
55	DA	2402	U
55	DA	2403	C
55	DA	2406	A
55	DA	2407	A
55	DA	2410	G
55	DA	2423	U
55	DA	2424	C
55	DA	2425	A
55	DA	2426	A
55	DA	2427	C
55	DA	2434	A
55	DA	2435	A
55	DA	2441	U
55	DA	2448	A
55	DA	2464	G
55	DA	2465	C
55	DA	2469	A
55	DA	2474	U
55	DA	2476	A
55	DA	2478	A
55	DA	2480	C
55	DA	2491	U
55	DA	2502	G

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Mol	Chain	Res	Type
55	DA	2505	G
55	DA	2518	A
55	DA	2520	C
55	DA	2529	G
55	DA	2535	G
55	DA	2547	A
55	DA	2564	A
55	DA	2566	A
55	DA	2567	G
55	DA	2573	C
55	DA	2578	G
55	DA	2582	G
55	DA	2585	U
55	DA	2586	U
55	DA	2596	U
55	DA	2603	G
55	DA	2609	U
55	DA	2613	U
55	DA	2621	G
55	DA	2629	U
55	DA	2630	G
55	DA	2661	G
55	DA	2663	G
55	DA	2673	G
55	DA	2689	U
55	DA	2690	U
55	DA	2706	A
55	DA	2714	G
55	DA	2719	G
55	DA	2720	U
55	DA	2721	A
55	DA	2726	A
55	DA	2729	G
55	DA	2733	A
55	DA	2744	G
55	DA	2748	A
55	DA	2762	C
55	DA	2765	A
55	DA	2769	U
55	DA	2778	A
55	DA	2791	G
55	DA	2798	U

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Mol	Chain	Res	Type
55	DA	2799	A
55	DA	2811	G
55	DA	2815	C
55	DA	2818	U
55	DA	2820	A
55	DA	2821	A
55	DA	2825	G
55	DA	2835	A
55	DA	2836	U
55	DA	2861	U
55	DA	2867	G
55	DA	2872	A
55	DA	2879	A
55	DA	2883	A

All (286) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	7	A
1	AA	30	U
1	AA	49	U
1	AA	70	U
1	AA	89	U
1	AA	142	G
1	AA	209	U
1	AA	250	A
1	AA	305	G
1	AA	327	A
1	AA	367	U
1	AA	413	G
1	AA	422	C
1	AA	438	U
1	AA	518	C
1	AA	559	A
1	AA	576	C
1	AA	641	U
1	AA	702	A
1	AA	733	G
1	AA	793	U
1	AA	841	C
1	AA	870	U

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Mol	Chain	Res	Type
1	AA	884	U
1	AA	965	U
1	AA	971	G
1	AA	974	A
1	AA	991	U
1	AA	992	U
1	AA	1053	G
1	AA	1129	C
1	AA	1136	C
1	AA	1137	C
1	AA	1140	C
1	AA	1141	C
1	AA	1195	C
1	AA	1197	A
1	AA	1224	U
1	AA	1225	A
1	AA	1278	G
1	AA	1281	C
1	AA	1319	A
1	AA	1345	U
1	AA	1380	U
1	AA	1397	C
1	AA	1432	G
1	AA	1452	C
1	BA	5	U
1	BA	7	A
1	BA	30	U
1	BA	49	U
1	BA	70	U
1	BA	83	C
1	BA	86	G
1	BA	89	U
1	BA	142	G
1	BA	209	U
1	BA	246	A
1	BA	250	A
1	BA	305	G
1	BA	327	A
1	BA	367	U
1	BA	422	C
1	BA	438	U
1	BA	518	C

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Mol	Chain	Res	Type
1	BA	559	A
1	BA	561	U
1	BA	576	C
1	BA	641	U
1	BA	702	A
1	BA	733	G
1	BA	793	U
1	BA	842	U
1	BA	870	U
1	BA	884	U
1	BA	965	U
1	BA	971	G
1	BA	974	A
1	BA	991	U
1	BA	992	U
1	BA	1008	U
1	BA	1053	G
1	BA	1129	C
1	BA	1136	C
1	BA	1137	C
1	BA	1140	C
1	BA	1141	C
1	BA	1196	A
1	BA	1224	U
1	BA	1225	A
1	BA	1278	G
1	BA	1281	C
1	BA	1319	A
1	BA	1345	U
1	BA	1362	A
1	BA	1363	A
1	BA	1380	U
1	BA	1397	C
1	BA	1452	C
28	CB	51	G
28	CB	89	U
31	CA	83	A
31	CA	137	U
31	CA	138	U
31	CA	139	U
31	CA	141	G
31	CA	177	G

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Mol	Chain	Res	Type
31	CA	196	A
31	CA	199	A
31	CA	215	G
31	CA	271	G
31	CA	278	A
31	CA	310	A
31	CA	345	A
31	CA	361	G
31	CA	386	G
31	CA	390	U
31	CA	403	U
31	CA	404	A
31	CA	411	G
31	CA	455	C
31	CA	503	A
31	CA	506	G
31	CA	527	C
31	CA	531	C
31	CA	571	U
31	CA	572	A
31	CA	573	U
31	CA	603	A
31	CA	620	G
31	CA	637	A
31	CA	669	G
31	CA	684	G
31	CA	685	A
31	CA	752	A
31	CA	764	A
31	CA	774	G
31	CA	781	A
31	CA	784	G
31	CA	827	U
31	CA	846	U
31	CA	913	U
31	CA	945	A
31	CA	957	C
31	CA	973	A
31	CA	984	A
31	CA	1021	A
31	CA	1045	C
31	CA	1061	U

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Mol	Chain	Res	Type
31	CA	1069	A
31	CA	1070	A
31	CA	1087	G
31	CA	1089	A
31	CA	1128	G
31	CA	1133	A
31	CA	1141	U
31	CA	1212	G
31	CA	1247	A
31	CA	1288	G
31	CA	1300	G
31	CA	1329	U
31	CA	1379	U
31	CA	1397	U
31	CA	1452	G
31	CA	1490	A
31	CA	1497	U
31	CA	1509	A
31	CA	1535	A
31	CA	1536	C
31	CA	1607	C
31	CA	1647	U
31	CA	1776	G
31	CA	1786	A
31	CA	1800	C
31	CA	1818	U
31	CA	1838	C
31	CA	1870	C
31	CA	1871	A
31	CA	1900	A
31	CA	1937	A
31	CA	1970	A
31	CA	2035	G
31	CA	2043	C
31	CA	2095	A
31	CA	2119	A
31	CA	2126	A
31	CA	2145	C
31	CA	2146	C
31	CA	2157	G
31	CA	2164	C
31	CA	2225	A

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Mol	Chain	Res	Type
31	CA	2238	G
31	CA	2282	G
31	CA	2286	G
31	CA	2324	U
31	CA	2326	C
31	CA	2423	U
31	CA	2425	A
31	CA	2426	A
31	CA	2448	A
31	CA	2468	A
31	CA	2542	A
31	CA	2572	A
31	CA	2645	G
31	CA	2680	U
31	CA	2776	A
31	CA	2778	A
31	CA	2779	U
31	CA	2849	U
31	CA	2873	A
31	CA	2893	A
28	DB	51	G
55	DA	119	A
55	DA	125	A
55	DA	137	U
55	DA	138	U
55	DA	141	G
55	DA	177	G
55	DA	196	A
55	DA	199	A
55	DA	215	G
55	DA	271	G
55	DA	278	A
55	DA	345	A
55	DA	361	G
55	DA	403	U
55	DA	411	G
55	DA	455	C
55	DA	503	A
55	DA	512	G
55	DA	603	A
55	DA	614	A
55	DA	620	G

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Mol	Chain	Res	Type
55	DA	764	A
55	DA	784	G
55	DA	858	G
55	DA	945	A
55	DA	984	A
55	DA	1061	U
55	DA	1069	A
55	DA	1070	A
55	DA	1087	G
55	DA	1089	A
55	DA	1128	G
55	DA	1133	A
55	DA	1171	G
55	DA	1300	G
55	DA	1329	U
55	DA	1396	U
55	DA	1397	U
55	DA	1420	A
55	DA	1427	A
55	DA	1490	A
55	DA	1509	A
55	DA	1535	A
55	DA	1558	C
55	DA	1607	C
55	DA	1647	U
55	DA	1786	A
55	DA	1800	C
55	DA	1870	C
55	DA	1871	A
55	DA	1900	A
55	DA	1939	5MU
55	DA	2035	G
55	DA	2051	A
55	DA	2097	A
55	DA	2119	A
55	DA	2126	A
55	DA	2127	G
55	DA	2146	C
55	DA	2157	G
55	DA	2158	A
55	DA	2164	C
55	DA	2238	G

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Mol	Chain	Res	Type
55	DA	2282	G
55	DA	2286	G
55	DA	2311	A
55	DA	2406	A
55	DA	2423	U
55	DA	2572	A
55	DA	2581	G
55	DA	2585	U
55	DA	2866	U
55	DA	2873	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
31	PSU	CA	2580	31	18,21,22	0.58	0	21,30,33	0.78	2 (9%)
1	MA6	AA	1518	1	23,26,27	0.50	0	33,38,41	1.21	4 (12%)
55	PSU	DA	955	55	18,21,22	0.69	0	21,30,33	0.50	0
1	2MG	AA	966	1	23,26,27	0.49	0	33,38,41	0.57	0
31	OMC	CA	2498	31,56	19,22,23	0.36	0	25,31,34	0.36	0
1	7MG	BA	527	1	23,26,27	4.22	2 (8%)	27,39,42	2.52	6 (22%)
55	PSU	DA	2457	55	18,21,22	0.56	0	21,30,33	0.52	0
31	OMG	CA	2251	31	23,26,27	0.46	0	32,38,41	0.42	0
41	4D4	DN	81[B]	-	9,11,12	1.82	2 (22%)	7,13,15	2.27	2 (28%)
55	5MU	DA	747	55	19,22,23	0.48	0	27,32,35	0.35	0
31	2MG	CA	1835	31	23,26,27	0.34	0	33,38,41	0.35	0
31	PSU	CA	955	31	18,21,22	0.39	0	21,30,33	0.57	1 (4%)
55	5MU	DA	1939	55	19,22,23	0.65	0	27,32,35	0.40	0
1	5MC	BA	1407	1	19,22,23	0.36	0	26,32,35	0.41	0
31	2MA	CA	2503	31	22,25,26	0.73	0	32,37,40	1.87	6 (18%)
1	PSU	BA	516	1	18,21,22	0.47	0	21,30,33	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UR3	AA	1498	1	19,22,23	0.60	0	26,32,35	0.60	1 (3%)
31	PSU	CA	2504	31	18,21,22	0.35	0	21,30,33	0.43	0
55	7MG	DA	2069	55	23,26,27	4.22	1 (4%)	27,39,42	2.25	6 (22%)
55	H2U	DA	2449	55	18,21,22	0.84	0	19,30,33	0.41	0
55	6MZ	DA	1618	55	22,25,26	0.66	0	29,36,39	1.32	1 (3%)
31	5MU	CA	747	31	19,22,23	0.26	0	27,32,35	0.28	0
55	OMU	DA	2552	55	19,22,23	0.51	0	25,31,34	0.33	0
55	PSU	DA	746	56,55	18,21,22	1.12	2 (11%)	21,30,33	0.39	0
55	2MA	DA	2503	56,55	22,25,26	0.70	0	32,37,40	1.62	6 (18%)
55	PSU	DA	2604	55	18,21,22	0.79	1 (5%)	21,30,33	0.51	0
1	MA6	BA	1519	1	23,26,27	0.49	0	33,38,41	1.05	3 (9%)
55	OMC	DA	2498	56,55	19,22,23	0.65	1 (5%)	25,31,34	0.46	0
31	7MG	CA	2069	31	23,26,27	4.21	4 (17%)	27,39,42	2.32	6 (22%)
31	PSU	CA	2457	31	18,21,22	0.83	1 (5%)	21,30,33	0.42	0
31	OMU	CA	2552	31	19,22,23	0.27	0	25,31,34	0.37	0
1	2MG	BA	1207	1	23,26,27	0.35	0	33,38,41	0.42	0
1	5MC	AA	1407	1	19,22,23	0.30	0	26,32,35	0.41	0
55	6MZ	DA	2030	55	22,25,26	0.39	0	29,36,39	0.67	1 (3%)
32	MEQ	DD	150[A]	32	8,9,10	0.40	0	5,10,12	0.54	0
1	2MG	AA	1516	1	23,26,27	0.33	0	33,38,41	0.46	0
1	7MG	AA	527	1	23,26,27	4.11	3 (13%)	27,39,42	2.49	6 (22%)
1	2MG	AA	1207	1	23,26,27	0.32	0	33,38,41	0.40	0
31	3TD	CA	1915	31	19,22,23	0.46	0	23,32,35	0.82	1 (4%)
55	5MC	DA	1962	55	19,22,23	0.67	0	26,32,35	0.45	0
55	OMG	DA	2251	55	23,26,27	0.42	0	32,38,41	0.38	0
55	2MG	DA	2445	55	23,26,27	0.47	0	33,38,41	0.44	0
55	PSU	DA	2605	55	18,21,22	0.48	0	21,30,33	0.51	0
1	2MG	BA	1516	1	23,26,27	0.33	0	33,38,41	0.47	0
1	MA6	BA	1518	1	23,26,27	0.49	0	33,38,41	1.27	4 (12%)
55	2MG	DA	1835	55	23,26,27	0.40	0	33,38,41	0.38	0
31	PSU	CA	746	31,56	18,21,22	0.70	1 (5%)	21,30,33	0.43	0
1	2MG	BA	966	1	23,26,27	0.49	0	33,38,41	0.48	0
12	D2T	AL	89	12	8,9,10	0.96	1 (12%)	6,11,13	0.75	0
31	PSU	CA	1911	31	18,21,22	0.37	0	21,30,33	0.42	0
31	6MZ	CA	1618	31	22,25,26	0.61	0	29,36,39	0.78	1 (3%)
31	6MZ	CA	2030	31	22,25,26	0.37	0	29,36,39	0.47	0
31	5MU	CA	1939	31	19,22,23	0.48	0	27,32,35	0.36	0
32	MEQ	DD	150[B]	32	8,9,10	1.47	1 (12%)	5,10,12	1.46	1 (20%)
55	PSU	DA	1917	55	18,21,22	0.50	0	21,30,33	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	AA	967	1	19,22,23	0.34	0	26,32,35	0.38	0
1	4OC	AA	1402	1	20,23,24	0.34	0	25,32,35	0.44	0
1	UR3	BA	1498	1	19,22,23	0.56	0	26,32,35	0.73	1 (3%)
12	D2T	BL	89	12	8,9,10	0.91	0	6,11,13	0.67	0
55	PSU	DA	2580	55	18,21,22	0.63	0	21,30,33	0.61	0
31	5MC	CA	1962	31	19,22,23	0.26	0	26,32,35	0.39	0
1	PSU	AA	516	56,1	18,21,22	0.44	0	21,30,33	0.48	0
31	2MG	CA	2445	31	23,26,27	0.36	0	33,38,41	0.45	0
31	1MG	CA	745	31	23,26,27	0.76	1 (4%)	33,39,42	0.70	1 (3%)
1	5MC	BA	967	1	19,22,23	0.34	0	26,32,35	0.37	0
55	3TD	DA	1915	55	19,22,23	0.43	0	23,32,35	0.80	1 (4%)
1	MA6	AA	1519	1	23,26,27	0.54	0	33,38,41	1.03	4 (12%)
31	PSU	CA	2605	31	18,21,22	0.35	0	21,30,33	0.50	0
41	4D4	CN	81	41	9,11,12	2.36	2 (22%)	7,13,15	2.40	2 (28%)
55	PSU	DA	1911	55	18,21,22	0.40	0	21,30,33	0.43	0
55	1MG	DA	745	55	23,26,27	0.95	1 (4%)	33,39,42	0.73	1 (3%)
55	PSU	DA	2504	55	18,21,22	0.45	0	21,30,33	0.39	0
31	PSU	CA	1917	31	18,21,22	0.40	0	21,30,33	0.39	0
41	4D4	DN	81[A]	-	9,11,12	1.67	1 (11%)	7,13,15	3.20	2 (28%)
1	4OC	BA	1402	1	20,23,24	0.40	0	25,32,35	0.46	0

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
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/11/29/30	0/3/3/3
55	PSU	DA	955	55	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/9/27/28	0/3/3/3
31	OMC	CA	2498	31,56	-	2/9/27/28	0/2/2/2
1	7MG	BA	527	1	-	2/7/37/38	0/3/3/3
55	PSU	DA	2457	55	-	0/7/25/26	0/2/2/2
31	OMG	CA	2251	31	-	0/9/27/28	0/3/3/3
41	4D4	DN	81[B]	-	-	3/11/12/14	-
55	5MU	DA	747	55	-	0/7/25/26	0/2/2/2
31	2MG	CA	1835	31	-	0/9/27/28	0/3/3/3
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
55	5MU	DA	1939	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
31	2MA	CA	2503	31	-	2/7/25/26	0/3/3/3
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
31	PSU	CA	2504	31	-	1/7/25/26	0/2/2/2
55	7MG	DA	2069	55	-	1/7/37/38	0/3/3/3
55	H2U	DA	2449	55	-	1/7/38/39	0/2/2/2
55	6MZ	DA	1618	55	-	0/9/27/28	0/3/3/3
31	5MU	CA	747	31	-	0/7/25/26	0/2/2/2
55	OMU	DA	2552	55	-	0/9/27/28	0/2/2/2
55	PSU	DA	746	56,55	-	2/7/25/26	0/2/2/2
55	2MA	DA	2503	56,55	-	2/7/25/26	0/3/3/3
55	PSU	DA	2604	55	-	1/7/25/26	0/2/2/2
1	MA6	BA	1519	1	-	3/11/29/30	0/3/3/3
55	OMC	DA	2498	56,55	-	0/9/27/28	0/2/2/2
31	7MG	CA	2069	31	-	0/7/37/38	0/3/3/3
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
31	OMU	CA	2552	31	-	0/9/27/28	0/2/2/2
1	2MG	BA	1207	1	-	0/9/27/28	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
55	6MZ	DA	2030	55	-	1/9/27/28	0/3/3/3
32	MEQ	DD	150[A]	32	-	5/8/9/11	-
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3
1	7MG	AA	527	1	-	2/7/37/38	0/3/3/3
1	2MG	AA	1207	1	-	0/9/27/28	0/3/3/3
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
55	5MC	DA	1962	55	-	1/7/25/26	0/2/2/2
55	OMG	DA	2251	55	-	0/9/27/28	0/3/3/3
55	2MG	DA	2445	55	-	2/9/27/28	0/3/3/3
55	PSU	DA	2605	55	-	0/7/25/26	0/2/2/2
1	2MG	BA	1516	1	-	0/9/27/28	0/3/3/3
1	MA6	BA	1518	1	-	0/11/29/30	0/3/3/3
55	2MG	DA	1835	55	-	0/9/27/28	0/3/3/3
31	PSU	CA	746	31,56	-	2/7/25/26	0/2/2/2
1	2MG	BA	966	1	-	0/9/27/28	0/3/3/3
12	D2T	AL	89	12	-	3/7/12/14	-
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
31	6MZ	CA	1618	31	-	1/9/27/28	0/3/3/3
31	6MZ	CA	2030	31	-	2/9/27/28	0/3/3/3
31	5MU	CA	1939	31	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MEQ	DD	150[B]	32	-	3/8/9/11	-
55	PSU	DA	1917	55	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
12	D2T	BL	89	12	-	6/7/12/14	-
55	PSU	DA	2580	55	-	1/7/25/26	0/2/2/2
31	5MC	CA	1962	31	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	56,1	-	0/7/25/26	0/2/2/2
31	2MG	CA	2445	31	-	0/9/27/28	0/3/3/3
31	1MG	CA	745	31	-	0/7/25/26	0/3/3/3
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
55	3TD	DA	1915	55	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	3/11/29/30	0/3/3/3
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
41	4D4	CN	81	41	-	1/11/12/14	-
55	PSU	DA	1911	55	-	0/7/25/26	0/2/2/2
55	1MG	DA	745	55	-	0/7/25/26	0/3/3/3
55	PSU	DA	2504	55	-	1/7/25/26	0/2/2/2
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
41	4D4	DN	81[A]	-	-	1/11/12/14	-
1	4OC	BA	1402	1	-	0/9/29/30	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	2069	7MG	C8-N9	-19.89	1.33	1.45
1	BA	527	7MG	C8-N9	-19.74	1.33	1.45
31	CA	2069	7MG	C8-N9	-19.20	1.33	1.45
1	AA	527	7MG	C8-N9	-19.14	1.33	1.45
41	CN	81	4D4	CZ-NE	6.34	1.45	1.33
41	DN	81[B]	4D4	CZ-NE	4.65	1.42	1.33
41	DN	81[A]	4D4	CZ-NE	4.44	1.41	1.33
31	CA	2069	7MG	C5-N7	3.96	1.40	1.35
55	DA	746	PSU	O4'-C1'	-3.91	1.38	1.43
32	DD	150[B]	MEQ	CB-CA	3.91	1.59	1.53
55	DA	745	1MG	C2-N1	3.63	1.43	1.37
31	CA	2069	7MG	C1'-N9	-3.59	1.40	1.46
1	AA	527	7MG	C5-N7	3.39	1.39	1.35
31	CA	745	1MG	C2-N1	3.01	1.42	1.37
41	CN	81	4D4	CZ-NH1	2.77	1.44	1.34
41	DN	81[B]	4D4	CZ-NH1	2.60	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	746	PSU	C2'-C1'	-2.36	1.50	1.53
31	CA	746	PSU	O4'-C1'	-2.26	1.40	1.43
55	DA	2604	PSU	O3'-C3'	-2.26	1.37	1.43
55	DA	2498	OMC	O5'-C5'	-2.21	1.37	1.44
1	BA	527	7MG	C1'-N9	-2.20	1.42	1.46
31	CA	2457	PSU	O5'-C5'	-2.11	1.38	1.44
31	CA	2069	7MG	C8-N7	-2.09	1.32	1.42
12	AL	89	D2T	CB-CG	2.04	1.55	1.52
1	AA	527	7MG	C8-N7	-2.03	1.32	1.42

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2503	2MA	N6-C6-N1	7.89	127.68	117.03
1	BA	527	7MG	C6-C5-C4	-6.80	110.43	122.40
41	DN	81[A]	4D4	NE-CZ-NH2	6.72	132.21	120.67
1	AA	527	7MG	C6-C5-N7	-6.66	121.61	131.93
55	DA	2503	2MA	N6-C6-N1	6.65	126.00	117.03
55	DA	1618	6MZ	C9-N6-C6	-6.63	116.70	122.85
1	BA	527	7MG	C6-C5-N7	-6.60	121.70	131.93
31	CA	2069	7MG	C6-C5-C4	-6.04	111.78	122.40
31	CA	2069	7MG	C6-C5-N7	-5.84	122.88	131.93
1	BA	527	7MG	O4'-C1'-N9	5.56	116.87	109.30
55	DA	2069	7MG	C5-C4-N3	-5.34	118.11	128.13
1	AA	527	7MG	C5-C4-N3	-5.33	118.12	128.13
41	CN	81	4D4	NE-CZ-NH2	5.29	129.75	120.67
1	AA	527	7MG	O4'-C1'-N9	5.14	116.30	109.30
31	CA	2069	7MG	N9-C8-N7	5.13	110.64	103.37
1	AA	527	7MG	C6-C5-C4	-5.07	113.49	122.40
55	DA	2069	7MG	C6-C5-N7	-5.05	124.11	131.93
55	DA	2069	7MG	C6-C5-C4	-5.04	113.54	122.40
55	DA	2069	7MG	O4'-C1'-N9	5.04	116.16	109.30
41	DN	81[B]	4D4	NE-CZ-NH2	4.98	129.22	120.67
1	AA	527	7MG	N9-C8-N7	4.92	110.33	103.37
41	DN	81[A]	4D4	NH1-CZ-NE	-4.59	108.84	119.27
1	BA	527	7MG	C5-C4-N3	-4.55	119.60	128.13
31	CA	2069	7MG	O4'-C1'-N9	4.41	115.30	109.30
1	BA	527	7MG	N9-C8-N7	4.33	109.50	103.37
55	DA	2069	7MG	N9-C8-N7	4.27	109.41	103.37
31	CA	2069	7MG	C5-C4-N3	-4.09	120.45	128.13
31	CA	2503	2MA	C2-N1-C6	4.04	124.32	118.10
1	BA	1518	MA6	N1-C6-N6	-4.01	111.97	116.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	1518	MA6	C4-C5-C6	-3.98	111.79	115.91
1	AA	1518	MA6	C4-C5-C6	-3.83	111.94	115.91
55	DA	2503	2MA	C2-N1-C6	3.75	123.87	118.10
1	AA	1518	MA6	N1-C6-N6	-3.52	112.57	116.86
55	DA	745	1MG	N2-C2-N1	-3.33	116.11	118.79
1	BA	1519	MA6	C4-C5-C6	-3.26	112.54	115.91
32	DD	150[B]	MEQ	CB-CG-CD	3.24	120.29	113.06
1	AA	527	7MG	C4-C5-N7	-3.12	101.69	105.38
31	CA	1915	3TD	C1'-C5-C4	2.98	122.12	117.61
31	CA	2069	7MG	C4-C5-N7	-2.96	101.87	105.38
1	AA	1519	MA6	C4-C5-C6	-2.96	112.85	115.91
1	BA	1498	UR3	C4-N3-C2	2.82	126.84	124.58
55	DA	1915	3TD	C1'-C5-C4	2.79	121.84	117.61
55	DA	2069	7MG	C4-C5-N7	-2.78	102.08	105.38
1	BA	527	7MG	C4-C5-N7	-2.77	102.10	105.38
41	DN	81[B]	4D4	NH1-CZ-NE	-2.72	113.09	119.27
1	BA	1519	MA6	C5-C6-N6	-2.70	121.06	125.33
1	BA	1518	MA6	C5-C6-N1	2.70	124.14	118.55
1	AA	1518	MA6	C5-C6-N1	2.64	124.02	118.55
31	CA	2503	2MA	C5-C6-N6	-2.58	116.90	123.29
1	BA	1518	MA6	C6-C5-N7	2.56	137.53	133.43
1	AA	1519	MA6	C5-C6-N6	-2.48	121.41	125.33
1	AA	1519	MA6	C5-C6-N1	2.46	123.65	118.55
1	AA	1518	MA6	C6-C5-N7	2.45	137.34	133.43
31	CA	745	1MG	C6-C5-C4	-2.42	117.23	119.97
1	BA	1519	MA6	C5-C6-N1	2.39	123.50	118.55
31	CA	2503	2MA	CM2-C2-N3	2.37	120.68	117.13
41	CN	81	4D4	NH1-CZ-NE	-2.36	113.90	119.27
31	CA	2503	2MA	N3-C2-N1	-2.34	121.64	125.77
55	DA	2503	2MA	CM2-C2-N3	2.29	120.56	117.13
31	CA	2503	2MA	C5-C6-N1	-2.26	115.38	118.90
55	DA	2503	2MA	N3-C2-N1	-2.24	121.82	125.77
1	AA	1498	UR3	C4-N3-C2	2.23	126.38	124.58
31	CA	2580	PSU	O4'-C1'-C2'	2.12	108.09	105.15
55	DA	2030	6MZ	C9-N6-C6	2.12	124.82	122.85
31	CA	1618	6MZ	C4-C5-C6	-2.12	115.02	116.78
55	DA	2503	2MA	C5-C6-N1	-2.09	115.65	118.90
31	CA	2580	PSU	C3'-C2'-C1'	2.07	104.14	101.69
1	AA	1519	MA6	C6-C5-N7	2.01	136.65	133.43
55	DA	2503	2MA	C5-C6-N6	-2.01	118.30	123.29
31	CA	955	PSU	C3'-C2'-C1'	-2.01	99.32	101.69

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	AL	89	D2T	O-C-CA-CB
12	AL	89	D2T	CG-CB-SB-CB1
12	BL	89	D2T	O-C-CA-CB
12	BL	89	D2T	CA-CB-SB-CB1
12	BL	89	D2T	CA-CB-CG-OD1
12	BL	89	D2T	CA-CB-CG-OD2
31	CA	746	PSU	C2'-C1'-C5-C4
31	CA	2030	6MZ	O4'-C4'-C5'-O5'
32	DD	150[A]	MEQ	N-CA-CB-CG
32	DD	150[A]	MEQ	C-CA-CB-CG
32	DD	150[A]	MEQ	O-C-CA-CB
32	DD	150[B]	MEQ	N-CA-CB-CG
32	DD	150[B]	MEQ	C-CA-CB-CG
41	CN	81	4D4	O-C-CA-CB
41	DN	81[A]	4D4	O-C-CA-CB
41	DN	81[B]	4D4	CA-CB-CG-CD
1	BA	527	7MG	C3'-C4'-C5'-O5'
1	BA	1519	MA6	O4'-C4'-C5'-O5'
31	CA	2030	6MZ	C3'-C4'-C5'-O5'
1	AA	527	7MG	O4'-C4'-C5'-O5'
1	AA	527	7MG	C3'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
1	BA	527	7MG	O4'-C4'-C5'-O5'
41	DN	81[B]	4D4	OB-CB-CG-CD
1	BA	1519	MA6	C3'-C4'-C5'-O5'
55	DA	2445	2MG	C3'-C4'-C5'-O5'
1	AA	1519	MA6	C3'-C4'-C5'-O5'
55	DA	2504	PSU	O4'-C4'-C5'-O5'
55	DA	2604	PSU	O4'-C4'-C5'-O5'
31	CA	2504	PSU	O4'-C4'-C5'-O5'
31	CA	746	PSU	O4'-C1'-C5-C4
55	DA	2030	6MZ	O4'-C4'-C5'-O5'
31	CA	1618	6MZ	C4'-C5'-O5'-P
55	DA	2069	7MG	C4'-C5'-O5'-P
32	DD	150[B]	MEQ	CA-CB-CG-CD
55	DA	2580	PSU	O4'-C4'-C5'-O5'
12	AL	89	D2T	CA-CB-SB-CB1
12	BL	89	D2T	SB-CB-CG-OD2
55	DA	746	PSU	O4'-C1'-C5-C6
32	DD	150[A]	MEQ	OE1-CD-CG-CB
31	CA	2498	OMC	O4'-C4'-C5'-O5'
31	CA	2503	2MA	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	AA	1519	MA6	C5-C6-N6-C9
1	BA	1519	MA6	C5-C6-N6-C9
31	CA	1939	5MU	O4'-C4'-C5'-O5'
55	DA	2503	2MA	O4'-C4'-C5'-O5'
55	DA	2503	2MA	C4'-C5'-O5'-P
12	BL	89	D2T	CG-CB-SB-CB1
55	DA	746	PSU	C2'-C1'-C5-C6
55	DA	2445	2MG	O4'-C4'-C5'-O5'
41	DN	81[B]	4D4	O-C-CA-CB
31	CA	2503	2MA	C4'-C5'-O5'-P
31	CA	2498	OMC	C2'-C1'-N1-C2
55	DA	2449	H2U	C4'-C5'-O5'-P
55	DA	1962	5MC	O4'-C4'-C5'-O5'
32	DD	150[A]	MEQ	NE2-CD-CG-CB

There are no ring outliers.

16 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1518	MA6	1	0
55	DA	747	5MU	1	0
31	CA	747	5MU	1	0
1	BA	1519	MA6	1	0
55	DA	2498	OMC	1	0
55	DA	2030	6MZ	2	0
32	DD	150[A]	MEQ	2	0
1	BA	1518	MA6	1	0
31	CA	2030	6MZ	5	0
31	CA	1939	5MU	1	0
32	DD	150[B]	MEQ	1	0
1	AA	1402	4OC	1	0
31	CA	745	1MG	1	0
1	BA	967	5MC	2	0
1	AA	1519	MA6	1	0
1	BA	1402	4OC	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 549 ligands modelled in this entry, 469 are monoatomic - leaving 80 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	$\# Z > 2$
59	PUT	AA	1672	-	5,5,5	0.06	0	4,4,4	0.11	0
57	PG4	DA	3216	-	12,12,12	0.14	0	11,11,11	0.14	0
58	MPD	AA	1676	-	7,7,7	0.65	0	9,10,10	0.59	0
58	MPD	DA	3192	-	7,7,7	0.74	0	9,10,10	0.69	0
61	PEG	DA	3226	-	6,6,6	0.20	0	5,5,5	0.06	0
66	ACY	DA	3196	-	3,3,3	2.84	1 (33%)	3,3,3	1.89	2 (66%)
58	MPD	DS	203	-	7,7,7	0.36	0	9,10,10	0.37	0
62	EDO	DA	3208	-	3,3,3	0.53	0	2,2,2	0.36	0
62	EDO	D1	101	-	3,3,3	0.62	0	2,2,2	0.26	0
59	PUT	DA	3221	-	5,5,5	0.25	0	4,4,4	0.17	0
59	PUT	DM	201	-	5,5,5	0.21	0	4,4,4	0.28	0
58	MPD	DE	302	-	7,7,7	0.86	0	9,10,10	0.76	0
61	PEG	DA	3200	-	6,6,6	0.24	0	5,5,5	0.09	0
57	PG4	AA	1670	-	12,12,12	0.18	0	11,11,11	0.20	0
62	EDO	DA	3003	-	3,3,3	0.61	0	2,2,2	0.36	0
64	SPD	DA	3187	-	9,9,9	0.12	0	8,8,8	0.22	0
64	SPD	DA	3183	-	9,9,9	0.21	0	8,8,8	0.36	0
58	MPD	AA	1671	-	7,7,7	0.36	0	9,10,10	0.54	0
61	PEG	DA	3227	-	6,6,6	0.25	0	5,5,5	0.15	0
64	SPD	DA	3224	-	9,9,9	0.12	0	8,8,8	0.25	0
59	PUT	DA	3212	-	5,5,5	0.24	0	4,4,4	0.16	0
63	PGE	DA	3217	-	9,9,9	0.22	0	8,8,8	0.19	0
63	PGE	DA	3214	-	9,9,9	0.24	0	8,8,8	0.33	0
58	MPD	DA	3210	-	7,7,7	0.71	0	9,10,10	0.37	0
62	EDO	DA	3002	-	3,3,3	0.56	0	2,2,2	0.21	0
59	PUT	AA	1673	-	5,5,5	0.13	0	4,4,4	0.06	0
63	PGE	DU	201	-	9,9,9	0.32	0	8,8,8	0.29	0
61	PEG	DA	3218	-	6,6,6	0.15	0	5,5,5	0.07	0
59	PUT	DA	3222	-	5,5,5	0.26	0	4,4,4	0.53	0
67	GUN	DA	3211	-	12,12,12	0.26	0	15,17,17	0.76	0
66	ACY	DA	3191	-	3,3,3	0.66	0	3,3,3	1.30	0
62	EDO	DA	3209	-	3,3,3	0.48	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
66	ACY	DA	3202	-	3,3,3	0.66	0	3,3,3	0.86	0
59	PUT	DA	3188	-	5,5,5	0.11	0	4,4,4	0.15	0
59	PUT	DA	3184	-	5,5,5	0.16	0	4,4,4	0.19	0
58	MPD	DK	201	-	7,7,7	0.92	1 (14%)	9,10,10	0.37	0
62	EDO	DA	3215	-	3,3,3	0.65	0	2,2,2	0.27	0
62	EDO	DA	3198	-	3,3,3	0.68	0	2,2,2	0.25	0
62	EDO	DB	210	-	3,3,3	0.62	0	2,2,2	0.20	0
59	PUT	DA	3219	-	5,5,5	0.20	0	4,4,4	0.17	0
61	PEG	D3	102	-	6,6,6	0.21	0	5,5,5	0.19	0
57	PG4	DA	3193	-	12,12,12	0.28	0	11,11,11	0.26	0
65	1PE	DA	3203	-	15,15,15	0.21	0	14,14,14	0.25	0
58	MPD	DN	201	-	7,7,7	1.06	1 (14%)	9,10,10	0.54	0
59	PUT	DA	3195	-	5,5,5	0.28	0	4,4,4	0.28	0
59	PUT	DA	3213	-	5,5,5	0.23	0	4,4,4	0.20	0
62	EDO	D0	101	-	3,3,3	0.57	0	2,2,2	0.57	0
62	EDO	DA	3194	-	3,3,3	0.67	0	2,2,2	0.07	0
61	PEG	DQ	201	-	6,6,6	0.22	0	5,5,5	0.12	0
58	MPD	DA	3204	-	7,7,7	0.64	0	9,10,10	0.49	0
63	PGE	D1	102	-	9,9,9	0.11	0	8,8,8	0.13	0
58	MPD	DT	201	-	7,7,7	0.69	0	9,10,10	0.33	0
59	PUT	AA	1674	-	5,5,5	0.13	0	4,4,4	0.10	0
61	PEG	DL	201	-	6,6,6	0.10	0	5,5,5	0.08	0
58	MPD	DA	3207	-	7,7,7	0.33	0	9,10,10	0.50	0
59	PUT	AA	1675	-	5,5,5	0.17	0	4,4,4	0.09	0
61	PEG	DA	3201	-	6,6,6	0.14	0	5,5,5	0.14	0
61	PEG	AL	201	-	6,6,6	0.19	0	5,5,5	0.15	0
63	PGE	D3	101	-	9,9,9	0.22	0	8,8,8	0.11	0
61	PEG	DA	3199	-	6,6,6	0.18	0	5,5,5	0.12	0
63	PGE	DA	3225	-	9,9,9	0.26	0	8,8,8	0.31	0
64	SPD	DA	3206	-	9,9,9	0.22	0	8,8,8	0.24	0
63	PGE	DA	3186	-	9,9,9	0.33	0	8,8,8	0.35	0
62	EDO	DB	211	-	3,3,3	0.52	0	2,2,2	0.35	0
58	MPD	DA	3190	-	7,7,7	0.47	0	9,10,10	0.46	0
57	PG4	DQ	202	-	12,12,12	0.13	0	11,11,11	0.15	0
59	PUT	DA	3223	-	5,5,5	0.19	0	4,4,4	0.18	0
68	TRS	DA	3220	-	7,7,7	0.28	0	9,9,9	0.27	0
61	PEG	DP	201	-	6,6,6	0.17	0	5,5,5	0.13	0
63	PGE	DS	201	-	9,9,9	0.22	0	8,8,8	0.18	0
59	PUT	DA	3205	-	5,5,5	0.17	0	4,4,4	0.16	0
57	PG4	BA	1642	-	12,12,12	0.23	0	11,11,11	0.18	0
62	EDO	DA	3197	-	3,3,3	0.60	0	2,2,2	0.19	0
65	1PE	DA	3185	-	15,15,15	0.20	0	14,14,14	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	MPD	DT	202	-	7,7,7	0.70	0	9,10,10	0.49	0
57	PG4	DR	201	-	12,12,12	0.22	0	11,11,11	0.25	0
63	PGE	DD	301	-	9,9,9	0.21	0	8,8,8	0.16	0
57	PG4	DS	202	-	12,12,12	0.19	0	11,11,11	0.23	0
59	PUT	DA	3189	-	5,5,5	0.08	0	4,4,4	0.19	0
58	MPD	DE	301	-	7,7,7	0.59	0	9,10,10	0.47	0

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
59	PUT	AA	1672	-	-	0/3/3/3	-
57	PG4	DA	3216	-	-	5/10/10/10	-
58	MPD	AA	1676	-	-	1/5/5/5	-
58	MPD	DA	3192	-	-	2/5/5/5	-
61	PEG	DA	3226	-	-	0/4/4/4	-
58	MPD	DS	203	-	-	1/5/5/5	-
62	EDO	DA	3208	-	-	0/1/1/1	-
62	EDO	D1	101	-	-	0/1/1/1	-
59	PUT	DA	3221	-	-	0/3/3/3	-
59	PUT	DM	201	-	-	0/3/3/3	-
58	MPD	DE	302	-	-	3/5/5/5	-
61	PEG	DA	3200	-	-	1/4/4/4	-
57	PG4	AA	1670	-	-	6/10/10/10	-
62	EDO	DA	3003	-	-	1/1/1/1	-
64	SPD	DA	3187	-	-	2/7/7/7	-
64	SPD	DA	3183	-	-	3/7/7/7	-
58	MPD	AA	1671	-	-	0/5/5/5	-
61	PEG	DA	3227	-	-	0/4/4/4	-
64	SPD	DA	3224	-	-	3/7/7/7	-
59	PUT	DA	3212	-	-	0/3/3/3	-
63	PGE	DA	3217	-	-	3/7/7/7	-
63	PGE	DA	3214	-	-	4/7/7/7	-
58	MPD	DA	3210	-	-	2/5/5/5	-
62	EDO	DA	3002	-	-	0/1/1/1	-
59	PUT	AA	1673	-	-	0/3/3/3	-
63	PGE	DU	201	-	-	4/7/7/7	-
61	PEG	DA	3218	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PUT	DA	3222	-	-	0/3/3/3	-
67	GUN	DA	3211	-	-	-	0/2/2/2
62	EDO	DA	3209	-	-	0/1/1/1	-
59	PUT	DA	3188	-	-	0/3/3/3	-
59	PUT	DA	3184	-	-	1/3/3/3	-
58	MPD	DK	201	-	-	4/5/5/5	-
62	EDO	DA	3215	-	-	0/1/1/1	-
62	EDO	DA	3198	-	-	1/1/1/1	-
62	EDO	DB	210	-	-	1/1/1/1	-
59	PUT	DA	3219	-	-	0/3/3/3	-
61	PEG	D3	102	-	-	1/4/4/4	-
57	PG4	DA	3193	-	-	4/10/10/10	-
65	1PE	DA	3203	-	-	5/13/13/13	-
58	MPD	DN	201	-	-	1/5/5/5	-
59	PUT	DA	3195	-	-	0/3/3/3	-
59	PUT	DA	3213	-	-	1/3/3/3	-
62	EDO	D0	101	-	-	0/1/1/1	-
62	EDO	DA	3194	-	-	0/1/1/1	-
61	PEG	DQ	201	-	-	2/4/4/4	-
58	MPD	DA	3204	-	-	3/5/5/5	-
63	PGE	D1	102	-	-	5/7/7/7	-
58	MPD	DT	201	-	-	2/5/5/5	-
59	PUT	AA	1674	-	-	0/3/3/3	-
61	PEG	DL	201	-	-	3/4/4/4	-
58	MPD	DA	3207	-	-	2/5/5/5	-
59	PUT	AA	1675	-	-	1/3/3/3	-
61	PEG	DA	3201	-	-	1/4/4/4	-
61	PEG	AL	201	-	-	2/4/4/4	-
63	PGE	D3	101	-	-	4/7/7/7	-
61	PEG	DA	3199	-	-	2/4/4/4	-
63	PGE	DA	3225	-	-	4/7/7/7	-
64	SPD	DA	3206	-	-	2/7/7/7	-
63	PGE	DA	3186	-	-	2/7/7/7	-
62	EDO	DB	211	-	-	0/1/1/1	-
58	MPD	DA	3190	-	-	1/5/5/5	-
57	PG4	DQ	202	-	-	1/10/10/10	-
59	PUT	DA	3223	-	-	1/3/3/3	-
68	TRS	DA	3220	-	-	0/9/9/9	-
61	PEG	DP	201	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PGE	DS	201	-	-	4/7/7/7	-
59	PUT	DA	3205	-	-	0/3/3/3	-
57	PG4	BA	1642	-	-	5/10/10/10	-
62	EDO	DA	3197	-	-	0/1/1/1	-
65	1PE	DA	3185	-	-	4/13/13/13	-
58	MPD	DT	202	-	-	3/5/5/5	-
57	PG4	DR	201	-	-	4/10/10/10	-
63	PGE	DD	301	-	-	5/7/7/7	-
57	PG4	DS	202	-	-	4/10/10/10	-
59	PUT	DA	3189	-	-	0/3/3/3	-
58	MPD	DE	301	-	-	2/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	DA	3196	ACY	O-C	4.72	1.42	1.22
58	DN	201	MPD	C3-C2	2.36	1.61	1.54
58	DK	201	MPD	C3-C2	2.04	1.60	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	DA	3196	ACY	OXT-C-CH3	2.45	125.31	115.05
66	DA	3196	ACY	O-C-CH3	-2.15	113.72	122.53

There are no chirality outliers.

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	DE	302	MPD	C1-C2-C3-C4
58	DE	302	MPD	O2-C2-C3-C4
63	DA	3225	PGE	O2-C3-C4-O3
57	BA	1642	PG4	O4-C7-C8-O5
63	DS	201	PGE	O2-C3-C4-O3
57	DA	3193	PG4	O3-C5-C6-O4
63	DA	3214	PGE	O2-C3-C4-O3
64	DA	3224	SPD	C3-C4-C5-N6
63	DA	3214	PGE	O3-C5-C6-O4
65	DA	3185	1PE	OH2-C12-C22-OH3

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Mol	Chain	Res	Type	Atoms
57	DS	202	PG4	O1-C1-C2-O2
61	DA	3199	PEG	O2-C3-C4-O4
63	DU	201	PGE	O3-C5-C6-O4
63	DA	3225	PGE	O1-C1-C2-O2
57	DR	201	PG4	O2-C3-C4-O3
64	DA	3183	SPD	C8-C7-N6-C5
57	AA	1670	PG4	O4-C7-C8-O5
63	DA	3214	PGE	O1-C1-C2-O2
62	DB	210	EDO	O1-C1-C2-O2
59	DA	3213	PUT	C1-C2-C3-C4
63	D1	102	PGE	O3-C5-C6-O4
63	DU	201	PGE	O1-C1-C2-O2
57	AA	1670	PG4	O1-C1-C2-O2
61	DL	201	PEG	O2-C3-C4-O4
61	DQ	201	PEG	O2-C3-C4-O4
62	DA	3198	EDO	O1-C1-C2-O2
61	DL	201	PEG	O1-C1-C2-O2
57	BA	1642	PG4	O2-C3-C4-O3
65	DA	3203	1PE	OH4-C13-C23-OH3
63	D1	102	PGE	O2-C3-C4-O3
65	DA	3203	1PE	OH5-C14-C24-OH4
59	DA	3184	PUT	C1-C2-C3-C4
57	DA	3193	PG4	C4-C3-O2-C2
57	DR	201	PG4	O3-C5-C6-O4
63	DD	301	PGE	C3-C4-O3-C5
63	DA	3186	PGE	C6-C5-O3-C4
61	DA	3201	PEG	C1-C2-O2-C3
61	DA	3218	PEG	C1-C2-O2-C3
63	DA	3225	PGE	C3-C4-O3-C5
63	DS	201	PGE	C4-C3-O2-C2
61	DA	3200	PEG	C1-C2-O2-C3
63	D3	101	PGE	C1-C2-O2-C3
57	DA	3216	PG4	C3-C4-O3-C5
57	BA	1642	PG4	C1-C2-O2-C3
57	DA	3193	PG4	C8-C7-O4-C6
57	DA	3216	PG4	C8-C7-O4-C6
63	D1	102	PGE	C4-C3-O2-C2
63	DS	201	PGE	C6-C5-O3-C4
63	DA	3217	PGE	C4-C3-O2-C2
57	DQ	202	PG4	O1-C1-C2-O2
57	DA	3216	PG4	C4-C3-O2-C2
65	DA	3185	1PE	C14-C24-OH4-C13

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Mol	Chain	Res	Type	Atoms
64	DA	3183	SPD	C4-C5-N6-C7
64	DA	3206	SPD	C8-C7-N6-C5
57	DR	201	PG4	C8-C7-O4-C6
63	DA	3214	PGE	C4-C3-O2-C2
61	DP	201	PEG	C1-C2-O2-C3
65	DA	3203	1PE	C12-C22-OH3-C23
57	AA	1670	PG4	C5-C6-O4-C7
63	DA	3217	PGE	C6-C5-O3-C4
63	DA	3217	PGE	C3-C4-O3-C5
63	DS	201	PGE	O3-C5-C6-O4
58	DA	3204	MPD	O2-C2-C3-C4
58	DA	3207	MPD	O2-C2-C3-C4
64	DA	3224	SPD	C8-C7-N6-C5
63	DU	201	PGE	C3-C4-O3-C5
57	DA	3216	PG4	C1-C2-O2-C3
63	DD	301	PGE	O3-C5-C6-O4
58	DE	302	MPD	CM-C2-C3-C4
58	DK	201	MPD	C1-C2-C3-C4
58	DK	201	MPD	CM-C2-C3-C4
58	DT	201	MPD	C1-C2-C3-C4
58	DA	3210	MPD	C1-C2-C3-C4
57	BA	1642	PG4	C8-C7-O4-C6
57	DS	202	PG4	C1-C2-O2-C3
63	D3	101	PGE	C3-C4-O3-C5
63	DA	3225	PGE	C1-C2-O2-C3
57	DS	202	PG4	C3-C4-O3-C5
57	AA	1670	PG4	C3-C4-O3-C5
63	D3	101	PGE	O3-C5-C6-O4
59	DA	3223	PUT	C1-C2-C3-C4
65	DA	3185	1PE	C16-C26-OH6-C15
57	AA	1670	PG4	C4-C3-O2-C2
61	AL	201	PEG	C1-C2-O2-C3
58	DE	301	MPD	C2-C3-C4-C5
58	DK	201	MPD	C2-C3-C4-C5
58	DT	202	MPD	C2-C3-C4-C5
58	DA	3190	MPD	C2-C3-C4-C5
58	DA	3192	MPD	C2-C3-C4-C5
58	DA	3204	MPD	C2-C3-C4-C5
61	AL	201	PEG	C4-C3-O2-C2
65	DA	3203	1PE	OH2-C12-C22-OH3
57	DS	202	PG4	C4-C3-O2-C2
61	DA	3199	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
61	DQ	201	PEG	C1-C2-O2-C3
63	D1	102	PGE	C1-C2-O2-C3
64	DA	3183	SPD	C2-C3-C4-C5
63	D1	102	PGE	C3-C4-O3-C5
63	DD	301	PGE	C1-C2-O2-C3
61	D3	102	PEG	C4-C3-O2-C2
63	DD	301	PGE	O2-C3-C4-O3
65	DA	3203	1PE	C14-C24-OH4-C13
57	DR	201	PG4	C5-C6-O4-C7
61	DL	201	PEG	C4-C3-O2-C2
63	DD	301	PGE	C4-C3-O2-C2
63	DA	3186	PGE	O3-C5-C6-O4
59	AA	1675	PUT	C1-C2-C3-C4
63	D3	101	PGE	C4-C3-O2-C2
64	DA	3224	SPD	C4-C5-N6-C7
65	DA	3185	1PE	C24-C14-OH5-C25
62	DA	3003	EDO	O1-C1-C2-O2
57	DA	3193	PG4	O2-C3-C4-O3
57	BA	1642	PG4	C3-C4-O3-C5
57	AA	1670	PG4	C1-C2-O2-C3
63	DU	201	PGE	C1-C2-O2-C3
58	DN	201	MPD	O2-C2-C3-C4
58	DT	202	MPD	O2-C2-C3-C4
57	DA	3216	PG4	O4-C7-C8-O5
64	DA	3206	SPD	C3-C4-C5-N6
64	DA	3187	SPD	C2-C3-C4-C5
58	AA	1676	MPD	C2-C3-C4-O4
58	DE	301	MPD	C2-C3-C4-O4
58	DK	201	MPD	C2-C3-C4-O4
58	DS	203	MPD	C2-C3-C4-O4
58	DA	3192	MPD	C2-C3-C4-O4
58	DA	3204	MPD	C2-C3-C4-O4
58	DA	3207	MPD	C2-C3-C4-O4
58	DT	201	MPD	CM-C2-C3-C4
58	DT	202	MPD	CM-C2-C3-C4
58	DA	3210	MPD	CM-C2-C3-C4
64	DA	3187	SPD	C7-C8-C9-N10

There are no ring outliers.

19 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	DA	3192	MPD	2	0
58	DS	203	MPD	3	0
59	DA	3212	PUT	1	0
63	DA	3214	PGE	1	0
62	DA	3002	EDO	1	0
63	DU	201	PGE	1	0
66	DA	3202	ACY	2	0
59	DA	3219	PUT	1	0
61	D3	102	PEG	1	0
59	DA	3213	PUT	1	0
62	DA	3194	EDO	3	0
61	DQ	201	PEG	1	0
61	DA	3201	PEG	1	0
63	DA	3225	PGE	4	0
59	DA	3223	PUT	1	0
68	DA	3220	TRS	1	0
57	BA	1642	PG4	1	0
65	DA	3185	1PE	1	0
57	DR	201	PG4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1523/1534 (99%)	-0.04	54 (3%) 47 31	65, 138, 270, 291	0
1	BA	1522/1534 (99%)	0.15	78 (5%) 33 22	86, 162, 293, 294	0
2	AB	224/224 (100%)	0.18	4 (1%) 67 49	108, 156, 231, 272	0
2	BB	224/224 (100%)	0.20	3 (1%) 75 57	138, 181, 229, 262	0
3	AC	206/206 (100%)	0.25	7 (3%) 48 32	138, 174, 208, 228	0
3	BC	206/206 (100%)	0.72	20 (9%) 13 11	223, 253, 269, 279	0
4	AD	205/205 (100%)	0.28	6 (2%) 53 35	100, 145, 174, 190	0
4	BD	205/205 (100%)	-0.27	1 (0%) 87 76	71, 100, 137, 174	0
5	AE	155/155 (100%)	-0.11	1 (0%) 85 73	83, 119, 150, 176	0
5	BE	150/155 (96%)	0.26	6 (4%) 42 28	92, 125, 168, 236	0
6	AF	106/106 (100%)	-0.10	1 (0%) 81 66	89, 126, 149, 187	0
6	BF	100/106 (94%)	0.18	3 (3%) 52 35	135, 162, 188, 196	0
7	AG	151/151 (100%)	0.35	10 (6%) 24 16	159, 186, 216, 229	0
7	BG	151/151 (100%)	0.91	17 (11%) 10 9	198, 247, 263, 268	0
8	AH	129/129 (100%)	0.01	2 (1%) 70 52	89, 122, 148, 158	0
8	BH	129/129 (100%)	0.12	3 (2%) 61 42	119, 151, 179, 192	0
9	AI	127/127 (100%)	0.70	13 (10%) 12 10	168, 196, 251, 270	0
9	BI	127/127 (100%)	0.85	16 (12%) 8 7	198, 234, 277, 283	0
10	AJ	99/99 (100%)	0.80	10 (10%) 12 10	169, 190, 228, 238	0
10	BJ	98/99 (98%)	1.12	18 (18%) 3 3	209, 248, 280, 287	0
11	AK	117/129 (90%)	0.02	3 (2%) 57 38	77, 139, 174, 190	0
11	BK	117/129 (90%)	0.65	13 (11%) 10 9	111, 166, 186, 202	0
12	AL	122/123 (99%)	0.18	3 (2%) 58 39	78, 112, 137, 178	0
12	BL	122/123 (99%)	0.20	2 (1%) 70 52	96, 121, 148, 177	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.46	4 (3%) 47 31	167, 198, 220, 233	0
13	BM	114/114 (100%)	0.83	7 (6%) 27 19	254, 271, 288, 292	0
14	AN	100/100 (100%)	0.95	11 (11%) 10 9	166, 188, 252, 260	0
14	BN	100/100 (100%)	1.08	16 (16%) 5 4	226, 252, 282, 288	0
15	AO	88/88 (100%)	-0.03	1 (1%) 78 61	75, 109, 142, 169	0
15	BO	88/88 (100%)	0.28	1 (1%) 78 61	127, 160, 180, 197	0
16	AP	82/82 (100%)	0.59	8 (9%) 13 11	88, 128, 168, 195	0
16	BP	82/82 (100%)	0.83	8 (9%) 13 11	106, 136, 168, 184	0
17	AQ	80/80 (100%)	0.07	1 (1%) 75 57	86, 115, 149, 157	0
17	BQ	80/80 (100%)	0.37	4 (5%) 34 23	120, 159, 182, 197	0
18	AR	55/55 (100%)	0.11	1 (1%) 67 49	86, 116, 172, 194	0
18	BR	55/55 (100%)	0.21	2 (3%) 46 31	126, 143, 173, 216	0
19	AS	79/79 (100%)	0.71	8 (10%) 12 10	180, 201, 215, 222	0
19	BS	79/79 (100%)	1.14	15 (18%) 3 3	229, 265, 274, 278	0
20	AT	86/86 (100%)	0.46	4 (4%) 36 24	91, 122, 151, 161	0
20	BT	85/86 (98%)	0.87	10 (11%) 9 8	136, 157, 183, 193	0
21	AU	56/56 (100%)	0.19	1 (1%) 67 49	114, 146, 208, 223	0
21	BU	56/56 (100%)	0.41	3 (5%) 31 21	112, 151, 191, 204	0
22	C1	56/56 (100%)	1.12	12 (21%) 2 2	131, 187, 206, 219	0
22	D1	56/56 (100%)	-0.62	0 100 100	31, 57, 81, 120	0
23	C2	50/51 (98%)	0.67	5 (10%) 12 11	179, 197, 215, 237	0
23	D2	51/51 (100%)	0.07	1 (1%) 65 46	81, 98, 130, 145	0
24	C3	46/46 (100%)	1.37	9 (19%) 3 3	129, 153, 170, 177	0
24	D3	46/46 (100%)	-0.50	1 (2%) 62 43	42, 51, 71, 143	0
25	C4	64/64 (100%)	1.99	27 (42%) 0 0	145, 165, 182, 187	0
25	D4	64/64 (100%)	-0.29	0 100 100	51, 64, 78, 105	0
26	C5	38/38 (100%)	1.10	6 (15%) 5 4	126, 153, 166, 174	0
26	D5	38/38 (100%)	-0.23	0 100 100	52, 68, 95, 120	0
27	C0	58/58 (100%)	0.67	6 (10%) 12 10	123, 142, 171, 180	0
27	D0	58/58 (100%)	-0.48	2 (3%) 48 32	30, 47, 85, 112	2 (3%)
28	CB	118/120 (98%)	0.13	3 (2%) 58 39	134, 208, 253, 258	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	120/120 (100%)	-0.67	1 (0%) 82 68	45, 87, 138, 167	0
29	CC	271/272 (99%)	0.58	27 (9%) 12 11	102, 130, 160, 176	0
29	DC	271/272 (99%)	-0.46	1 (0%) 88 79	42, 75, 106, 142	0
30	CD	209/209 (100%)	0.84	32 (15%) 5 5	100, 154, 179, 193	0
31	CA	2876/2904 (99%)	0.30	95 (3%) 49 33	92, 184, 267, 286	0
32	DD	208/209 (99%)	-0.65	1 (0%) 87 76	27, 55, 93, 121	0
33	CE	201/201 (100%)	0.83	19 (9%) 14 11	133, 193, 233, 243	0
33	DE	201/201 (100%)	-0.54	0 100 100	30, 82, 132, 150	0
34	CF	177/178 (99%)	0.30	3 (1%) 69 50	212, 233, 249, 254	0
34	DF	177/178 (99%)	0.00	3 (1%) 69 50	78, 120, 170, 188	0
35	CG	176/176 (100%)	0.27	2 (1%) 78 61	168, 196, 232, 244	0
35	DG	176/176 (100%)	-0.25	3 (1%) 69 50	57, 93, 122, 156	0
36	CH	149/149 (100%)	0.11	2 (1%) 75 57	131, 172, 197, 208	0
36	DH	149/149 (100%)	0.10	5 (3%) 48 32	82, 173, 211, 231	0
37	CJ	134/135 (99%)	0.95	21 (15%) 5 4	259, 279, 289, 291	0
37	DJ	134/135 (99%)	0.76	16 (11%) 9 8	228, 249, 266, 272	0
38	CK	142/142 (100%)	0.73	17 (11%) 9 8	115, 144, 168, 182	0
38	DK	142/142 (100%)	-0.67	0 100 100	28, 49, 82, 106	0
39	CL	122/123 (99%)	0.44	5 (4%) 41 27	105, 133, 168, 181	0
39	DL	123/123 (100%)	-0.54	1 (0%) 82 68	43, 62, 95, 135	0
40	CM	144/144 (100%)	1.05	21 (14%) 6 5	131, 195, 243, 260	0
40	DM	144/144 (100%)	-0.26	6 (4%) 40 26	26, 78, 114, 152	0
41	CN	135/136 (99%)	0.42	6 (4%) 39 25	107, 145, 176, 205	0
41	DN	135/136 (99%)	-0.66	0 100 100	24, 59, 90, 112	1 (0%)
42	CO	120/127 (94%)	0.88	14 (11%) 9 8	127, 158, 186, 233	0
42	DO	125/127 (98%)	-0.61	0 100 100	33, 52, 96, 155	0
43	CP	116/117 (99%)	0.46	4 (3%) 48 32	165, 195, 217, 223	0
43	DP	117/117 (100%)	-0.28	1 (0%) 81 66	56, 84, 121, 136	0
44	CQ	114/114 (100%)	0.52	4 (3%) 47 31	124, 150, 174, 186	0
44	DQ	114/114 (100%)	-0.40	1 (0%) 81 66	47, 72, 105, 135	0
45	CR	117/117 (100%)	1.02	17 (14%) 6 5	117, 144, 166, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	DR	117/117 (100%)	-0.70	0 100 100	24, 41, 63, 114	0
46	CS	103/103 (100%)	0.72	12 (11%) 9 8	117, 159, 195, 202	0
46	DS	103/103 (100%)	-0.56	1 (0%) 79 63	30, 55, 92, 126	0
47	CT	110/110 (100%)	1.27	24 (21%) 2 2	140, 171, 196, 207	0
47	DT	110/110 (100%)	-0.55	1 (0%) 81 66	26, 45, 79, 128	0
48	CU	93/100 (93%)	1.11	13 (13%) 6 6	159, 194, 219, 229	0
48	DU	93/100 (93%)	-0.24	1 (1%) 78 61	51, 73, 136, 154	0
49	CV	102/103 (99%)	1.04	14 (13%) 6 6	157, 198, 231, 242	0
49	DV	102/103 (99%)	-0.28	0 100 100	57, 82, 126, 156	0
50	CW	94/94 (100%)	0.21	3 (3%) 50 33	132, 172, 186, 192	0
50	DW	94/94 (100%)	-0.36	1 (1%) 78 61	43, 73, 110, 119	0
51	CX	75/76 (98%)	0.61	6 (8%) 18 14	129, 161, 175, 206	0
51	DX	76/76 (100%)	-0.30	0 100 100	24, 62, 92, 157	1 (1%)
52	CY	77/77 (100%)	0.65	5 (6%) 25 17	120, 145, 173, 185	0
52	DY	77/77 (100%)	-0.17	0 100 100	56, 76, 111, 130	0
53	CZ	62/62 (100%)	0.64	1 (1%) 70 52	177, 199, 210, 217	0
53	DZ	62/62 (100%)	-0.22	0 100 100	64, 97, 136, 174	0
54	DI	135/135 (100%)	0.74	16 (11%) 9 8	98, 179, 244, 266	1 (0%)
55	DA	2873/2904 (98%)	-0.87	27 (0%) 81 66	29, 65, 231, 294	11 (0%)
All	All	20634/20795 (99%)	0.08	924 (4%) 38 25	24, 144, 266, 294	16 (0%)

All (924) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	121	U	8.8
1	BA	1243	C	8.7
1	BA	1305	G	8.5
55	DA	2120	G	8.1
40	CM	81	ASP	8.0
55	DA	2172	U	7.6
1	BA	1242	G	7.5
7	BG	62	PHE	7.1
37	CJ	13	VAL	7.0
9	BI	124	ARG	6.9
54	DI	2	ALA	6.6

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Mol	Chain	Res	Type	RSRZ
44	DQ	2	SER	6.5
1	BA	1302	C	6.3
30	CD	200	ASP	6.3
55	DA	2886[A]	A	6.2
31	CA	331	C	6.2
1	AA	1364	U	6.1
7	AG	5	ARG	6.1
40	DM	104	GLN	6.0
31	CA	2449	U	5.9
1	BA	1244	G	5.8
1	AA	1127	G	5.8
9	BI	122	ARG	5.7
31	CA	2172	U	5.7
29	CC	242	LYS	5.7
47	CT	97	LEU	5.7
1	BA	1241	G	5.6
31	CA	931	U	5.6
37	CJ	11	LEU	5.5
1	AA	1126	U	5.5
31	CA	2666	C	5.5
1	AA	1281	C	5.5
37	CJ	23	PRO	5.4
54	DI	3	LEU	5.3
25	C4	37	ALA	5.3
3	BC	196	ILE	5.3
10	AJ	8	ILE	5.3
11	BK	110	ILE	5.3
30	CD	198	GLY	5.3
31	CA	2383	G	5.2
46	CS	96	VAL	5.2
10	BJ	41	PRO	5.2
9	BI	16	ALA	5.2
31	CA	1068	G	5.1
10	BJ	74	VAL	5.1
1	BA	121	U	5.1
29	CC	210	ALA	5.1
1	BA	1240	U	5.0
30	CD	6	GLY	5.0
51	CX	54	GLY	4.9
14	BN	60	GLN	4.8
25	C4	36	LYS	4.8
46	CS	75	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
31	CA	1067	A	4.8
47	CT	85	ILE	4.7
1	BA	1304	G	4.6
1	AA	1148	U	4.6
22	C1	2	ALA	4.6
31	CA	2402	U	4.5
1	AA	1092	A	4.5
10	BJ	8	ILE	4.5
39	CL	2	ILE	4.5
31	CA	829	A	4.5
33	CE	73	ILE	4.5
19	BS	49	ILE	4.5
1	AA	1128	C	4.5
31	CA	2667	C	4.5
29	CC	18	LYS	4.5
30	CD	26	VAL	4.5
48	CU	43	ILE	4.4
25	C4	14	PHE	4.4
54	DI	83	ALA	4.4
29	CC	202	LEU	4.4
1	AA	984	C	4.4
1	AA	1286	U	4.4
20	BT	4	ILE	4.4
38	CK	81	ILE	4.4
45	CR	9	ILE	4.4
37	CJ	24	VAL	4.4
42	CO	25	ALA	4.3
30	CD	130	GLN	4.3
47	CT	82	MET	4.3
1	BA	1387	G	4.3
19	BS	13	LEU	4.3
1	BA	1067	A	4.2
10	AJ	6	ILE	4.2
40	CM	100	ILE	4.2
31	CA	2126	A	4.2
25	C4	40	ARG	4.2
21	BU	57	ALA	4.2
20	BT	6	SER	4.2
1	BA	954	G	4.2
1	BA	1274	A	4.2
19	BS	71	LEU	4.1
10	BJ	75	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	AA	974	A	4.1
1	AA	1354	U	4.1
37	DJ	53	LEU	4.1
17	BQ	70	THR	4.1
1	AA	962	C	4.0
47	CT	45	VAL	4.0
8	BH	2	SER	4.0
29	CC	3	VAL	4.0
1	BA	1204	A	4.0
1	BA	985	C	4.0
9	AI	120	LYS	4.0
9	BI	68	LYS	4.0
20	AT	16	LYS	4.0
31	CA	2627	G	4.0
30	CD	65	ALA	4.0
31	CA	2174	C	4.0
1	BA	1331	G	3.9
31	CA	1984	G	3.9
33	CE	32	VAL	3.9
26	C5	23	ILE	3.9
44	CQ	110	ILE	3.9
30	CD	192	ALA	3.9
23	C2	36	LEU	3.9
1	AA	1125	U	3.9
30	CD	142	VAL	3.9
37	DJ	13	VAL	3.9
22	C1	8	PRO	3.9
40	CM	35	HIS	3.9
25	C4	44	LEU	3.9
26	C5	21	GLY	3.8
1	AA	1030	U	3.8
33	CE	33	VAL	3.8
9	AI	89	GLU	3.8
20	BT	5	LYS	3.8
31	CA	1066	U	3.8
14	BN	47	LYS	3.8
40	DM	72	ALA	3.8
45	CR	99	ALA	3.8
30	CD	131	ASP	3.8
1	AA	540	G	3.8
21	AU	57	ALA	3.8
25	C4	28	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
24	D3	46	LYS	3.8
26	C5	18	LYS	3.8
31	CA	2149	U	3.8
14	AN	71	HIS	3.7
33	CE	72	SER	3.7
23	C2	24	THR	3.7
13	BM	106	ALA	3.7
48	CU	36	LYS	3.7
9	BI	125	PRO	3.7
30	CD	151	THR	3.7
10	AJ	36	VAL	3.7
10	AJ	75	ASP	3.7
47	CT	94	ASP	3.7
9	AI	72	ILE	3.7
45	CR	65	ILE	3.7
17	AQ	53	CYS	3.7
30	CD	8	LYS	3.7
2	AB	30	PHE	3.7
1	AA	1244	G	3.6
31	CA	1084	A	3.6
29	CC	232	HIS	3.6
4	AD	2	ALA	3.6
18	BR	51	TYR	3.6
25	C4	7	VAL	3.6
14	AN	12	LYS	3.6
54	DI	38	MET	3.6
31	CA	2668	G	3.6
1	AA	1243	C	3.6
27	C0	10	THR	3.6
47	CT	47	VAL	3.6
8	AH	2	SER	3.6
49	CV	31	SER	3.5
42	CO	26	GLY	3.5
1	AA	1280	A	3.5
55	DA	2116	G	3.5
55	DA	2885[A]	G	3.5
1	BA	1086	U	3.5
49	CV	13	VAL	3.5
49	CV	80	ALA	3.5
34	DF	32	GLU	3.5
31	CA	1167	C	3.5
14	AN	8	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
24	C3	35	ARG	3.5
14	BN	11	VAL	3.5
45	CR	8	VAL	3.5
55	DA	1731	G	3.5
30	CD	9	VAL	3.4
3	BC	198	VAL	3.4
3	AC	74	GLY	3.4
47	CT	46	LEU	3.4
7	BG	39	ALA	3.4
39	CL	83	ALA	3.4
54	DI	111	ALA	3.4
2	BB	67	ILE	3.4
13	BM	96	PRO	3.4
20	AT	19	LYS	3.4
1	BA	1386	G	3.4
13	BM	89	LEU	3.4
37	DJ	79	LEU	3.4
41	CN	8	LYS	3.4
31	CA	2245	U	3.4
42	CO	21	PHE	3.4
7	BG	4	ARG	3.4
48	CU	79	ASP	3.4
23	D2	54	ILE	3.4
1	BA	1049	U	3.3
14	AN	55	SER	3.3
48	CU	62	VAL	3.3
30	CD	154	LYS	3.3
37	DJ	54	PRO	3.3
9	AI	122	ARG	3.3
42	CO	46	ARG	3.3
10	BJ	26	VAL	3.3
30	CD	62	LYS	3.3
35	CG	175	LYS	3.3
7	BG	43	VAL	3.3
1	BA	933	G	3.3
3	BC	197	GLY	3.3
7	BG	45	SER	3.3
38	CK	103	ILE	3.3
1	BA	983	A	3.3
11	BK	111	THR	3.3
24	C3	42	LEU	3.3
37	CJ	14	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
22	C1	16	ARG	3.3
1	AA	1353	G	3.3
40	CM	19	LEU	3.3
11	BK	86	VAL	3.3
1	BA	1289	A	3.3
3	BC	162	ILE	3.3
9	AI	125	PRO	3.2
9	BI	120	LYS	3.2
29	CC	220	VAL	3.2
12	BL	70	GLU	3.2
45	CR	29	SER	3.2
48	CU	93	LEU	3.2
40	CM	92	LEU	3.2
31	CA	386	G	3.2
29	CC	33	LEU	3.2
30	CD	186	LEU	3.2
37	CJ	79	LEU	3.2
19	BS	30	PRO	3.2
39	CL	122	VAL	3.2
37	CJ	12	GLN	3.2
9	AI	119	ARG	3.2
1	AA	951	G	3.2
25	C4	39	LYS	3.2
31	CA	776	G	3.2
31	CA	2363	G	3.2
1	BA	632	U	3.1
38	CK	111	LYS	3.1
54	DI	7	ASP	3.1
15	AO	57	LEU	3.1
1	BA	1306	A	3.1
31	CA	32	C	3.1
47	CT	86	MET	3.1
52	CY	56	MET	3.1
3	AC	78	GLY	3.1
19	BS	76	PRO	3.1
16	AP	1	MET	3.1
9	BI	116	VAL	3.1
1	BA	955	U	3.1
10	BJ	58	ASN	3.1
47	CT	48	LYS	3.1
37	DJ	76	ALA	3.1
37	CJ	28	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
29	CC	234	GLY	3.1
40	DM	102	GLY	3.1
19	BS	17	LYS	3.1
1	BA	1353	G	3.1
31	CA	2067	G	3.1
40	DM	103	ILE	3.1
30	CD	75	ALA	3.1
33	CE	36	ALA	3.1
30	CD	10	GLY	3.1
33	CE	28	VAL	3.1
49	CV	70	VAL	3.1
43	DP	1	MET	3.1
42	CO	28	LEU	3.0
50	DW	12	GLN	3.0
29	CC	241	GLY	3.0
6	BF	8	PHE	3.0
16	AP	24	SER	3.0
3	BC	120	ILE	3.0
42	CO	23	ASN	3.0
3	BC	159	GLY	3.0
55	DA	2150	C	3.0
55	DA	2174	C	3.0
11	BK	14	LYS	3.0
25	C4	41	LYS	3.0
1	BA	982	U	3.0
25	C4	63	PRO	3.0
31	CA	12	U	3.0
55	DA	2149	U	3.0
31	CA	1026	G	3.0
19	BS	15	LEU	3.0
40	CM	27	LEU	3.0
16	AP	29	ASN	3.0
1	AA	199	A	3.0
1	BA	1201	A	3.0
46	CS	20	VAL	3.0
11	BK	96	THR	3.0
30	CD	156	PHE	3.0
31	CA	2248	C	3.0
9	BI	128	SER	3.0
38	CK	42	ALA	3.0
49	CV	67	VAL	3.0
26	C5	13	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
30	CD	23	PRO	3.0
9	BI	119	ARG	3.0
16	BP	12	LYS	3.0
14	AN	11	VAL	3.0
30	CD	158	GLY	3.0
3	AC	162	ILE	3.0
11	AK	97	ILE	3.0
9	AI	118	LEU	2.9
47	CT	36	LEU	2.9
34	CF	32	GLU	2.9
25	C4	65	ALA	2.9
16	AP	23	ASP	2.9
1	AA	1119	C	2.9
31	CA	2066	C	2.9
1	BA	1148	U	2.9
22	C1	12	LYS	2.9
5	BE	127	ALA	2.9
55	DA	2152	G	2.9
2	AB	9	MET	2.9
14	BN	16	LEU	2.9
45	CR	4	VAL	2.9
25	C4	32	ILE	2.9
13	AM	19	LEU	2.9
43	CP	48	LEU	2.9
25	C4	5	LYS	2.9
14	AN	50	THR	2.9
1	BA	976	G	2.9
47	CT	43	ALA	2.9
54	DI	93	ALA	2.9
55	DA	879	G	2.9
1	AA	1120	C	2.9
1	BA	980	C	2.9
1	BA	1354	U	2.9
25	C4	57	LEU	2.9
40	CM	73	ILE	2.9
47	CT	98	LYS	2.9
29	CC	223	THR	2.9
30	CD	143	PRO	2.9
36	DH	87	GLU	2.9
49	CV	36	VAL	2.9
41	CN	40	ARG	2.9
31	CA	2435	A	2.9

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Mol	Chain	Res	Type	RSRZ
51	CX	75	LYS	2.9
47	CT	44	ALA	2.8
1	AA	983	A	2.8
1	AA	1285	A	2.8
31	CA	2173	A	2.8
1	BA	1355	G	2.8
10	BJ	39	PRO	2.8
55	DA	2141	G	2.8
39	DL	37	ASP	2.8
1	AA	985	C	2.8
1	AA	1149	C	2.8
10	AJ	74	VAL	2.8
16	AP	25	ARG	2.8
14	AN	97	LYS	2.8
40	CM	14	LYS	2.8
9	BI	127	PHE	2.8
10	AJ	76	ILE	2.8
46	CS	50	GLY	2.8
38	CK	44	TYR	2.8
46	CS	73	LYS	2.8
48	CU	64	LYS	2.8
54	DI	40	GLU	2.8
31	CA	1134	A	2.8
29	CC	47	GLY	2.8
25	C4	61	CYS	2.8
20	BT	63	ALA	2.8
40	CM	59	ARG	2.8
11	BK	84	VAL	2.8
38	CK	72	LYS	2.8
40	CM	80	SER	2.8
51	CX	44	LYS	2.8
5	BE	24	THR	2.8
1	BA	1236	A	2.8
1	BA	1217	C	2.8
45	CR	37	GLN	2.8
31	CA	512	G	2.8
31	CA	2877	G	2.8
46	CS	51	VAL	2.8
55	DA	277	G	2.8
14	BN	46	LEU	2.8
17	BQ	8	LEU	2.8
33	CE	143	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
49	CV	39	ILE	2.8
51	CX	55	ARG	2.7
24	C3	20	ALA	2.7
30	CD	7	LYS	2.7
31	CA	2070	A	2.7
13	BM	22	ILE	2.7
19	BS	33	THR	2.7
25	C4	54	ASP	2.7
42	CO	22	ARG	2.7
47	CT	95	ARG	2.7
9	BI	108	ALA	2.7
25	C4	43	HIS	2.7
42	CO	18	GLN	2.7
48	CU	61	LEU	2.7
1	BA	1364	U	2.7
55	DA	2151	U	2.7
1	BA	1219	A	2.7
15	BO	25	THR	2.7
54	DI	131	THR	2.7
17	BQ	69	LYS	2.7
25	C4	15	LYS	2.7
27	D0	3[A]	LYS	2.7
44	CQ	111	LYS	2.7
1	BA	962	C	2.7
14	AN	54	ASP	2.7
26	C5	20	ASP	2.7
51	CX	56	ASP	2.7
11	BK	109	ASN	2.7
48	CU	41	ALA	2.7
37	DJ	24	VAL	2.7
9	BI	118	LEU	2.7
36	DH	12	LEU	2.7
1	AA	973	G	2.7
1	AA	1260	G	2.7
31	CA	1238	G	2.7
40	CM	77	ILE	2.7
11	BK	94	GLU	2.7
40	CM	36	LYS	2.7
31	CA	328	U	2.7
1	AA	539	A	2.7
29	CC	245	VAL	2.7
31	CA	33	C	2.7

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Mol	Chain	Res	Type	RSRZ
19	AS	49	ILE	2.7
28	CB	98	G	2.7
55	DA	2107	G	2.7
13	BM	60	VAL	2.7
38	CK	100	VAL	2.7
42	CO	29	VAL	2.7
33	CE	51	GLU	2.6
9	BI	17	ALA	2.6
38	CK	47	HIS	2.6
1	AA	1305	G	2.6
1	BA	107	G	2.6
10	AJ	25	ILE	2.6
34	CF	67	ILE	2.6
14	AN	21	PHE	2.6
1	BA	959	A	2.6
1	BA	1016	A	2.6
10	BJ	61	ALA	2.6
54	DI	25	ALA	2.6
54	DI	126	LEU	2.6
12	AL	116	LYS	2.6
49	CV	33	LYS	2.6
31	CA	767	U	2.6
40	CM	51	GLU	2.6
1	BA	202	G	2.6
1	BA	1356	G	2.6
31	CA	2046	G	2.6
38	CK	40	HIS	2.6
33	CE	200	LEU	2.6
37	CJ	80	LEU	2.6
42	CO	10	LEU	2.6
45	CR	18	LEU	2.6
35	DG	113	VAL	2.6
1	AA	632	U	2.6
10	BJ	50	THR	2.6
35	CG	176	LYS	2.6
47	CT	83	LYS	2.6
11	AK	110	ILE	2.6
47	CT	96	ILE	2.6
30	CD	199	SER	2.6
55	DA	2121	G	2.6
31	CA	1103	A	2.6
37	DJ	12	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
19	AS	68	GLY	2.6
40	CM	52	GLY	2.6
31	CA	2045	C	2.6
20	AT	2	ALA	2.6
24	C3	33	ARG	2.6
36	CH	27	ARG	2.6
48	CU	66	LYS	2.6
49	CV	103	ILE	2.5
27	C0	18	PRO	2.5
29	CC	231	PRO	2.5
3	BC	178	LEU	2.5
52	CY	49	LEU	2.5
1	AA	1094	G	2.5
1	BA	108	G	2.5
5	BE	114	VAL	2.5
9	AI	18	ARG	2.5
7	BG	106	GLU	2.5
19	AS	60	VAL	2.5
31	CA	1106	G	2.5
31	CA	2125	G	2.5
31	CA	2525	G	2.5
31	CA	764	A	2.5
3	BC	177	THR	2.5
4	AD	64	ILE	2.5
1	BA	979	C	2.5
1	BA	1352	C	2.5
31	CA	1986	C	2.5
3	BC	158	GLY	2.5
7	AG	4	ARG	2.5
14	BN	14	VAL	2.5
54	DI	26	VAL	2.5
14	BN	10	GLU	2.5
29	CC	49	ILE	2.5
49	CV	35	ILE	2.5
2	AB	136	MET	2.5
37	DJ	117	MET	2.5
1	AA	959	A	2.5
1	BA	262	A	2.5
31	CA	1214	A	2.5
1	AA	971	G	2.5
1	BA	1048	G	2.5
1	BA	1370	G	2.5

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Mol	Chain	Res	Type	RSRZ
55	DA	2110	G	2.5
1	BA	1388	C	2.5
22	C1	5	GLN	2.5
43	CP	52	SER	2.5
10	AJ	61	ALA	2.5
43	CP	107	ALA	2.5
48	CU	35	ALA	2.5
31	CA	2743	U	2.5
5	BE	141	ILE	2.5
16	BP	23	ASP	2.5
22	C1	15	MET	2.5
29	CC	30	PHE	2.5
18	AR	51	TYR	2.5
26	C5	31	PRO	2.5
11	AK	100	LEU	2.5
24	C3	31	LEU	2.5
25	C4	35	LYS	2.5
31	CA	1213	A	2.5
35	DG	116	GLN	2.5
1	BA	988	G	2.5
1	BA	1220	G	2.5
52	CY	35	SER	2.5
54	DI	24	SER	2.5
20	BT	67	ILE	2.5
1	BA	470	C	2.5
55	DA	2153	C	2.5
7	BG	15	ASP	2.5
10	BJ	60	ASP	2.5
29	CC	240	PHE	2.5
1	BA	1126	U	2.5
44	CQ	97	LEU	2.5
25	C4	9	GLY	2.5
17	BQ	29	VAL	2.5
31	CA	631	A	2.4
21	BU	19	PHE	2.4
25	C4	22	PHE	2.4
1	BA	984	C	2.4
1	BA	1303	C	2.4
20	BT	86	LEU	2.4
24	C3	24	THR	2.4
37	DJ	80	LEU	2.4
28	DB	25	U	2.4

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Mol	Chain	Res	Type	RSRZ
30	CD	144	GLY	2.4
19	BS	35	SER	2.4
29	DC	272	SER	2.4
7	BG	35	LYS	2.4
14	AN	9	ARG	2.4
16	AP	14	ARG	2.4
47	CT	84	ARG	2.4
30	CD	167	ASN	2.4
10	AJ	43	PRO	2.4
16	AP	41	PRO	2.4
12	BL	4	VAL	2.4
45	CR	34	VAL	2.4
11	BK	97	ILE	2.4
31	CA	183	C	2.4
45	CR	10	ALA	2.4
31	CA	2650	U	2.4
14	BN	7	LYS	2.4
19	AS	32	ARG	2.4
24	C3	14	ARG	2.4
27	C0	11	ARG	2.4
7	BG	93	PRO	2.4
9	AI	116	VAL	2.4
25	C4	58	VAL	2.4
13	AM	15	ALA	2.4
27	D0	2[A]	ALA	2.4
1	AA	977	A	2.4
31	CA	2346	A	2.4
33	CE	49	ARG	2.4
40	CM	70	LYS	2.4
1	BA	1237	C	2.4
1	BA	1366	C	2.4
16	BP	52	LEU	2.4
31	CA	766	U	2.4
31	CA	1065	U	2.4
6	AF	42	TRP	2.4
22	C1	3	VAL	2.4
9	AI	90	TYR	2.4
16	AP	17	TYR	2.4
30	CD	27	ILE	2.4
37	CJ	101	ILE	2.4
7	BG	36	LYS	2.4
14	BN	4	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
14	BN	96	LEU	2.4
7	AG	106	GLU	2.4
29	CC	236	GLU	2.4
31	CA	1085	A	2.4
31	CA	2800	A	2.4
31	CA	1963	U	2.4
36	DH	78	VAL	2.4
1	BA	1066	C	2.3
7	BG	38	THR	2.3
25	C4	25	LYS	2.3
3	BC	179	ARG	2.3
33	CE	175	ILE	2.3
39	CL	7	MET	2.3
31	CA	1216	G	2.3
19	BS	31	LEU	2.3
19	BS	41	PHE	2.3
30	CD	201	LEU	2.3
37	CJ	22	PRO	2.3
37	DJ	128	SER	2.3
40	CM	101	ILE	2.3
45	CR	50	ARG	2.3
28	CB	74	U	2.3
31	CA	34	U	2.3
1	AA	1096	C	2.3
11	BK	112	ASP	2.3
45	CR	52	GLN	2.3
1	BA	212	G	2.3
7	AG	32	VAL	2.3
31	CA	1168	G	2.3
45	CR	11	ARG	2.3
10	BJ	76	ILE	2.3
29	CC	64	ILE	2.3
33	CE	50	ALA	2.3
33	CE	104	ALA	2.3
7	AG	50	LEU	2.3
37	DJ	11	LEU	2.3
31	CA	508	A	2.3
37	DJ	38	PHE	2.3
31	CA	1105	U	2.3
4	AD	121	LYS	2.3
7	BG	32	VAL	2.3
10	BJ	84	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
12	AL	93	VAL	2.3
33	CE	178	VAL	2.3
47	CT	42	LYS	2.3
52	CY	7	VAL	2.3
55	DA	2175	C	2.3
13	AM	33	ILE	2.3
38	CK	101	ILE	2.3
42	CO	105	GLY	2.3
47	CT	74	ILE	2.3
24	C3	40	ALA	2.3
33	CE	39	ALA	2.3
40	DM	75	ALA	2.3
46	DS	103	ALA	2.3
19	AS	33	THR	2.3
19	BS	66	MET	2.3
14	BN	37	SER	2.3
40	CM	30	THR	2.3
3	BC	43	LEU	2.3
29	CC	243	HIS	2.3
35	DG	111	HIS	2.3
48	DU	70	HIS	2.3
55	DA	2125	G	2.3
34	DF	81	GLN	2.3
1	AA	1019	A	2.3
1	BA	1363	A	2.3
48	CU	47	VAL	2.3
48	CU	63	VAL	2.3
55	DA	2108	A	2.3
1	AA	1090	U	2.3
47	CT	103	ILE	2.3
20	BT	72	ALA	2.3
1	BA	1245	C	2.3
31	CA	2000	C	2.3
31	CA	2575	C	2.3
20	AT	20	HIS	2.3
12	AL	5	ASN	2.3
20	BT	33	LYS	2.3
31	CA	830	G	2.2
31	CA	2128	G	2.2
3	AC	81	GLY	2.2
54	DI	112	ALA	2.2
1	BA	1235	U	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	1194	A	2.2
10	BJ	22	THR	2.2
22	C1	11	SER	2.2
1	BA	1218	C	2.2
31	CA	765	C	2.2
46	CS	79	ARG	2.2
30	CD	168	GLU	2.2
37	CJ	55	ILE	2.2
9	BI	121	ALA	2.2
29	CC	208	ALA	2.2
38	CK	8	PRO	2.2
38	CK	104	ALA	2.2
47	CT	87	PRO	2.2
19	AS	71	LEU	2.2
19	BS	16	LEU	2.2
45	CR	60	LEU	2.2
7	AG	49	THR	2.2
31	CA	329	G	2.2
34	DF	72	LYS	2.2
4	AD	4	TYR	2.2
55	DA	1729	U	2.2
1	AA	958	A	2.2
1	AA	1346	A	2.2
42	CO	15	SER	2.2
16	BP	57	ILE	2.2
1	AA	1031	C	2.2
4	AD	11	LEU	2.2
5	BE	96	MET	2.2
10	AJ	52	LEU	2.2
10	BJ	52	LEU	2.2
13	AM	32	ALA	2.2
30	CD	138	LEU	2.2
37	CJ	106	LEU	2.2
47	DT	82	MET	2.2
54	DI	130	PRO	2.2
14	BN	12	LYS	2.2
38	CK	106	LYS	2.2
9	AI	124	ARG	2.2
10	BJ	62	ARG	2.2
16	BP	3	THR	2.2
46	CS	82	HIS	2.2
1	BA	981	U	2.2

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Mol	Chain	Res	Type	RSRZ
37	CJ	109	ILE	2.2
1	AA	1032	G	2.2
7	BG	50	LEU	2.2
23	C2	51	GLU	2.2
38	CK	43	GLU	2.2
53	CZ	18	LEU	2.2
55	DA	2117	A	2.2
22	C1	21	ALA	2.2
30	CD	57	ALA	2.2
39	CL	94	PRO	2.2
40	CM	26	GLY	2.2
40	CM	28	GLY	2.2
29	CC	255	LYS	2.2
1	AA	972	C	2.2
1	AA	980	C	2.2
1	BA	1203	C	2.2
31	CA	318	C	2.2
31	CA	1104	C	2.2
31	CA	1961	C	2.2
55	DA	2165	C	2.2
3	BC	68	ILE	2.2
10	BJ	25	ILE	2.2
37	DJ	55	ILE	2.2
46	CS	86	GLN	2.2
49	CV	5	ILE	2.2
3	BC	137	ALA	2.2
9	AI	121	ALA	2.2
21	BU	54	LYS	2.2
29	CC	211	ALA	2.2
31	CA	1396	U	2.2
55	DA	2109	U	2.2
33	CE	61	ARG	2.2
2	BB	126	PHE	2.2
31	CA	515	A	2.2
31	CA	2127	G	2.2
9	BI	9	THR	2.1
37	DJ	118	THR	2.1
23	C2	21	TYR	2.1
1	AA	136	C	2.1
31	CA	1985	C	2.1
7	AG	23	LEU	2.1
11	BK	64	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
8	BH	3	MET	2.1
27	C0	21	LYS	2.1
46	CS	81	LYS	2.1
49	CV	44	LYS	2.1
33	CE	182	ALA	2.1
36	CH	23	ALA	2.1
29	CC	212	ARG	2.1
40	DM	106	GLU	2.1
40	CM	114	GLY	2.1
10	BJ	51	VAL	2.1
37	CJ	9	VAL	2.1
33	CE	131	THR	2.1
1	AA	1000	A	2.1
3	BC	193	TYR	2.1
13	BM	86	TYR	2.1
34	CF	156	ILE	2.1
20	BT	76	LYS	2.1
38	CK	109	LEU	2.1
41	CN	20	LEU	2.1
1	AA	1316	G	2.1
1	BA	971	G	2.1
1	BA	1221	G	2.1
42	CO	1	MET	2.1
55	DA	2124	G	2.1
14	BN	15	ALA	2.1
30	CD	132	ALA	2.1
37	CJ	76	ALA	2.1
6	BF	100	SER	2.1
9	AI	40	GLY	2.1
45	CR	23	GLY	2.1
50	CW	84	PRO	2.1
51	CX	17	GLU	2.1
31	CA	2150	C	2.1
3	BC	116	VAL	2.1
3	BC	173	VAL	2.1
38	CK	48	VAL	2.1
3	BC	10	ILE	2.1
14	BN	20	TYR	2.1
37	CJ	10	LYS	2.1
3	BC	172	ARG	2.1
7	AG	10	ARG	2.1
20	BT	13	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
22	C1	4	GLN	2.1
33	CE	34	ALA	2.1
41	CN	79	ALA	2.1
1	BA	325	A	2.1
7	AG	8	GLY	2.1
31	CA	2665	A	2.1
1	BA	953	G	2.1
1	BA	987	G	2.1
4	AD	130	VAL	2.1
31	CA	289	G	2.1
31	CA	1514	G	2.1
31	CA	1627	G	2.1
1	AA	504	C	2.1
31	CA	1005	C	2.1
31	CA	2628	C	2.1
7	BG	11	LYS	2.1
7	BG	104	ILE	2.1
19	BS	12	ASP	2.1
29	CC	229	ASP	2.1
41	CN	133	LYS	2.1
50	CW	14	LYS	2.1
38	CK	25	LEU	2.1
44	CQ	4	ILE	2.1
2	AB	46	THR	2.1
6	BF	92	THR	2.1
14	BN	59	ARG	2.1
14	BN	67	THR	2.1
11	BK	85	MET	2.1
36	DH	25	TYR	2.1
7	BG	65	ALA	2.1
31	CA	2690	U	2.1
29	CC	244	PRO	2.1
47	CT	12	SER	2.1
3	BC	151	VAL	2.1
14	AN	7	LYS	2.1
31	CA	330	A	2.1
36	DH	35	LYS	2.1
43	CP	3	LYS	2.1
7	BG	29	ILE	2.1
8	BH	99	LEU	2.1
41	CN	73	ILE	2.1
19	BS	48	THR	2.1

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Mol	Chain	Res	Type	RSRZ
24	C3	4	THR	2.1
25	C4	49	MET	2.1
37	CJ	60	THR	2.1
45	CR	32	TYR	2.1
1	AA	1140	C	2.1
1	BA	932	C	2.1
1	BA	1028	C	2.1
1	BA	1208	C	2.1
28	CB	97	C	2.1
31	CA	343	C	2.1
37	DJ	77	ALA	2.1
49	CV	75	ALA	2.1
55	DA	2161	C	2.1
5	AE	27	GLY	2.1
3	AC	105	GLU	2.1
19	AS	76	PRO	2.1
1	AA	981	U	2.0
22	C1	7	LYS	2.0
47	CT	71	VAL	2.0
3	AC	207	ILE	2.0
3	BC	47	LEU	2.0
4	BD	131	ASN	2.0
5	BE	30	ILE	2.0
16	BP	9	HIS	2.0
25	C4	24	HIS	2.0
1	BA	1275	A	2.0
16	BP	17	TYR	2.0
32	DD	54	ALA	2.0
46	CS	36	ALA	2.0
7	AG	62	PHE	2.0
10	BJ	55	PRO	2.0
19	AS	74	PHE	2.0
1	BA	1296	C	2.0
1	BA	1369	C	2.0
47	CT	49	LYS	2.0
54	DI	55	VAL	2.0
13	BM	34	LEU	2.0
29	CC	14	ARG	2.0
31	CA	930	G	2.0
31	CA	1087	G	2.0
31	CA	1166	G	2.0
3	AC	77	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
22	C1	55	ILE	2.0
37	CJ	59	ILE	2.0
52	CY	64	ILE	2.0
1	AA	1017	U	2.0
1	BA	956	U	2.0
11	BK	67	ALA	2.0
25	C4	60	ALA	2.0
50	CW	22	ALA	2.0
49	CV	18	ASP	2.0
8	AH	82	GLY	2.0
37	CJ	42	PHE	2.0
46	CS	88	GLY	2.0
23	C2	37	LYS	2.0
25	C4	47	LYS	2.0
30	CD	159	LYS	2.0
45	CR	59	GLN	2.0
2	BB	145	GLU	2.0
9	BI	111	VAL	2.0
18	BR	20	GLU	2.0
31	CA	2860	A	2.0
37	CJ	140	VAL	2.0
48	CU	10	VAL	2.0
16	BP	54	LEU	2.0
27	C0	17	LEU	2.0
27	C0	29	LEU	2.0
37	DJ	138	LEU	2.0
40	CM	82	LEU	2.0
42	CO	51	LEU	2.0
1	AA	948	C	2.0
31	CA	1152	C	2.0
31	CA	2078	C	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	2MG	BA	966	24/25	0.33	0.14	258,264,268,268	0
1	2MG	AA	1207	24/25	0.62	0.10	234,239,241,243	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	2MG	BA	1207	24/25	0.62	0.13	256,257,258,259	0
1	5MC	BA	967	21/22	0.66	0.14	258,263,266,266	0
1	2MG	AA	966	24/25	0.71	0.12	211,213,215,216	0
31	PSU	CA	1917	20/21	0.76	0.09	132,140,149,149	0
1	PSU	AA	516	20/21	0.81	0.11	135,138,139,141	0
31	3TD	CA	1915	21/22	0.82	0.08	162,165,170,171	0
1	5MC	AA	967	21/22	0.82	0.10	214,216,219,220	0
31	PSU	CA	2580	20/21	0.83	0.11	118,125,130,131	0
31	PSU	CA	955	20/21	0.85	0.11	126,130,135,136	0
31	PSU	CA	2457	20/21	0.88	0.11	118,122,126,127	0
31	PSU	CA	1911	20/21	0.88	0.06	152,158,159,161	0
41	4D4	CN	81	12/13	0.88	0.14	118,121,132,133	0
31	PSU	CA	746	20/21	0.89	0.10	135,137,142,142	0
1	PSU	BA	516	20/21	0.89	0.08	111,121,128,129	0
31	6MZ	CA	1618	23/24	0.89	0.12	160,164,168,172	0
31	PSU	CA	2504	20/21	0.90	0.11	106,114,117,120	0
31	5MC	CA	1962	21/22	0.90	0.12	103,106,110,112	0
31	2MA	CA	2503	23/24	0.90	0.12	117,126,137,138	0
1	UR3	BA	1498	21/22	0.91	0.10	118,122,126,127	0
1	2MG	BA	1516	24/25	0.91	0.09	105,110,116,117	0
31	OMG	CA	2251	24/25	0.92	0.14	111,114,115,116	0
12	D2T	BL	89	10/11	0.92	0.17	106,110,113,114	0
31	1MG	CA	745	24/25	0.92	0.09	123,126,132,134	0
1	5MC	BA	1407	21/22	0.92	0.09	111,121,124,125	0
31	6MZ	CA	2030	23/24	0.92	0.09	117,125,134,134	0
55	PSU	DA	1911	20/21	0.92	0.06	107,118,120,121	0
55	3TD	DA	1915	21/22	0.92	0.07	133,140,146,147	0
55	PSU	DA	1917	20/21	0.92	0.07	109,113,119,119	0
31	7MG	CA	2069	24/25	0.92	0.15	104,111,124,124	0
31	2MG	CA	1835	24/25	0.93	0.10	100,103,106,110	0
31	5MU	CA	1939	21/22	0.93	0.10	95,99,105,107	0
1	7MG	AA	527	24/25	0.94	0.09	102,109,115,118	0
1	7MG	BA	527	24/25	0.94	0.08	100,108,118,120	0
31	2MG	CA	2445	24/25	0.94	0.14	103,109,112,114	0
31	5MU	CA	747	21/22	0.94	0.08	131,134,136,137	0
31	OMC	CA	2498	21/22	0.94	0.12	116,124,130,132	0
12	D2T	AL	89	10/11	0.94	0.10	109,114,125,128	0
31	OMU	CA	2552	21/22	0.95	0.18	106,111,115,116	0
1	MA6	BA	1518	24/25	0.95	0.08	91,97,102,103	0
1	4OC	AA	1402	22/23	0.96	0.09	94,99,103,104	0
55	5MC	DA	1962	21/22	0.96	0.09	46,61,65,66	0
31	PSU	CA	2605	20/21	0.96	0.07	97,101,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	5MC	AA	1407	21/22	0.97	0.06	80,88,90,91	0
1	4OC	BA	1402	22/23	0.97	0.07	111,116,127,128	0
1	UR3	AA	1498	21/22	0.97	0.07	86,92,97,100	0
1	2MG	AA	1516	24/25	0.97	0.06	74,82,84,86	0
1	MA6	AA	1518	24/25	0.97	0.07	67,77,81,85	0
1	MA6	AA	1519	24/25	0.97	0.08	72,76,80,81	0
55	PSU	DA	2604	20/21	0.97	0.06	58,63,70,72	0
55	PSU	DA	2605	20/21	0.97	0.08	51,59,64,65	0
1	MA6	BA	1519	24/25	0.97	0.08	100,102,107,110	0
41	4D4	DN	81[A]	12/13	0.97	0.10	49,59,65,66	9
41	4D4	DN	81[B]	12/13	0.97	0.10	37,45,50,50	9
55	5MU	DA	1939	21/22	0.98	0.06	53,58,65,69	0
55	2MG	DA	1835	24/25	0.98	0.06	59,65,71,72	0
55	H2U	DA	2449	20/21	0.98	0.11	33,39,46,46	0
55	PSU	DA	2504	20/21	0.98	0.07	50,51,54,56	0
55	OMU	DA	2552	21/22	0.98	0.06	45,48,52,57	0
55	7MG	DA	2069	24/25	0.99	0.06	41,48,53,53	0
55	OMG	DA	2251	24/25	0.99	0.05	29,48,54,62	0
55	2MG	DA	2445	24/25	0.99	0.06	39,45,50,62	0
55	6MZ	DA	1618	23/24	0.99	0.06	34,42,47,49	0
55	PSU	DA	2457	20/21	0.99	0.05	44,46,52,53	0
55	OMC	DA	2498	21/22	0.99	0.05	37,39,46,47	0
55	2MA	DA	2503	23/24	0.99	0.05	44,51,58,62	0
32	MEQ	DD	150[A]	10/11	0.99	0.09	31,32,37,37	10
32	MEQ	DD	150[B]	10/11	0.99	0.09	35,38,44,45	10
55	PSU	DA	2580	20/21	0.99	0.06	30,35,41,43	0
55	1MG	DA	745	24/25	0.99	0.04	31,37,42,44	0
55	PSU	DA	746	20/21	0.99	0.04	38,44,46,47	0
55	5MU	DA	747	21/22	0.99	0.05	41,43,52,58	0
55	PSU	DA	955	20/21	0.99	0.06	32,35,39,41	0
55	6MZ	DA	2030	23/24	0.99	0.06	27,33,38,40	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3139	1/1	0.35	0.20	140,140,140,140	0
56	MG	AA	1628	1/1	0.37	0.17	137,137,137,137	0
56	MG	BA	1624	1/1	0.40	0.12	293,293,293,293	0
56	MG	AA	1606	1/1	0.46	0.18	124,124,124,124	0
56	MG	CA	3132	1/1	0.48	0.14	157,157,157,157	0
56	MG	CA	3123	1/1	0.49	0.09	142,142,142,142	0
56	MG	BA	1626	1/1	0.50	0.13	255,255,255,255	0
56	MG	CA	3124	1/1	0.53	0.16	159,159,159,159	0
56	MG	BA	1641	1/1	0.56	0.15	140,140,140,140	0
56	MG	BA	1625	1/1	0.58	0.20	288,288,288,288	0
56	MG	CA	3061	1/1	0.58	0.14	270,270,270,270	0
56	MG	CA	3155	1/1	0.60	0.17	181,181,181,181	0
56	MG	AA	1622	1/1	0.63	0.18	106,106,106,106	0
56	MG	AA	1616	1/1	0.64	0.40	105,105,105,105	0
56	MG	CA	3104	1/1	0.65	0.14	249,249,249,249	0
56	MG	DA	3130	1/1	0.66	0.21	109,109,109,109	0
56	MG	AA	1609	1/1	0.67	0.28	107,107,107,107	0
56	MG	CA	3077	1/1	0.68	0.12	244,244,244,244	0
56	MG	AA	1608	1/1	0.68	0.22	128,128,128,128	0
56	MG	AA	1660	1/1	0.69	0.12	283,283,283,283	0
56	MG	CA	3140	1/1	0.69	0.15	108,108,108,108	0
56	MG	CA	3075	1/1	0.70	0.20	231,231,231,231	0
56	MG	CA	3007	1/1	0.70	0.06	257,257,257,257	0
56	MG	CA	3126	1/1	0.71	0.14	115,115,115,115	0
56	MG	DA	3171	1/1	0.71	0.23	111,111,111,111	0
61	PEG	DP	201	7/7	0.71	0.15	149,153,164,165	0
62	EDO	DA	3003	4/4	0.72	0.27	135,137,140,141	0
56	MG	BA	1604	1/1	0.73	0.12	257,257,257,257	0
56	MG	AA	1605	1/1	0.73	0.27	87,87,87,87	0
56	MG	DA	3168	1/1	0.73	0.17	119,119,119,119	0
56	MG	CA	3130	1/1	0.75	0.16	84,84,84,84	0
56	MG	CA	3115	1/1	0.75	0.19	111,111,111,111	0
56	MG	DA	3062	1/1	0.76	0.09	269,269,269,269	0
56	MG	AA	1626	1/1	0.76	0.14	120,120,120,120	0
56	MG	CA	3021	1/1	0.76	0.29	253,253,253,253	0
56	MG	CA	3060	1/1	0.76	0.10	238,238,238,238	0
56	MG	CA	3142	1/1	0.76	0.10	102,102,102,102	0
56	MG	AA	1658	1/1	0.76	0.13	212,212,212,212	0
56	MG	BA	1607	1/1	0.77	0.14	280,280,280,280	0
56	MG	BA	1619	1/1	0.77	0.19	228,228,228,228	0
56	MG	CA	3056	1/1	0.77	0.61	77,77,77,77	0
56	MG	CA	3014	1/1	0.78	0.11	273,273,273,273	0
56	MG	DA	3152	1/1	0.78	0.29	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3148	1/1	0.79	0.28	43,43,43,43	1
56	MG	CA	3112	1/1	0.79	0.12	103,103,103,103	0
56	MG	BA	1629	1/1	0.79	0.30	217,217,217,217	0
59	PUT	DA	3221	6/6	0.80	0.20	112,120,122,122	0
56	MG	CA	3111	1/1	0.80	0.13	103,103,103,103	0
58	MPD	DE	301	8/8	0.80	0.20	172,174,179,179	0
56	MG	CA	3009	1/1	0.81	0.15	259,259,259,259	0
56	MG	DA	3176	1/1	0.81	0.20	81,81,81,81	0
56	MG	AA	1603	1/1	0.81	0.19	111,111,111,111	0
56	MG	CA	3083	1/1	0.81	0.12	254,254,254,254	0
56	MG	CA	3145	1/1	0.81	0.33	78,78,78,78	0
56	MG	CA	3067	1/1	0.81	0.08	274,274,274,274	0
56	MG	CA	3154	1/1	0.82	0.16	110,110,110,110	0
56	MG	BA	1638	1/1	0.82	0.23	65,65,65,65	0
56	MG	AA	1627	1/1	0.82	0.13	115,115,115,115	0
62	EDO	DB	210	4/4	0.82	0.36	125,126,126,127	0
56	MG	BA	1623	1/1	0.82	0.30	277,277,277,277	0
56	MG	CA	3002	1/1	0.83	0.14	224,224,224,224	0
56	MG	CA	3003	1/1	0.83	0.32	272,272,272,272	0
56	MG	CA	3110	1/1	0.83	0.16	129,129,129,129	0
59	PUT	AA	1673	6/6	0.83	0.10	142,145,148,150	0
56	MG	DA	3131	1/1	0.83	0.30	83,83,83,83	0
56	MG	DA	3147	1/1	0.83	0.17	108,108,108,108	0
56	MG	CA	3135	1/1	0.83	0.11	78,78,78,78	0
56	MG	AA	1615	1/1	0.83	0.69	129,129,129,129	0
56	MG	CA	3072	1/1	0.84	0.18	258,258,258,258	0
56	MG	AA	1623	1/1	0.84	0.22	87,87,87,87	0
56	MG	CA	3026	1/1	0.84	0.21	245,245,245,245	0
56	MG	BA	1639	1/1	0.84	0.07	117,117,117,117	0
56	MG	BA	1606	1/1	0.85	0.10	270,270,270,270	0
56	MG	CB	203	1/1	0.85	0.09	237,237,237,237	0
56	MG	CA	3105	1/1	0.85	0.09	252,252,252,252	0
58	MPD	DK	201	8/8	0.85	0.11	125,126,127,127	0
56	MG	CA	3125	1/1	0.85	0.10	136,136,136,136	0
56	MG	DA	3137	1/1	0.85	0.13	61,61,61,61	0
61	PEG	AL	201	7/7	0.85	0.12	132,133,135,136	0
56	MG	CA	3034	1/1	0.85	0.16	228,228,228,228	0
61	PEG	DQ	201	7/7	0.85	0.28	162,166,170,170	0
56	MG	CA	3001	1/1	0.85	0.15	291,291,291,291	0
56	MG	BA	1635	1/1	0.85	0.12	209,209,209,209	0
56	MG	CA	3048	1/1	0.86	0.11	147,147,147,147	0
56	MG	CA	3137	1/1	0.86	0.16	164,164,164,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3028	1/1	0.86	0.11	284,284,284,284	0
56	MG	CA	3129	1/1	0.86	0.13	135,135,135,135	0
56	MG	AA	1659	1/1	0.86	0.07	273,273,273,273	0
56	MG	CA	3087	1/1	0.86	0.13	232,232,232,232	0
56	MG	CA	3146	1/1	0.86	0.08	174,174,174,174	0
56	MG	CA	3038	1/1	0.87	0.09	252,252,252,252	0
56	MG	BA	1627	1/1	0.87	0.28	203,203,203,203	0
56	MG	DA	3170	1/1	0.87	0.21	59,59,59,59	0
56	MG	CA	3152	1/1	0.87	0.07	160,160,160,160	0
56	MG	AA	1618	1/1	0.87	0.44	172,172,172,172	0
57	PG4	AA	1670	13/13	0.87	0.12	111,116,118,119	0
56	MG	AA	1604	1/1	0.87	0.26	79,79,79,79	0
56	MG	CA	3156	1/1	0.87	0.11	263,263,263,263	0
56	MG	CA	3138	1/1	0.87	0.13	98,98,98,98	0
56	MG	BA	1637	1/1	0.87	0.34	121,121,121,121	0
56	MG	AA	1613	1/1	0.87	0.14	80,80,80,80	0
56	MG	CA	3109	1/1	0.87	0.10	67,67,67,67	0
56	MG	DA	3138	1/1	0.87	0.38	29,29,29,29	1
56	MG	DA	3142	1/1	0.87	0.32	80,80,80,80	0
56	MG	AA	1665	1/1	0.87	0.23	274,274,274,274	0
56	MG	CA	3016	1/1	0.88	0.34	218,218,218,218	0
56	MG	AA	1601	1/1	0.88	0.24	62,62,62,62	0
56	MG	CA	3022	1/1	0.88	0.15	259,259,259,259	0
56	MG	DA	3123	1/1	0.88	0.18	84,84,84,84	0
56	MG	DA	3127	1/1	0.88	0.34	69,69,69,69	0
56	MG	CA	3088	1/1	0.88	0.19	86,86,86,86	0
58	MPD	DA	3204	8/8	0.88	0.16	116,119,125,127	0
59	PUT	AA	1672	6/6	0.88	0.23	149,150,150,150	0
56	MG	CA	3141	1/1	0.88	0.23	78,78,78,78	0
59	PUT	AA	1674	6/6	0.88	0.26	109,113,116,117	0
56	MG	AA	1630	1/1	0.88	0.09	205,205,205,205	0
56	MG	CB	201	1/1	0.88	0.06	235,235,235,235	0
56	MG	CA	3107	1/1	0.88	0.20	81,81,81,81	0
56	MG	CA	3071	1/1	0.88	0.09	228,228,228,228	0
56	MG	AA	1642	1/1	0.88	0.13	275,275,275,275	0
56	MG	AA	1624	1/1	0.88	0.11	82,82,82,82	0
68	TRS	DA	3220	8/8	0.88	0.15	184,187,190,191	0
56	MG	CA	3134	1/1	0.89	0.08	167,167,167,167	0
56	MG	CA	3070	1/1	0.89	0.11	234,234,234,234	0
56	MG	DA	3008	1/1	0.89	0.10	280,280,280,280	0
57	PG4	BA	1642	13/13	0.89	0.10	113,117,132,132	0
56	MG	CA	3118	1/1	0.89	0.22	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3119	1/1	0.89	0.16	100,100,100,100	0
58	MPD	DA	3190	8/8	0.89	0.12	100,102,103,106	0
56	MG	CA	3122	1/1	0.89	0.16	89,89,89,89	0
56	MG	BA	1633	1/1	0.89	0.13	237,237,237,237	0
56	MG	CA	3023	1/1	0.89	0.20	255,255,255,255	0
56	MG	CA	3004	1/1	0.89	0.09	192,192,192,192	0
59	PUT	AA	1675	6/6	0.89	0.22	172,174,174,175	0
56	MG	AA	1614	1/1	0.89	0.16	83,83,83,83	0
56	MG	CA	3032	1/1	0.89	0.06	197,197,197,197	0
56	MG	CA	3147	1/1	0.89	0.17	36,36,36,36	1
56	MG	CA	3084	1/1	0.89	0.10	172,172,172,172	0
56	MG	DA	3153	1/1	0.89	0.59	102,102,102,102	0
62	EDO	DA	3002	4/4	0.89	0.48	176,176,176,177	0
56	MG	CA	3131	1/1	0.89	0.13	123,123,123,123	0
66	ACY	DA	3196	4/4	0.89	0.14	61,69,69,72	0
56	MG	CA	3008	1/1	0.89	0.12	202,202,202,202	0
56	MG	AA	1656	1/1	0.90	0.09	274,274,274,274	0
56	MG	CA	3010	1/1	0.90	0.12	259,259,259,259	0
56	MG	CA	3121	1/1	0.90	0.13	83,83,83,83	0
56	MG	BA	1636	1/1	0.90	0.16	77,77,77,77	0
56	MG	AA	1664	1/1	0.90	0.14	265,265,265,265	0
56	MG	AA	1612	1/1	0.90	0.14	77,77,77,77	0
56	MG	DA	3120	1/1	0.90	0.26	66,66,66,66	0
56	MG	AA	1669	1/1	0.90	0.14	239,239,239,239	0
56	MG	AA	1621	1/1	0.90	0.38	97,97,97,97	0
56	MG	BA	1634	1/1	0.90	0.11	216,216,216,216	0
57	PG4	DQ	202	13/13	0.90	0.10	84,89,100,101	0
56	MG	CA	3113	1/1	0.90	0.26	76,76,76,76	0
56	MG	CA	3064	1/1	0.90	0.10	271,271,271,271	0
56	MG	CA	3116	1/1	0.90	0.15	92,92,92,92	0
56	MG	CA	3150	1/1	0.91	0.14	79,79,79,79	0
58	MPD	DN	201	8/8	0.91	0.13	109,117,119,121	0
56	MG	BA	1612	1/1	0.91	0.34	262,262,262,262	0
56	MG	CA	3076	1/1	0.91	0.10	218,218,218,218	0
56	MG	AA	1639	1/1	0.91	0.10	225,225,225,225	0
56	MG	CA	3006	1/1	0.91	0.07	221,221,221,221	0
56	MG	CA	3068	1/1	0.91	0.13	174,174,174,174	0
56	MG	DA	3160	1/1	0.91	0.25	64,64,64,64	0
56	MG	CA	3051	1/1	0.91	0.15	248,248,248,248	0
56	MG	AA	1625	1/1	0.91	0.24	83,83,83,83	0
56	MG	CA	3090	1/1	0.91	0.09	187,187,187,187	0
56	MG	DA	3126	1/1	0.91	0.21	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3093	1/1	0.91	0.06	143,143,143,143	0
56	MG	DA	3128	1/1	0.91	0.37	57,57,57,57	0
56	MG	CA	3099	1/1	0.91	0.08	174,174,174,174	0
57	PG4	DA	3193	13/13	0.91	0.22	109,113,119,120	0
56	MG	AA	1663	1/1	0.91	0.10	230,230,230,230	0
56	MG	AA	1607	1/1	0.92	0.17	90,90,90,90	0
56	MG	CA	3092	1/1	0.92	0.05	163,163,163,163	0
56	MG	DA	3111	1/1	0.92	0.24	283,283,283,283	0
56	MG	DA	3155	1/1	0.92	0.18	86,86,86,86	0
56	MG	DA	3157	1/1	0.92	0.20	74,74,74,74	0
56	MG	AA	1636	1/1	0.92	0.13	209,209,209,209	0
56	MG	AA	1661	1/1	0.92	0.21	223,223,223,223	0
56	MG	CA	3100	1/1	0.92	0.18	243,243,243,243	0
59	PUT	DA	3195	6/6	0.92	0.27	100,104,108,108	0
59	PUT	DA	3205	6/6	0.92	0.37	106,108,108,109	0
56	MG	BA	1614	1/1	0.92	0.11	217,217,217,217	0
56	MG	DA	3172	1/1	0.92	0.11	85,85,85,85	0
56	MG	CA	3082	1/1	0.92	0.12	168,168,168,168	0
56	MG	CA	3039	1/1	0.92	0.10	190,190,190,190	0
61	PEG	DA	3226	7/7	0.92	0.39	125,126,131,131	0
62	EDO	D1	101	4/4	0.92	0.09	70,71,73,75	0
56	MG	BA	1603	1/1	0.92	0.07	278,278,278,278	0
56	MG	AA	1610	1/1	0.92	0.15	99,99,99,99	0
56	MG	CA	3054	1/1	0.92	0.08	122,122,122,122	0
63	PGE	D1	102	10/10	0.92	0.18	142,145,152,153	0
63	PGE	DA	3214	10/10	0.92	0.18	67,87,91,92	0
64	SPD	DA	3183	10/10	0.92	0.12	80,95,97,98	0
58	MPD	AA	1676	8/8	0.92	0.29	145,146,148,148	0
56	MG	DA	3006	1/1	0.92	0.20	266,266,266,266	0
59	PUT	DA	3184	6/6	0.93	0.22	65,70,74,74	0
56	MG	CA	3149	1/1	0.93	0.21	76,76,76,76	0
57	PG4	DR	201	13/13	0.93	0.26	156,168,173,173	0
59	PUT	DA	3212	6/6	0.93	0.24	114,115,117,117	0
56	MG	DA	3158	1/1	0.93	0.10	107,107,107,107	0
56	MG	CA	3036	1/1	0.93	0.09	227,227,227,227	0
61	PEG	DL	201	7/7	0.93	0.14	102,103,109,110	0
56	MG	DA	3162	1/1	0.93	0.07	79,79,79,79	0
58	MPD	DE	302	8/8	0.93	0.18	101,102,103,104	0
61	PEG	DA	3199	7/7	0.93	0.18	99,106,112,113	0
61	PEG	DA	3200	7/7	0.93	0.23	124,124,125,125	0
56	MG	DA	3079	1/1	0.93	0.07	179,179,179,179	0
56	MG	CA	3019	1/1	0.93	0.07	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	EDO	D0	101	4/4	0.93	0.17	79,80,85,89	0
58	MPD	DT	201	8/8	0.93	0.23	110,115,125,126	0
56	MG	AA	1654	1/1	0.93	0.16	178,178,178,178	0
56	MG	CA	3081	1/1	0.93	0.10	254,254,254,254	0
58	MPD	DA	3207	8/8	0.93	0.17	121,125,128,129	0
63	PGE	DD	301	10/10	0.93	0.21	120,122,129,130	0
63	PGE	DS	201	10/10	0.93	0.09	96,99,101,101	0
56	MG	AA	1634	1/1	0.93	0.18	179,179,179,179	0
56	MG	DA	3180	1/1	0.93	0.11	77,77,77,77	0
56	MG	DR	202	1/1	0.93	0.20	269,269,269,269	0
67	GUN	DA	3211	11/11	0.93	0.16	116,122,123,124	0
56	MG	BA	1609	1/1	0.93	0.12	156,156,156,156	0
56	MG	CA	3106	1/1	0.94	0.08	74,74,74,74	0
59	PUT	DA	3219	6/6	0.94	0.19	100,102,103,103	0
56	MG	DA	3001	1/1	0.94	0.16	47,47,47,47	0
59	PUT	DA	3222	6/6	0.94	0.16	77,81,83,83	0
56	MG	DA	3146	1/1	0.94	0.28	76,76,76,76	0
61	PEG	D3	102	7/7	0.94	0.15	136,138,140,140	0
57	PG4	DA	3216	13/13	0.94	0.13	111,122,132,134	0
58	MPD	AA	1671	8/8	0.94	0.20	143,144,147,148	0
56	MG	CA	3047	1/1	0.94	0.10	100,100,100,100	0
56	MG	CA	3018	1/1	0.94	0.08	147,147,147,147	0
56	MG	CA	3031	1/1	0.94	0.05	128,128,128,128	0
61	PEG	DA	3201	7/7	0.94	0.27	146,150,151,152	0
56	MG	AA	1644	1/1	0.94	0.13	180,180,180,180	0
61	PEG	DA	3227	7/7	0.94	0.20	109,114,120,120	0
56	MG	CA	3127	1/1	0.94	0.17	73,73,73,73	0
56	MG	AA	1662	1/1	0.94	0.07	164,164,164,164	0
58	MPD	DT	202	8/8	0.94	0.23	138,139,144,145	0
56	MG	DA	3121	1/1	0.94	0.11	111,111,111,111	0
56	MG	CA	3059	1/1	0.94	0.08	118,118,118,118	0
62	EDO	DA	3209	4/4	0.94	0.32	94,96,98,99	0
56	MG	CA	3005	1/1	0.94	0.08	233,233,233,233	0
63	PGE	D3	101	10/10	0.94	0.15	121,123,125,126	0
56	MG	AA	1602	1/1	0.94	0.12	78,78,78,78	0
56	MG	CA	3117	1/1	0.94	0.08	59,59,59,59	0
56	MG	DA	3129	1/1	0.94	0.18	51,51,51,51	0
63	PGE	DA	3225	10/10	0.94	0.20	100,120,131,131	0
56	MG	CA	3080	1/1	0.94	0.10	108,108,108,108	0
56	MG	CA	3062	1/1	0.94	0.07	168,168,168,168	0
56	MG	DA	3134	1/1	0.94	0.17	98,98,98,98	0
56	MG	AA	1617	1/1	0.94	0.14	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3141	1/1	0.95	0.24	80,80,80,80	0
56	MG	CA	3073	1/1	0.95	0.06	139,139,139,139	0
56	MG	DA	3144	1/1	0.95	0.07	79,79,79,79	0
56	MG	AA	1657	1/1	0.95	0.17	134,134,134,134	0
56	MG	CA	3063	1/1	0.95	0.09	155,155,155,155	0
56	MG	DA	3151	1/1	0.95	0.14	48,48,48,48	0
56	MG	BA	1618	1/1	0.95	0.06	172,172,172,172	0
56	MG	DA	3080	1/1	0.95	0.13	195,195,195,195	0
61	PEG	DA	3218	7/7	0.95	0.26	179,180,181,181	0
56	MG	CA	3055	1/1	0.95	0.07	193,193,193,193	0
56	MG	CA	3094	1/1	0.95	0.09	132,132,132,132	0
56	MG	CA	3128	1/1	0.95	0.12	116,116,116,116	0
56	MG	CA	3114	1/1	0.95	0.16	67,67,67,67	0
56	MG	BA	1630	1/1	0.95	0.09	197,197,197,197	0
62	EDO	DB	211	4/4	0.95	0.25	131,131,132,133	0
56	MG	DA	3163	1/1	0.95	0.16	87,87,87,87	0
56	MG	DA	3166	1/1	0.95	0.11	74,74,74,74	0
62	EDO	DA	3197	4/4	0.95	0.09	75,76,77,77	0
56	MG	BA	1602	1/1	0.95	0.05	102,102,102,102	0
62	EDO	DA	3215	4/4	0.95	0.10	64,67,70,73	0
56	MG	DA	3169	1/1	0.95	0.09	41,41,41,41	0
56	MG	CA	3101	1/1	0.95	0.05	239,239,239,239	0
56	MG	CA	3133	1/1	0.95	0.08	110,110,110,110	0
56	MG	BA	1620	1/1	0.95	0.08	172,172,172,172	0
56	MG	DA	3175	1/1	0.95	0.26	115,115,115,115	0
56	MG	BA	1640	1/1	0.95	0.07	103,103,103,103	0
56	MG	DA	3178	1/1	0.95	0.17	93,93,93,93	0
56	MG	CA	3120	1/1	0.95	0.10	130,130,130,130	0
56	MG	DB	207	1/1	0.95	0.17	92,92,92,92	0
56	MG	CA	3086	1/1	0.95	0.08	106,106,106,106	0
60	ZN	C5	101	1/1	0.96	0.06	175,175,175,175	0
56	MG	AA	1620	1/1	0.96	0.23	116,116,116,116	0
57	PG4	DS	202	13/13	0.96	0.10	72,73,85,86	0
56	MG	DA	3125	1/1	0.96	0.09	51,51,51,51	0
56	MG	CA	3103	1/1	0.96	0.06	176,176,176,176	0
56	MG	BA	1605	1/1	0.96	0.05	136,136,136,136	0
56	MG	DB	205	1/1	0.96	0.40	148,148,148,148	0
56	MG	DA	3159	1/1	0.96	0.12	131,131,131,131	0
56	MG	CA	3050	1/1	0.96	0.07	166,166,166,166	0
56	MG	BA	1622	1/1	0.96	0.07	240,240,240,240	0
56	MG	BA	1628	1/1	0.96	0.05	120,120,120,120	0
56	MG	DA	3164	1/1	0.96	0.18	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3132	1/1	0.96	0.12	56,56,56,56	0
56	MG	DA	3167	1/1	0.96	0.14	97,97,97,97	0
58	MPD	DA	3192	8/8	0.96	0.22	84,90,92,94	0
56	MG	CA	3108	1/1	0.96	0.09	89,89,89,89	0
56	MG	DA	3136	1/1	0.96	0.10	72,72,72,72	0
56	MG	CA	3078	1/1	0.96	0.07	198,198,198,198	0
62	EDO	DA	3194	4/4	0.96	0.13	89,90,90,90	0
56	MG	CA	3037	1/1	0.96	0.12	234,234,234,234	0
62	EDO	DA	3198	4/4	0.96	0.25	109,110,112,112	0
56	MG	AA	1655	1/1	0.96	0.04	152,152,152,152	0
56	MG	DA	3098	1/1	0.96	0.16	246,246,246,246	0
59	PUT	DM	201	6/6	0.96	0.16	63,66,74,75	0
56	MG	CA	3151	1/1	0.96	0.12	102,102,102,102	0
59	PUT	DA	3189	6/6	0.96	0.07	49,55,59,62	0
56	MG	DA	3177	1/1	0.96	0.14	52,52,52,52	0
63	PGE	DU	201	10/10	0.96	0.14	135,141,147,147	0
56	MG	DA	3117	1/1	0.96	0.14	70,70,70,70	0
63	PGE	DA	3217	10/10	0.96	0.11	87,89,93,94	0
56	MG	CA	3057	1/1	0.96	0.06	111,111,111,111	0
59	PUT	DA	3213	6/6	0.96	0.22	156,156,157,157	0
64	SPD	DA	3206	10/10	0.96	0.23	142,143,144,144	0
65	1PE	DA	3185	16/16	0.96	0.10	74,89,123,123	0
56	MG	DA	3148	1/1	0.96	0.16	67,67,67,67	0
56	MG	DA	3149	1/1	0.96	0.08	96,96,96,96	0
56	MG	AA	1647	1/1	0.96	0.06	145,145,145,145	0
59	PUT	DA	3223	6/6	0.97	0.13	75,81,84,84	0
56	MG	DA	3182	1/1	0.97	0.07	55,55,55,55	0
56	MG	CA	3030	1/1	0.97	0.05	82,82,82,82	0
56	MG	CA	3017	1/1	0.97	0.10	192,192,192,192	0
56	MG	DA	3054	1/1	0.97	0.09	167,167,167,167	0
56	MG	CA	3053	1/1	0.97	0.06	86,86,86,86	0
56	MG	AA	1645	1/1	0.97	0.05	70,70,70,70	0
56	MG	AA	1632	1/1	0.97	0.07	162,162,162,162	0
56	MG	DA	3095	1/1	0.97	0.10	65,65,65,65	0
56	MG	CA	3074	1/1	0.97	0.06	145,145,145,145	0
56	MG	DA	3154	1/1	0.97	0.27	60,60,60,60	0
56	MG	CA	3143	1/1	0.97	0.04	72,72,72,72	0
56	MG	BA	1608	1/1	0.97	0.08	144,144,144,144	0
56	MG	AA	1650	1/1	0.97	0.11	115,115,115,115	0
56	MG	CA	3058	1/1	0.97	0.08	124,124,124,124	0
58	MPD	DS	203	8/8	0.97	0.16	62,64,65,67	0
56	MG	AA	1611	1/1	0.97	0.07	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3161	1/1	0.97	0.13	73,73,73,73	0
56	MG	CA	3079	1/1	0.97	0.07	131,131,131,131	0
56	MG	CA	3025	1/1	0.97	0.06	133,133,133,133	0
56	MG	CA	3040	1/1	0.97	0.04	122,122,122,122	0
56	MG	CA	3042	1/1	0.97	0.06	96,96,96,96	0
58	MPD	DA	3210	8/8	0.97	0.16	110,118,123,125	0
56	MG	CA	3153	1/1	0.97	0.12	77,77,77,77	0
56	MG	CA	3045	1/1	0.97	0.05	167,167,167,167	0
56	MG	AA	1619	1/1	0.97	0.15	122,122,122,122	0
56	MG	CA	3085	1/1	0.97	0.04	116,116,116,116	0
56	MG	CA	3065	1/1	0.97	0.08	115,115,115,115	0
56	MG	DB	201	1/1	0.97	0.06	121,121,121,121	0
59	PUT	DA	3188	6/6	0.97	0.22	89,93,93,94	0
56	MG	DA	3173	1/1	0.97	0.18	100,100,100,100	0
56	MG	CA	3066	1/1	0.97	0.08	91,91,91,91	0
56	MG	BA	1615	1/1	0.97	0.05	103,103,103,103	0
64	SPD	DA	3187	10/10	0.97	0.14	78,82,85,85	0
56	MG	DA	3139	1/1	0.97	0.07	42,42,42,42	0
64	SPD	DA	3224	10/10	0.97	0.11	58,71,88,88	0
56	MG	DB	208	1/1	0.97	0.07	57,57,57,57	0
65	1PE	DA	3203	16/16	0.97	0.13	98,105,109,109	0
56	MG	DA	3179	1/1	0.97	0.07	85,85,85,85	0
56	MG	CA	3136	1/1	0.97	0.14	107,107,107,107	0
56	MG	DA	3181	1/1	0.97	0.15	66,66,66,66	0
56	MG	BA	1617	1/1	0.98	0.05	165,165,165,165	0
56	MG	DA	3085	1/1	0.98	0.07	100,100,100,100	0
56	MG	DA	3165	1/1	0.98	0.23	63,63,63,63	0
56	MG	DA	3088	1/1	0.98	0.06	75,75,75,75	0
56	MG	AA	1635	1/1	0.98	0.06	220,220,220,220	0
56	MG	DA	3097	1/1	0.98	0.04	75,75,75,75	0
56	MG	AA	1646	1/1	0.98	0.06	80,80,80,80	0
56	MG	CA	3020	1/1	0.98	0.06	116,116,116,116	0
56	MG	CA	3144	1/1	0.98	0.06	66,66,66,66	0
60	ZN	AB	301	1/1	0.98	0.03	165,165,165,165	0
56	MG	CA	3044	1/1	0.98	0.05	113,113,113,113	0
56	MG	AA	1641	1/1	0.98	0.05	122,122,122,122	0
56	MG	DA	3174	1/1	0.98	0.05	87,87,87,87	0
56	MG	CA	3091	1/1	0.98	0.05	81,81,81,81	0
56	MG	DA	3124	1/1	0.98	0.13	90,90,90,90	0
56	MG	CA	3046	1/1	0.98	0.07	99,99,99,99	0
56	MG	CA	3069	1/1	0.98	0.04	107,107,107,107	0
56	MG	AA	1668	1/1	0.98	0.11	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3095	1/1	0.98	0.05	174,174,174,174	0
56	MG	CA	3097	1/1	0.98	0.09	112,112,112,112	0
56	MG	CA	3098	1/1	0.98	0.04	98,98,98,98	0
56	MG	DA	3230	1/1	0.98	0.05	76,76,76,76	0
56	MG	AA	1633	1/1	0.98	0.04	116,116,116,116	0
56	MG	CA	3024	1/1	0.98	0.11	85,85,85,85	0
56	MG	DA	3133	1/1	0.98	0.06	52,52,52,52	0
56	MG	BA	1610	1/1	0.98	0.04	107,107,107,107	0
56	MG	DM	202	1/1	0.98	0.07	90,90,90,90	0
56	MG	CA	3102	1/1	0.98	0.03	99,99,99,99	0
56	MG	CA	3052	1/1	0.98	0.06	124,124,124,124	0
56	MG	AA	1651	1/1	0.98	0.07	75,75,75,75	0
56	MG	DB	206	1/1	0.98	0.09	73,73,73,73	0
62	EDO	DA	3208	4/4	0.98	0.22	111,113,113,113	0
56	MG	BA	1613	1/1	0.98	0.14	149,149,149,149	0
56	MG	DA	3143	1/1	0.98	0.10	63,63,63,63	0
56	MG	CA	3029	1/1	0.98	0.05	143,143,143,143	0
56	MG	DB	209	1/1	0.98	0.10	83,83,83,83	0
56	MG	AA	1643	1/1	0.98	0.05	70,70,70,70	0
56	MG	CA	3011	1/1	0.98	0.05	95,95,95,95	0
56	MG	CA	3012	1/1	0.98	0.06	115,115,115,115	0
63	PGE	DA	3186	10/10	0.98	0.07	58,65,71,71	0
56	MG	DA	3012	1/1	0.98	0.07	141,141,141,141	0
56	MG	DA	3026	1/1	0.98	0.09	228,228,228,228	0
56	MG	DA	3037	1/1	0.98	0.09	13,13,13,13	0
56	MG	DA	3042	1/1	0.98	0.06	87,87,87,87	0
56	MG	DA	3044	1/1	0.98	0.09	124,124,124,124	0
56	MG	DA	3156	1/1	0.98	0.12	83,83,83,83	0
56	MG	DA	3052	1/1	0.98	0.08	251,251,251,251	0
56	MG	CA	3013	1/1	0.98	0.04	71,71,71,71	0
56	MG	AA	1638	1/1	0.98	0.04	142,142,142,142	0
66	ACY	DA	3191	4/4	0.98	0.09	79,80,81,81	0
56	MG	DA	3067	1/1	0.98	0.05	75,75,75,75	0
66	ACY	DA	3202	4/4	0.98	0.10	93,96,96,97	0
56	MG	DA	3070	1/1	0.98	0.08	151,151,151,151	0
56	MG	BA	1616	1/1	0.98	0.07	151,151,151,151	0
56	MG	DA	3030	1/1	0.99	0.04	88,88,88,88	0
56	MG	DA	3031	1/1	0.99	0.03	51,51,51,51	0
56	MG	AA	1631	1/1	0.99	0.03	75,75,75,75	0
56	MG	CA	3043	1/1	0.99	0.03	90,90,90,90	0
56	MG	DA	3135	1/1	0.99	0.07	146,146,146,146	0
56	MG	CA	3096	1/1	0.99	0.03	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3027	1/1	0.99	0.06	88,88,88,88	0
56	MG	DA	3231	1/1	0.99	0.07	70,70,70,70	0
56	MG	DA	3053	1/1	0.99	0.03	54,54,54,54	0
56	MG	CA	3015	1/1	0.99	0.14	84,84,84,84	0
56	MG	DA	3140	1/1	0.99	0.07	51,51,51,51	0
56	MG	DA	3055	1/1	0.99	0.07	52,52,52,52	0
56	MG	AA	1666	1/1	0.99	0.05	100,100,100,100	0
56	MG	DA	3063	1/1	0.99	0.08	111,111,111,111	0
56	MG	BA	1611	1/1	0.99	0.03	84,84,84,84	0
56	MG	DA	3069	1/1	0.99	0.07	64,64,64,64	0
56	MG	AA	1667	1/1	0.99	0.09	76,76,76,76	0
56	MG	DA	3071	1/1	0.99	0.03	56,56,56,56	0
56	MG	DA	3074	1/1	0.99	0.03	54,54,54,54	0
56	MG	CA	3049	1/1	0.99	0.05	53,53,53,53	0
56	MG	DB	203	1/1	0.99	0.08	88,88,88,88	0
56	MG	DA	3084	1/1	0.99	0.09	55,55,55,55	0
56	MG	DB	204	1/1	0.99	0.03	85,85,85,85	0
56	MG	AA	1648	1/1	0.99	0.03	84,84,84,84	0
56	MG	CA	3033	1/1	0.99	0.11	150,150,150,150	0
56	MG	BA	1631	1/1	0.99	0.07	132,132,132,132	0
56	MG	BA	1632	1/1	0.99	0.06	74,74,74,74	0
56	MG	DA	3099	1/1	0.99	0.07	45,45,45,45	0
56	MG	DA	3103	1/1	0.99	0.02	59,59,59,59	0
56	MG	CB	202	1/1	0.99	0.08	116,116,116,116	0
56	MG	DA	3113	1/1	0.99	0.08	113,113,113,113	0
56	MG	CA	3089	1/1	0.99	0.08	64,64,64,64	0
56	MG	DA	3118	1/1	0.99	0.03	31,31,31,31	0
56	MG	DA	3119	1/1	0.99	0.08	41,41,41,41	0
56	MG	DA	3005	1/1	0.99	0.07	67,67,67,67	0
56	MG	AA	1640	1/1	0.99	0.05	131,131,131,131	0
56	MG	DA	3122	1/1	0.99	0.29	48,48,48,48	0
56	MG	DA	3007	1/1	0.99	0.04	127,127,127,127	0
56	MG	AA	1677	1/1	0.99	0.04	101,101,101,101	0
56	MG	BA	1601	1/1	0.99	0.04	135,135,135,135	0
56	MG	DA	3015	1/1	0.99	0.03	78,78,78,78	0
56	MG	DA	3018	1/1	0.99	0.07	95,95,95,95	0
56	MG	CA	3041	1/1	0.99	0.09	50,50,50,50	0
56	MG	DA	3027	1/1	0.99	0.02	49,49,49,49	0
56	MG	DA	3028	1/1	0.99	0.04	116,116,116,116	0
56	MG	AA	1629	1/1	1.00	0.06	110,110,110,110	0
56	MG	DA	3096	1/1	1.00	0.03	28,28,28,28	0
56	MG	DA	3228	1/1	1.00	0.01	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3229	1/1	1.00	0.05	107,107,107,107	0
56	MG	AA	1652	1/1	1.00	0.12	42,42,42,42	0
56	MG	DA	3004	1/1	1.00	0.03	149,149,149,149	0
56	MG	DA	3029	1/1	1.00	0.08	44,44,44,44	0
56	MG	DA	3100	1/1	1.00	0.03	34,34,34,34	0
56	MG	DA	3101	1/1	1.00	0.03	90,90,90,90	0
56	MG	DA	3102	1/1	1.00	0.01	32,32,32,32	0
56	MG	DB	202	1/1	1.00	0.03	56,56,56,56	0
56	MG	DA	3104	1/1	1.00	0.07	43,43,43,43	0
56	MG	DA	3105	1/1	1.00	0.04	33,33,33,33	0
56	MG	DA	3106	1/1	1.00	0.07	45,45,45,45	0
56	MG	DA	3107	1/1	1.00	0.02	50,50,50,50	0
56	MG	DA	3108	1/1	1.00	0.02	36,36,36,36	0
56	MG	DA	3109	1/1	1.00	0.02	38,38,38,38	0
56	MG	DA	3110	1/1	1.00	0.02	31,31,31,31	0
56	MG	AA	1653	1/1	1.00	0.02	108,108,108,108	0
56	MG	DA	3112	1/1	1.00	0.01	46,46,46,46	0
56	MG	DA	3032	1/1	1.00	0.04	33,33,33,33	0
56	MG	DA	3114	1/1	1.00	0.02	52,52,52,52	0
56	MG	DA	3115	1/1	1.00	0.02	52,52,52,52	0
56	MG	DA	3116	1/1	1.00	0.03	72,72,72,72	0
56	MG	DA	3033	1/1	1.00	0.02	46,46,46,46	0
56	MG	DA	3034	1/1	1.00	0.03	44,44,44,44	0
56	MG	DA	3035	1/1	1.00	0.01	24,24,24,24	0
56	MG	DA	3036	1/1	1.00	0.04	32,32,32,32	0
56	MG	CA	3035	1/1	1.00	0.11	100,100,100,100	0
56	MG	DA	3038	1/1	1.00	0.02	35,35,35,35	0
56	MG	DA	3039	1/1	1.00	0.04	34,34,34,34	0
56	MG	DA	3040	1/1	1.00	0.02	55,55,55,55	0
56	MG	DA	3041	1/1	1.00	0.11	22,22,22,22	0
56	MG	AA	1649	1/1	1.00	0.03	111,111,111,111	0
56	MG	DA	3043	1/1	1.00	0.04	40,40,40,40	0
56	MG	DA	3009	1/1	1.00	0.03	39,39,39,39	0
56	MG	DA	3045	1/1	1.00	0.07	73,73,73,73	0
56	MG	DA	3046	1/1	1.00	0.04	27,27,27,27	0
56	MG	DA	3047	1/1	1.00	0.04	42,42,42,42	0
56	MG	DA	3048	1/1	1.00	0.03	59,59,59,59	0
56	MG	DA	3049	1/1	1.00	0.04	52,52,52,52	0
56	MG	DA	3050	1/1	1.00	0.02	41,41,41,41	0
56	MG	DA	3051	1/1	1.00	0.01	37,37,37,37	0
56	MG	DA	3010	1/1	1.00	0.05	48,48,48,48	0
56	MG	DA	3011	1/1	1.00	0.02	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	ZN	D5	101	1/1	1.00	0.01	84,84,84,84	0
56	MG	AA	1637	1/1	1.00	0.07	106,106,106,106	0
56	MG	DA	3013	1/1	1.00	0.01	13,13,13,13	0
56	MG	DA	3056	1/1	1.00	0.03	55,55,55,55	0
56	MG	DA	3057	1/1	1.00	0.01	28,28,28,28	0
56	MG	DA	3058	1/1	1.00	0.01	66,66,66,66	0
56	MG	DA	3059	1/1	1.00	0.03	25,25,25,25	0
56	MG	DA	3060	1/1	1.00	0.01	23,23,23,23	0
56	MG	DA	3145	1/1	1.00	0.03	45,45,45,45	0
56	MG	DA	3061	1/1	1.00	0.01	44,44,44,44	0
56	MG	DA	3014	1/1	1.00	0.02	31,31,31,31	0
56	MG	DD	302	1/1	1.00	0.04	62,62,62,62	0
56	MG	DA	3064	1/1	1.00	0.06	75,75,75,75	0
56	MG	DA	3150	1/1	1.00	0.02	72,72,72,72	0
56	MG	DA	3065	1/1	1.00	0.01	41,41,41,41	0
56	MG	DA	3066	1/1	1.00	0.03	43,43,43,43	0
56	MG	DA	3016	1/1	1.00	0.02	74,74,74,74	0
56	MG	DA	3068	1/1	1.00	0.05	43,43,43,43	0
56	MG	DA	3017	1/1	1.00	0.01	34,34,34,34	0
56	MG	BA	1621	1/1	1.00	0.07	45,45,45,45	0
56	MG	DA	3019	1/1	1.00	0.11	16,16,16,16	0
56	MG	DA	3072	1/1	1.00	0.04	86,86,86,86	0
56	MG	DA	3073	1/1	1.00	0.02	40,40,40,40	0
56	MG	DA	3020	1/1	1.00	0.04	69,69,69,69	0
56	MG	DA	3075	1/1	1.00	0.05	25,25,25,25	0
56	MG	DA	3076	1/1	1.00	0.05	46,46,46,46	0
56	MG	DA	3077	1/1	1.00	0.03	71,71,71,71	0
56	MG	DA	3078	1/1	1.00	0.02	47,47,47,47	0
56	MG	DA	3021	1/1	1.00	0.03	31,31,31,31	0
56	MG	DA	3022	1/1	1.00	0.04	40,40,40,40	0
56	MG	DA	3081	1/1	1.00	0.02	46,46,46,46	0
56	MG	DA	3082	1/1	1.00	0.03	109,109,109,109	0
56	MG	DA	3083	1/1	1.00	0.02	57,57,57,57	0
56	MG	DA	3023	1/1	1.00	0.06	57,57,57,57	0
56	MG	DA	3024	1/1	1.00	0.04	44,44,44,44	0
56	MG	DA	3086	1/1	1.00	0.03	82,82,82,82	0
56	MG	DA	3087	1/1	1.00	0.02	32,32,32,32	0
56	MG	DA	3025	1/1	1.00	0.01	57,57,57,57	0
56	MG	DA	3089	1/1	1.00	0.01	24,24,24,24	0
56	MG	DA	3090	1/1	1.00	0.01	26,26,26,26	0
56	MG	DA	3091	1/1	1.00	0.02	29,29,29,29	0
56	MG	DA	3092	1/1	1.00	0.02	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3093	1/1	1.00	0.03	23,23,23,23	0
56	MG	DA	3094	1/1	1.00	0.09	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.