



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 04:56 PM EDT

PDB ID : 5J7L
Title : Structure of the 70S E coli ribosome with the U1052G mutation in the 16S rRNA bound to tetracycline
Authors : Cocozaki, A.; Ferguson, A.
Deposited on : 2016-04-06
Resolution : 3.00 Å(reported)

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

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

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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

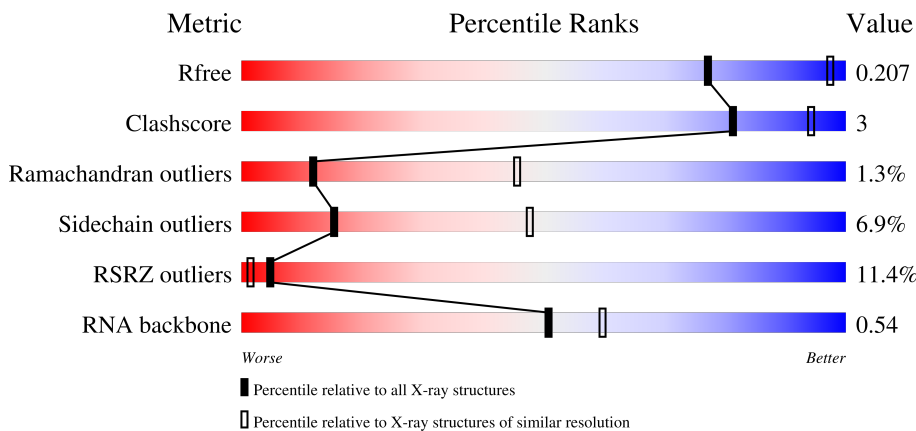
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



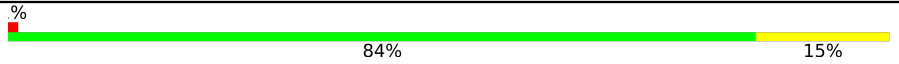
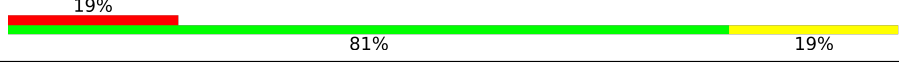
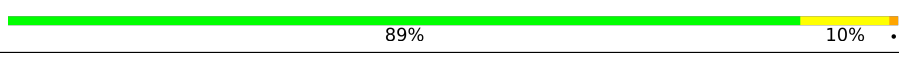


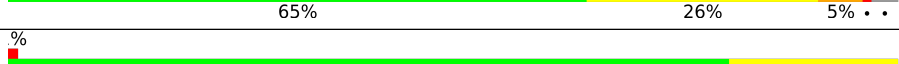
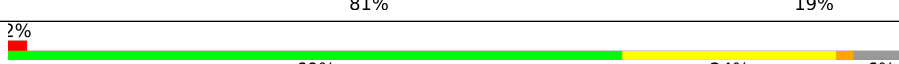
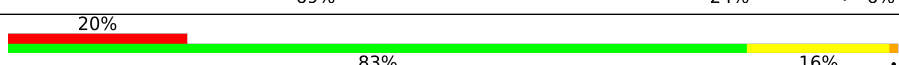



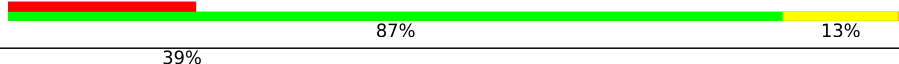
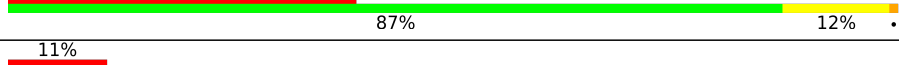

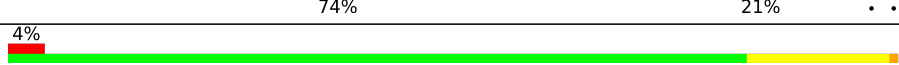




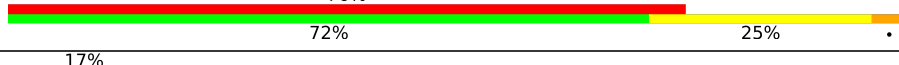

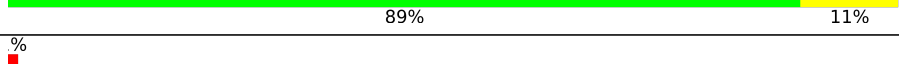
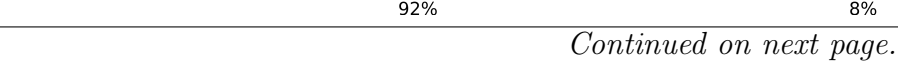


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	
1	BA	1534	
2	AB	224	
2	BB	224	

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Mol	Chain	Length	Quality of chain
3	AC	206	 % 84% 15%
3	BC	206	 19% 81% 19%
4	AD	205	 89% 10% .
4	BD	205	 86% 12% .
5	AE	155	 78% 19% .
5	BE	155	 % 65% 26% 5% . .
6	AF	106	 % 81% 19%
6	BF	106	 2% 69% 24% . 6%
7	AG	151	 20% 83% 16% .
7	BG	151	 51% 83% 17%
8	AH	129	 % 83% 16% .
8	BH	129	 3% 83% 17%
9	AI	127	 21% 87% 13% .
9	BI	127	 39% 87% 12% .
10	AJ	99	 11% 77% 21% .
10	BJ	99	 60% 74% 21% . .
11	AK	117	 4% 83% 16% .
11	BK	117	 3% 76% 23% .
12	AL	123	 % 88% 11% .
12	BL	123	 3% 83% 14% .
13	AM	114	 30% 80% 18% .
13	BM	114	 76% 72% 25% .
14	AN	100	 17% 87% 12% .
14	BN	100	 52% 89% 11%
15	AO	88	 % 92% 8%

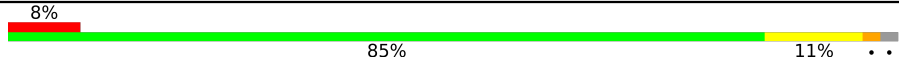















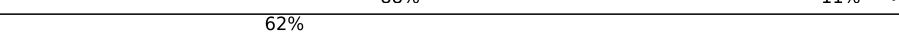

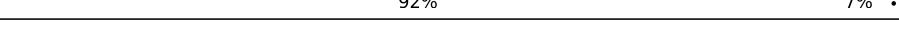
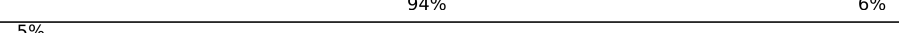





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Mol	Chain	Length	Quality of chain
15	BO	88	7% 91% 8%
16	AP	82	4% 90% 10%
16	BP	82	23% 82% 17%
17	AQ	80	2% 78% 21%
17	BQ	80	21% 61% 31% 6%
18	AR	55	2% 87% 13%
18	BR	55	5% 93% 7%
19	AS	79	14% 82% 16%
19	BS	79	76% 84% 14%
20	AT	86	90% 7%
20	BT	86	26% 79% 15% 5%
21	AU	56	4% 88% 12%
21	BU	56	2% 88% 12%
22	C1	56	21% 84% 12%
22	D1	56	84% 16%
23	C2	51	67% 69% 27%
23	D2	51	73% 25%
24	C3	46	28% 85% 15%
24	D3	46	89% 11%
25	C4	64	14% 84% 16%
25	D4	64	91% 9%
26	C5	38	24% 79% 18%
26	D5	38	87% 13%
27	C0	58	16% 76% 22%
27	D0	58	83% 16%

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Mol	Chain	Length	Quality of chain
28	CB	120	 8% 85% 11% . .
28	DB	120	 91% 8% .
29	CC	271	 6% 82% 16% .
29	DC	271	 90% 8% .
30	CD	209	 15% 88% 11%
30	DD	209	 90% 10%
31	CA	2904	 9% 73% 23% .
32	CE	201	 23% 83% 14% .
32	DE	201	 91% 8% .
33	CF	177	 63% 83% 15% .
33	DF	177	 % 81% 18% .
34	CG	176	 44% 89% 11%
34	DG	176	 % 90% 10%
35	CH	149	 26% 79% 20% .
35	DH	149	 18% 82% 18%
36	CJ	134	 90% 88% 11% .
36	DJ	134	 62% 88% 11% .
37	CK	142	 3% 92% 7% .
37	DK	142	 94% 6% .
38	CL	123	 5% 85% 11% . . .
38	DL	123	 87% 11% .
39	CM	144	 38% 79% 19% .
39	DM	144	 92% 8% .
40	CN	136	 4% 85% 15% .
40	DN	136	 84% 15% .

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Mol	Chain	Length	Quality of chain
41	CO	125	22% 82% 12% . .
41	DO	125	91% 6% .
42	CP	117	40% 87% 10% . .
42	DP	117	85% 12% .
43	CQ	114	21% 90% 8% .
43	DQ	114	90% 9% .
44	CR	117	16% 87% 13%
44	DR	117	% 89% 11%
45	CS	103	32% 80% 17% . .
45	DS	103	90% 10%
46	CT	110	13% 82% 16% .
46	DT	110	85% 15%
47	CU	93	32% 80% 16% .
47	DU	93	2% 87% 13%
48	CV	102	57% 80% 19% .
48	DV	102	2% 85% 14% .
49	CW	94	32% 86% 14%
49	DW	94	89% 11%
50	CX	76	30% 88% 11% .
50	DX	76	% 87% 9% .
51	CY	77	4% 82% 18%
51	DY	77	91% 9%
52	CZ	62	52% 82% 18%
52	DZ	62	2% 92% 8%
53	DI	135	22% 75% 22% .

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Mol	Chain	Length	Quality of chain
54	DA	2904	

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
55	MG	AA	1616	-	-	-	X
55	MG	AA	1621	-	-	-	X
55	MG	AA	1622	-	-	-	X
55	MG	AA	1624	-	-	-	X
55	MG	AA	1626	-	-	-	X
55	MG	BA	1637	-	-	-	X
55	MG	BA	1638	-	-	-	X
55	MG	BA	1639	-	-	-	X
55	MG	CA	3003	-	-	-	X
55	MG	CA	3005	-	-	-	X
55	MG	CA	3060	-	-	-	X
55	MG	CA	3075	-	-	-	X
55	MG	CA	3077	-	-	-	X
55	MG	CA	3113	-	-	-	X
55	MG	CA	3116	-	-	-	X
55	MG	CA	3122	-	-	-	X
55	MG	CA	3123	-	-	-	X
55	MG	CA	3131	-	-	-	X
55	MG	CA	3133	-	-	-	X
55	MG	CA	3134	-	-	-	X
55	MG	CA	3135	-	-	-	X
55	MG	CA	3154	-	-	-	X
55	MG	DA	3144	-	-	-	X
55	MG	DA	3170	-	-	-	X
57	MPD	AA	1676	-	-	-	X
57	MPD	DE	301	-	-	-	X
57	MPD	DN	201	-	-	-	X
58	PUT	AA	1672	-	-	-	X
58	PUT	AA	1674	-	-	-	X
58	PUT	AA	1675	-	-	-	X
58	PUT	DA	3195	-	-	-	X
59	TAC	BA	1644	-	-	-	X
61	PEG	D1	103	-	-	-	X
61	PEG	D3	101	-	-	-	X
61	PEG	DP	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	PEG	DQ	201	-	-	-	X
63	PGE	D1	102	-	-	-	X
63	PGE	DA	3001	-	-	-	X
66	ACY	DA	3196	-	X	-	-

2 Entry composition [i](#)

There are 69 unique types of molecules in this entry. The entry contains 295261 atoms, of which 2 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
			Total	C	N	O	P			
1	AA	1534	Total	C	N	O	P	0	0	0
			32933	14695	6044	10660	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32911	14685	6039	10654	1533			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1052	G	U	engineered mutation	GB 595593103
BA	1052	G	U	engineered mutation	GB 595593103

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	AE	155	1144	711	216	211	6	0	0	0
5	BE	150	1105	687	211	201	6	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	AF	106	862	545	156	154	7	0	0	0
6	BF	100	817	515	148	148	6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	AG	151	1182	735	227	216	4	0	0	0
7	BG	151	1182	735	227	216	4	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	AJ	99	Total 796	C 498	N 152	O 145	S 1	0	0	0
10	BJ	98	Total 787	C 493	N 150	O 143	S 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	AL	123	Total 957	C 591	N 196	O 165	S 5	0	0	0
12	BL	123	Total 957	C 591	N 196	O 165	S 5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	AM	114	Total 884	C 546	N 178	O 157	S 3	0	0	0
13	BM	114	Total 884	C 546	N 178	O 157	S 3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	AN	100	Total 805	C 499	N 164	O 139	S 3	0	0	0
14	BN	100	Total 805	C 499	N 164	O 139	S 3	0	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	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
			2083	1288	423	365	7			
29	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	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			
30	DD	209	Total	C	N	O	S	0	1	0
			1576	986	290	296	4			

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

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

- Molecule 32 is a protein called 50S ribosomal protein L4.

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

- Molecule 33 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	CF	177	1411	899	249	257	6	0	0	0
33	DF	177	1411	899	249	257	6	0	0	0

- Molecule 34 is a protein called 50S ribosomal protein L6.

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

- Molecule 35 is a protein called 50S ribosomal protein L9.

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

- Molecule 36 is a protein called 50S ribosomal protein L11.

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

- Molecule 37 is a protein called 50S ribosomal protein L13.

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

- Molecule 38 is a protein called 50S ribosomal protein L14.

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

- Molecule 39 is a protein called 50S ribosomal protein L15.

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

- Molecule 40 is a protein called 50S ribosomal protein L16.

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

- Molecule 41 is a protein called 50S ribosomal protein L17.

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

- Molecule 42 is a protein called 50S ribosomal protein L18.

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

- Molecule 43 is a protein called 50S ribosomal protein L19.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L21.

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

- Molecule 46 is a protein called 50S ribosomal protein L22.

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

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
47	CU	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	DU	93	739	466	139	132	2	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
48	CV	102	780	492	146	142	0	0	0
48	DV	102	780	492	146	142	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L25.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

- Molecule 52 is a protein called 50S ribosomal protein L29.

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

- Molecule 53 is a protein called 50S ribosomal protein L10.

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

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

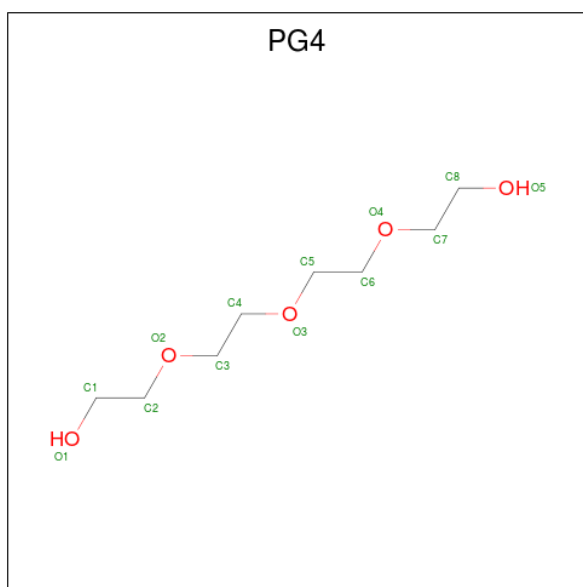
- Molecule 54 is a RNA chain called 23S rRNA.

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

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

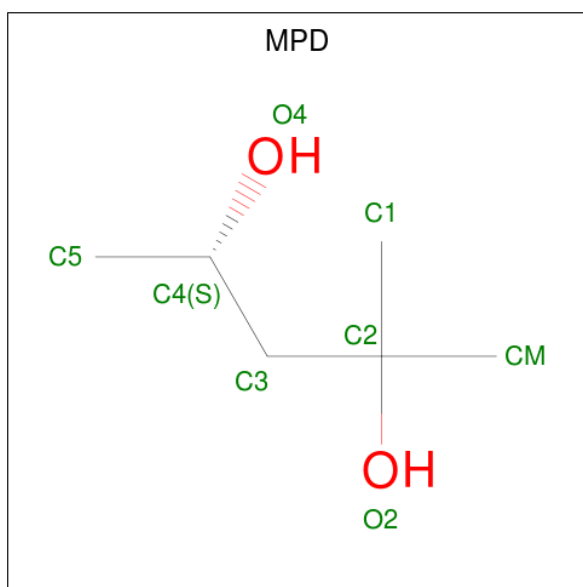
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	72	Total 72	Mg 72	0	0
55	BA	45	Total 45	Mg 45	0	0
55	CB	3	Total 3	Mg 3	0	0
55	CA	156	Total 156	Mg 156	0	0
55	DD	1	Total 1	Mg 1	0	0
55	DM	1	Total 1	Mg 1	0	0
55	DR	2	Total 2	Mg 2	0	0
55	DB	9	Total 9	Mg 9	0	0
55	DA	183	Total 183	Mg 183	0	0

- Molecule 56 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



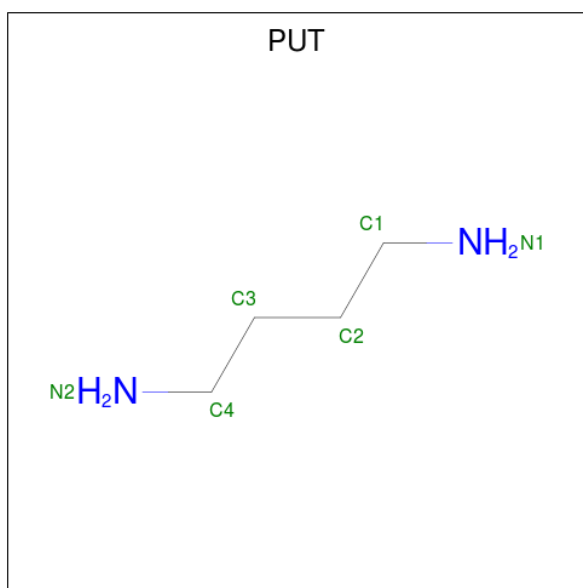
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AA	1	Total C O 13 8 5	0	0
56	BA	1	Total C O 13 8 5	0	0
56	DQ	1	Total C O 13 8 5	0	0
56	DR	1	Total C O 13 8 5	0	0
56	DS	1	Total C O 13 8 5	0	0
56	DA	1	Total C O 13 8 5	0	0
56	DA	1	Total C O 13 8 5	0	0

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 58 is 1,4-DIAMINOBTUTANE (three-letter code: PUT) (formula: C₄H₁₂N₂).



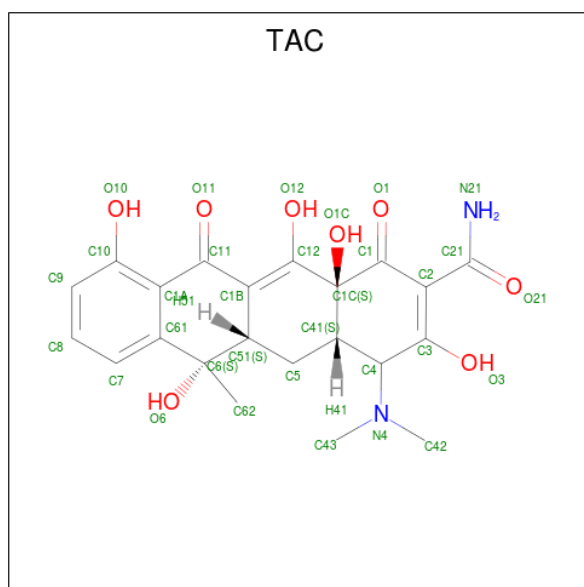
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AA	1	Total C N 6 4 2	0	0
58	AA	1	Total C N 6 4 2	0	0
58	AA	1	Total C N 6 4 2	0	0
58	AA	1	Total C N 6 4 2	0	0
58	DM	1	Total C N 6 4 2	0	0
58	DA	1	Total C N 6 4 2	0	0
58	DA	1	Total C N 6 4 2	0	0
58	DA	1	Total C N 6 4 2	0	0
58	DA	1	Total C N 6 4 2	0	0
58	DA	1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

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

- Molecule 59 is TETRACYCLINE (three-letter code: TAC) (formula: $C_{22}H_{24}N_2O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
59	AA	1	Total	C	N	O	0	0	
			32	22	2	8			
59	AA	1	Total	C	H	N	O	0	0
			33	22	1	2	8		
59	BA	1	Total	C	N	O	0	0	
			32	22	2	8			
59	BA	1	Total	C	H	N	O	0	0
			33	22	1	2	8		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

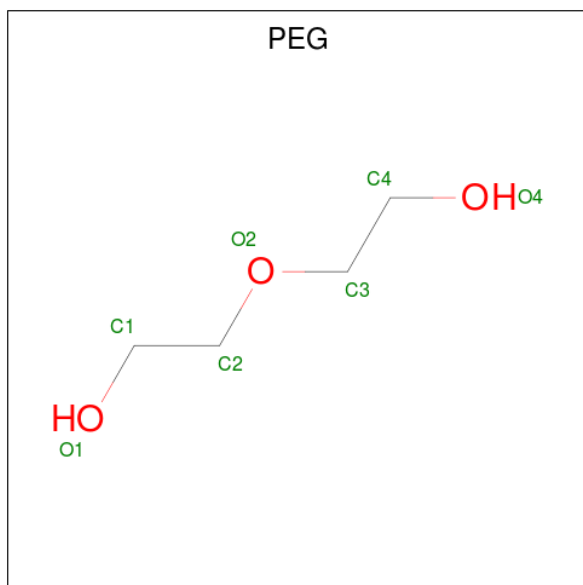
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AB	1	Total	Zn	0	0
			1	1		
60	C5	1	Total	Zn	0	0
			1	1		

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

- Molecule 61 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



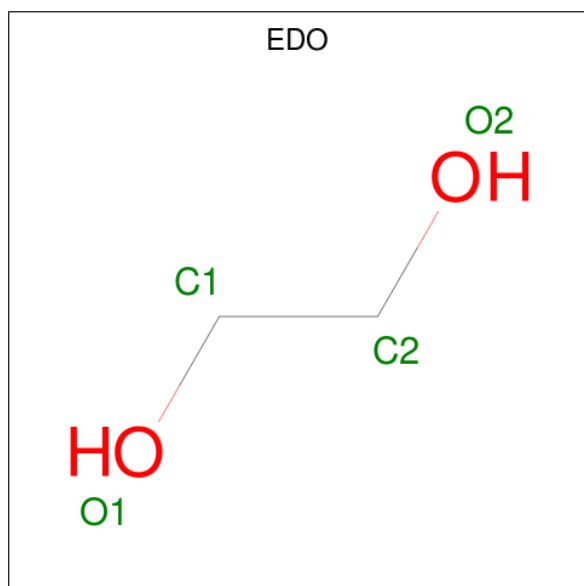
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	D1	1	Total	C	O	0	0
			7	4	3		
61	D3	1	Total	C	O	0	0
			7	4	3		
61	DL	1	Total	C	O	0	0
			7	4	3		
61	DP	1	Total	C	O	0	0
			7	4	3		
61	DQ	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 62 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



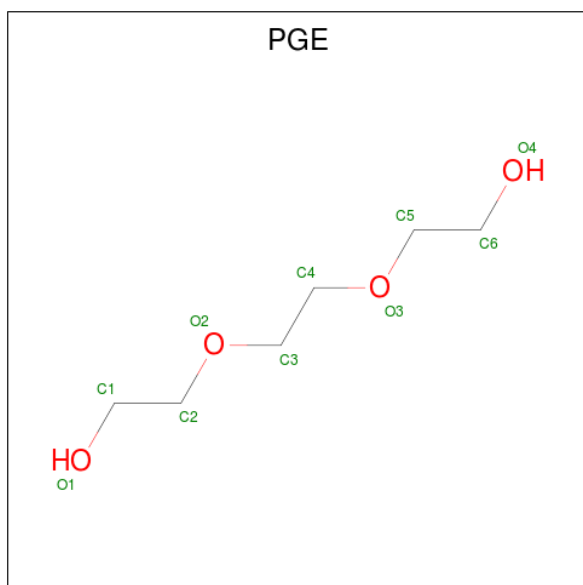
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	D1	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4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

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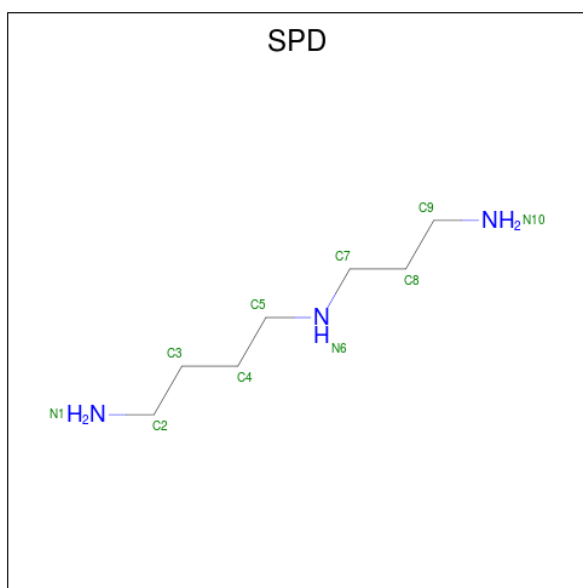
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	DA	1	Total C O 4 2 2	0	0
62	DA	1	Total C O 4 2 2	0	0

- Molecule 63 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



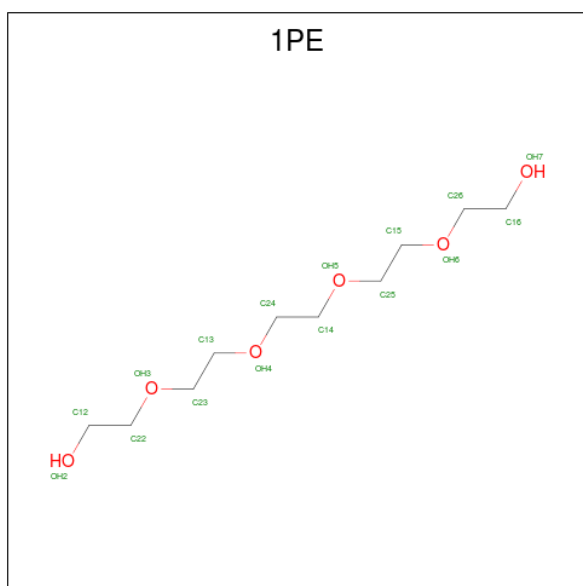
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	D1	1	Total C O 10 6 4	0	0
63	DS	1	Total C O 10 6 4	0	0
63	DU	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0
63	DA	1	Total C O 10 6 4	0	0

- Molecule 64 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



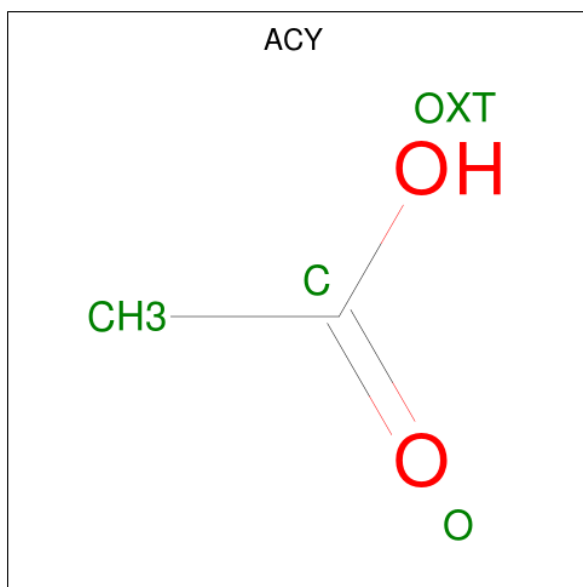
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0
64	DA	1	Total C N 10 7 3	0	0

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



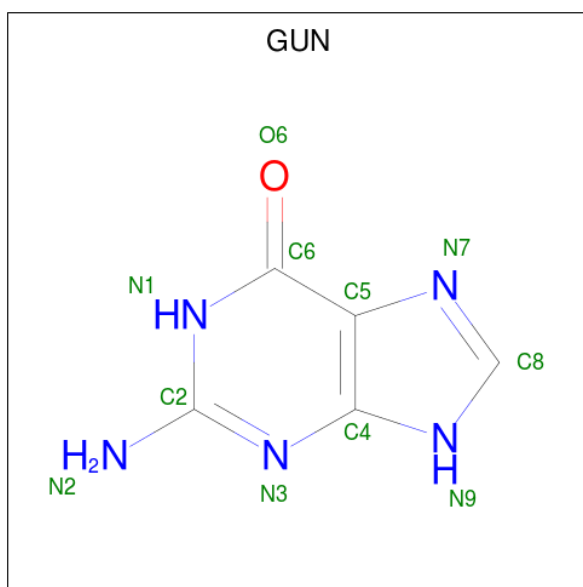
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
65	DA	1	Total	C	O	0	0
			16	10	6		
65	DA	1	Total	C	O	0	0
			16	10	6		

- Molecule 66 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



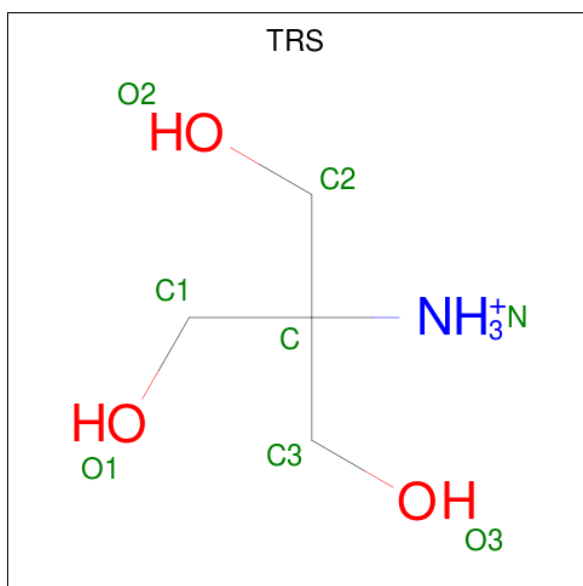
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 67 is GUANINE (three-letter code: GUN) (formula: C₅H₅N₅O).



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

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



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

- Molecule 69 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AA	501	Total 501	O 501	0	0
69	AC	4	Total 4	O 4	0	0
69	AD	2	Total 2	O 2	0	0
69	AE	5	Total 5	O 5	0	0
69	AG	1	Total 1	O 1	0	0
69	AH	1	Total 1	O 1	0	0
69	AJ	2	Total 2	O 2	0	0
69	AK	6	Total 6	O 6	0	0
69	AL	10	Total 10	O 10	0	0
69	AM	5	Total 5	O 5	0	0
69	AN	6	Total 6	O 6	0	0
69	AO	2	Total 2	O 2	0	0
69	AP	2	Total 2	O 2	0	0
69	AR	1	Total 1	O 1	0	0
69	AT	3	Total 3	O 3	0	0
69	AU	3	Total 3	O 3	0	0
69	C3	4	Total 4	O 4	0	0
69	C4	1	Total 1	O 1	0	0
69	BA	287	Total 287	O 287	0	0
69	BD	13	Total 13	O 13	0	0
69	BE	1	Total 1	O 1	0	0
69	BF	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	BK	2	Total O 2 2	0	0
69	BL	4	Total O 4 4	0	0
69	BN	2	Total O 2 2	0	0
69	BO	1	Total O 1 1	0	0
69	BP	3	Total O 3 3	0	0
69	BT	2	Total O 2 2	0	0
69	BU	2	Total O 2 2	0	0
69	D1	43	Total O 43 43	0	0
69	D2	6	Total O 6 6	0	0
69	D3	22	Total O 22 22	0	0
69	D4	39	Total O 39 39	0	0
69	D5	8	Total O 8 8	0	0
69	D0	24	Total O 24 24	0	0
69	CB	13	Total O 13 13	0	0
69	CC	10	Total O 10 10	0	0
69	CD	6	Total O 6 6	0	0
69	CA	691	Total O 691 691	0	0
69	DC	100	Total O 100 100	0	0
69	DD	98	Total O 98 98	0	0
69	CE	5	Total O 5 5	0	0
69	CL	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	CM	4	Total 4	O 4	0	0
69	CO	2	Total 2	O 2	0	0
69	CU	3	Total 3	O 3	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	61	Total 61	O 61	0	0
69	DF	15	Total 15	O 15	0	0
69	DG	6	Total 6	O 6	0	0
69	DH	2	Total 2	O 2	0	0
69	DK	65	Total 65	O 65	0	0
69	DL	52	Total 52	O 52	0	0
69	DM	63	Total 63	O 63	0	0
69	DN	72	Total 72	O 72	0	0
69	DO	44	Total 44	O 44	0	0
69	DP	38	Total 38	O 38	0	0
69	DQ	33	Total 33	O 33	0	0
69	DR	62	Total 62	O 62	0	0
69	DS	46	Total 46	O 46	0	0
69	DT	69	Total 69	O 69	0	0
69	DU	18	Total 18	O 18	0	0

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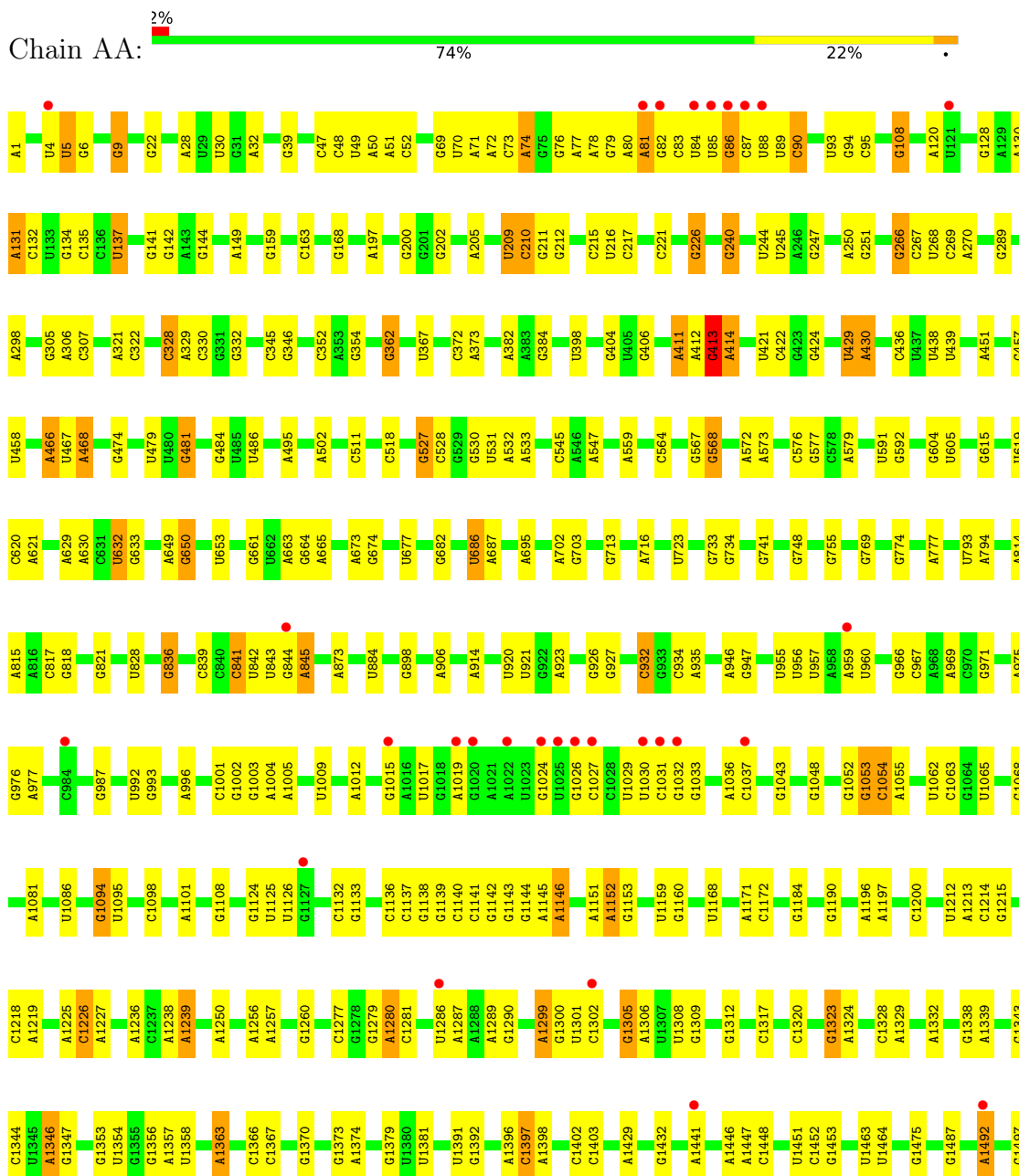
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	DV	20	Total O 20 20	0	0
69	DW	31	Total O 31 31	0	0
69	DX	25	Total O 25 25	0	0
69	DY	9	Total O 9 9	0	0
69	DZ	8	Total O 8 8	0	0
69	DB	209	Total O 209 209	0	0
69	DA	4840	Total O 4840 4840	0	0

3 Residue-property plots [i](#)

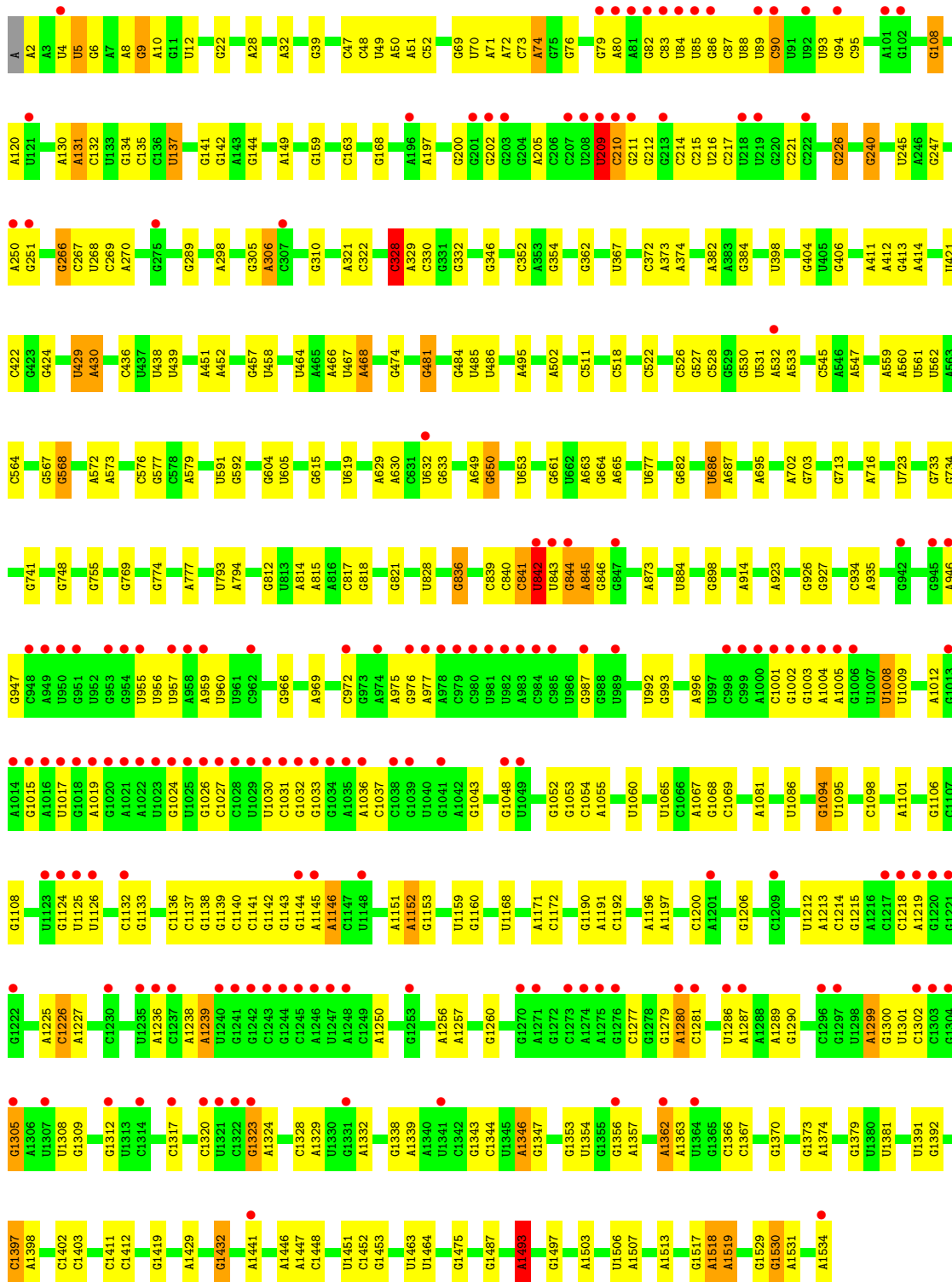
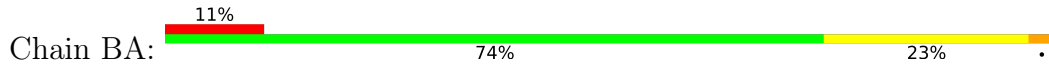
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 16S rRNA

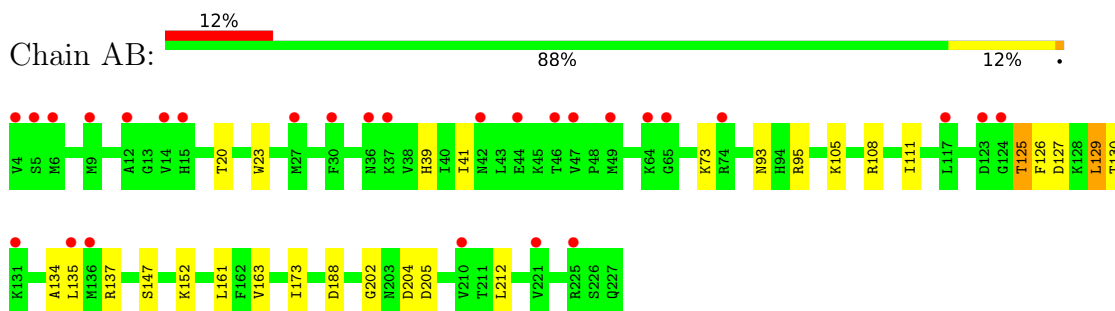




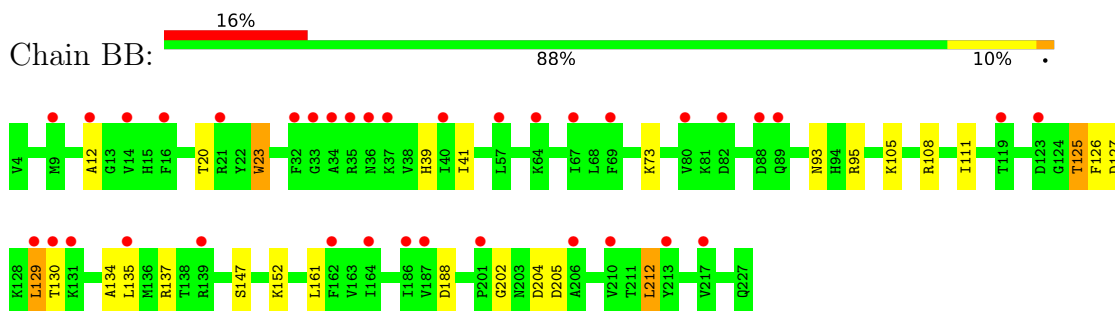
• Molecule 1: 16S rRNA



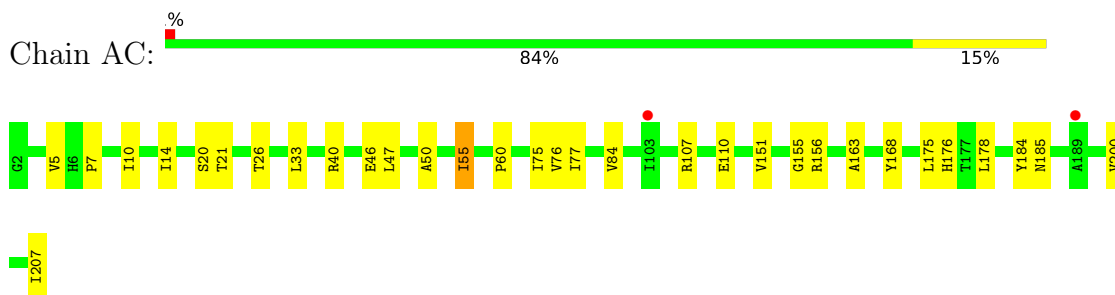
- Molecule 2: 30S ribosomal protein S2



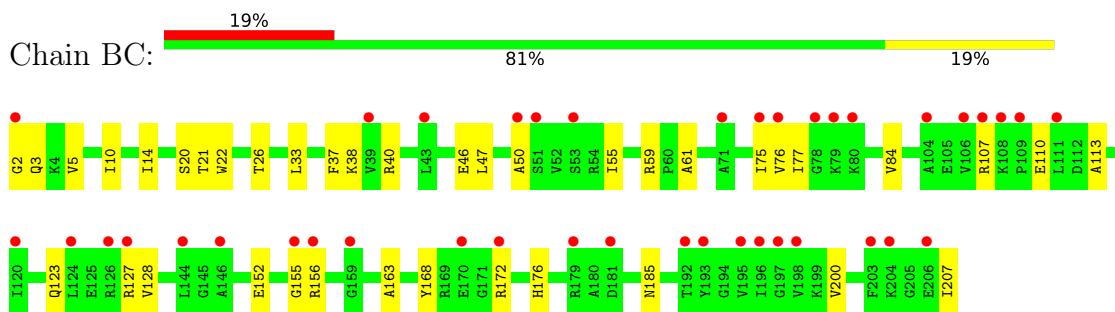
- Molecule 2: 30S ribosomal protein S2



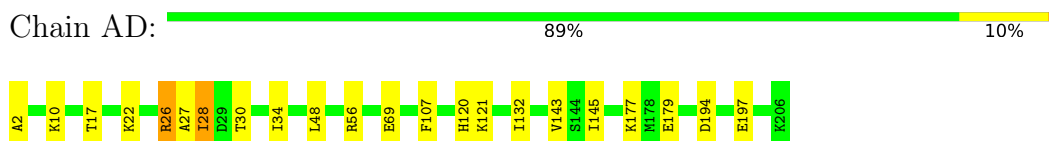
- Molecule 3: 30S ribosomal protein S3




- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4




- Molecule 4: 30S ribosomal protein S4

Chain BD:  86% 12%



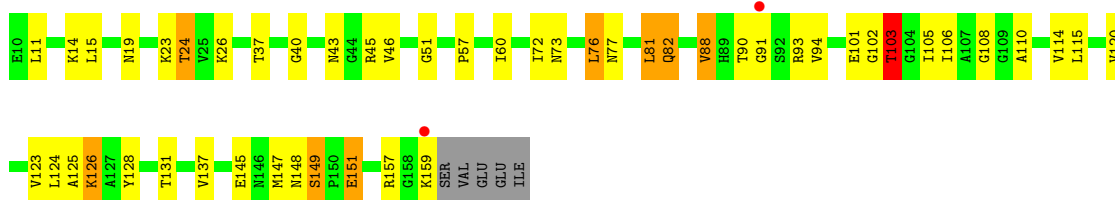
- Molecule 5: 30S ribosomal protein S5

Chain AE:  78% 19%




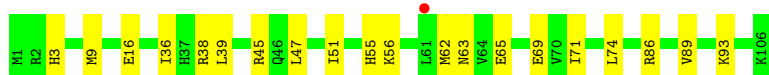
- Molecule 5: 30S ribosomal protein S5

Chain BE:  65% 26% 5%



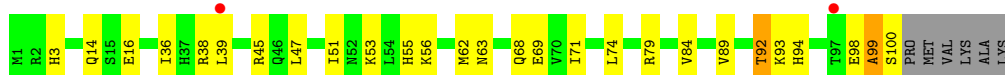
- Molecule 6: 30S ribosomal protein S6

Chain AF:  81% 19%




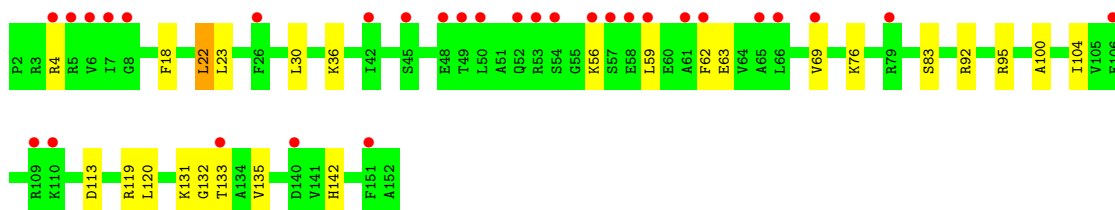
- Molecule 6: 30S ribosomal protein S6

Chain BF:  69% 24% 6%

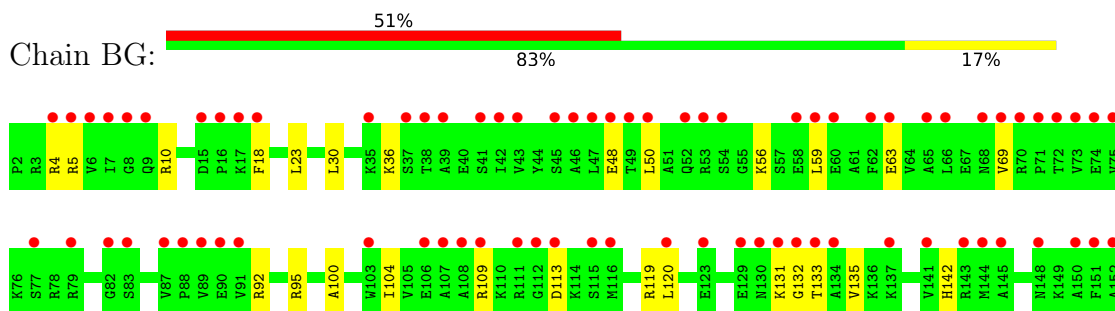


- Molecule 7: 30S ribosomal protein S7

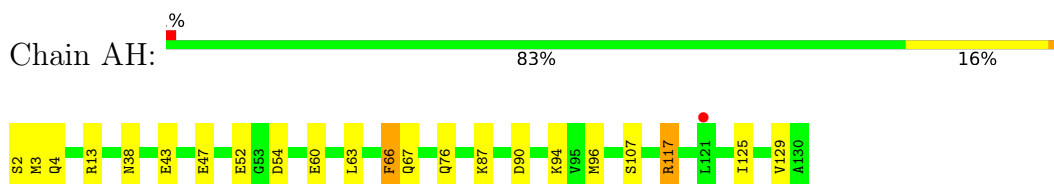
Chain AG:  20% 83% 16%



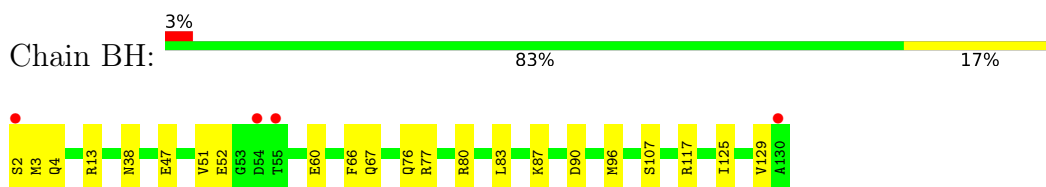
- Molecule 7: 30S ribosomal protein S7



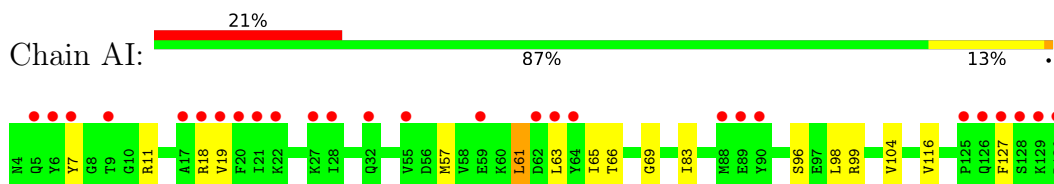
- Molecule 8: 30S ribosomal protein S8



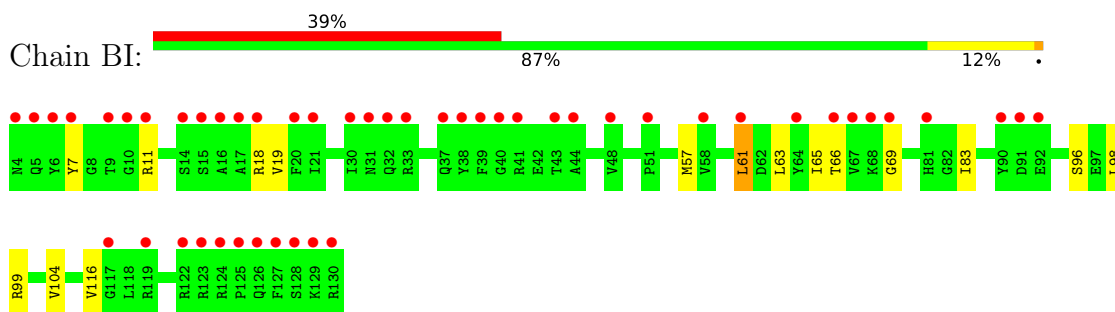
- Molecule 8: 30S ribosomal protein S8



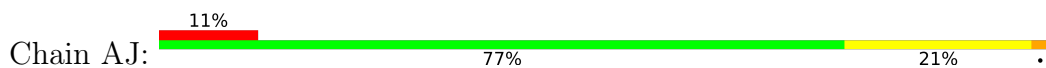
- Molecule 9: 30S ribosomal protein S9

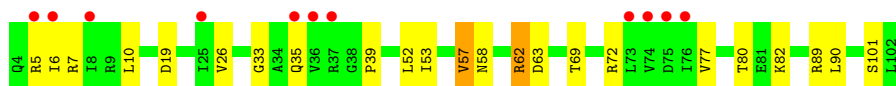


- Molecule 9: 30S ribosomal protein S9

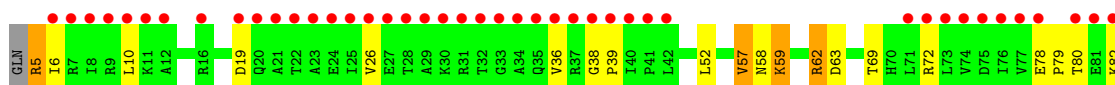
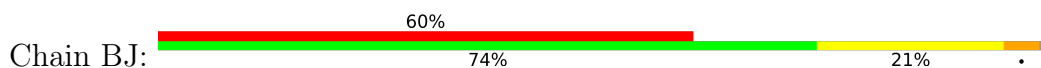


- Molecule 10: 30S ribosomal protein S10

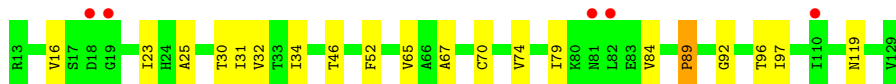
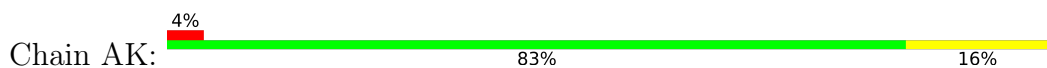




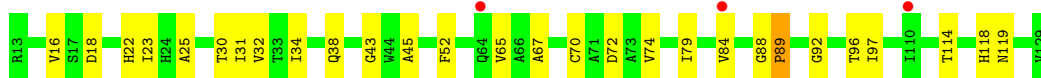
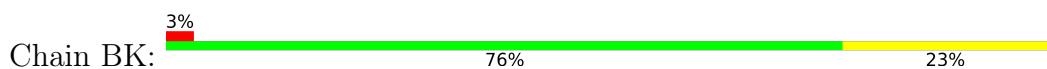
- Molecule 10: 30S ribosomal protein S10



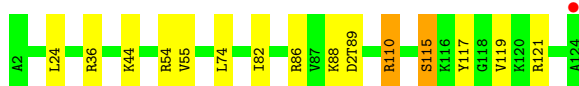
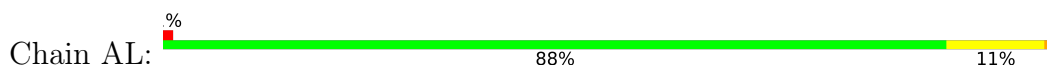
- Molecule 11: 30S ribosomal protein S11



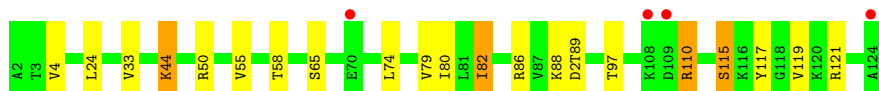
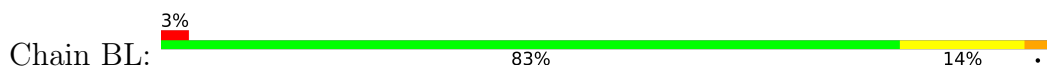
- Molecule 11: 30S ribosomal protein S11



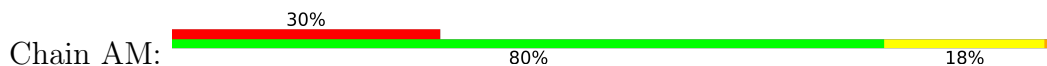
- Molecule 12: 30S ribosomal protein S12

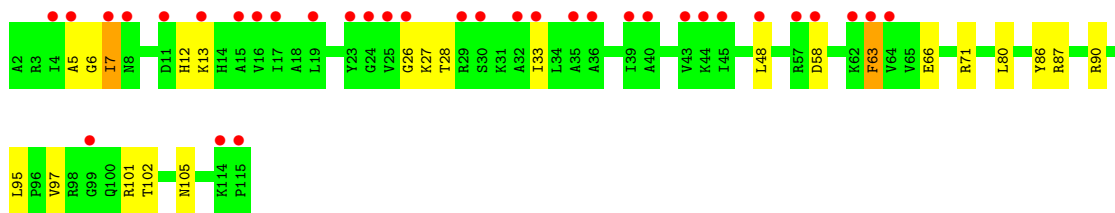


- Molecule 12: 30S ribosomal protein S12

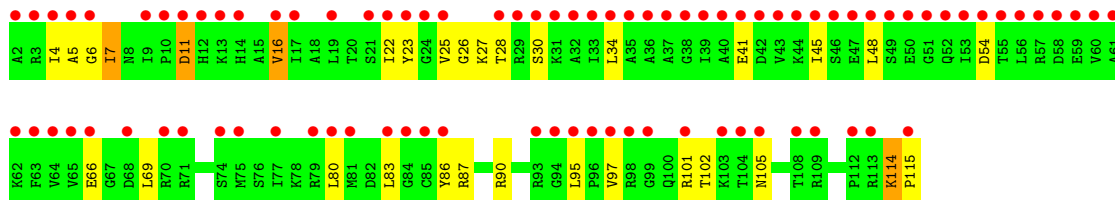
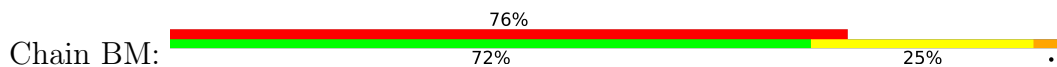


- Molecule 13: 30S ribosomal protein S13

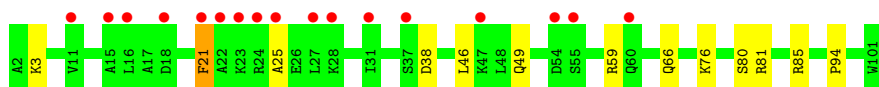
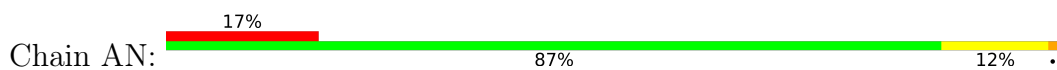




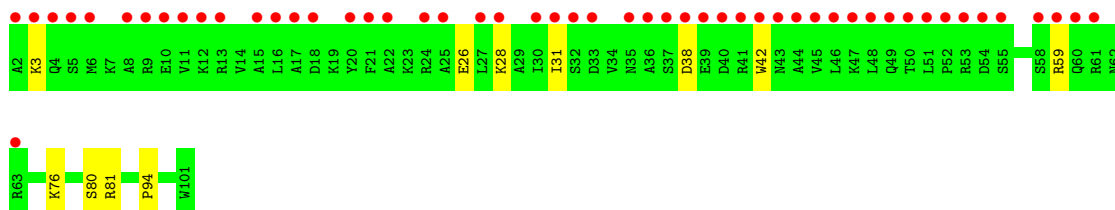
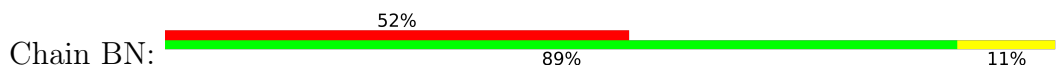
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14



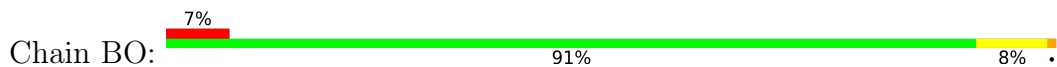
- Molecule 14: 30S ribosomal protein S14



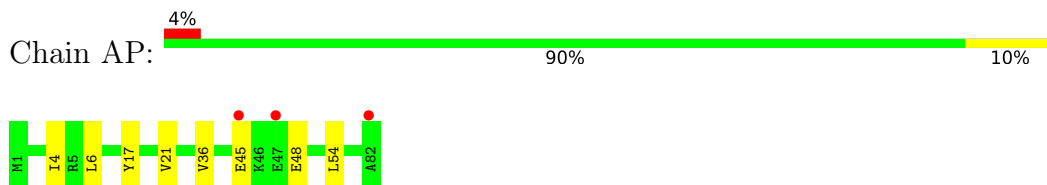
- Molecule 15: 30S ribosomal protein S15



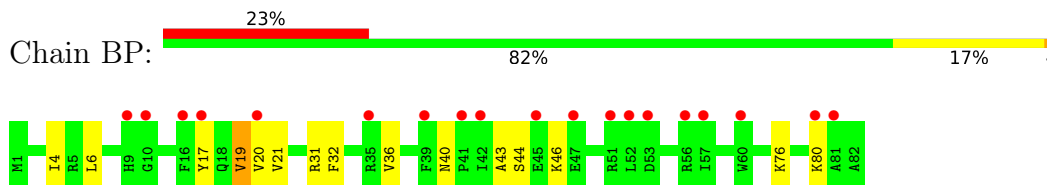
- Molecule 15: 30S ribosomal protein S15



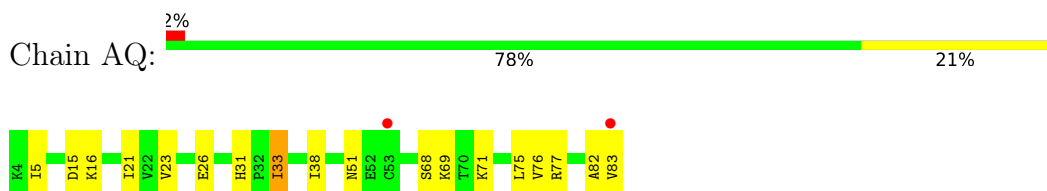
- Molecule 16: 30S ribosomal protein S16



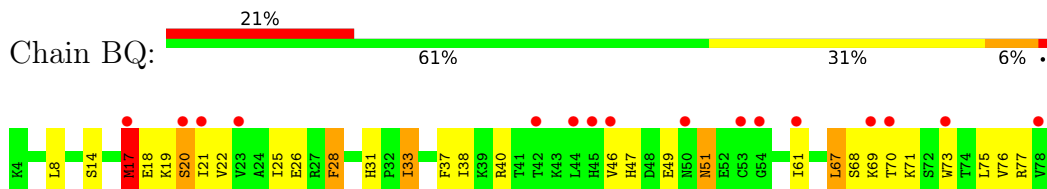
- Molecule 16: 30S ribosomal protein S16



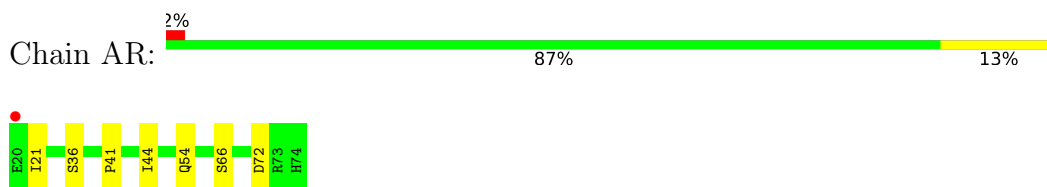
- Molecule 17: 30S ribosomal protein S17



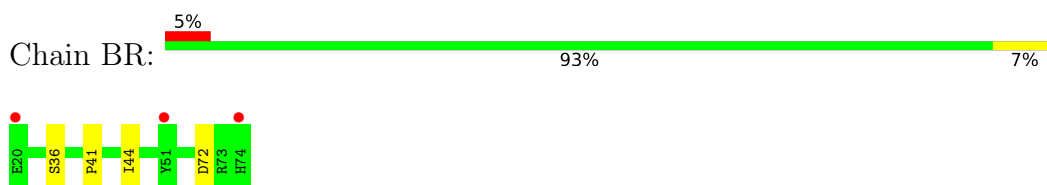
- Molecule 17: 30S ribosomal protein S17



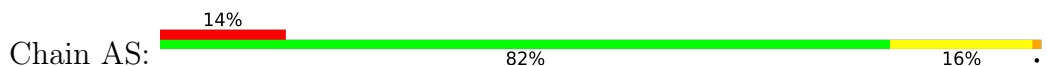
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

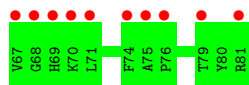
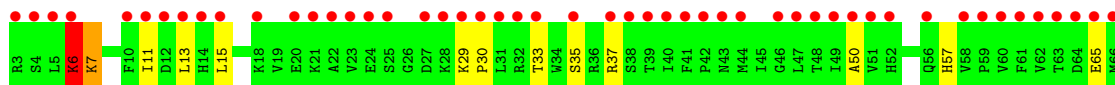
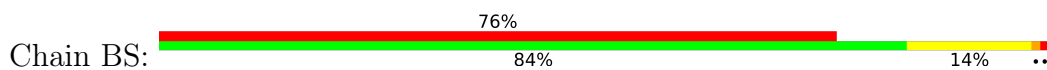


- Molecule 19: 30S ribosomal protein S19





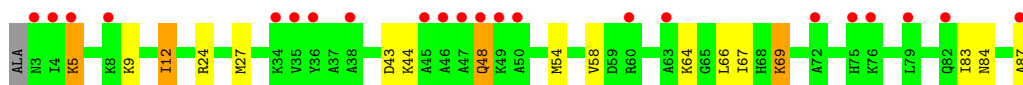
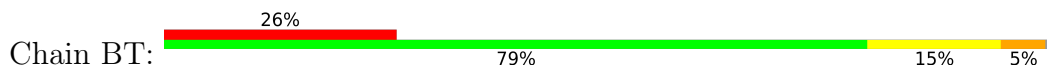
- Molecule 19: 30S ribosomal protein S19



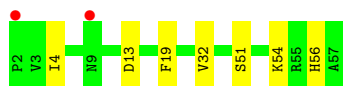
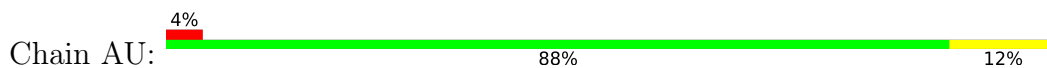
- Molecule 20: 30S ribosomal protein S20



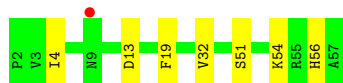
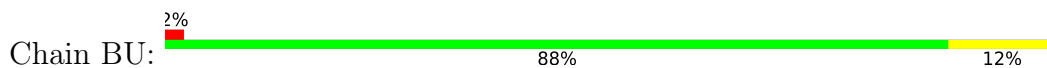
- Molecule 20: 30S ribosomal protein S20



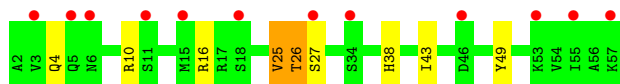
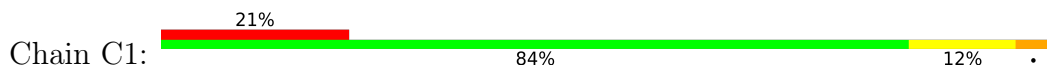
- Molecule 21: 30S ribosomal protein S21




- Molecule 21: 30S ribosomal protein S21

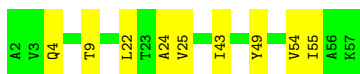


- Molecule 22: 50S ribosomal protein L32



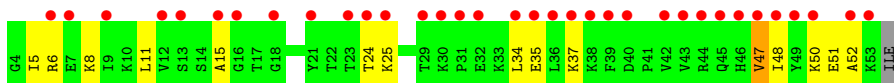
- Molecule 22: 50S ribosomal protein L32

Chain D1:  84% 16%




- Molecule 23: 50S ribosomal protein L33

Chain C2:  67% 69% 27%




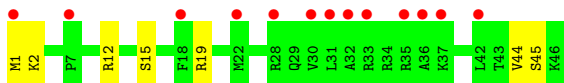
- Molecule 23: 50S ribosomal protein L33

Chain D2:  73% 25%



- Molecule 24: 50S ribosomal protein L34

Chain C3:  28% 85% 15%




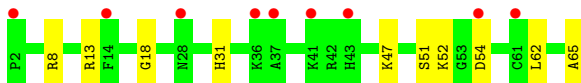
- Molecule 24: 50S ribosomal protein L34

Chain D3:  89% 11%



- Molecule 25: 50S ribosomal protein L35

Chain C4:  14% 84% 16%

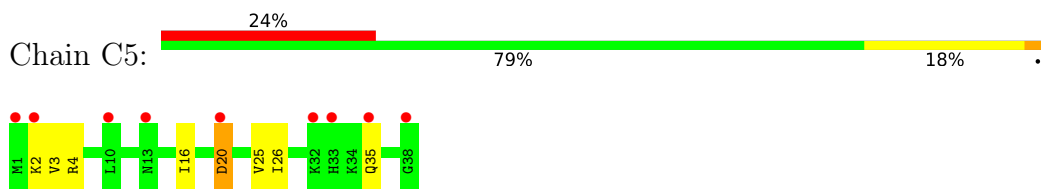


- Molecule 25: 50S ribosomal protein L35

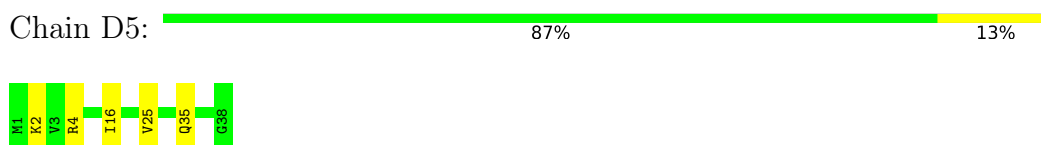
Chain D4:  91% 9%



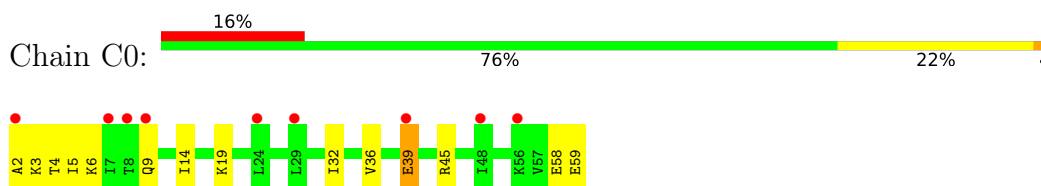
- Molecule 26: 50S ribosomal protein L36



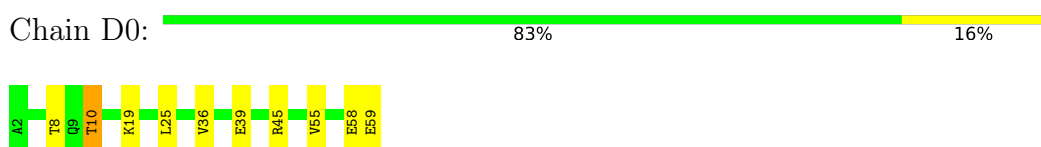
- Molecule 26: 50S ribosomal protein L36



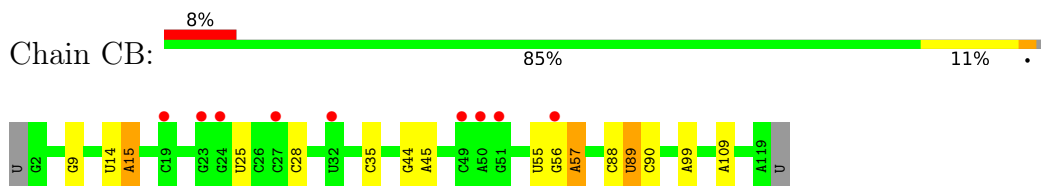
- Molecule 27: 50S ribosomal protein L30



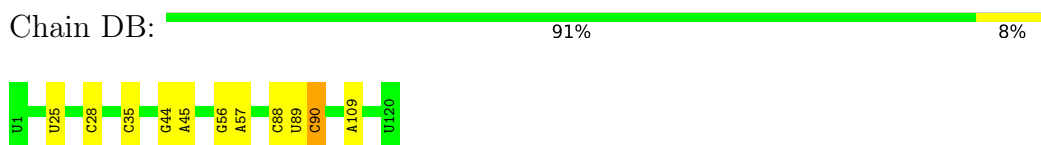
- Molecule 27: 50S ribosomal protein L30



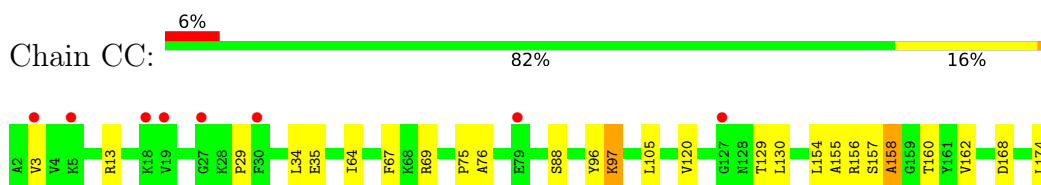
- Molecule 28: 5S rRNA



- Molecule 28: 5S rRNA



- Molecule 29: 50S ribosomal protein L2

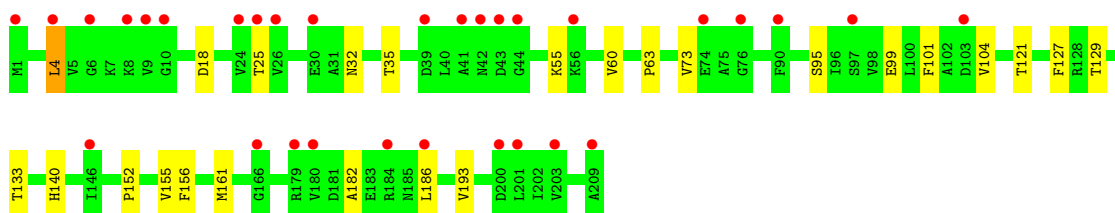
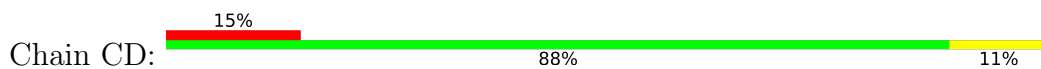




- Molecule 29: 50S ribosomal protein L2



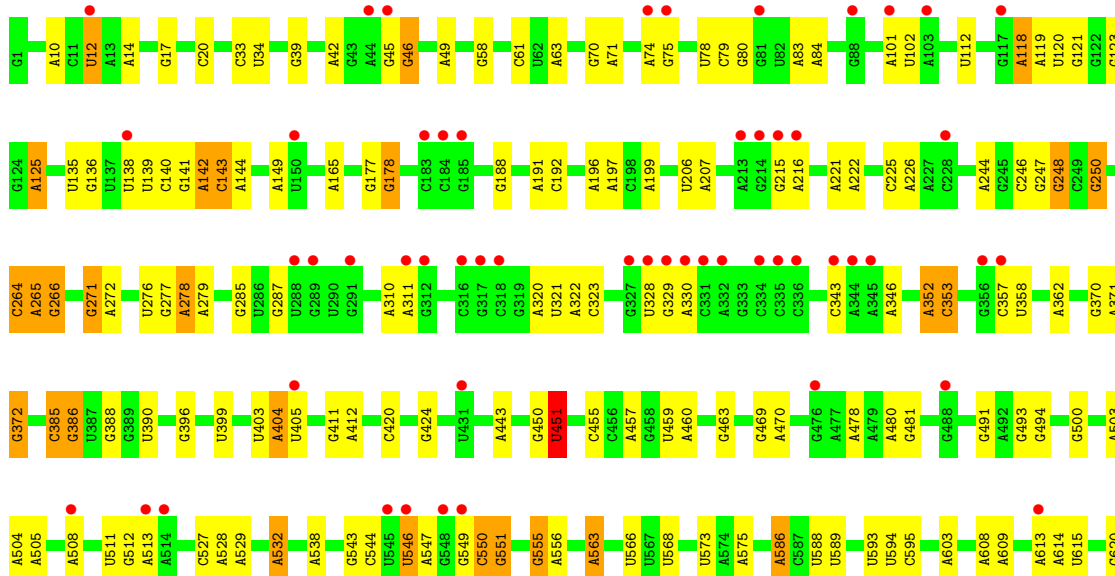
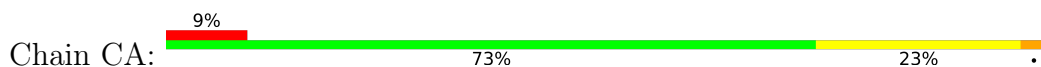
- Molecule 30: 50S ribosomal protein L3

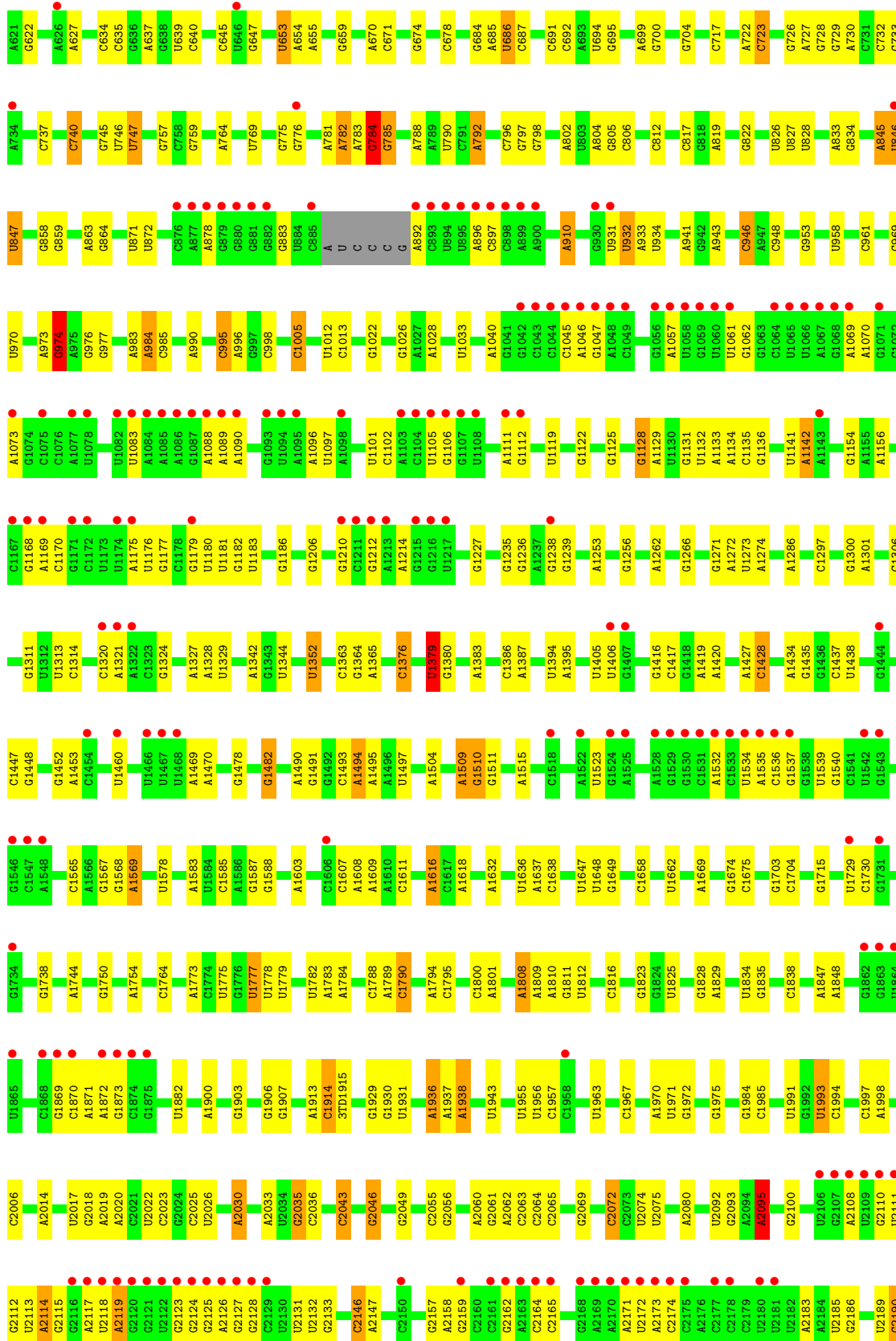


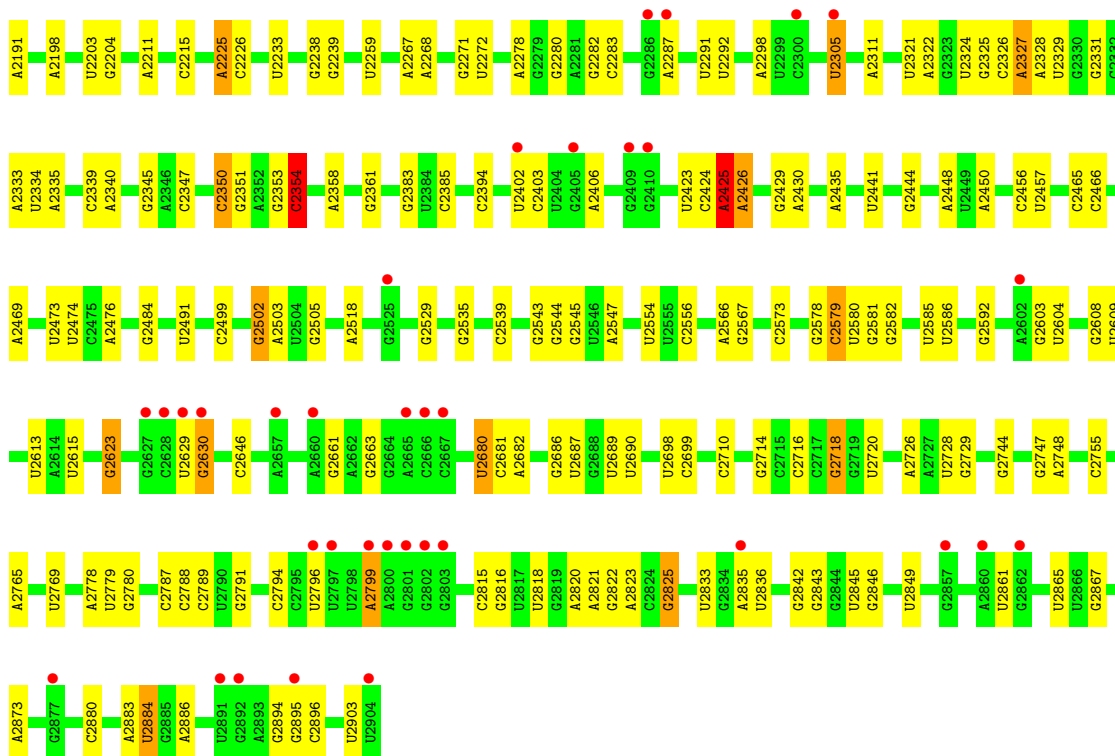
- Molecule 30: 50S ribosomal protein L3



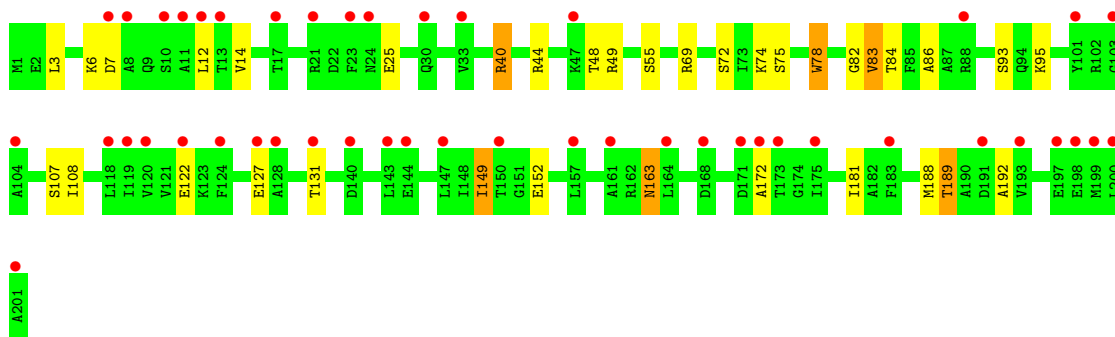
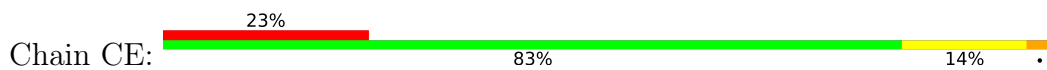
- Molecule 31: 23S rRNA



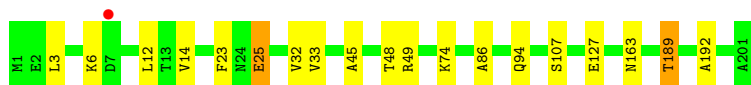




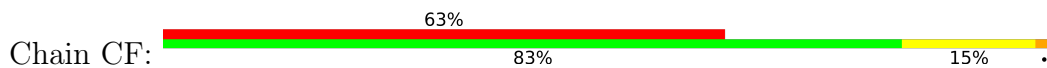
• Molecule 32: 50S ribosomal protein L4

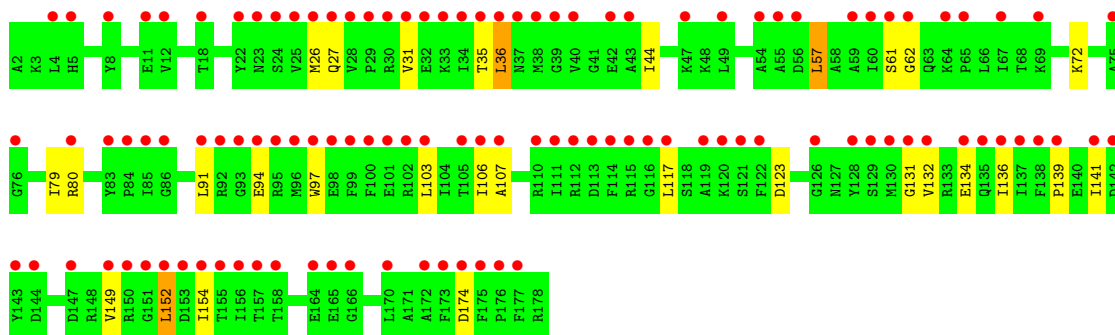


• Molecule 32: 50S ribosomal protein L4

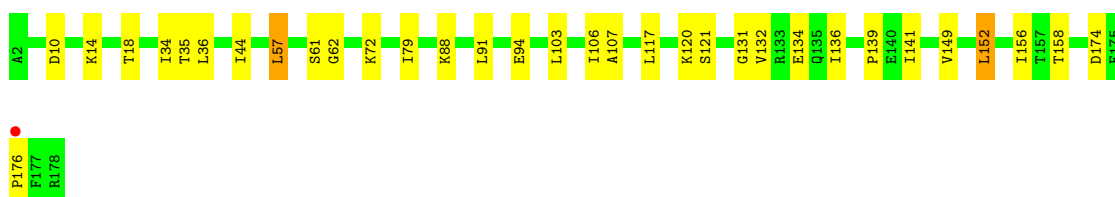
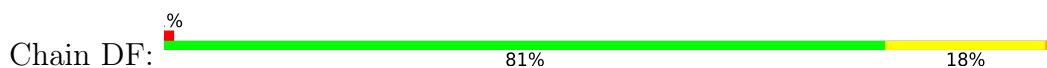


• Molecule 33: 50S ribosomal protein L5

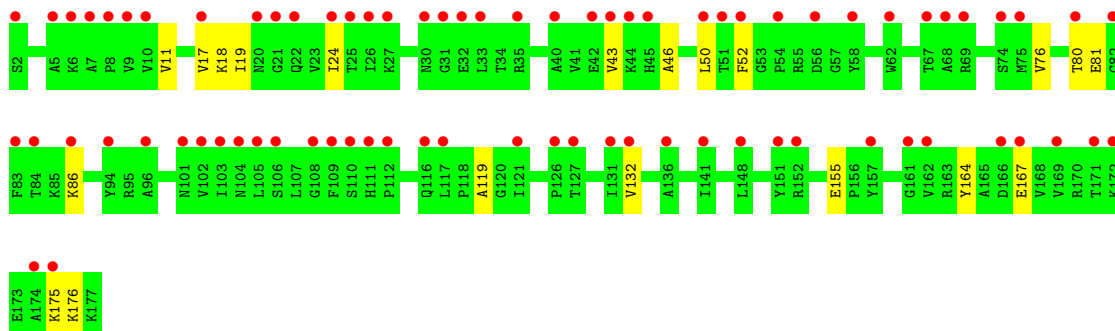
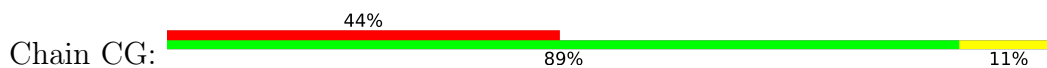




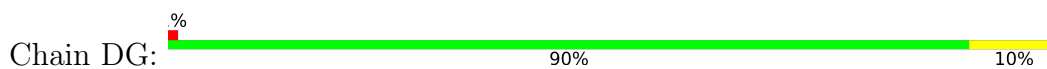
- Molecule 33: 50S ribosomal protein L5



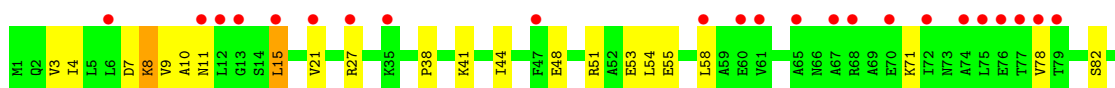
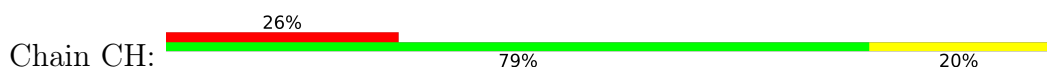
- Molecule 34: 50S ribosomal protein L6

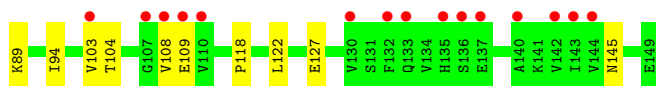


- Molecule 34: 50S ribosomal protein L6

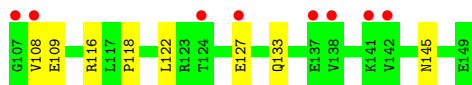
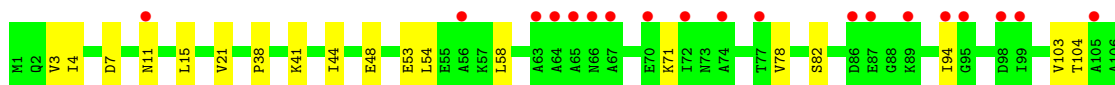
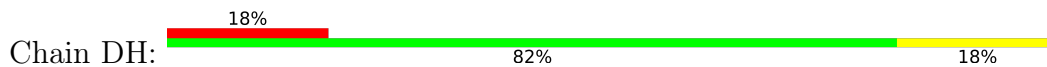


- Molecule 35: 50S ribosomal protein L9

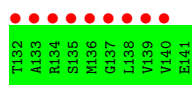
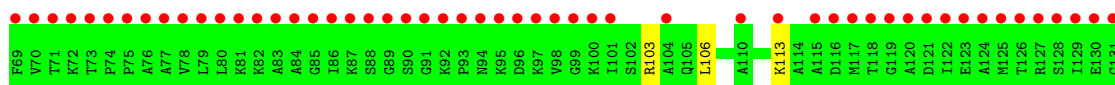
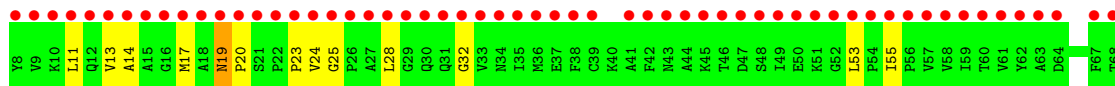
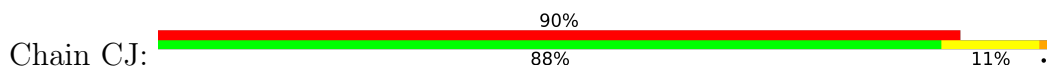




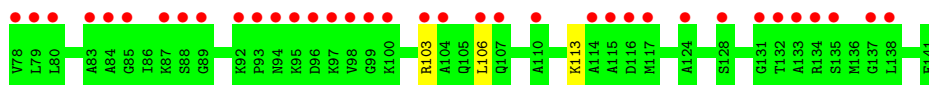
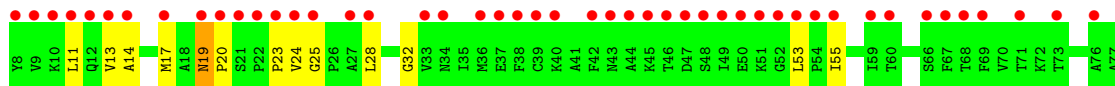
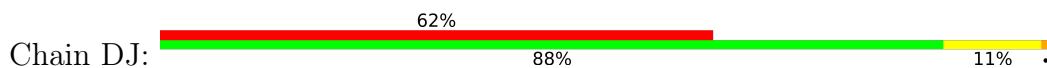
- Molecule 35: 50S ribosomal protein L9



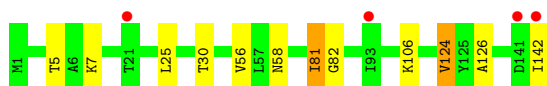
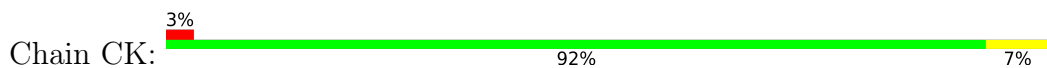
- Molecule 36: 50S ribosomal protein L11



- Molecule 36: 50S ribosomal protein L11



- Molecule 37: 50S ribosomal protein L13

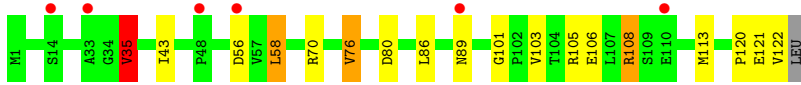
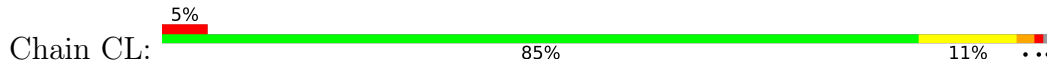


- Molecule 37: 50S ribosomal protein L13

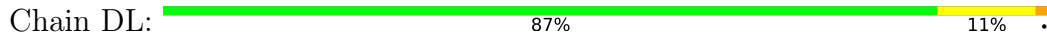




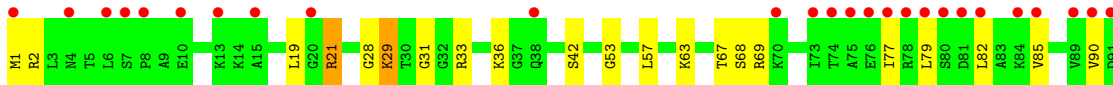
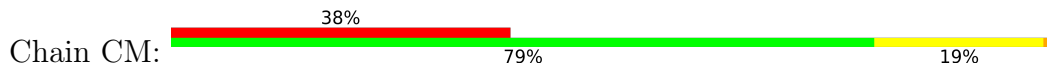
- Molecule 38: 50S ribosomal protein L14



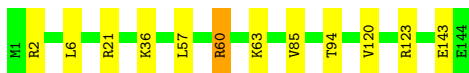
- Molecule 38: 50S ribosomal protein L14



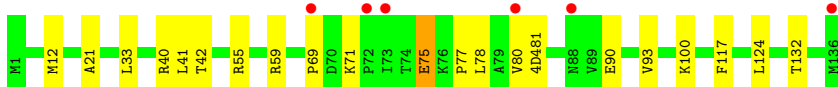
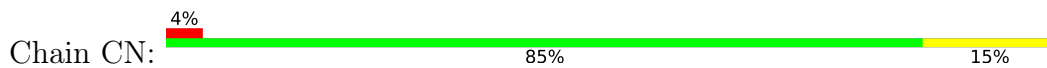
- Molecule 39: 50S ribosomal protein L15



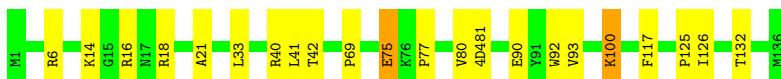
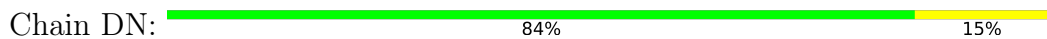
- Molecule 39: 50S ribosomal protein L15



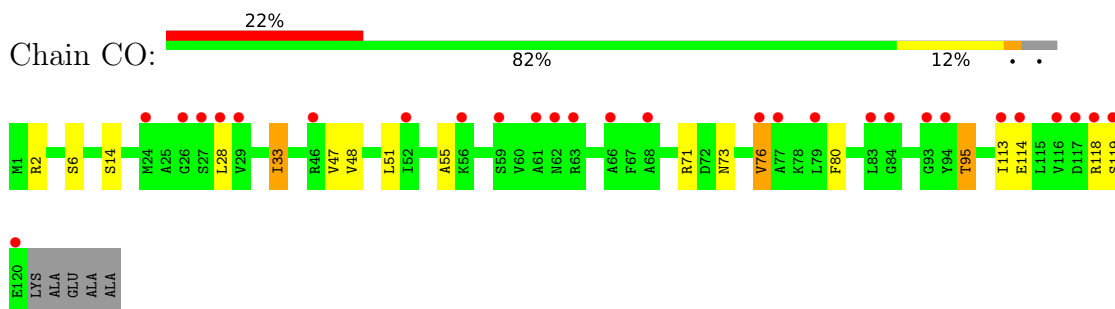
- Molecule 40: 50S ribosomal protein L16



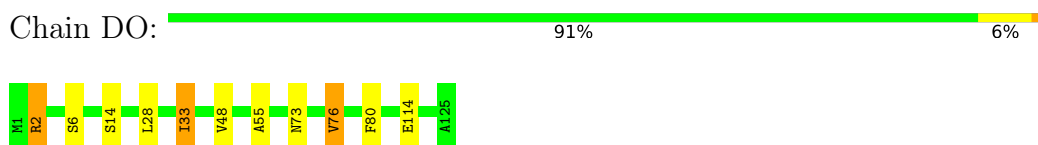
- Molecule 40: 50S ribosomal protein L16



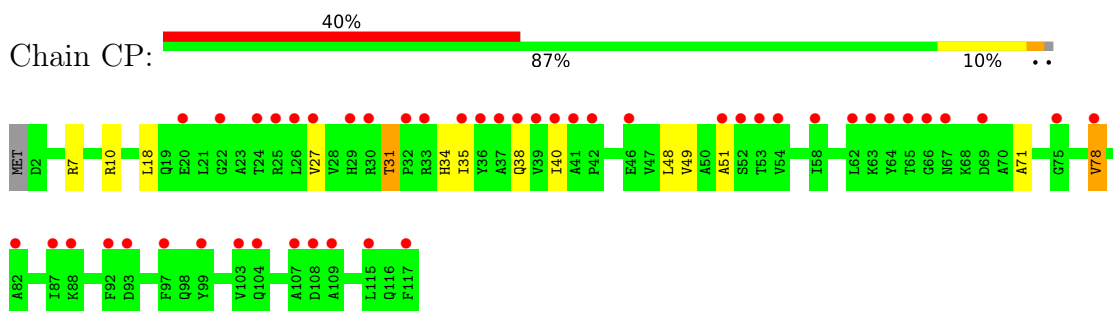
- Molecule 41: 50S ribosomal protein L17



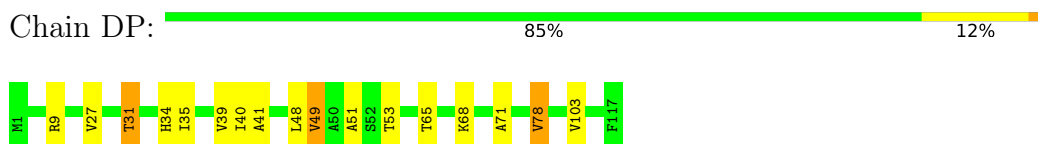
- Molecule 41: 50S ribosomal protein L17



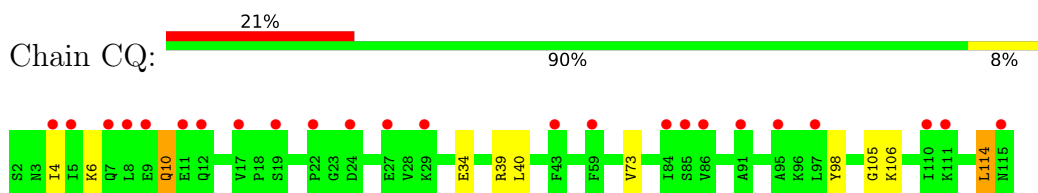
- Molecule 42: 50S ribosomal protein L18



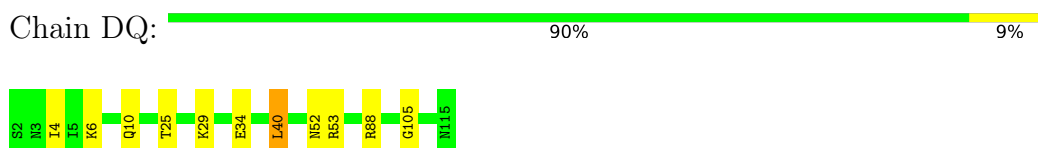
- Molecule 42: 50S ribosomal protein L18



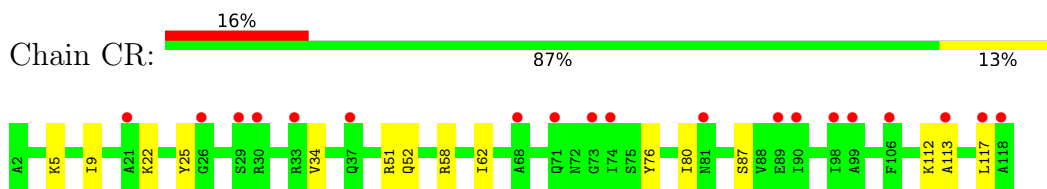
- Molecule 43: 50S ribosomal protein L19



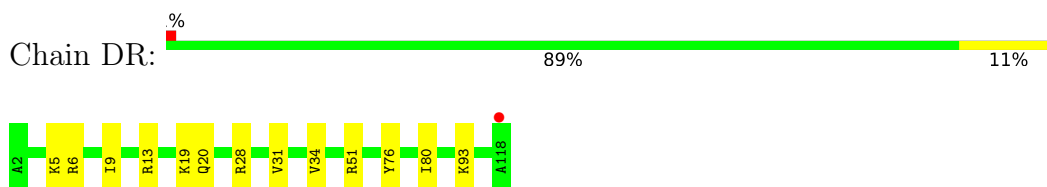
- Molecule 43: 50S ribosomal protein L19



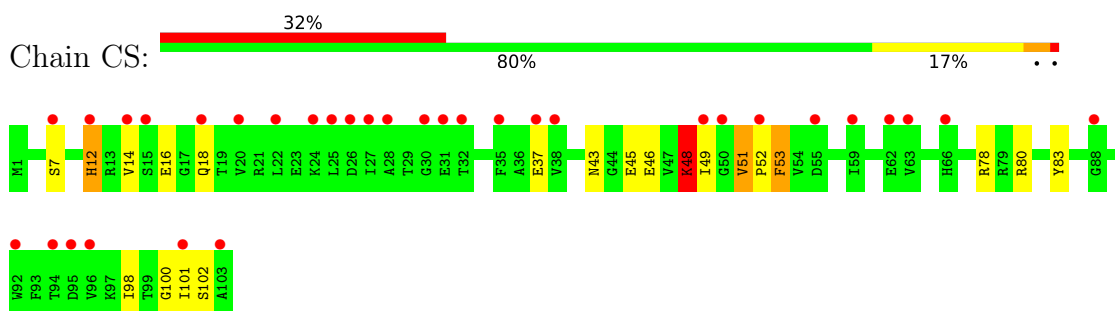
- Molecule 44: 50S ribosomal protein L20



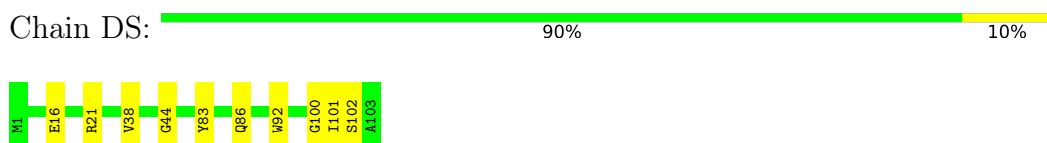
- Molecule 44: 50S ribosomal protein L20



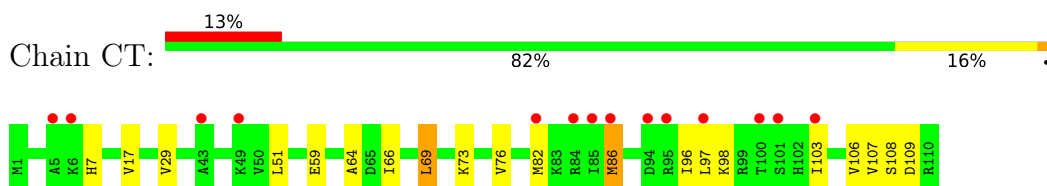
- Molecule 45: 50S ribosomal protein L21



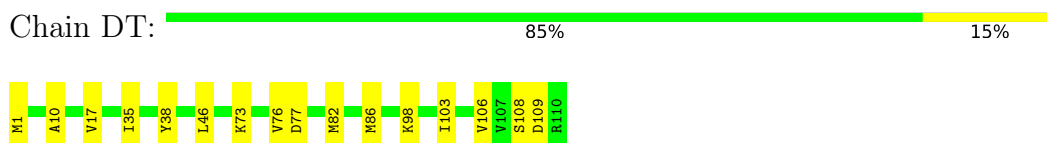
- Molecule 45: 50S ribosomal protein L21



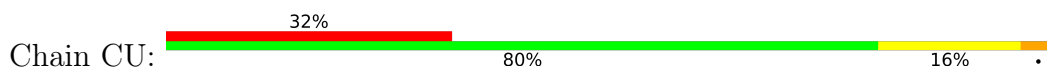
- Molecule 46: 50S ribosomal protein L22

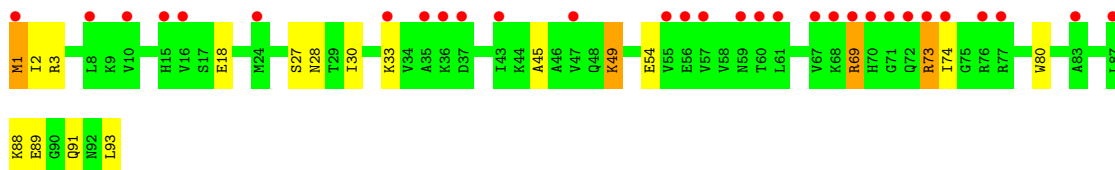


- Molecule 46: 50S ribosomal protein L22

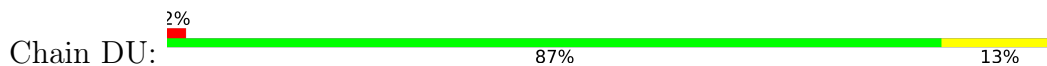


- Molecule 47: 50S ribosomal protein L23

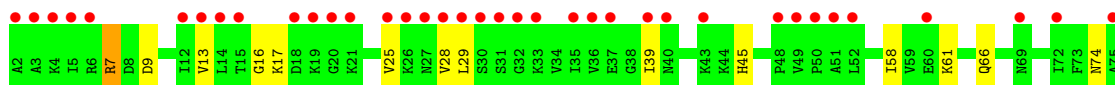




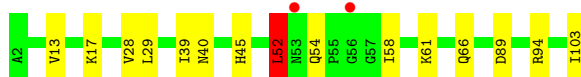
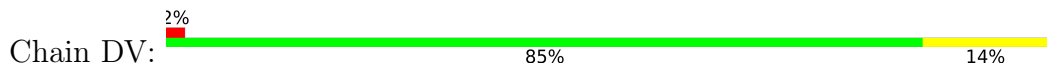
- Molecule 47: 50S ribosomal protein L23



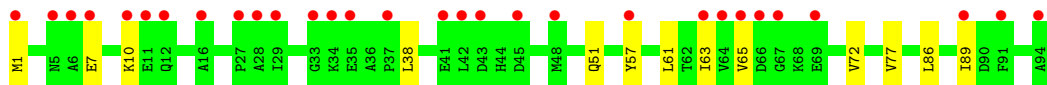
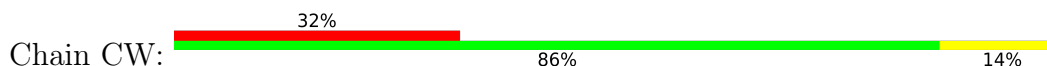
- Molecule 48: 50S ribosomal protein L24



- Molecule 48: 50S ribosomal protein L24



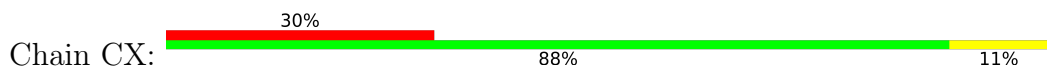
- Molecule 49: 50S ribosomal protein L25

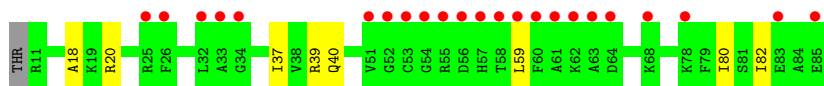


- Molecule 49: 50S ribosomal protein L25

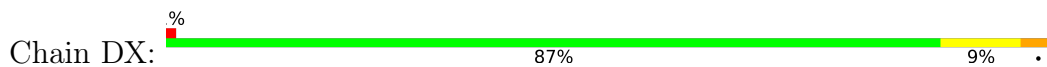


- Molecule 50: 50S ribosomal protein L27

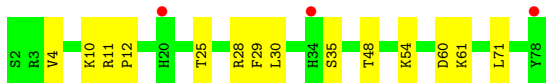
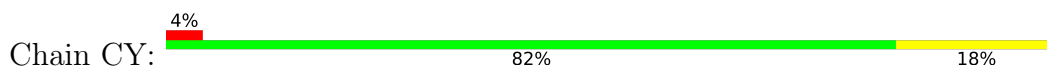




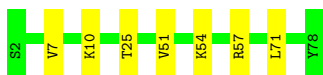
- Molecule 50: 50S ribosomal protein L27



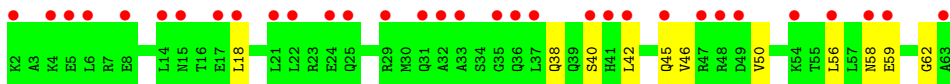
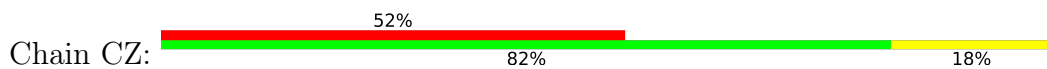
- Molecule 51: 50S ribosomal protein L28



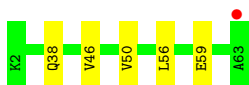
- Molecule 51: 50S ribosomal protein L28



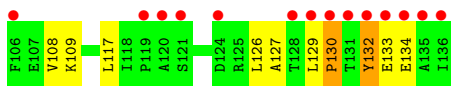
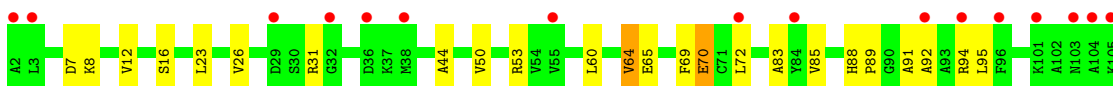
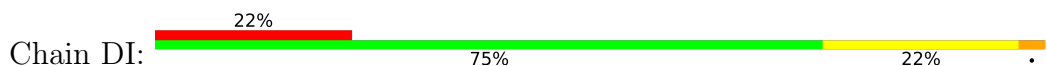
- Molecule 52: 50S ribosomal protein L29



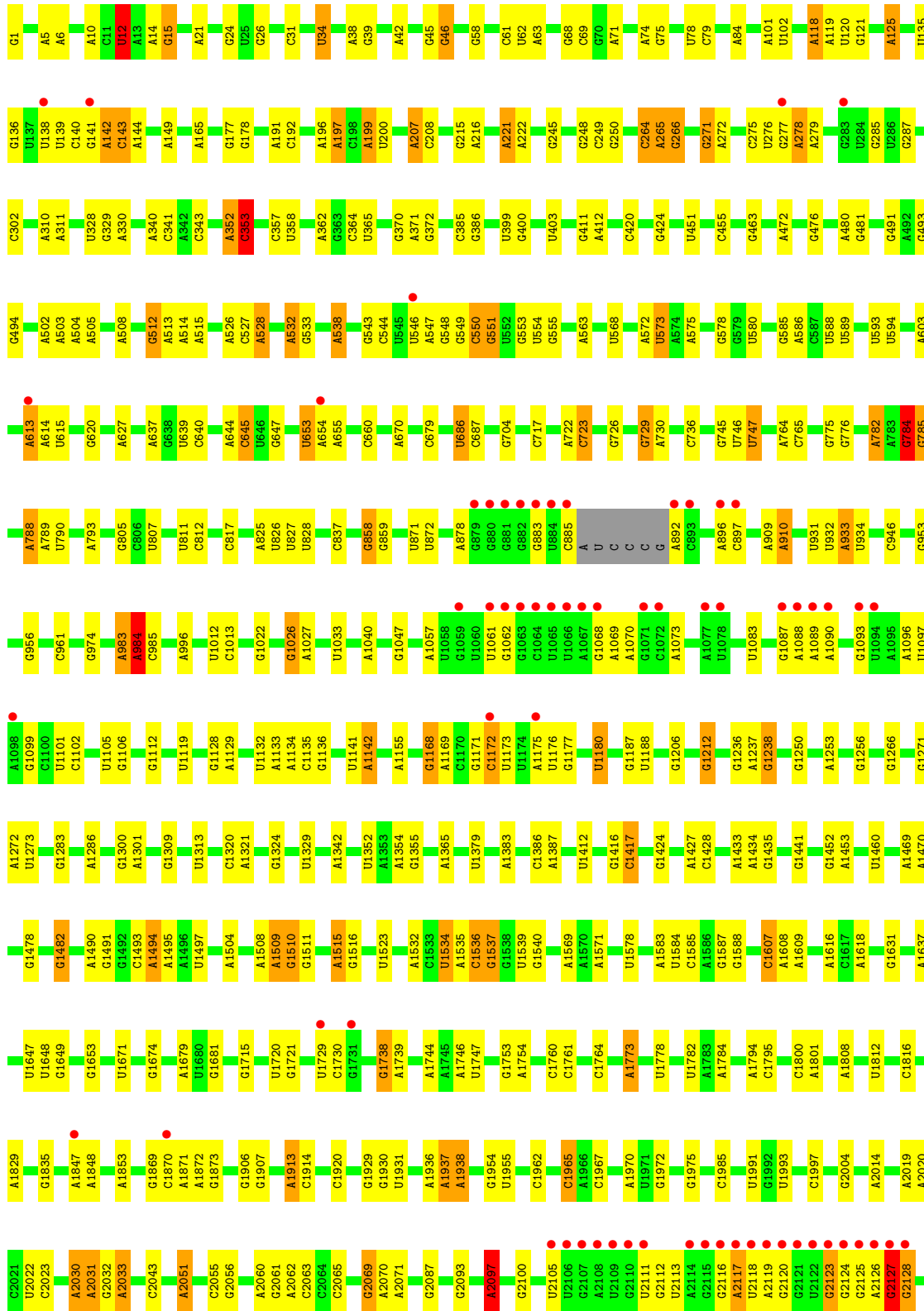
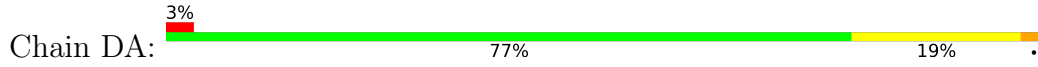
- Molecule 52: 50S ribosomal protein L29

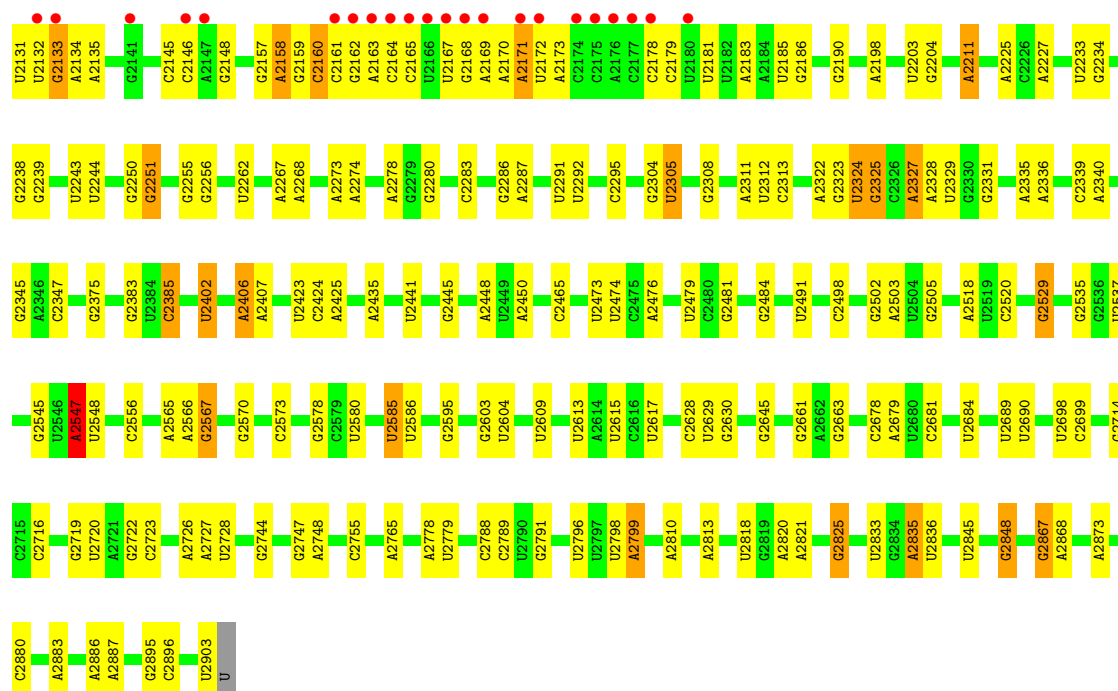


- Molecule 53: 50S ribosomal protein L10



• Molecule 54: 23S rRNA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.41Å 435.70Å 625.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 3.00 48.61 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.61-3.00) 99.2 (48.61-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.01Å)	Xtrriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, R_{free}	0.172 , 0.193 0.184 , 0.207	Depositor DCC
R_{free} test set	4504 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtrriage
Anisotropy	0.311	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 84.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	295261	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% 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: PG4, OMG, PGE, 4OC, ZN, 1MG, PSU, 2MG, ACY, D2T, PUT, 4D4, OMU, MEQ, MPD, TAC, MG, 2MA, UR3, H2U, 6MZ, 5MU, TRS, PEG, G7M, 1PE, OMC, EDO, MA6, GUN, SPD, 3TD, 5MC

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	0.97	8/36597 (0.0%)	0.86	4/57088 (0.0%)
1	BA	0.99	13/36572 (0.0%)	0.86	7/57049 (0.0%)
2	AB	0.45	0/1784	0.64	0/2403
2	BB	0.44	0/1784	0.64	0/2403
3	AC	0.46	0/1652	0.66	0/2225
3	BC	0.45	0/1652	0.68	0/2225
4	AD	0.43	0/1665	0.66	0/2227
4	BD	0.44	0/1665	0.67	0/2227
5	AE	0.47	0/1157	0.75	0/1557
5	BE	0.50	0/1118	0.80	0/1504
6	AF	0.45	0/881	0.70	1/1189 (0.1%)
6	BF	0.46	0/835	0.79	1/1128 (0.1%)
7	AG	0.45	0/1196	0.62	0/1602
7	BG	0.45	0/1196	0.62	0/1602
8	AH	0.43	0/989	0.70	0/1326
8	BH	0.42	0/989	0.69	0/1326
9	AI	0.44	0/1034	0.65	0/1375
9	BI	0.44	0/1034	0.65	0/1375
10	AJ	0.42	0/806	0.66	0/1089
10	BJ	0.48	0/797	0.70	0/1077
11	AK	0.43	0/893	0.63	0/1205
11	BK	0.42	0/893	0.67	0/1205
12	AL	0.44	0/960	0.72	0/1286
12	BL	0.44	0/960	0.73	0/1286
13	AM	0.50	0/893	0.73	0/1193
13	BM	0.49	0/893	0.72	0/1193
14	AN	0.45	0/817	0.64	0/1088
14	BN	0.43	0/817	0.63	0/1088
15	AO	0.45	0/722	0.61	0/964
15	BO	0.43	0/722	0.61	0/964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	AP	0.45	0/659	0.69	0/884
16	BP	0.48	0/659	0.76	0/884
17	AQ	0.46	0/658	0.72	0/881
17	BQ	0.50	0/658	0.76	0/881
18	AR	0.47	0/463	0.65	0/621
18	BR	0.48	0/463	0.65	0/621
19	AS	0.46	0/653	0.60	0/877
19	BS	0.46	0/653	0.61	0/877
20	AT	0.48	0/676	0.67	0/895
20	BT	0.53	0/671	0.69	0/888
21	AU	0.40	0/472	0.61	0/627
21	BU	0.38	0/472	0.62	0/627
22	C1	0.48	0/450	0.67	0/599
22	D1	0.58	0/450	0.72	0/599
23	C2	0.48	0/416	0.70	0/554
23	D2	0.47	0/421	0.69	0/561
24	C3	0.45	0/380	0.68	0/498
24	D3	0.56	0/380	0.76	0/498
25	C4	0.43	0/513	0.65	0/676
25	D4	0.50	0/513	0.68	0/676
26	C5	0.41	0/303	0.79	0/397
26	D5	0.50	0/303	0.78	0/397
27	C0	0.48	0/453	0.77	0/605
27	D0	0.62	0/467	0.79	1/623 (0.2%)
28	CB	0.91	0/2828	0.88	1/4410 (0.0%)
28	DB	1.01	0/2872	0.88	0/4478
29	CC	0.43	0/2122	0.73	0/2852
29	DC	0.48	0/2122	0.74	1/2852 (0.0%)
30	CD	0.42	0/1576	0.67	0/2119
30	DD	0.51	0/1576	0.68	0/2119
31	CA	1.02	39/69143 (0.1%)	0.87	11/107862 (0.0%)
32	CE	0.43	0/1571	0.70	0/2113
32	DE	0.49	0/1571	0.68	0/2113
33	CF	0.41	0/1435	0.67	0/1926
33	DF	0.46	0/1435	0.70	0/1926
34	CG	0.39	0/1343	0.66	0/1816
34	DG	0.43	0/1343	0.64	0/1816
35	CH	0.46	0/1121	0.68	1/1515 (0.1%)
35	DH	0.46	0/1121	0.67	0/1515
36	CJ	0.49	0/993	0.62	0/1341
36	DJ	0.49	0/993	0.62	0/1341
37	CK	0.41	0/1152	0.68	0/1551
37	DK	0.53	0/1152	0.71	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	CL	0.45	0/947	0.71	0/1268
38	DL	0.51	0/955	0.72	0/1279
39	CM	0.45	0/1062	0.73	1/1413 (0.1%)
39	DM	0.47	0/1062	0.70	0/1413
40	CN	0.45	0/1081	0.72	0/1443
40	DN	0.54	0/1092	0.76	0/1457
41	CO	0.44	0/973	0.68	0/1301
41	DO	0.54	0/1006	0.74	0/1345
42	CP	0.42	0/902	0.71	0/1209
42	DP	0.49	0/910	0.71	0/1219
43	CQ	0.40	0/929	0.69	1/1242 (0.1%)
43	DQ	0.45	0/929	0.69	0/1242
44	CR	0.43	0/960	0.65	0/1278
44	DR	0.54	0/960	0.68	0/1278
45	CS	0.42	0/829	0.73	0/1107
45	DS	0.51	0/829	0.74	0/1107
46	CT	0.41	0/864	0.70	0/1156
46	DT	0.53	0/864	0.69	0/1156
47	CU	0.44	0/745	0.71	0/994
47	DU	0.48	0/745	0.72	0/994
48	CV	0.44	0/788	0.75	0/1051
48	DV	0.47	0/788	0.75	0/1051
49	CW	0.40	0/766	0.65	0/1025
49	DW	0.49	0/766	0.68	0/1025
50	CX	0.40	0/576	0.65	0/762
50	DX	0.55	0/598	0.74	0/790
51	CY	0.41	0/635	0.70	0/848
51	DY	0.46	0/635	0.70	0/848
52	CZ	0.42	0/502	0.59	0/667
52	DZ	0.45	0/502	0.59	0/667
53	DI	0.50	0/1037	0.76	1/1402 (0.1%)
54	DA	1.14	49/69364 (0.1%)	0.91	15/108207 (0.0%)
All	All	0.91	109/309249 (0.0%)	0.84	46/462175 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	3
1	BA	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	CA	0	8
40	CN	0	1
40	DN	0	1
54	DA	0	41
All	All	0	56

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2095	A	O5'-C5'	-9.26	1.28	1.42
54	DA	12	U	C1'-N1	8.76	1.61	1.48
31	CA	1936	A	N9-C4	-8.51	1.32	1.37
54	DA	2097	A	O5'-C5'	-8.36	1.29	1.42
31	CA	2425	A	C3'-O3'	8.30	1.53	1.42
54	DA	1237	A	C3'-O3'	-7.96	1.31	1.42
31	CA	769	U	C1'-N1	7.92	1.60	1.48
31	CA	12	U	C1'-N1	7.83	1.60	1.48
31	CA	2225	A	C3'-O3'	7.82	1.53	1.42
54	DA	2585	U	C3'-O3'	7.54	1.52	1.42
31	CA	1777	U	C1'-N1	7.22	1.59	1.48
1	BA	5	U	C1'-N1	6.74	1.58	1.48
31	CA	2233	U	C1'-N1	6.72	1.58	1.48
54	DA	788	A	N7-C5	-6.68	1.35	1.39
31	CA	1379	U	C3'-O3'	6.61	1.51	1.42
1	AA	5	U	C1'-N1	6.58	1.58	1.48
31	CA	1658	C	C1'-N1	6.40	1.58	1.48
31	CA	692	C	C1'-N1	6.35	1.58	1.48
1	BA	1493	A	C3'-O3'	6.34	1.51	1.42
54	DA	1607	C	N1-C6	6.22	1.40	1.37
54	DA	12	U	P-O5'	6.16	1.66	1.59
31	CA	946	C	C1'-N1	6.15	1.57	1.48
1	AA	1354	U	C1'-N1	6.12	1.57	1.48
54	DA	1607	C	P-O5'	-6.10	1.53	1.59
54	DA	2585	U	C1'-N1	6.10	1.57	1.48
54	DA	2585	U	N1-C2	6.07	1.44	1.38
31	CA	1825	U	C1'-N1	6.07	1.57	1.48
54	DA	21	A	N3-C4	6.05	1.38	1.34
54	DA	1965	C	C3'-O3'	-6.05	1.33	1.42
31	CA	451	U	C1'-N1	5.96	1.57	1.48
54	DA	12	U	N1-C2	5.95	1.44	1.38
31	CA	404	A	C3'-O3'	5.91	1.50	1.42
1	AA	956	U	C1'-N1	5.89	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2017	U	C1'-N1	5.89	1.57	1.48
31	CA	546	U	C1'-N1	5.88	1.57	1.48
54	DA	2547	A	O5'-C5'	-5.83	1.33	1.42
1	BA	1008	U	O5'-C5'	-5.82	1.33	1.42
54	DA	613	A	N9-C4	5.80	1.41	1.37
1	BA	1397	C	N1-C2	5.76	1.46	1.40
31	CA	1790	C	C1'-N1	5.75	1.57	1.48
54	DA	1188	U	C3'-O3'	-5.74	1.34	1.42
54	DA	1679	A	N7-C5	-5.72	1.35	1.39
54	DA	653	U	C1'-N1	5.72	1.57	1.48
54	DA	578	G	N7-C5	-5.70	1.35	1.39
31	CA	20	C	C1'-N1	5.70	1.57	1.48
1	BA	306	A	C5-C6	5.67	1.46	1.41
1	BA	306	A	N3-C4	5.66	1.38	1.34
54	DA	2127	G	C3'-O3'	5.65	1.50	1.42
54	DA	2867	G	C3'-O3'	5.64	1.50	1.42
31	CA	1314	C	C1'-N1	5.63	1.57	1.48
54	DA	1313	U	C1'-N1	5.61	1.57	1.48
1	AA	632	U	C1'-N1	5.59	1.57	1.48
54	DA	2051	A	N7-C5	-5.59	1.35	1.39
31	CA	653	U	C1'-N1	5.58	1.57	1.48
31	CA	2146	C	C3'-O3'	5.58	1.50	1.42
1	AA	1397	C	N1-C6	5.54	1.40	1.37
1	AA	955	U	C1'-N1	5.51	1.57	1.48
31	CA	691	C	C1'-N1	5.50	1.57	1.48
1	BA	209	U	C1'-N1	5.50	1.57	1.48
54	DA	2402	U	P-O5'	5.50	1.65	1.59
1	BA	842	U	C3'-O3'	5.50	1.49	1.42
31	CA	817	C	C1'-N1	5.49	1.56	1.48
31	CA	2456	C	C1'-N1	5.47	1.56	1.48
54	DA	2402	U	N1-C2	5.46	1.43	1.38
54	DA	271	G	C3'-O3'	5.45	1.49	1.42
54	DA	784	G	C3'-O3'	5.43	1.49	1.42
54	DA	736	C	C3'-O3'	-5.42	1.34	1.42
31	CA	1376	C	C1'-N1	5.41	1.56	1.48
54	DA	1441	G	O5'-C5'	-5.41	1.34	1.42
31	CA	995	C	O5'-C5'	-5.41	1.34	1.42
1	BA	956	U	C1'-N1	5.38	1.56	1.48
1	BA	1354	U	C1'-N1	5.38	1.56	1.48
1	BA	955	U	C1'-N1	5.37	1.56	1.48
54	DA	2004	G	N3-C4	5.37	1.39	1.35
31	CA	2354	C	C1'-N1	5.36	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	221	C	C1'-N1	5.30	1.56	1.48
54	DA	1571	A	N7-C5	-5.30	1.36	1.39
54	DA	538	A	N7-C5	-5.30	1.36	1.39
54	DA	2402	U	C1'-N1	5.29	1.56	1.48
31	CA	1788	C	C1'-N1	5.28	1.56	1.48
31	CA	790	U	C1'-N1	5.26	1.56	1.48
31	CA	1352	U	C1'-N1	5.23	1.56	1.48
31	CA	1994	C	C1'-N1	5.23	1.56	1.48
1	AA	221	C	C1'-N1	5.20	1.56	1.48
1	AA	532	A	N9-C4	5.19	1.41	1.37
54	DA	2211	A	C3'-O3'	5.19	1.49	1.42
31	CA	1838	C	N1-C2	5.18	1.45	1.40
31	CA	2680	U	C3'-O3'	5.18	1.49	1.42
54	DA	817	C	C3'-O3'	-5.18	1.34	1.42
54	DA	1920	C	C1'-N1	5.15	1.56	1.48
31	CA	1306	C	C1'-N1	5.14	1.56	1.48
54	DA	1534	U	C1'-N1	5.13	1.56	1.48
54	DA	2810	A	N7-C5	-5.11	1.36	1.39
54	DA	532	A	N7-C5	-5.11	1.36	1.39
31	CA	1938	A	N9-C4	5.09	1.41	1.37
54	DA	2617	U	O5'-C5'	-5.09	1.34	1.42
54	DA	275	C	C1'-N1	5.09	1.56	1.48
31	CA	1971	U	C1'-N1	5.07	1.56	1.48
54	DA	1412	U	C1'-N1	5.07	1.56	1.48
54	DA	1584	U	C1'-N1	5.06	1.56	1.48
1	BA	1067	A	C3'-O3'	5.06	1.49	1.42
31	CA	678	C	C1'-N1	5.06	1.56	1.48
54	DA	2868	A	N7-C5	-5.04	1.36	1.39
54	DA	207	A	C3'-O3'	-5.04	1.35	1.42
54	DA	2227	A	N7-C5	-5.04	1.36	1.39
31	CA	2215	C	C1'-N1	5.02	1.56	1.48
54	DA	353	C	C1'-N1	5.02	1.56	1.48
54	DA	2570	G	C6-N1	-5.00	1.36	1.39
54	DA	34	U	O3'-P	-5.00	1.55	1.61

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	CB	15	A	O4'-C1'-N9	10.03	116.22	108.20
54	DA	1936	A	O4'-C1'-N9	8.20	114.76	108.20
1	BA	1362	A	C1'-O4'-C4'	-7.38	104.00	109.90
1	AA	1	A	OP1-P-OP2	-7.19	108.81	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	271	G	P-O3'-C3'	7.11	128.24	119.70
54	DA	892	A	OP1-P-OP2	-7.08	108.98	119.60
53	DI	132	TYR	C-N-CA	7.07	139.38	121.70
31	CA	892	A	OP1-P-OP2	-6.99	109.12	119.60
54	DA	1	G	OP1-P-OP2	-6.95	109.18	119.60
1	AA	413	G	C1'-O4'-C4'	-6.88	104.40	109.90
1	BA	2	A	OP1-P-OP2	-6.85	109.33	119.60
54	DA	2825	G	O4'-C1'-N9	6.82	113.66	108.20
54	DA	271	G	P-O3'-C3'	6.63	127.66	119.70
54	DA	784	G	P-O3'-C3'	6.62	127.65	119.70
31	CA	2035	G	C1'-O4'-C4'	-6.60	104.62	109.90
29	DC	156	ARG	CB-CG-CD	-6.40	94.96	111.60
31	CA	974	G	N9-C1'-C2'	6.39	122.31	114.00
54	DA	2406	A	C5'-C4'-O4'	-5.91	102.01	109.10
31	CA	2225	A	P-O3'-C3'	5.84	126.70	119.70
31	CA	512	G	O4'-C1'-N9	5.80	112.84	108.20
31	CA	784	G	P-O3'-C3'	5.80	126.66	119.70
31	CA	451	U	C1'-O4'-C4'	-5.70	105.34	109.90
54	DA	1985	C	O4'-C1'-N1	5.69	112.75	108.20
31	CA	1128	G	C1'-O4'-C4'	-5.59	105.42	109.90
54	DA	199	A	C1'-O4'-C4'	-5.52	105.48	109.90
27	D0	10	THR	N-CA-CB	-5.52	99.81	110.30
54	DA	1266	G	C3'-C2'-C1'	-5.46	97.13	101.50
1	BA	328	C	C1'-O4'-C4'	-5.41	105.57	109.90
54	DA	2848	G	O4'-C1'-N9	5.40	112.52	108.20
1	BA	485	U	O4'-C1'-N1	5.38	112.51	108.20
39	CM	68	SER	C-N-CA	5.37	135.13	121.70
54	DA	807	U	C4'-C3'-C2'	-5.35	97.25	102.60
6	AF	55	HIS	N-CA-C	-5.19	97.00	111.00
54	DA	512	G	O4'-C1'-N9	5.18	112.35	108.20
1	AA	841	C	P-O3'-C3'	5.15	125.88	119.70
54	DA	679	C	O4'-C1'-N1	5.15	112.32	108.20
31	CA	2680	U	P-O3'-C3'	5.11	125.83	119.70
1	AA	686	U	C1'-O4'-C4'	-5.10	105.82	109.90
54	DA	729	G	C1'-O4'-C4'	-5.10	105.82	109.90
6	BF	55	HIS	N-CA-C	-5.09	97.25	111.00
31	CA	404	A	P-O3'-C3'	5.06	125.77	119.70
43	CQ	114	LEU	CA-CB-CG	5.05	126.92	115.30
1	BA	686	U	C1'-O4'-C4'	-5.05	105.86	109.90
35	CH	8	LYS	C-N-CA	5.03	134.28	121.70
1	BA	842	U	P-O3'-C3'	5.02	125.73	119.70
1	BA	1362	A	O4'-C1'-N9	5.01	112.21	108.20

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1432	G	Sidechain
1	AA	362	G	Sidechain
1	AA	898	G	Sidechain
1	BA	1432	G	Sidechain
1	BA	898	G	Sidechain
31	CA	2267	A	Sidechain
31	CA	2444	G	Sidechain
31	CA	250	G	Sidechain
31	CA	463	G	Sidechain
31	CA	555	G	Sidechain
31	CA	704	G	Sidechain
31	CA	726	G	Sidechain
31	CA	757	G	Sidechain
40	CN	69	PRO	Mainchain
54	DA	1142	A	Sidechain
54	DA	1212	G	Sidechain
54	DA	1283	G	Sidechain
54	DA	1324	G	Sidechain
54	DA	15	G	Sidechain
54	DA	1631	G	Sidechain
54	DA	1681	G	Sidechain
54	DA	1753	G	Sidechain
54	DA	1761	C	Sidechain
54	DA	177	G	Sidechain
54	DA	1937	A	Sidechain
54	DA	1938	A	Sidechain
54	DA	1954	G	Sidechain
54	DA	221	A	Sidechain
54	DA	2250	G	Sidechain
54	DA	2267	A	Sidechain
54	DA	2323	G	Sidechain
54	DA	2375	G	Sidechain
54	DA	2481	G	Sidechain
54	DA	249	C	Sidechain
54	DA	250	G	Sidechain
54	DA	2529	G	Sidechain
54	DA	2578	G	Sidechain
54	DA	2595	G	Sidechain
54	DA	2645	G	Sidechain
54	DA	2719	G	Sidechain

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Mol	Chain	Res	Type	Group
54	DA	2727	A	Sidechain
54	DA	2728	U	Sidechain
54	DA	2835	A	Sidechain
54	DA	2848	G	Sidechain
54	DA	463	G	Sidechain
54	DA	512	G	Sidechain
54	DA	515	A	Sidechain
54	DA	555	G	Sidechain
54	DA	670	A	Sidechain
54	DA	704	G	Sidechain
54	DA	726	G	Sidechain
54	DA	858	G	Sidechain
54	DA	956	G	Sidechain
54	DA	983	A	Sidechain
54	DA	984	A	Sidechain
40	DN	69	PRO	Mainchain

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	32933	0	16592	113	0
1	BA	32911	0	16581	115	0
2	AB	1753	0	1780	7	0
2	BB	1753	0	1780	9	0
3	AC	1625	0	1696	13	0
3	BC	1625	0	1696	17	0
4	AD	1643	0	1707	11	0
4	BD	1643	0	1707	17	0
5	AE	1144	0	1185	14	0
5	BE	1105	0	1148	25	0
6	AF	862	0	864	7	0
6	BF	817	0	808	7	0
7	AG	1182	0	1238	7	0
7	BG	1182	0	1238	4	0
8	AH	979	0	1031	6	0
8	BH	979	0	1031	3	0
9	AI	1022	0	1070	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	BI	1022	0	1070	7	0
10	AJ	796	0	836	11	0
10	BJ	787	0	828	8	0
11	AK	877	0	887	13	0
11	BK	877	0	887	15	0
12	AL	957	0	1017	5	0
12	BL	957	0	1017	8	0
13	AM	884	0	941	13	0
13	BM	884	0	941	18	0
14	AN	805	0	844	8	0
14	BN	805	0	844	7	0
15	AO	714	0	734	0	0
15	BO	714	0	734	0	0
16	AP	649	0	666	2	0
16	BP	649	0	666	7	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	13	0
18	AR	456	0	478	3	0
18	BR	456	0	478	2	0
19	AS	638	0	665	4	0
19	BS	638	0	665	6	0
20	AT	670	0	719	3	0
20	BT	665	0	714	4	0
21	AU	465	0	491	3	0
21	BU	465	0	491	3	0
22	C1	444	0	458	5	0
22	D1	444	0	458	9	0
23	C2	409	0	440	6	0
23	D2	414	0	442	6	0
24	C3	377	0	418	3	0
24	D3	377	0	418	3	0
25	C4	504	0	572	2	0
25	D4	504	0	572	2	0
26	C5	302	0	340	6	0
26	D5	302	0	340	2	0
27	C0	449	0	488	3	0
27	D0	463	0	504	2	0
28	CB	2529	0	1281	6	0
28	DB	2569	0	1301	3	0
29	CC	2083	0	2154	24	0
29	DC	2083	0	2154	12	0
30	CD	1565	0	1614	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	DD	1576	0	1627	15	0
31	CA	62229	0	31318	224	0
32	CE	1552	0	1619	18	0
32	DE	1552	0	1619	9	0
33	CF	1411	0	1444	14	0
33	DF	1411	0	1444	11	0
34	CG	1323	0	1371	8	0
34	DG	1323	0	1371	8	0
35	CH	1110	0	1148	10	0
35	DH	1110	0	1148	9	0
36	CJ	979	0	1028	5	0
36	DJ	979	0	1028	5	0
37	CK	1129	0	1162	8	0
37	DK	1129	0	1162	4	0
38	CL	938	0	1012	8	0
38	DL	946	0	1023	7	0
39	CM	1053	0	1129	19	0
39	DM	1053	0	1129	6	0
40	CN	1075	0	1154	9	0
40	DN	1092	0	1177	13	0
41	CO	960	0	1000	6	0
41	DO	993	0	1034	5	0
42	CP	892	0	923	6	0
42	DP	900	0	935	11	0
43	CQ	917	0	962	6	0
43	DQ	917	0	962	7	0
44	CR	947	0	1019	11	0
44	DR	947	0	1019	13	0
45	CS	816	0	839	12	0
45	DS	816	0	839	7	0
46	CT	857	0	922	9	0
46	DT	857	0	922	9	0
47	CU	739	0	807	8	0
47	DU	739	0	807	7	0
48	CV	780	0	831	7	0
48	DV	780	0	831	6	0
49	CW	753	0	780	5	0
49	DW	753	0	780	4	0
50	CX	569	0	581	3	0
50	DX	591	0	606	10	0
51	CY	625	0	652	8	0
51	DY	625	0	652	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	CZ	501	0	531	3	0
52	DZ	501	0	531	2	0
53	DI	1023	0	1052	15	0
54	DA	62423	0	31411	176	0
55	AA	72	0	0	0	0
55	BA	45	0	0	0	0
55	CA	156	0	0	0	0
55	CB	3	0	0	0	0
55	DA	183	0	0	0	0
55	DB	9	0	0	0	0
55	DD	1	0	0	0	0
55	DM	1	0	0	0	0
55	DR	2	0	0	0	0
56	AA	13	0	18	1	0
56	BA	13	0	18	1	0
56	DA	26	0	36	3	0
56	DQ	13	0	18	0	0
56	DR	13	0	18	5	0
56	DS	13	0	18	3	0
57	AA	16	0	28	3	0
57	DA	40	0	70	3	0
57	DE	16	0	28	0	0
57	DK	8	0	14	0	0
57	DN	8	0	14	1	0
57	DS	8	0	14	0	0
57	DT	16	0	28	0	0
58	AA	24	0	48	0	0
58	DA	66	0	132	7	0
58	DM	6	0	12	0	0
59	AA	64	1	42	2	0
59	BA	64	1	42	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	D1	7	0	10	1	0
61	D3	7	0	10	0	0
61	DA	35	0	50	0	0
61	DL	7	0	10	0	0
61	DP	7	0	10	1	0
61	DQ	7	0	10	0	0
62	D1	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	DA	32	0	48	1	0
62	DB	12	0	18	0	0
63	D1	10	0	14	2	0
63	DA	60	0	84	4	0
63	DS	10	0	14	1	0
63	DU	10	0	14	3	0
64	DA	40	0	76	2	0
65	DA	32	0	44	1	0
66	DA	12	0	9	0	0
67	DA	11	0	5	0	0
68	DA	8	0	12	1	0
69	AA	501	0	0	0	0
69	AC	4	0	0	0	0
69	AD	2	0	0	0	0
69	AE	5	0	0	0	0
69	AG	1	0	0	0	0
69	AH	1	0	0	0	0
69	AJ	2	0	0	0	0
69	AK	6	0	0	0	0
69	AL	10	0	0	0	0
69	AM	5	0	0	2	0
69	AN	6	0	0	1	0
69	AO	2	0	0	0	0
69	AP	2	0	0	0	0
69	AR	1	0	0	0	0
69	AT	3	0	0	0	0
69	AU	3	0	0	0	0
69	BA	287	0	0	1	0
69	BD	13	0	0	0	0
69	BE	1	0	0	0	0
69	BF	2	0	0	0	0
69	BK	2	0	0	0	0
69	BL	4	0	0	0	0
69	BN	2	0	0	0	0
69	BO	1	0	0	0	0
69	BP	3	0	0	0	0
69	BT	2	0	0	0	0
69	BU	2	0	0	0	0
69	C3	4	0	0	0	0
69	C4	1	0	0	0	0
69	CA	691	0	0	3	0
69	CB	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	CC	10	0	0	0	0
69	CD	6	0	0	0	0
69	CE	5	0	0	0	0
69	CL	1	0	0	0	0
69	CM	4	0	0	0	0
69	CO	2	0	0	0	0
69	CU	3	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	0	0
69	D1	43	0	0	0	0
69	D2	6	0	0	0	0
69	D3	22	0	0	0	0
69	D4	39	0	0	0	0
69	D5	8	0	0	0	0
69	DA	4840	0	0	15	0
69	DB	209	0	0	1	0
69	DC	100	0	0	1	0
69	DD	98	0	0	2	0
69	DE	61	0	0	0	0
69	DF	15	0	0	0	0
69	DG	6	0	0	0	0
69	DH	2	0	0	0	0
69	DK	65	0	0	1	0
69	DL	52	0	0	1	0
69	DM	63	0	0	0	0
69	DN	72	0	0	0	0
69	DO	44	0	0	0	0
69	DP	38	0	0	0	0
69	DQ	33	0	0	0	0
69	DR	62	0	0	1	0
69	DS	46	0	0	2	0
69	DT	69	0	0	1	0
69	DU	18	0	0	0	0
69	DV	20	0	0	0	0
69	DW	31	0	0	0	0
69	DX	25	0	0	1	0
69	DY	9	0	0	0	0
69	DZ	8	0	0	0	0
All	All	295259	2	194494	1263	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 3.

All (1263) 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)
45:CS:14:VAL:HG21	45:CS:98:ILE:HG13	1.27	1.10
31:CA:1005:C:O2'	37:CK:30:THR:HG21	1.61	1.00
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.46	0.97
31:CA:1847:A:HO2'	31:CA:1848:A:H8	0.98	0.95
31:CA:528:A:C2	31:CA:2043:C:H4'	2.00	0.95
54:DA:2796:U:H3	54:DA:2799:A:H61	1.11	0.95
54:DA:1847:A:HO2'	54:DA:1848:A:H8	0.98	0.94
26:C5:3:VAL:HG11	31:CA:2539:C:H5'	1.50	0.94
2:BB:20:THR:HA	2:BB:39:HIS:CE1	2.02	0.94
11:BK:88:GLY:H	11:BK:114:THR:HG22	1.34	0.93
31:CA:2796:U:H3	31:CA:2799:A:H61	1.14	0.93
39:CM:77:ILE:HD11	39:CM:108:ALA:HB1	1.50	0.92
31:CA:1936:A:H2	31:CA:1943:U:H3	0.96	0.91
14:AN:66:GLN:HB2	69:AN:206:HOH:O	1.70	0.90
45:CS:14:VAL:CG2	45:CS:98:ILE:HG13	2.00	0.90
1:AA:1492:A:H5''	12:AL:44:LYS:HG2	1.53	0.89
1:AA:307:C:N4	57:AA:1676:MPD:H12	1.88	0.88
12:BL:80:ILE:HD12	12:BL:97:THR:HG22	1.54	0.88
54:DA:1913:A:H4'	54:DA:1913:A:OP1	1.72	0.87
31:CA:135:U:H3	31:CA:144:A:H61	1.20	0.87
54:DA:135:U:H3	54:DA:144:A:H61	1.20	0.87
46:CT:86:MET:HB2	46:CT:96:ILE:HD11	1.54	0.86
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.59	0.85
54:DA:2255:G:H21	68:DA:3220:TRS:H12	1.42	0.85
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.58	0.84
44:DR:20:GLN:HG3	56:DR:202:PG4:H42	1.58	0.84
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.59	0.83
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.61	0.82
31:CA:740:C:H5'	31:CA:1784:A:H3'	1.61	0.82
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.59	0.81
45:CS:14:VAL:HG21	45:CS:98:ILE:CG1	2.10	0.81
1:BA:841:C:H3'	1:BA:842:U:H5''	1.62	0.80
1:BA:664:G:H22	1:BA:741:G:H1	1.29	0.80
2:BB:20:THR:HA	2:BB:39:HIS:HE1	1.46	0.80
31:CA:1779:U:H5	31:CA:1784:A:N7	1.80	0.79
13:BM:6:GLY:HA3	13:BM:66:GLU:HG3	1.63	0.79
1:BA:1052:G:H22	1:BA:1206:G:H1	1.30	0.79
3:BC:123:GLN:HB3	3:BC:128:VAL:HG21	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1305:G:H21	1:AA:1332:A:H2	1.32	0.78
13:AM:33:ILE:HD11	13:AM:63:PHE:HE1	1.48	0.78
44:DR:28:ARG:HD3	69:DR:302:HOH:O	1.85	0.77
1:AA:664:G:H22	1:AA:741:G:H1	1.31	0.77
31:CA:1936:A:H2	31:CA:1943:U:N3	1.80	0.77
8:BH:87:LYS:HB2	8:BH:125:ILE:HD11	1.67	0.77
13:BM:114:LYS:HB3	13:BM:115:PRO:HD3	1.67	0.76
32:DE:33:VAL:HG22	57:DA:3192:MPD:H12	1.66	0.76
17:BQ:14:SER:HB3	17:BQ:22:VAL:HG12	1.68	0.76
1:BA:1305:G:H21	1:BA:1332:A:H2	1.32	0.76
10:AJ:7:ARG:HB3	10:AJ:101:SER:HB2	1.67	0.75
1:AA:202:G:HO2'	1:AA:468:A:H8	1.33	0.75
1:BA:522:C:H5	12:BL:50:ARG:HH12	1.33	0.75
31:CA:846:U:H1'	31:CA:847:U:H5	1.52	0.74
8:AH:87:LYS:HB2	8:AH:125:ILE:HD11	1.69	0.74
30:CD:133:THR:HG22	31:CA:1993:U:H4'	1.68	0.73
54:DA:2127:G:H4'	54:DA:2128:G:OP1	1.89	0.72
1:BA:841:C:H3'	1:BA:842:U:C5'	2.19	0.72
54:DA:568:U:H1'	54:DA:2030:6MZ:H9C1	1.72	0.71
24:C3:12:ARG:HD2	24:C3:44:VAL:HG11	1.71	0.71
69:DD:443:HOH:O	54:DA:1671:U:H4'	1.90	0.71
34:CG:24:ILE:HD11	34:CG:43:VAL:HG11	1.71	0.71
31:CA:1105:U:H2'	31:CA:1106:G:H8	1.56	0.71
34:DG:24:ILE:HD11	34:DG:43:VAL:HG11	1.74	0.70
54:DA:1105:U:H2'	54:DA:1106:G:H8	1.56	0.70
4:AD:107:PHE:HB3	4:AD:145:ILE:HD11	1.74	0.70
5:AE:77:ASN:HB2	5:AE:82:GLN:NE2	2.07	0.69
22:C1:16:ARG:HA	31:CA:2046:G:H5'	1.73	0.69
1:BA:1060:U:C5	3:BC:2:GLY:HA3	2.28	0.69
34:CG:76:VAL:O	34:CG:80:THR:HG22	1.92	0.69
11:BK:89:PRO:HG3	21:BU:32:VAL:HG11	1.74	0.69
29:CC:29:PRO:HG2	29:CC:34:LEU:HD11	1.74	0.69
46:CT:59:GLU:HA	46:CT:64:ALA:HA	1.73	0.69
1:BA:502:A:OP1	12:BL:115:SER:HB2	1.93	0.68
5:BE:72:ILE:HG12	5:BE:145:GLU:HG3	1.75	0.68
35:DH:41:LYS:HA	35:DH:44:ILE:HG12	1.76	0.68
65:DA:3202:1PE:H231	69:DA:3678:HOH:O	1.92	0.68
38:DL:70:ARG:HD3	38:DL:76:VAL:HG22	1.76	0.68
6:BF:38:ARG:HH12	6:BF:99:ALA:HB3	1.59	0.68
29:DC:29:PRO:HG2	29:DC:34:LEU:HD11	1.75	0.68
4:BD:107:PHE:HB3	4:BD:145:ILE:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:502:A:OP1	12:AL:115:SER:HB2	1.94	0.67
31:CA:2291:U:H2'	31:CA:2292:U:C6	2.28	0.67
47:CU:54:GLU:HB3	47:CU:88:LYS:HD2	1.77	0.67
35:CH:41:LYS:HA	35:CH:44:ILE:HG12	1.75	0.67
29:CC:105:LEU:H	29:CC:105:LEU:HD12	1.59	0.67
12:BL:65:SER:HB2	12:BL:82:ILE:HD11	1.75	0.67
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.77	0.67
5:BE:77:ASN:HB2	5:BE:82:GLN:NE2	2.09	0.67
31:CA:1105:U:H2'	31:CA:1106:G:C8	2.30	0.67
54:DA:2033:A:H5'	69:DA:3362:HOH:O	1.96	0.66
13:AM:33:ILE:HD11	13:AM:63:PHE:CE1	2.29	0.66
69:DK:315:HOH:O	44:DR:93:LYS:HD2	1.93	0.66
31:CA:1394:U:H4'	31:CA:1603:A:H4'	1.78	0.66
35:CH:15:LEU:HD22	35:CH:15:LEU:H	1.60	0.66
5:AE:90:THR:HG22	5:AE:91:GLY:H	1.60	0.66
47:DU:54:GLU:HB3	47:DU:88:LYS:HD2	1.77	0.66
46:CT:73:LYS:HB2	46:CT:106:VAL:HB	1.78	0.66
5:BE:90:THR:HG22	5:BE:91:GLY:H	1.60	0.66
20:BT:9:LYS:O	20:BT:12:ILE:HG13	1.95	0.66
25:D4:8:ARG:HD3	54:DA:245:G:O6	1.96	0.66
48:CV:7:ARG:O	48:CV:25:VAL:HB	1.95	0.66
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.32	0.65
5:AE:157:ARG:HD2	8:AH:43:GLU:O	1.95	0.65
42:DP:39:VAL:HB	42:DP:49:VAL:HG23	1.77	0.65
31:CA:528:A:H2	31:CA:2043:C:H4'	1.57	0.65
1:BA:1323:G:H2'	1:BA:1324:A:C8	2.32	0.65
40:CN:41:LEU:HD21	40:CN:124:LEU:HD22	1.78	0.65
54:DA:1105:U:H2'	54:DA:1106:G:C8	2.30	0.65
39:CM:21:ARG:CG	39:CM:21:ARG:HH21	2.09	0.65
31:CA:528:A:H2'	31:CA:529:A:H5''	1.77	0.65
39:CM:82:LEU:HD11	39:CM:116:VAL:HG23	1.78	0.65
31:CA:2728:U:HO2'	31:CA:2729:G:H8	1.45	0.65
1:AA:1226:C:H2'	13:AM:102:THR:HB	1.80	0.64
31:CA:674:G:H1'	32:CE:69:ARG:HH11	1.62	0.64
31:CA:1311:G:H21	31:CA:1603:A:H62	1.44	0.64
58:DA:3195:PUT:H21	69:DA:5832:HOH:O	1.96	0.64
44:DR:20:GLN:CG	56:DR:202:PG4:H42	2.26	0.64
1:BA:1226:C:H2'	13:BM:102:THR:HB	1.79	0.64
46:DT:73:LYS:HB2	46:DT:106:VAL:HB	1.79	0.64
54:DA:2128:G:H1	54:DA:2160:C:H42	1.44	0.64
26:C5:3:VAL:HG11	31:CA:2539:C:C5'	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:DN:18[B]:ARG:HG3	28:DB:90:C:H5''	1.79	0.63
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.80	0.63
34:CG:80:THR:HG23	34:CG:81:GLU:H	1.62	0.63
54:DA:1853:A:N1	54:DA:2087:G:H1'	2.14	0.63
1:BA:451:A:H2'	69:BA:1701:HOH:O	1.98	0.63
16:BP:20:VAL:HG13	16:BP:32:PHE:HB2	1.81	0.62
7:AG:22:LEU:HD12	7:AG:62:PHE:HE2	1.64	0.62
54:DA:45:G:H5''	54:DA:46:G:H5'	1.82	0.62
16:BP:4:ILE:HG12	16:BP:21:VAL:HG22	1.82	0.62
1:BA:1012:A:H61	1:BA:1017:U:H3	1.48	0.62
31:CA:1131:G:OP1	37:CK:82:GLY:HA2	1.99	0.61
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.81	0.61
33:CF:36:LEU:HD21	33:CF:91:LEU:HD11	1.82	0.61
1:AA:1012:A:H61	1:AA:1017:U:H3	1.49	0.61
48:DV:52:LEU:HB3	48:DV:54:GLN:HB2	1.81	0.61
11:BK:88:GLY:N	11:BK:114:THR:HG22	2.10	0.61
38:CL:43:ILE:HD12	38:CL:56:ASP:HB2	1.82	0.61
41:CO:33:ILE:HD12	41:CO:114:GLU:HB3	1.82	0.61
40:DN:16:ARG:HG3	40:DN:18[B]:ARG:HH11	1.64	0.61
31:CA:45:G:H5''	31:CA:46:G:H5'	1.82	0.61
31:CA:118:A:N3	31:CA:178:G:H1'	2.16	0.60
46:CT:17:VAL:HG11	46:CT:103:ILE:HG12	1.83	0.60
45:DS:83:TYR:CE1	54:DA:1187:G:H5''	2.36	0.60
31:CA:784:G:H5'	31:CA:785:G:OP1	2.01	0.60
40:DN:77:PRO:HG2	40:DN:80:VAL:HG21	1.84	0.60
46:DT:17:VAL:HG11	46:DT:103:ILE:HG12	1.83	0.60
54:DA:2256:G:H21	56:DA:3193:PG4:H31	1.67	0.60
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.37	0.60
3:BC:40:ARG:HH11	3:BC:55:ILE:HG23	1.67	0.60
1:BA:1151:A:HO2'	1:BA:1152:A:H8	1.48	0.60
30:DD:114:LYS:HE2	54:DA:2681:C:OP2	2.02	0.60
17:BQ:68:SER:OG	17:BQ:71:LYS:HB3	2.02	0.60
53:DI:69:PHE:HB3	53:DI:72:LEU:HD12	1.83	0.60
19:AS:15:LEU:HD13	19:AS:33:THR:HG21	1.84	0.60
38:DL:113:MET:CE	38:DL:116:ILE:HD11	2.32	0.60
1:AA:1396:A:H3'	59:AA:1681:TAC:H433	1.84	0.59
31:CA:674:G:H1'	32:CE:69:ARG:HD2	1.85	0.59
42:DP:31:THR:HG21	28:DB:28:C:OP1	2.02	0.59
1:BA:619:U:H3	4:BD:131:ASN:HB3	1.67	0.59
1:BA:1218:C:H2'	1:BA:1219:A:C8	2.37	0.59
48:CV:13:VAL:HG21	48:CV:39:ILE:HG21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DL:43:ILE:HD12	38:DL:56:ASP:HB2	1.84	0.59
3:AC:40:ARG:HG2	3:AC:55:ILE:HG21	1.83	0.59
1:BA:108:G:H5''	1:BA:108:G:N3	2.18	0.59
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	1.85	0.59
53:DI:23:LEU:HD13	53:DI:89:PRO:HD3	1.84	0.59
31:CA:457:A:N1	31:CA:470:A:H5''	2.17	0.59
41:DO:33:ILE:HD12	41:DO:114:GLU:HB3	1.83	0.59
43:DQ:53:ARG:NH2	54:DA:2720:U:OP1	2.36	0.59
39:CM:79:LEU:HD11	39:CM:112:LEU:HD12	1.84	0.59
44:CR:112:LYS:HD3	45:CS:48:LYS:HG3	1.84	0.59
48:CV:45:HIS:HD2	48:CV:58:ILE:HG12	1.68	0.59
48:DV:13:VAL:HG21	48:DV:39:ILE:HG21	1.84	0.59
54:DA:2796:U:H3	54:DA:2799:A:N6	1.92	0.59
31:CA:910:A:H62	40:CN:12:MET:HA	1.67	0.59
31:CA:1638:C:H5''	31:CA:2710:C:O2'	2.03	0.59
1:AA:108:G:N3	1:AA:108:G:H5''	2.17	0.59
4:BD:201:VAL:HG11	5:BE:103:THR:HB	1.85	0.59
13:BM:83:LEU:HD21	19:BS:65:GLU:HB2	1.85	0.59
37:CK:81:ILE:HG23	37:CK:82:GLY:H	1.67	0.59
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.85	0.58
11:BK:23:ILE:HG22	11:BK:32:VAL:HG13	1.86	0.58
50:DX:21:LEU:HD11	50:DX:41[A]:ARG:HE	1.68	0.58
31:CA:974:G:H8	31:CA:990:A:H62	1.52	0.58
31:CA:206:U:H2'	31:CA:207:A:H8	1.69	0.58
30:DD:186:LEU:HD21	43:DQ:4:ILE:HG21	1.85	0.58
11:AK:23:ILE:HG22	11:AK:32:VAL:HG13	1.86	0.58
31:CA:2796:U:H3	31:CA:2799:A:N6	1.94	0.58
54:DA:62:U:O4'	57:DA:3204:MPD:H31	2.03	0.58
50:CX:37:ILE:HG21	50:CX:80:ILE:HG21	1.85	0.58
24:C3:2:LYS:HE2	31:CA:687:C:H5''	1.85	0.58
39:CM:77:ILE:CD1	39:CM:108:ALA:HB1	2.29	0.58
30:DD:99:GLU:HG2	30:DD:182:ALA:HB2	1.86	0.58
50:DX:41[A]:ARG:HH11	50:DX:41[A]:ARG:HG2	1.69	0.58
46:CT:82:MET:HB2	46:CT:98:LYS:HB2	1.85	0.57
48:CV:74:ASN:HD22	48:CV:77:THR:H	1.51	0.57
43:DQ:29:LYS:HB3	43:DQ:40:LEU:HD13	1.85	0.57
46:DT:82:MET:HB2	46:DT:98:LYS:HB2	1.86	0.57
47:DU:80:TRP:HB3	63:DU:101:PGE:H32	1.85	0.57
7:BG:113:ASP:HB2	7:BG:119:ARG:HG3	1.85	0.57
30:DD:140:HIS:HB3	69:DD:487:HOH:O	2.02	0.57
30:CD:4:LEU:HD22	30:CD:101:PHE:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:129:LEU:HD13	2:AB:134:ALA:HB2	1.87	0.57
29:CC:227:PRO:HA	29:CC:233:GLY:HA2	1.86	0.57
35:CH:4:ILE:HD11	35:CH:44:ILE:HG22	1.86	0.57
38:CL:58:LEU:HD11	38:CL:86:LEU:HD13	1.86	0.57
1:BA:1106:G:H5''	3:BC:172:ARG:HG3	1.87	0.57
54:DA:1975:G:H21	63:DA:3225:PGE:C2	2.18	0.57
31:CA:1936:A:H62	31:CA:1963:U:H3	1.50	0.57
50:DX:59:LEU:HD12	50:DX:80:ILE:HD12	1.87	0.57
54:DA:1417:C:H5'	54:DA:1588:G:H1'	1.87	0.57
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.85	0.57
24:D3:19:ARG:HD3	54:DA:125:A:OP2	2.04	0.57
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.51	0.57
5:AE:38:VAL:HG11	5:AE:114:VAL:HG22	1.87	0.57
1:AA:86:G:H21	1:AA:87:C:H41	1.53	0.57
2:AB:20:THR:HG22	2:AB:39:HIS:CE1	2.40	0.57
11:AK:31:ILE:HG12	11:AK:46:THR:HG22	1.86	0.57
1:BA:1277:C:HO2'	1:BA:1279:G:H8	1.53	0.57
17:BQ:17:MET:HB3	17:BQ:20:SER:HB3	1.86	0.57
42:DP:31:THR:HG22	42:DP:34:HIS:H	1.69	0.57
1:AA:774:G:H21	56:AA:1670:PG4:H51	1.70	0.56
11:AK:67:ALA:HB2	11:AK:96:THR:HG23	1.87	0.56
42:CP:31:THR:HG22	42:CP:34:HIS:H	1.69	0.56
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.87	0.56
1:BA:202:G:H1	1:BA:215:C:H42	1.51	0.56
1:BA:686:U:HO2'	1:BA:687:A:H8	1.52	0.56
33:CF:31:VAL:CG1	33:CF:97:TRP:CH2	2.88	0.56
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.88	0.56
1:BA:9:G:H5'	5:BE:108:GLY:HA3	1.86	0.56
2:BB:129:LEU:HD13	2:BB:134:ALA:HB2	1.87	0.56
3:BC:77:ILE:HA	3:BC:84:VAL:HG23	1.87	0.56
30:CD:99:GLU:HG2	30:CD:182:ALA:HB2	1.86	0.56
31:CA:1156:A:H5''	69:CA:3399:HOH:O	2.05	0.56
50:DX:37:ILE:HG21	50:DX:80:ILE:HG21	1.87	0.56
5:BE:88:VAL:HG12	5:BE:93:ARG:HG2	1.86	0.56
31:CA:244:A:H5''	39:CM:67:THR:HG21	1.87	0.56
54:DA:1746:A:H2'	54:DA:1747:U:C6	2.41	0.56
1:AA:81:A:H61	1:AA:86:G:H1	1.54	0.56
6:BF:38:ARG:NH1	6:BF:99:ALA:HB3	2.20	0.56
11:BK:67:ALA:HB2	11:BK:96:THR:HG23	1.87	0.56
29:CC:210:ALA:HA	29:CC:213:TRP:CE2	2.40	0.56
54:DA:526:A:H2'	69:DA:3716:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DA:1975:G:H21	63:DA:3225:PGE:H22	1.70	0.56
25:C4:54:ASP:HB3	39:CM:57:LEU:HD22	1.86	0.56
26:C5:3:VAL:CG1	31:CA:2539:C:H5'	2.31	0.56
11:BK:16:VAL:HG13	11:BK:79:ILE:HG13	1.88	0.56
12:BL:110:ARG:HB2	12:BL:119:VAL:HG21	1.88	0.56
22:D1:4:GLN:HA	54:DA:2615:U:C2	2.41	0.56
36:CJ:19:ASN:H	36:CJ:20:PRO:HD2	1.71	0.56
47:CU:18:GLU:H	47:CU:18:GLU:CD	2.08	0.56
23:C2:25:LYS:HD2	23:C2:52:ALA:HB1	1.87	0.56
38:DL:58:LEU:HD11	38:DL:86:LEU:HD13	1.88	0.56
1:AA:137:U:H3	1:AA:226:G:H1	1.53	0.56
1:AA:209:U:H4'	1:AA:210:C:OP2	2.06	0.56
17:BQ:19:LYS:HG2	17:BQ:49:GLU:HA	1.87	0.56
31:CA:2019:A:H4'	44:CR:34:VAL:HG21	1.88	0.56
40:CN:77:PRO:HG2	40:CN:80:VAL:HG21	1.87	0.56
5:BE:40:GLY:HA2	5:BE:45:ARG:O	2.06	0.55
22:D1:9:THR:CG2	54:DA:2020:A:H5'	2.36	0.55
30:CD:129:THR:HG23	30:CD:140:HIS:O	2.06	0.55
32:DE:189:THR:HG22	32:DE:192:ALA:H	1.71	0.55
1:AA:202:G:H1	1:AA:215:C:H42	1.54	0.55
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.88	0.55
48:DV:45:HIS:HD2	48:DV:58:ILE:HG12	1.71	0.55
1:BA:240:G:H4'	1:BA:240:G:OP1	2.06	0.55
31:CA:396:G:H1'	51:CY:29:PHE:HB3	1.87	0.55
31:CA:2502:G:H5''	31:CA:2503:2MA:H5''	1.89	0.55
32:DE:48:THR:HG22	32:DE:86:ALA:HB3	1.88	0.55
44:DR:6:ARG:NH1	54:DA:585:G:N7	2.53	0.55
6:BF:45:ARG:O	6:BF:56:LYS:HA	2.07	0.55
8:BH:87:LYS:HB2	8:BH:125:ILE:CD1	2.36	0.55
38:CL:35:VAL:HG12	38:CL:106:GLU:HG2	1.87	0.55
50:CX:59:LEU:HD12	50:CX:80:ILE:HD12	1.87	0.55
9:AI:116:VAL:HG21	10:AJ:62:ARG:HB2	1.89	0.55
1:BA:137:U:H3	1:BA:226:G:H1	1.54	0.55
29:CC:88:SER:HB2	29:CC:158:ALA:HB2	1.88	0.55
31:CA:460:A:H5'	47:CU:73:ARG:HH22	1.72	0.55
29:DC:227:PRO:HA	29:DC:233:GLY:HA2	1.87	0.55
36:DJ:19:ASN:H	36:DJ:20:PRO:HD2	1.71	0.55
2:BB:23:TRP:HB3	2:BB:39:HIS:CE1	2.41	0.55
40:DN:16:ARG:HG3	40:DN:18[B]:ARG:NH1	2.22	0.55
1:AA:1329:A:H5''	13:AM:26:GLY:H	1.71	0.55
10:AJ:35:GLN:HB2	10:AJ:77:VAL:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:374:A:H5''	1:BA:452:A:C2	2.41	0.55
12:BL:80:ILE:HD12	12:BL:97:THR:CG2	2.30	0.55
23:D2:35:GLU:HG2	23:D2:50:LYS:HG2	1.89	0.55
31:CA:1028:A:N6	31:CA:1125:G:H2'	2.22	0.55
32:CE:3:LEU:HD12	32:CE:14:VAL:HG11	1.89	0.55
22:D1:54:VAL:HG23	22:D1:55:ILE:HG12	1.89	0.54
31:CA:699:A:H2'	31:CA:700:G:O4'	2.07	0.54
46:CT:66:ILE:HA	46:CT:69:LEU:HD22	1.89	0.54
1:AA:1144:G:H21	1:AA:1146:A:H62	1.54	0.54
31:CA:247:G:H4'	31:CA:386:G:C5	2.41	0.54
31:CA:2043:C:C6	31:CA:2043:C:H5''	2.42	0.54
45:CS:78:ARG:HB2	45:CS:83:TYR:HD1	1.71	0.54
54:DA:789:A:OP1	58:DA:3222:PUT:H11	2.07	0.54
31:CA:822:G:O6	31:CA:943:A:H2	1.89	0.54
31:CA:863:A:H2'	31:CA:864:G:C8	2.42	0.54
54:DA:2065:C:H4'	54:DA:2251:OMG:HM22	1.89	0.54
54:DA:1482:G:H1'	54:DA:1509:A:H61	1.73	0.54
6:AF:45:ARG:O	6:AF:56:LYS:HA	2.07	0.54
1:BA:769:G:H4'	1:BA:1513:A:H4'	1.88	0.54
1:BA:1329:A:H5''	13:BM:26:GLY:H	1.73	0.54
5:BE:106:ILE:HD11	5:BE:124:LEU:HD23	1.88	0.54
28:CB:55:U:H1'	33:CF:26:MET:HG3	1.88	0.54
1:AA:1343:G:H2'	1:AA:1344:C:C6	2.42	0.54
1:BA:1144:G:H21	1:BA:1146:A:H62	1.54	0.54
17:BQ:76:VAL:HG12	17:BQ:77:ARG:HG3	1.89	0.54
63:D1:102:PGE:H4	69:DT:311:HOH:O	2.08	0.54
32:CE:149:ILE:HG12	32:CE:188:MET:HG2	1.90	0.54
52:CZ:56:LEU:HA	52:CZ:59:GLU:HG2	1.89	0.54
54:DA:1180:U:H5''	54:DA:1180:U:H6	1.73	0.54
22:C1:43:ILE:HG22	22:C1:49:TYR:HB2	1.89	0.54
32:DE:3:LEU:HD12	32:DE:14:VAL:HG11	1.90	0.54
41:DO:2:ARG:HG3	54:DA:1653:G:H3'	1.90	0.54
1:AA:412:A:H3'	1:AA:413:G:H5'	1.90	0.54
1:AA:307:C:N4	57:AA:1676:MPD:C1	2.68	0.53
31:CA:550:C:H2'	31:CA:551:G:H5''	1.90	0.53
10:BJ:5:ARG:HG2	10:BJ:79:PRO:HG3	1.90	0.53
30:CD:133:THR:CG2	31:CA:1993:U:H4'	2.38	0.53
31:CA:2425:A:H4'	31:CA:2426:A:O5'	2.08	0.53
31:CA:2815:C:H2'	31:CA:2816:G:O4'	2.08	0.53
33:CF:61:SER:HB2	33:CF:91:LEU:HD21	1.90	0.53
54:DA:1847:A:O2'	54:DA:1848:A:H8	1.78	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:73:C:HO2'	1:AA:74:A:H8	1.56	0.53
12:AL:110:ARG:HB2	12:AL:119:VAL:HG21	1.90	0.53
17:AQ:76:VAL:HG12	17:AQ:77:ARG:HG3	1.89	0.53
47:CU:28:ASN:HD21	47:CU:91:GLN:HB3	1.74	0.53
47:CU:69:ARG:HB2	47:CU:74:ILE:HG22	1.90	0.53
11:AK:84:VAL:HG11	11:AK:97:ILE:HG12	1.90	0.53
22:C1:4:GLN:HA	31:CA:2615:U:C2	2.43	0.53
5:BE:72:ILE:HG13	5:BE:73:ASN:N	2.23	0.53
31:CA:782:A:H5'	31:CA:783:A:C2	2.44	0.53
31:CA:2190:G:H2'	31:CA:2191:A:H8	1.73	0.53
33:DF:61:SER:HB2	33:DF:91:LEU:HD21	1.90	0.53
52:DZ:56:LEU:HA	52:DZ:59:GLU:HG2	1.89	0.53
1:BA:374:A:H5''	1:BA:452:A:N1	2.23	0.53
46:CT:69:LEU:HG	46:CT:107:VAL:HG22	1.91	0.53
22:C1:38:HIS:HE1	31:CA:2884:U:O4	1.91	0.53
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	1.90	0.53
24:D3:2:LYS:HE2	54:DA:687:C:H5''	1.90	0.53
1:AA:404:G:N7	4:AD:2:ALA:HB3	2.23	0.53
7:AG:22:LEU:HD12	7:AG:62:PHE:CE2	2.42	0.53
46:CT:29:VAL:HG22	46:CT:51:LEU:HD11	1.89	0.53
33:DF:132:VAL:HG22	33:DF:152:LEU:HG	1.91	0.53
1:BA:73:C:HO2'	1:BA:74:A:H8	1.55	0.53
5:BE:90:THR:HG22	5:BE:91:GLY:N	2.23	0.53
31:CA:1363:C:H2'	31:CA:1364:G:C8	2.44	0.53
32:CE:189:THR:HG22	32:CE:192:ALA:H	1.73	0.53
33:CF:44:ILE:HG21	33:CF:79:ILE:HG22	1.91	0.53
37:DK:9:GLU:HG2	69:DA:5751:HOH:O	2.09	0.53
4:BD:85:ASN:HA	5:BE:102:GLY:CA	2.34	0.52
34:DG:17:VAL:HG11	34:DG:50:LEU:HD21	1.90	0.52
1:BA:209:U:H4'	1:BA:210:C:OP2	2.08	0.52
11:BK:84:VAL:HG11	11:BK:97:ILE:HG12	1.91	0.52
30:DD:152:PRO:HG3	30:DD:156:PHE:CZ	2.45	0.52
56:DS:202:PG4:H21	69:DS:315:HOH:O	2.09	0.52
54:DA:550:C:H2'	54:DA:551:G:H5''	1.91	0.52
10:AJ:52:LEU:HB2	14:AN:81:ARG:HD2	1.91	0.52
1:BA:12:U:H4'	1:BA:526:C:H4'	1.91	0.52
1:BA:404:G:N7	4:BD:2:ALA:HB3	2.24	0.52
9:BI:19:VAL:HG22	9:BI:65:ILE:HG22	1.91	0.52
34:CG:17:VAL:HG11	34:CG:50:LEU:HD21	1.90	0.52
5:AE:90:THR:HG22	5:AE:91:GLY:N	2.22	0.52
17:BQ:8:LEU:HD23	17:BQ:25:ILE:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DH:4:ILE:HD11	35:DH:44:ILE:HG22	1.91	0.52
53:DI:8:LYS:O	53:DI:12:VAL:HG23	2.09	0.52
1:AA:1126:U:O2	1:AA:1280:A:H5'	2.09	0.52
41:CO:73:ASN:HA	41:CO:76:VAL:HG13	1.92	0.52
33:DF:44:ILE:HG21	33:DF:79:ILE:HG22	1.91	0.52
28:CB:28:C:OP1	42:CP:31:THR:HG21	2.10	0.52
31:CA:2718:G:OP1	43:CQ:98:TYR:HD2	1.93	0.52
32:CE:48:THR:HG22	32:CE:86:ALA:HB3	1.91	0.52
50:DX:18:ALA:HB3	50:DX:20:ARG:NH1	2.24	0.52
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.44	0.52
17:BQ:8:LEU:HD13	17:BQ:73:TRP:CH2	2.45	0.52
54:DA:2291:U:H2'	54:DA:2292:U:C6	2.45	0.52
18:AR:36:SER:HA	18:AR:72:ASP:HB3	1.91	0.52
19:BS:15:LEU:HD13	19:BS:33:THR:HG21	1.91	0.52
31:CA:1274:A:N3	31:CA:1297:C:H1'	2.24	0.52
31:CA:1482:G:H1'	31:CA:1509:A:H61	1.75	0.52
54:DA:551:G:H5''	54:DA:551:G:H8	1.75	0.52
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	1.91	0.52
1:BA:1126:U:O2	1:BA:1280:A:H5'	2.09	0.52
1:BA:1343:G:H2'	1:BA:1344:C:C6	2.44	0.52
31:CA:846:U:H1'	31:CA:847:U:C5	2.40	0.52
31:CA:1636:U:H2'	31:CA:1637:A:C8	2.45	0.52
38:CL:121:GLU:HG2	38:CL:122:VAL:HG23	1.92	0.52
45:DS:16:GLU:HG2	45:DS:100:GLY:HA2	1.92	0.52
9:AI:19:VAL:HG22	9:AI:65:ILE:HG22	1.91	0.51
23:C2:35:GLU:HG2	23:C2:50:LYS:HG2	1.91	0.51
31:CA:566:U:O4	45:CS:80:ARG:HD3	2.10	0.51
54:DA:837:C:H5	69:DA:6614:HOH:O	1.93	0.51
1:AA:673:A:H2'	1:AA:674:G:C8	2.45	0.51
53:DI:132:TYR:H	53:DI:133:GLU:HB2	1.75	0.51
31:CA:784:G:H3'	69:CA:3435:HOH:O	2.10	0.51
31:CA:1363:C:H2'	31:CA:1364:G:H8	1.76	0.51
51:CY:4:VAL:HG22	51:CY:11:ARG:HG3	1.91	0.51
1:AA:686:U:HO2'	1:AA:687:A:H8	1.58	0.51
1:AA:1151:A:O2'	1:AA:1152:A:H8	1.94	0.51
1:BA:1068:G:N7	1:BA:1094:G:H2'	2.25	0.51
33:CF:36:LEU:HB2	33:CF:57:LEU:HD21	1.92	0.51
33:DF:36:LEU:HB2	33:DF:57:LEU:HD21	1.92	0.51
54:DA:793:A:OP1	64:DA:3224:SPD:H81	2.10	0.51
1:AA:528:C:H5''	1:AA:528:C:H6	1.76	0.51
5:AE:107:ALA:HB2	5:AE:125:ALA:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AH:2:SER:HB2	8:AH:4:GLN:HE21	1.76	0.51
10:BJ:52:LEU:HB2	14:BN:81:ARG:HD2	1.92	0.51
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.40	0.51
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.41	0.51
8:AH:87:LYS:HB2	8:AH:125:ILE:CD1	2.39	0.51
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.76	0.51
29:CC:208:ALA:HB2	31:CA:1790:C:O2'	2.11	0.51
39:CM:21:ARG:HH21	39:CM:21:ARG:HG2	1.75	0.51
37:DK:56:VAL:HB	37:DK:124:VAL:HB	1.93	0.51
43:DQ:52:ASN:O	54:DA:2845:U:H5''	2.10	0.51
56:DA:3216:PG4:H31	69:DA:4497:HOH:O	2.11	0.51
13:AM:12:HIS:HB3	69:AM:305:HOH:O	2.10	0.51
31:CA:1810:A:H2'	31:CA:1811:G:O4'	2.08	0.51
40:CN:40:ARG:HD3	40:CN:93:VAL:HG21	1.93	0.51
44:DR:6:ARG:HD3	54:DA:1250:G:C5'	2.41	0.51
54:DA:2273:A:H2'	54:DA:2274:A:C8	2.45	0.51
9:BI:116:VAL:HG21	10:BJ:62:ARG:HB2	1.93	0.51
31:CA:1447:C:H2'	31:CA:1448:G:C8	2.46	0.51
42:DP:68:LYS:HB3	61:DP:201:PEG:H22	1.92	0.51
26:C5:2:LYS:HE3	26:C5:4:ARG:HH11	1.76	0.51
4:BD:177:LYS:HB3	4:BD:179:GLU:HG2	1.92	0.51
53:DI:50:VAL:HG13	53:DI:85:VAL:HG22	1.93	0.51
64:DA:3224:SPD:H82	69:DA:5291:HOH:O	2.10	0.51
13:AM:86:TYR:CZ	13:AM:90:ARG:HD2	2.46	0.50
13:BM:90:ARG:HH21	13:BM:95:LEU:HB3	1.76	0.50
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.47	0.50
32:CE:149:ILE:HD12	32:CE:172:ALA:HA	1.93	0.50
34:DG:164:TYR:HB2	34:DG:167:GLU:HB2	1.93	0.50
1:AA:1328:C:H5''	13:AM:28:THR:HG21	1.93	0.50
4:AD:177:LYS:HB3	4:AD:179:GLU:HG2	1.93	0.50
13:BM:22:ILE:HB	13:BM:25:VAL:HG12	1.93	0.50
41:DO:73:ASN:HA	41:DO:76:VAL:HG13	1.93	0.50
1:BA:1151:A:O2'	1:BA:1152:A:H8	1.94	0.50
1:BA:1518:MA6:H103	1:BA:1519:MA6:C10	2.39	0.50
54:DA:12:U:H6	69:DA:4057:HOH:O	1.93	0.50
1:AA:845:A:O4'	1:AA:845:A:P	2.69	0.50
6:AF:47:LEU:HD13	6:AF:51:ILE:HG12	1.94	0.50
13:AM:90:ARG:HD3	13:AM:97:VAL:HA	1.92	0.50
30:CD:152:PRO:HG3	30:CD:156:PHE:CZ	2.46	0.50
31:CA:792:A:H1'	31:CA:2072:C:O2'	2.11	0.50
33:CF:132:VAL:HG22	33:CF:152:LEU:HG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:781:A:H2'	31:CA:1777:U:O2'	2.11	0.50
30:DD:150[A]:MEQ:HE3	54:DA:2032:G:C8	2.47	0.50
37:CK:81:ILE:CG2	37:CK:82:GLY:H	2.24	0.50
34:DG:86:LYS:HG2	34:DG:132:VAL:HG22	1.93	0.50
46:DT:10:ALA:HB1	46:DT:46:LEU:HD13	1.94	0.50
54:DA:287:G:H1	54:DA:353:C:H42	1.60	0.50
31:CA:1405:U:H2'	31:CA:1406:U:C6	2.47	0.50
31:CA:1809:A:H2'	31:CA:1810:A:C8	2.45	0.50
54:DA:1738:G:HO2'	54:DA:1739:A:H8	1.58	0.50
1:BA:374:A:OP1	1:BA:452:A:N1	2.44	0.50
1:BA:1493:A:H1'	31:CA:1913:A:H61	1.77	0.50
13:BM:86:TYR:CZ	13:BM:90:ARG:HD2	2.46	0.50
31:CA:328:U:O3'	48:CV:66:GLN:HG3	2.11	0.50
35:CH:27:ARG:HH11	51:CY:60:ASP:HA	1.77	0.50
36:DJ:14:ALA:HB3	36:DJ:17:MET:HB2	1.94	0.50
54:DA:2886[A]:A:C2	54:DA:2887[A]:A:H1'	2.46	0.50
1:AA:412:A:H3'	1:AA:413:G:C5'	2.42	0.50
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	1.94	0.50
31:CA:1469:A:H2'	31:CA:1470:A:C8	2.47	0.50
38:CL:76:VAL:HG12	43:CQ:73:VAL:HB	1.93	0.50
13:BM:90:ARG:HD3	13:BM:97:VAL:HA	1.93	0.49
1:BA:202:G:O2'	1:BA:468:A:H8	1.94	0.49
5:BE:81:LEU:HB3	5:BE:147:MET:SD	2.52	0.49
35:CH:94:ILE:HB	35:CH:122:LEU:HB2	1.95	0.49
37:CK:81:ILE:HG23	37:CK:82:GLY:N	2.27	0.49
33:DF:88:LYS:HD3	54:DA:2313:C:H5''	1.93	0.49
1:BA:518:C:H2'	1:BA:530:G:C8	2.48	0.49
1:BA:1328:C:H5''	13:BM:28:THR:HG21	1.95	0.49
31:CA:593:U:H2'	31:CA:594:U:C6	2.47	0.49
54:DA:118:A:N3	54:DA:178:G:H1'	2.26	0.49
54:DA:1172:C:C5	54:DA:1173:U:H1'	2.47	0.49
54:DA:1515:A:H2'	54:DA:1516:G:O4'	2.12	0.49
31:CA:2189:U:H2'	31:CA:2190:G:H8	1.78	0.49
53:DI:64:VAL:HG22	53:DI:69:PHE:HB2	1.95	0.49
1:AA:131:A:H2'	1:AA:132:C:C6	2.48	0.49
1:BA:845:A:O5'	1:BA:845:A:H8	1.96	0.49
5:BE:72:ILE:HG13	5:BE:73:ASN:H	1.77	0.49
31:CA:1847:A:O2'	31:CA:1848:A:H8	1.78	0.49
30:DD:161:MET:HG2	69:DA:6194:HOH:O	2.12	0.49
36:CJ:14:ALA:HB3	36:CJ:17:MET:HB2	1.93	0.49
21:AU:51:SER:HA	21:AU:54:LYS:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:8:A:C6	4:BD:206:LYS:HB3	2.48	0.49
26:D5:25:VAL:HB	26:D5:35:GLN:HB2	1.94	0.49
31:CA:1775:U:O4	31:CA:1789:A:H2	1.95	0.49
20:AT:43:ASP:HB3	20:AT:46:ALA:HB3	1.95	0.49
30:DD:150[A]:MEQ:HG2	69:DA:3634:HOH:O	2.13	0.49
41:CO:95:THR:HG21	41:CO:113:ILE:HD11	1.94	0.49
53:DI:126:LEU:HA	53:DI:129:LEU:HD12	1.94	0.49
54:DA:136:G:H1	54:DA:143:C:H42	1.61	0.49
54:DA:593:U:H2'	54:DA:594:U:C6	2.48	0.49
31:CA:551:G:H5''	31:CA:551:G:H8	1.76	0.49
34:CG:86:LYS:HG2	34:CG:132:VAL:HG22	1.95	0.49
38:CL:103:VAL:O	38:CL:122:VAL:HB	2.13	0.49
6:AF:3:HIS:CE1	6:AF:65:GLU:HG3	2.48	0.49
10:BJ:26:VAL:HG21	10:BJ:39:PRO:HD3	1.95	0.49
11:BK:52:PHE:HE2	11:BK:65:VAL:HG21	1.78	0.49
13:BM:16:VAL:HG13	13:BM:34:LEU:HD12	1.94	0.49
41:DO:55:ALA:HA	41:DO:80:PHE:CE2	2.48	0.49
44:DR:31:VAL:HG13	54:DA:580:U:O3'	2.13	0.49
48:DV:94:ARG:HB3	48:DV:103:ILE:HD12	1.95	0.49
54:DA:2327:A:H2'	54:DA:2328:A:C8	2.48	0.49
54:DA:2813:A:C2	54:DA:2887[B]:A:N6	2.80	0.49
1:AA:439:U:H5''	4:AD:121:LYS:HD2	1.95	0.48
1:AA:1518:MA6:H103	1:AA:1519:MA6:C10	2.37	0.48
2:AB:111:ILE:HD12	2:AB:152:LYS:HA	1.95	0.48
10:AJ:5:ARG:HE	10:AJ:77:VAL:HG22	1.78	0.48
11:AK:16:VAL:HG23	11:AK:79:ILE:HG13	1.94	0.48
1:BA:1190:G:H5'	3:BC:176:HIS:NE2	2.28	0.48
22:D1:24:ALA:HB3	63:D1:102:PGE:H5	1.95	0.48
45:CS:49:ILE:HB	45:CS:51:VAL:O	2.13	0.48
54:DA:12:U:O2	54:DA:12:U:H2'	2.13	0.48
54:DA:572:A:H5''	54:DA:573:U:OP2	2.13	0.48
54:DA:784:G:H5'	54:DA:785:G:OP1	2.13	0.48
54:DA:1536:C:H4'	54:DA:1537:G:H5''	1.94	0.48
1:AA:1277:C:HO2'	1:AA:1279:G:H8	1.61	0.48
54:DA:1773:A:H5''	69:DA:4750:HOH:O	2.12	0.48
6:AF:16:GLU:HB3	4:BD:189:SER:HA	1.95	0.48
11:AK:52:PHE:HE2	11:AK:65:VAL:HG21	1.78	0.48
1:BA:1001:C:H2'	1:BA:1002:G:H8	1.78	0.48
8:BH:2:SER:HB2	8:BH:4:GLN:HE21	1.78	0.48
29:CC:67:PHE:CD1	29:CC:105:LEU:HD11	2.48	0.48
31:CA:1379:U:H5'	31:CA:1379:U:H6	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1956:U:O2	31:CA:1985:C:H4'	2.13	0.48
40:DN:21:ALA:HB1	40:DN:100:LYS:HG2	1.95	0.48
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.79	0.48
3:AC:20:SER:HB3	14:AN:94:PRO:HG3	1.95	0.48
29:CC:3:VAL:HG21	29:CC:202:LEU:HD23	1.96	0.48
31:CA:12:U:H2'	31:CA:12:U:O2	2.14	0.48
29:DC:233:GLY:HA3	69:DC:309:HOH:O	2.12	0.48
33:CF:106:ILE:HD12	33:CF:139:PRO:HG2	1.95	0.48
37:CK:56:VAL:HB	37:CK:124:VAL:HB	1.93	0.48
33:DF:131:GLY:HA3	54:DA:2305:U:H5''	1.95	0.48
35:DH:94:ILE:HB	35:DH:122:LEU:HB2	1.95	0.48
40:DN:18[B]:ARG:HG3	28:DB:90:C:C5'	2.43	0.48
1:AA:413:G:H5''	1:AA:414:A:H5'	1.96	0.48
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	1.96	0.48
32:CE:108:ILE:HG22	39:CM:1:MET:SD	2.54	0.48
36:CJ:103:ARG:HA	36:CJ:106:LEU:HD12	1.95	0.48
42:DP:35:ILE:HG21	42:DP:71:ALA:HA	1.94	0.48
54:DA:1794:A:H2'	54:DA:1795:C:C6	2.47	0.48
54:DA:2628:C:H5'	58:DA:3195:PUT:H11	1.95	0.48
1:AA:1250:A:O3'	9:AI:69:GLY:HA2	2.14	0.48
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.48	0.48
21:AU:4:ILE:HG13	21:AU:19:PHE:HA	1.96	0.48
19:BS:6:LYS:HD2	19:BS:7:LYS:H	1.78	0.48
31:CA:287:G:H1	31:CA:353:C:H42	1.61	0.48
33:DF:106:ILE:HD12	33:DF:139:PRO:HG2	1.94	0.48
1:AA:1346:A:H61	1:AA:1374:A:H3'	1.77	0.48
13:AM:26:GLY:HA2	69:AM:303:HOH:O	2.13	0.48
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	1.95	0.48
31:CA:747:5MU:O2	31:CA:2014:A:H1'	2.14	0.48
36:DJ:103:ARG:HA	36:DJ:106:LEU:HD12	1.95	0.48
26:C5:25:VAL:HB	26:C5:35:GLN:HB2	1.95	0.48
1:BA:131:A:H2'	1:BA:132:C:C6	2.49	0.48
31:CA:136:G:H1	31:CA:143:C:H42	1.62	0.48
31:CA:450:G:H2'	31:CA:451:U:H5''	1.96	0.48
45:CS:16:GLU:HG2	45:CS:100:GLY:HA2	1.95	0.48
53:DI:50:VAL:HG11	53:DI:92:ALA:HB2	1.94	0.48
54:DA:588:U:H2'	54:DA:589:U:C6	2.49	0.48
54:DA:2628:C:H5'	58:DA:3195:PUT:C1	2.44	0.48
1:BA:1493:A:H8	1:BA:1493:A:OP2	1.97	0.48
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.79	0.48
31:CA:323:C:H5'	32:CE:163:ASN:HD21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DS:92:TRP:CZ2	63:DS:201:PGE:H2	2.49	0.48
1:AA:451:A:H61	1:AA:481:G:H5'	1.79	0.48
13:BM:11:ASP:HA	13:BM:45:ILE:HD13	1.94	0.48
13:BM:22:ILE:HB	13:BM:25:VAL:CG1	2.44	0.48
31:CA:538:A:H4'	37:CK:7:LYS:HG2	1.96	0.48
31:CA:674:G:H2'	31:CA:804:A:H61	1.79	0.48
31:CA:796:C:H2'	31:CA:797:G:C8	2.49	0.48
54:DA:2031:A:C6	54:DA:2498:OMC:H1'	2.48	0.48
54:DA:2262:U:H4'	54:DA:2328:A:C2	2.49	0.48
54:DA:2262:U:H4'	54:DA:2328:A:H2	1.79	0.48
29:CC:228:VAL:HG21	69:CA:3410:HOH:O	2.13	0.47
31:CA:1783:A:H5'	31:CA:2608:G:H4'	1.95	0.47
31:CA:2271:G:H2'	31:CA:2272:U:C6	2.49	0.47
35:CH:82:SER:HB2	35:CH:94:ILE:HD11	1.96	0.47
48:DV:17:LYS:HE3	48:DV:40:ASN:HA	1.96	0.47
1:BA:1346:A:H61	1:BA:1374:A:H3'	1.78	0.47
21:BU:4:ILE:HG13	21:BU:19:PHE:HA	1.95	0.47
41:CO:55:ALA:HA	41:CO:80:PHE:CE2	2.49	0.47
42:CP:35:ILE:HG21	42:CP:71:ALA:HA	1.96	0.47
54:DA:1433:A:O2'	54:DA:1434:A:H5'	2.14	0.47
20:AT:24:ARG:HD3	20:AT:24:ARG:N	2.30	0.47
6:BF:47:LEU:HD13	6:BF:51:ILE:HG12	1.96	0.47
34:CG:164:TYR:HB2	34:CG:167:GLU:HB2	1.95	0.47
44:CR:58:ARG:HH11	44:CR:62:ILE:HD11	1.79	0.47
52:CZ:42:LEU:HD23	52:CZ:45:GLN:HE21	1.79	0.47
40:DN:33:LEU:HD13	40:DN:117:PHE:HB3	1.95	0.47
54:DA:1509:A:HO2'	54:DA:1510:G:H8	1.62	0.47
1:AA:1190:G:H5'	3:AC:176:HIS:NE2	2.30	0.47
11:AK:30:THR:HG21	11:AK:92:GLY:HA3	1.97	0.47
31:CA:804:A:H2'	31:CA:806:C:C4	2.49	0.47
53:DI:44:ALA:HB1	53:DI:95:LEU:HD11	1.96	0.47
1:AA:518:C:H2'	1:AA:530:G:C8	2.48	0.47
17:BQ:31:HIS:HE1	17:BQ:33:ILE:HD12	1.79	0.47
31:CA:588:U:H2'	31:CA:589:U:C6	2.49	0.47
31:CA:634:C:H2'	31:CA:635:C:C6	2.50	0.47
31:CA:2822:G:H2'	31:CA:2823:A:H5''	1.97	0.47
29:DC:3:VAL:HG21	29:DC:202:LEU:HD23	1.96	0.47
39:CM:85:VAL:HG11	39:CM:90:VAL:HG22	1.96	0.47
42:DP:9:ARG:HH22	54:DA:2295:C:P	2.38	0.47
44:DR:19:LYS:HD3	56:DR:202:PG4:H22	1.96	0.47
54:DA:2520:C:C6	54:DA:2567:G:H1'	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1305:G:HO2'	1:AA:1306:A:H8	1.63	0.47
17:AQ:15:ASP:HA	17:AQ:21:ILE:HG22	1.96	0.47
2:BB:41:ILE:HD13	2:BB:202:GLY:HA2	1.96	0.47
3:BC:26:THR:HG23	14:BN:76:LYS:HD2	1.96	0.47
22:D1:43:ILE:HG22	22:D1:49:TYR:HB2	1.95	0.47
24:D3:7:PRO:HB2	54:DA:1309:G:H4'	1.95	0.47
31:CA:70:G:H5''	31:CA:112:U:O2	2.14	0.47
31:CA:737:C:H42	31:CA:759:G:H1	1.63	0.47
31:CA:2350:C:H2'	31:CA:2351:G:O4'	2.15	0.47
31:CA:2686:G:H2'	31:CA:2687:U:C6	2.50	0.47
39:CM:19:LEU:HD23	39:CM:31:GLY:O	2.15	0.47
39:CM:28:GLY:O	39:CM:29:LYS:O	2.33	0.47
44:CR:87:SER:HB3	45:CS:52:PRO:HD3	1.96	0.47
49:CW:51:GLN:HG2	49:CW:86:LEU:HD11	1.97	0.47
54:DA:2324:U:H3'	54:DA:2325:G:H5''	1.97	0.47
1:AA:946:A:H2'	1:AA:947:G:C8	2.50	0.47
2:AB:41:ILE:HD13	2:AB:202:GLY:HA2	1.95	0.47
1:BA:10:A:OP2	5:BE:131:THR:HG21	2.15	0.47
1:BA:1391:U:H2'	1:BA:1392:G:C8	2.49	0.47
29:CC:155:ALA:HB2	29:CC:162:VAL:HG23	1.96	0.47
1:BA:214:C:H2'	1:BA:215:C:H6	1.80	0.47
1:BA:946:A:H2'	1:BA:947:G:C8	2.50	0.47
1:BA:957:U:O2	1:BA:959:A:H8	1.98	0.47
31:CA:248:G:H5'	31:CA:250:G:N7	2.29	0.47
31:CA:2623:G:H4'	31:CA:2825:G:H8	1.80	0.47
40:CN:21:ALA:HB1	40:CN:100:LYS:HG2	1.97	0.47
48:CV:94:ARG:HB3	48:CV:103:ILE:HD12	1.97	0.47
54:DA:5:A:H2'	54:DA:6:A:C8	2.50	0.47
22:D1:22:LEU:HD23	61:D1:103:PEG:H31	1.96	0.47
29:CC:75:PRO:HG2	29:CC:97:LYS:HD3	1.97	0.47
31:CA:1182:G:H2'	31:CA:1183:U:O4'	2.15	0.47
31:CA:1914:C:H2'	31:CA:1915:3TD:H6	1.96	0.47
31:CA:2025:C:H2'	31:CA:2026:U:C6	2.50	0.47
31:CA:2328:A:H2'	31:CA:2329:U:C6	2.51	0.47
41:CO:47:VAL:O	41:CO:51:LEU:HD23	2.15	0.47
39:DM:21:ARG:HA	54:DA:811:U:H2'	1.96	0.47
1:AA:620:C:H2'	1:AA:621:A:O4'	2.14	0.46
10:AJ:26:VAL:HG21	10:AJ:39:PRO:HD3	1.97	0.46
11:AK:84:VAL:HG21	11:AK:97:ILE:HG23	1.97	0.46
1:BA:1250:A:O3'	9:BI:69:GLY:HA2	2.15	0.46
1:BA:1356:G:H2'	1:BA:1357:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:976:G:H2'	31:CA:977:G:H8	1.80	0.46
31:CA:1494:A:H2'	31:CA:1495:A:C8	2.50	0.46
31:CA:2327:A:H2'	31:CA:2328:A:C8	2.50	0.46
35:DH:82:SER:HB2	35:DH:94:ILE:HD11	1.95	0.46
54:DA:933:A:H5'	54:DA:934:U:OP2	2.14	0.46
2:AB:129:LEU:H	2:AB:129:LEU:HG	1.54	0.46
1:BA:1069:C:H4'	1:BA:1192:C:O2	2.16	0.46
31:CA:443:A:H2'	32:CE:40:ARG:NH1	2.29	0.46
39:CM:21:ARG:CG	39:CM:21:ARG:NH2	2.76	0.46
54:DA:2128:G:H1	54:DA:2160:C:N4	2.12	0.46
1:AA:429:U:H1'	1:AA:430:A:H5''	1.97	0.46
7:BG:69:VAL:HG23	7:BG:100:ALA:HB1	1.98	0.46
42:CP:7:ARG:HA	42:CP:10:ARG:HE	1.79	0.46
19:AS:32:ARG:HE	19:AS:57:HIS:CE1	2.34	0.46
1:BA:411:A:P	4:BD:26:ARG:HH12	2.38	0.46
1:BA:429:U:H1'	1:BA:430:A:H5''	1.98	0.46
1:BA:1152:A:H2'	1:BA:1153:G:C8	2.51	0.46
31:CA:727:A:H2'	31:CA:728:G:C8	2.50	0.46
31:CA:833:A:H2'	31:CA:834:G:C8	2.50	0.46
29:DC:207:LYS:HB2	54:DA:729:G:C6	2.50	0.46
7:AG:132:GLY:H	7:AG:135:VAL:HG22	1.80	0.46
31:CA:933:A:H5'	31:CA:934:U:OP2	2.16	0.46
31:CA:1386:C:H2'	31:CA:1387:A:C8	2.51	0.46
34:DG:52:PHE:CD1	34:DG:52:PHE:N	2.84	0.46
38:DL:101:GLY:O	38:DL:120:PRO:HD2	2.16	0.46
54:DA:265:A:H4'	54:DA:266:G:OP1	2.16	0.46
54:DA:2895:G:H2'	54:DA:2896:C:C6	2.51	0.46
1:AA:1053:G:H4'	1:AA:1054:C:H5'	1.97	0.46
12:BL:110:ARG:NH2	12:BL:117:TYR:CE2	2.84	0.46
18:BR:36:SER:HA	18:BR:72:ASP:HB3	1.96	0.46
20:BT:44:LYS:HB3	20:BT:87:ALA:HB2	1.98	0.46
42:CP:51:ALA:HB3	42:CP:78:VAL:HG13	1.98	0.46
51:DY:10:LYS:HE3	51:DY:54:LYS:HG2	1.97	0.46
18:BR:41:PRO:HG2	18:BR:44:ILE:HD12	1.97	0.46
29:CC:35:GLU:HG3	29:CC:64:ILE:HD11	1.98	0.46
29:DC:35:GLU:HG3	29:DC:64:ILE:HD11	1.96	0.46
30:DD:121:THR:HB	30:DD:127:PHE:CD2	2.51	0.46
40:CN:33:LEU:HD13	40:CN:117:PHE:HB3	1.97	0.46
44:CR:22:LYS:HE2	44:CR:22:LYS:HA	1.97	0.46
49:DW:51:GLN:HG2	49:DW:86:LEU:HD11	1.98	0.46
54:DA:2243:U:H2'	54:DA:2244:U:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:76:G:H22	1:AA:93:U:H3	1.64	0.46
3:BC:5:VAL:HG21	3:BC:10:ILE:HD13	1.98	0.46
31:CA:686:U:H2'	31:CA:788:A:N1	2.31	0.46
31:CA:2728:U:O2'	31:CA:2729:G:H8	1.98	0.46
31:CA:2788:C:H2'	31:CA:2789:C:C6	2.51	0.46
45:CS:7:SER:HB3	45:CS:12:HIS:HE1	1.79	0.46
54:DA:1168:G:H2'	54:DA:1169:A:O4'	2.15	0.46
1:AA:619:U:C2	4:AD:132:ILE:HD11	2.51	0.46
1:AA:1239:A:H62	1:AA:1299:A:N6	2.14	0.46
14:BN:31:ILE:HG23	14:BN:42:TRP:HZ2	1.81	0.46
23:D2:10:LYS:HE3	23:D2:53:LYS:O	2.16	0.46
31:CA:493:G:H2'	31:CA:494:G:O4'	2.16	0.46
31:CA:2030:6MZ:C2	31:CA:2499:C:H5''	2.46	0.46
31:CA:2353:G:H2'	31:CA:2354:C:O4'	2.15	0.46
38:DL:76:VAL:CG2	54:DA:2684:U:H4'	2.46	0.46
54:DA:493:G:H2'	54:DA:494:G:O4'	2.16	0.46
54:DA:1738:G:O2'	54:DA:1739:A:H8	1.99	0.46
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.51	0.46
31:CA:1510:G:H2'	31:CA:1511:G:O4'	2.16	0.46
31:CA:1638:C:H4'	31:CA:2710:C:O2	2.16	0.46
31:CA:2630:G:O4'	31:CA:2894:G:H1'	2.15	0.46
31:CA:2845:U:H2'	31:CA:2846:G:O4'	2.16	0.46
33:CF:31:VAL:HG11	33:CF:97:TRP:CH2	2.51	0.46
50:DX:11:ARG:HH11	54:DA:2256:G:H4'	1.81	0.46
1:AA:957:U:O2	1:AA:959:A:H8	1.98	0.45
1:AA:1289:A:H3'	1:AA:1290:G:H8	1.82	0.45
8:AH:66:PHE:CD2	8:AH:67:GLN:HG2	2.51	0.45
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.80	0.45
1:BA:439:U:H5''	4:BD:121:LYS:HD2	1.97	0.45
3:BC:20:SER:HB3	14:BN:94:PRO:HG3	1.97	0.45
40:DN:75:GLU:HB2	40:DN:90:GLU:HG3	1.97	0.45
54:DA:68:G:H2'	54:DA:69:C:O4'	2.16	0.45
54:DA:1510:G:H2'	54:DA:1511:G:O4'	2.16	0.45
54:DA:2133:G:H21	54:DA:2158:A:N6	2.14	0.45
3:AC:26:THR:HG23	14:AN:76:LYS:HD2	1.97	0.45
5:AE:15:LEU:HA	5:AE:37:THR:HG22	1.98	0.45
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.97	0.45
13:BM:6:GLY:O	13:BM:7:ILE:HG13	2.15	0.45
30:CD:25:THR:HG21	30:CD:193:VAL:HG22	1.98	0.45
51:CY:10:LYS:HE3	51:CY:54:LYS:HG2	1.96	0.45
50:DX:39:ARG:HD3	69:DX:118:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DA:722:A:H2'	54:DA:723:C:O4'	2.16	0.45
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	1.98	0.45
5:BE:15:LEU:HA	5:BE:37:THR:HG22	1.98	0.45
31:CA:998:C:OP2	44:CR:58:ARG:NH2	2.49	0.45
31:CA:2095:A:H8	31:CA:2095:A:H5''	1.81	0.45
31:CA:2895:G:H2'	31:CA:2896:C:C6	2.51	0.45
54:DA:2547:A:H2'	54:DA:2548:U:C6	2.52	0.45
1:BA:76:G:H22	1:BA:93:U:H3	1.64	0.45
6:BF:99:ALA:O	6:BF:100:SER:HB3	2.16	0.45
31:CA:722:A:H2'	31:CA:723:C:O4'	2.17	0.45
31:CA:969:G:H2'	31:CA:970:U:C6	2.52	0.45
54:DA:1386:C:H2'	54:DA:1387:A:C8	2.51	0.45
54:DA:2328:A:H2'	54:DA:2329:U:C6	2.51	0.45
10:AJ:5:ARG:HG3	10:AJ:77:VAL:HA	1.99	0.45
27:D0:45:ARG:HH12	27:D0:59:GLU:CD	2.20	0.45
31:CA:1936:A:N6	31:CA:1963:U:H3	2.14	0.45
30:DD:150[B]:MEQ:HE2	54:DA:2033:A:O5'	2.16	0.45
54:DA:686:U:H2'	54:DA:788:A:N1	2.31	0.45
54:DA:788:A:H5''	58:DA:3222:PUT:H12	1.99	0.45
12:AL:110:ARG:NH2	12:AL:117:TYR:CE2	2.85	0.45
18:AR:41:PRO:HG2	18:AR:44:ILE:HD12	1.98	0.45
1:BA:451:A:H61	1:BA:481:G:H5'	1.81	0.45
1:BA:545:C:H5'	4:BD:69:GLU:HB2	1.98	0.45
1:BA:1239:A:H62	1:BA:1299:A:N6	2.14	0.45
11:BK:45:ALA:HB3	11:BK:70:CYS:HB2	1.97	0.45
20:BT:48:GLN:HE21	20:BT:83:ILE:HD13	1.81	0.45
31:CA:278:A:N3	31:CA:278:A:H2'	2.32	0.45
38:CL:101:GLY:O	38:CL:120:PRO:HD2	2.15	0.45
1:AA:604:G:H2'	1:AA:605:U:O4'	2.17	0.45
3:AC:7:PRO:HD2	3:AC:184:TYR:CD1	2.51	0.45
1:BA:328:C:H2'	1:BA:328:C:O2	2.17	0.45
4:BD:48:LEU:HD21	4:BD:56:ARG:HG3	1.97	0.45
30:CD:129:THR:CG2	30:CD:140:HIS:O	2.65	0.45
31:CA:1936:A:C2	31:CA:1943:U:N3	2.61	0.45
44:DR:34:VAL:HG21	54:DA:2019:A:H4'	1.98	0.45
54:DA:747:5MU:O2	54:DA:2014:A:H1'	2.17	0.45
54:DA:788:A:H3'	58:DA:3222:PUT:H41	1.98	0.45
54:DA:1494:A:H2'	54:DA:1495:A:C8	2.51	0.45
1:AA:411:A:P	4:AD:26:ARG:HH12	2.40	0.45
1:AA:1239:A:H62	1:AA:1299:A:H62	1.64	0.45
1:BA:972:C:H4'	10:BJ:59:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1003:G:H21	1:BA:1005:A:H5'	1.82	0.45
5:BE:76:LEU:HD21	5:BE:120:VAL:HG22	1.99	0.45
11:BK:30:THR:HG21	11:BK:92:GLY:HA3	1.98	0.45
31:CA:1324:G:H1'	31:CA:1616:A:N6	2.32	0.45
48:CV:45:HIS:CD2	48:CV:58:ILE:HG12	2.50	0.45
33:DF:121:SER:HB2	54:DA:2304:G:H5'	1.98	0.45
42:DP:51:ALA:HB3	42:DP:78:VAL:HG13	1.99	0.45
54:DA:136:G:H1	54:DA:143:C:N4	2.15	0.45
1:AA:528:C:H5''	1:AA:528:C:C6	2.52	0.45
1:BA:49:U:O2	1:BA:362:G:H1'	2.17	0.45
7:BG:132:GLY:H	7:BG:135:VAL:HG22	1.81	0.45
31:CA:639:U:H2'	31:CA:640:C:C6	2.51	0.45
40:DN:14:LYS:HE2	69:DA:3581:HOH:O	2.16	0.45
1:AA:1068:G:N7	1:AA:1094:G:H2'	2.32	0.45
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.82	0.45
1:BA:604:G:H2'	1:BA:605:U:O4'	2.17	0.45
1:BA:1289:A:H3'	1:BA:1290:G:H8	1.81	0.45
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	1.98	0.45
31:CA:2842:G:H2'	31:CA:2843:G:O4'	2.17	0.45
54:DA:278:A:N3	54:DA:278:A:H2'	2.32	0.45
54:DA:825:A:H2'	54:DA:826:U:O4'	2.17	0.45
54:DA:2788:C:H2'	54:DA:2789:C:C6	2.52	0.45
23:C2:15:ALA:HB2	23:C2:47:VAL:HG21	1.99	0.44
1:BA:1081:A:H5'	5:BE:23:LYS:HG3	1.98	0.44
3:BC:47:LEU:HD22	3:BC:76:VAL:HG22	1.99	0.44
9:BI:7:TYR:HE1	9:BI:18:ARG:HB2	1.81	0.44
9:BI:57:MET:HG3	9:BI:61:LEU:HG	1.99	0.44
17:BQ:51:ASN:N	17:BQ:51:ASN:HD22	2.15	0.44
22:D1:25:VAL:HG11	46:DT:38:TYR:HB2	1.99	0.44
29:CC:105:LEU:HD12	29:CC:105:LEU:N	2.30	0.44
31:CA:1327:A:H2'	31:CA:1328:A:O4'	2.17	0.44
54:DA:639:U:H2'	54:DA:640:C:C6	2.52	0.44
1:AA:545:C:H5'	4:AD:69:GLU:HB2	1.98	0.44
20:BT:69:LYS:H	20:BT:69:LYS:HG3	1.54	0.44
31:CA:1214:A:H4'	31:CA:1239:G:H4'	2.00	0.44
54:DA:1101:U:H2'	54:DA:1102:C:C6	2.52	0.44
1:AA:79:G:H22	1:AA:90:C:H42	1.66	0.44
3:AC:5:VAL:HG21	3:AC:10:ILE:HD13	1.98	0.44
4:AD:48:LEU:HD21	4:AD:56:ARG:HG3	2.00	0.44
17:AQ:31:HIS:HE1	17:AQ:33:ILE:HD12	1.81	0.44
23:D2:15:ALA:HB2	23:D2:47:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:CR:58:ARG:NH1	44:CR:62:ILE:HD11	2.32	0.44
54:DA:455:C:N3	54:DA:472:A:H2'	2.31	0.44
7:AG:69:VAL:HG21	7:AG:104:ILE:HD11	1.98	0.44
1:BA:134:G:H2'	1:BA:135:C:O4'	2.18	0.44
1:BA:1069:C:O4'	1:BA:1191:A:H2	2.00	0.44
14:BN:31:ILE:HG23	14:BN:42:TRP:CZ2	2.52	0.44
23:D2:11:LEU:HD21	23:D2:34:LEU:HD23	1.99	0.44
31:CA:320:A:H4'	31:CA:322:A:N7	2.31	0.44
31:CA:1509:A:HO2'	31:CA:1510:G:H8	1.66	0.44
31:CA:2030:6MZ:N3	31:CA:2499:C:H5''	2.33	0.44
31:CA:2339:C:H2'	31:CA:2340:A:C8	2.53	0.44
40:DN:41:LEU:CD2	40:DN:125:PRO:HD2	2.47	0.44
54:DA:2722:G:H2'	54:DA:2723:C:C6	2.53	0.44
54:DA:2747:G:O6	54:DA:2755:C:H5''	2.17	0.44
1:AA:345:C:H5''	43:DQ:34:GLU:O	2.17	0.44
1:AA:1329:A:H5''	13:AM:26:GLY:N	2.33	0.44
9:AI:57:MET:HG3	9:AI:61:LEU:HG	1.99	0.44
2:BB:129:LEU:H	2:BB:129:LEU:HG	1.54	0.44
6:BF:3:HIS:H	6:BF:92:THR:HG23	1.82	0.44
31:CA:136:G:H1	31:CA:143:C:N4	2.16	0.44
34:CG:52:PHE:CD2	34:CG:52:PHE:N	2.86	0.44
40:CN:75:GLU:HB2	40:CN:90:GLU:HG3	2.00	0.44
50:DX:11:ARG:H	50:DX:11:ARG:HE	1.65	0.44
53:DI:132:TYR:N	53:DI:133:GLU:HB2	2.32	0.44
54:DA:2339:C:H2'	54:DA:2340:A:C8	2.53	0.44
11:BK:84:VAL:HG21	11:BK:97:ILE:HG23	1.99	0.44
29:CC:219:THR:O	31:CA:1789:A:H5''	2.17	0.44
31:CA:694:U:OP1	31:CA:1569:A:H1'	2.17	0.44
31:CA:1587:G:H2'	31:CA:1588:G:H8	1.83	0.44
41:CO:28:LEU:HD23	41:CO:48:VAL:HG21	1.99	0.44
39:DM:85:VAL:HB	39:DM:94:THR:HG22	1.99	0.44
45:DS:21:ARG:HH21	56:DS:202:PG4:H71	1.81	0.44
54:DA:1637:A:H5'	54:DA:1760:C:O2'	2.17	0.44
54:DA:2723:C:O5'	54:DA:2723:C:H6	2.01	0.44
1:AA:1003:G:H21	1:AA:1005:A:H5'	1.82	0.44
3:BC:47:LEU:HB3	3:BC:50:ALA:HB3	1.99	0.44
7:BG:69:VAL:HG21	7:BG:104:ILE:HD11	1.99	0.44
30:CD:121:THR:HB	30:CD:127:PHE:CD2	2.53	0.44
31:CA:17:G:H4'	44:CR:25:TYR:HE2	1.81	0.44
31:CA:1434:A:H2'	31:CA:1435:G:C8	2.52	0.44
31:CA:2298:A:C2	31:CA:2321:U:N3	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2394:C:H5''	39:CM:63:LYS:HE2	2.00	0.44
30:DD:55:LYS:HD3	30:DD:60:VAL:HG22	2.00	0.44
35:CH:104:THR:HG22	35:CH:109:GLU:HA	2.00	0.44
53:DI:50:VAL:HG22	53:DI:85:VAL:HG13	1.99	0.44
54:DA:2117:A:H61	54:DA:2171:A:H61	1.66	0.44
21:BU:51:SER:HA	21:BU:54:LYS:HE3	2.00	0.44
31:CA:142:A:H1'	47:CU:1:MET:HB3	1.99	0.44
31:CA:671:C:C5	39:CM:33:ARG:NH2	2.86	0.44
31:CA:1101:U:H2'	31:CA:1102:C:C6	2.52	0.44
31:CA:2074:U:H2'	31:CA:2075:U:C6	2.52	0.44
40:CN:42:THR:HA	40:CN:93:VAL:HG12	2.00	0.44
35:DH:104:THR:HG22	35:DH:109:GLU:HA	1.99	0.44
54:DA:2473:U:O2	54:DA:2473:U:H2'	2.18	0.44
1:AA:240:G:H4'	1:AA:240:G:OP1	2.17	0.44
1:AA:328:C:H2'	1:AA:328:C:O2	2.17	0.44
2:AB:188:ASP:HB2	2:AB:204:ASP:OD2	2.17	0.44
1:BA:677:U:H3	1:BA:713:G:H22	1.66	0.44
1:BA:1432:G:H3'	43:CQ:106:LYS:HE2	1.99	0.44
28:CB:89:U:C6	31:CA:958:U:H2'	2.52	0.44
31:CA:2747:G:O6	31:CA:2755:C:H5''	2.17	0.44
47:DU:33:LYS:HG3	47:DU:80:TRP:CE3	2.52	0.44
54:DA:352:A:H5''	54:DA:352:A:H8	1.82	0.44
1:AA:1152:A:H2'	1:AA:1153:G:C8	2.53	0.43
3:AC:47:LEU:HD22	3:AC:76:VAL:HG22	2.00	0.43
5:AE:133:PRO:O	5:AE:137:VAL:HG13	2.18	0.43
1:BA:1239:A:H62	1:BA:1299:A:H62	1.64	0.43
3:BC:22:TRP:HB3	3:BC:59:ARG:H	1.83	0.43
17:BQ:28:PHE:HD2	17:BQ:37:PHE:HB3	1.83	0.43
48:DV:66:GLN:HG3	54:DA:328:U:O3'	2.17	0.43
54:DA:142:A:H2'	54:DA:143:C:C6	2.52	0.43
54:DA:207:A:H2'	54:DA:208:C:O4'	2.17	0.43
54:DA:1180:U:H5''	54:DA:1180:U:C6	2.52	0.43
22:C1:25:VAL:HG13	22:C1:26:THR:H	1.83	0.43
1:BA:774:G:H21	56:BA:1642:PG4:H62	1.84	0.43
30:DD:25:THR:HG21	30:DD:193:VAL:HG22	2.00	0.43
38:CL:105:ARG:HH21	43:CQ:34:GLU:HG2	1.84	0.43
47:CU:33:LYS:HG3	47:CU:80:TRP:CE3	2.53	0.43
40:DN:42:THR:HG22	40:DN:93:VAL:HG12	1.99	0.43
42:DP:27:VAL:HG21	42:DP:40:ILE:HD12	2.00	0.43
44:DR:19:LYS:HB3	56:DR:202:PG4:H41	2.00	0.43
54:DA:31:C:O3'	54:DA:1238:G:H5''	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:844:G:H2'	1:BA:844:G:N3	2.32	0.43
29:CC:154:LEU:HD13	29:CC:176:LEU:HD21	1.99	0.43
30:CD:35:THR:HG22	30:CD:73:VAL:HG21	1.99	0.43
35:CH:78:VAL:HG21	35:CH:103:VAL:HG22	2.00	0.43
49:DW:51:GLN:HB2	49:DW:57:TYR:OH	2.18	0.43
54:DA:553:G:H2'	54:DA:554:U:O4'	2.18	0.43
1:AA:1358:U:H3	1:AA:1363:A:H62	1.66	0.43
1:BA:1329:A:H5''	13:BM:26:GLY:N	2.33	0.43
31:CA:2473:U:O2	31:CA:2473:U:H2'	2.18	0.43
1:AA:202:G:H21	1:AA:466:A:H61	1.65	0.43
27:C0:2:ALA:CB	27:C0:39:GLU:HB3	2.49	0.43
1:BA:1152:A:H2'	1:BA:1153:G:H8	1.82	0.43
2:BB:188:ASP:HB2	2:BB:204:ASP:OD2	2.18	0.43
28:CB:57:A:C4'	33:CF:27:GLN:HG3	2.49	0.43
28:CB:57:A:O4'	33:CF:27:GLN:HG3	2.17	0.43
31:CA:142:A:H2'	31:CA:143:C:C6	2.53	0.43
31:CA:265:A:H4'	31:CA:266:G:OP1	2.19	0.43
31:CA:2114:A:N6	31:CA:2119:A:H62	2.16	0.43
32:DE:45:ALA:HB3	54:DA:38:A:H5'	2.01	0.43
40:DN:40:ARG:HD3	40:DN:93:VAL:HG21	2.00	0.43
53:DI:94:ARG:HG2	53:DI:127:ALA:HA	2.01	0.43
1:AA:923:A:OP1	5:AE:26:LYS:HG2	2.18	0.43
23:C2:11:LEU:HD21	23:C2:34:LEU:HD23	2.00	0.43
23:C2:37:LYS:HG2	23:C2:48:ILE:HG13	2.01	0.43
1:BA:8:A:H5'	5:BE:125:ALA:O	2.18	0.43
1:BA:322:C:H5	1:BA:328:C:C5	2.36	0.43
13:BM:23:TYR:HD1	13:BM:69:LEU:HD23	1.84	0.43
16:BP:20:VAL:CG1	16:BP:32:PHE:HB2	2.48	0.43
31:CA:459:U:C5	31:CA:469:G:N2	2.87	0.43
31:CA:871:U:H2'	31:CA:872:U:C6	2.53	0.43
30:DD:150[B]:MEQ:HG3	54:DA:2032:G:N3	2.33	0.43
33:CF:103:LEU:HA	33:CF:107:ALA:HB3	2.01	0.43
54:DA:26:G:H1'	54:DA:514:A:N6	2.33	0.43
1:AA:1338:G:H2'	1:AA:1339:A:C8	2.54	0.43
4:AD:27:ALA:HB3	4:AD:30:THR:HG23	2.00	0.43
5:BE:126:LYS:HG2	5:BE:128:TYR:CZ	2.54	0.43
31:CA:532:A:N1	31:CA:2020:A:H1'	2.34	0.43
31:CA:1794:A:H2'	31:CA:1795:C:C6	2.54	0.43
31:CA:2064:C:H2'	31:CA:2065:C:C6	2.53	0.43
54:DA:984:A:N3	54:DA:984:A:H2'	2.33	0.43
54:DA:1778:U:H2'	54:DA:1784:A:N6	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:216:U:H2'	1:AA:217:C:C6	2.53	0.43
11:AK:34:ILE:HG12	11:AK:70:CYS:SG	2.59	0.43
5:BE:88:VAL:CG1	5:BE:93:ARG:HG2	2.48	0.43
19:BS:29:LYS:HB3	19:BS:30:PRO:HD2	2.01	0.43
31:CA:321:U:H5''	32:CE:131:THR:HG23	2.01	0.43
29:DC:155:ALA:HB2	29:DC:162:VAL:HG23	2.00	0.43
32:DE:23:PHE:HE2	32:DE:25:GLU:HG3	1.84	0.43
33:DF:103:LEU:HA	33:DF:107:ALA:HB3	2.00	0.43
54:DA:1469:A:H2'	54:DA:1470:A:C8	2.54	0.43
54:DA:1587:G:H2'	54:DA:1588:G:H8	1.84	0.43
54:DA:2233:U:H2'	54:DA:2234:G:C8	2.54	0.43
1:AA:567:G:H2'	1:AA:568:G:O4'	2.19	0.43
4:BD:27:ALA:HB3	4:BD:30:THR:HG23	2.00	0.43
31:CA:1028:A:H61	31:CA:1125:G:H2'	1.84	0.43
32:CE:75:SER:O	32:CE:78:TRP:HB2	2.18	0.43
49:CW:77:VAL:HG23	49:CW:89:ILE:HG12	2.00	0.43
36:DJ:19:ASN:N	36:DJ:20:PRO:HD2	2.33	0.43
54:DA:644:A:H2'	54:DA:645:C:O4'	2.19	0.43
54:DA:2097:A:H8	54:DA:2097:A:H5''	1.84	0.43
17:AQ:68:SER:OG	17:AQ:71:LYS:HB2	2.19	0.43
25:C4:62:LEU:HB3	25:C4:65:ALA:HB2	2.01	0.43
1:BA:8:A:H1'	5:BE:108:GLY:HA2	2.00	0.43
1:BA:663:A:H5'	1:BA:836:G:OP1	2.19	0.43
29:CC:258:ARG:NH1	29:CC:264:ASP:OD1	2.52	0.43
31:CA:1101:U:H2'	31:CA:1102:C:H6	1.84	0.43
31:CA:1427:A:H4'	31:CA:1428:C:O4'	2.18	0.43
31:CA:1662:U:H3	31:CA:1998:A:H61	1.66	0.43
33:CF:36:LEU:HD12	33:CF:154:ILE:HG12	2.01	0.43
43:DQ:6:LYS:O	43:DQ:10:GLN:HG2	2.19	0.43
47:DU:28:ASN:OD1	47:DU:91:GLN:HB3	2.19	0.43
1:BA:1171:A:H2'	1:BA:1172:C:C6	2.53	0.42
4:BD:28:ILE:HG12	4:BD:34:ILE:HD13	2.01	0.42
29:CC:69:ARG:HB2	29:CC:129:THR:HG21	2.00	0.42
29:CC:160:THR:HG22	29:CC:177:ARG:HG2	1.99	0.42
29:CC:174:LEU:HD21	29:CC:184:VAL:HB	2.00	0.42
34:CG:19:ILE:HG12	34:CG:24:ILE:HG12	2.01	0.42
52:CZ:46:VAL:O	52:CZ:50:VAL:HG23	2.19	0.42
50:DX:41[B]:ARG:HA	50:DX:41[B]:ARG:HD3	1.77	0.42
51:DY:57:ARG:NH1	54:DA:400:G:N7	2.55	0.42
1:AA:268:U:H2'	1:AA:269:C:C6	2.54	0.42
1:AA:1081:A:H5'	5:AE:23:LYS:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1366:C:H2'	1:AA:1367:C:C6	2.54	0.42
5:AE:81:LEU:HB3	5:AE:147:MET:SD	2.59	0.42
13:AM:80:LEU:HD22	13:AM:87:ARG:HB3	2.02	0.42
1:BA:1411:C:H2'	1:BA:1412:C:C6	2.54	0.42
25:D4:13:ARG:HG3	39:DM:63:LYS:HA	2.01	0.42
28:CB:14:U:H2'	28:CB:15:A:C2	2.53	0.42
31:CA:352:A:H8	31:CA:352:A:H5''	1.84	0.42
31:CA:2543:G:H2'	31:CA:2544:G:C8	2.55	0.42
39:CM:77:ILE:HD11	39:CM:108:ALA:CB	2.35	0.42
45:CS:16:GLU:HG3	45:CS:101:ILE:HG12	1.99	0.42
51:DY:7:VAL:HG23	51:DY:51:VAL:HG12	2.00	0.42
54:DA:476:G:H4'	54:DA:502:A:N1	2.34	0.42
54:DA:1026:G:H2'	54:DA:1027:A:C8	2.54	0.42
4:AD:28:ILE:HG12	4:AD:34:ILE:HD13	2.01	0.42
8:AH:94:LYS:HB3	8:AH:117:ARG:HH22	1.85	0.42
10:BJ:10:LEU:HB2	10:BJ:72:ARG:HB2	2.01	0.42
30:DD:35:THR:HG22	30:DD:73:VAL:HG21	2.01	0.42
35:CH:3:VAL:HG12	35:CH:38:PRO:HA	2.00	0.42
45:CS:37:GLU:HB3	45:CS:53:PHE:CD1	2.54	0.42
32:DE:94:GLN:HG2	54:DA:660:C:H5''	2.02	0.42
41:DO:28:LEU:HD23	41:DO:48:VAL:HG21	2.00	0.42
54:DA:2051:A:H8	54:DA:2051:A:OP2	2.02	0.42
1:AA:134:G:H2'	1:AA:135:C:O4'	2.19	0.42
1:AA:663:A:H5'	1:AA:836:G:OP1	2.19	0.42
9:BI:19:VAL:HG11	9:BI:83:ILE:HA	2.02	0.42
9:BI:98:LEU:HB3	9:BI:104:VAL:HG13	2.01	0.42
31:CA:123:G:H4'	31:CA:1376:C:O5'	2.20	0.42
31:CA:948:C:H1'	31:CA:984:A:C8	2.54	0.42
36:CJ:19:ASN:N	36:CJ:20:PRO:HD2	2.33	0.42
37:CK:58:ASN:HA	37:CK:126:ALA:O	2.19	0.42
54:DA:2813:A:H2	54:DA:2887[B]:A:N6	2.17	0.42
1:AA:967:5MC:O3'	9:AI:127:PHE:HE1	2.03	0.42
16:BP:6:LEU:HB3	16:BP:17:TYR:HB3	2.01	0.42
29:CC:208:ALA:CB	31:CA:1790:C:H4'	2.50	0.42
31:CA:478:A:H61	31:CA:500:G:H4'	1.84	0.42
31:CA:2579:C:H2'	31:CA:2580:PSU:O4'	2.19	0.42
47:CU:45:ALA:O	47:CU:49:LYS:HG2	2.19	0.42
49:CW:38:LEU:HD21	49:CW:65:VAL:HG11	2.01	0.42
50:CX:18:ALA:HB3	50:CX:20:ARG:NH1	2.33	0.42
53:DI:130:PRO:HG2	53:DI:134:GLU:HG2	2.01	0.42
6:AF:38:ARG:HE	6:AF:63:ASN:ND2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:34:ILE:HB	11:AK:74:VAL:HG11	2.02	0.42
11:BK:34:ILE:HB	11:BK:74:VAL:HG11	2.01	0.42
30:CD:55:LYS:HD3	30:CD:60:VAL:HG22	2.02	0.42
30:CD:101:PHE:O	30:CD:104:VAL:HG22	2.19	0.42
30:CD:186:LEU:HD21	43:CQ:4:ILE:HG21	2.01	0.42
31:CA:121:G:H4'	31:CA:149:A:H5'	2.02	0.42
31:CA:608:A:H2'	31:CA:609:A:C8	2.55	0.42
43:CQ:6:LYS:O	43:CQ:10:GLN:HG2	2.20	0.42
34:DG:19:ILE:HG12	34:DG:24:ILE:HG12	2.00	0.42
54:DA:191:A:H2'	54:DA:192:C:C6	2.55	0.42
19:AS:29:LYS:HB3	19:AS:30:PRO:HD2	2.02	0.42
1:BA:1338:G:H2'	1:BA:1339:A:C8	2.54	0.42
16:BP:6:LEU:HD23	16:BP:19:VAL:HB	2.00	0.42
31:CA:659:G:H4'	32:CE:95:LYS:HD3	2.02	0.42
31:CA:732:C:H2'	31:CA:733:G:O4'	2.20	0.42
31:CA:785:G:H4'	31:CA:1779:U:H4'	2.00	0.42
31:CA:1539:U:H2'	31:CA:1540:G:C8	2.55	0.42
31:CA:1957:C:H5'	31:CA:1984:G:O2'	2.20	0.42
29:DC:69:ARG:HB2	29:DC:129:THR:HG21	2.01	0.42
35:DH:116:ARG:HH21	35:DH:133:GLN:HB2	1.85	0.42
53:DI:26:VAL:HB	53:DI:83:ALA:HB3	2.00	0.42
54:DA:1168:G:H8	54:DA:1168:G:H5''	1.84	0.42
1:AA:1171:A:H2'	1:AA:1172:C:C6	2.54	0.42
27:C0:6:LYS:HB2	27:C0:58:GLU:HG3	2.02	0.42
1:BA:216:U:H2'	1:BA:217:C:C6	2.54	0.42
1:BA:923:A:OP1	5:BE:26:LYS:HG2	2.19	0.42
23:D2:6:ARG:HG2	23:D2:24:THR:HB	2.02	0.42
31:CA:191:A:H2'	31:CA:192:C:C6	2.55	0.42
31:CA:528:A:H8	31:CA:528:A:H3'	1.84	0.42
31:CA:1703:G:H2'	31:CA:1704:C:C6	2.55	0.42
42:CP:27:VAL:HG21	42:CP:40:ILE:HD12	2.00	0.42
54:DA:1236:G:N7	58:DA:3189:PUT:H41	2.35	0.42
1:AA:202:G:O2'	1:AA:468:A:H8	1.95	0.42
6:AF:9:MET:HG2	6:AF:86:ARG:HB3	2.01	0.42
9:AI:98:LEU:HB3	9:AI:104:VAL:HG13	2.01	0.42
10:AJ:10:LEU:HB2	10:AJ:72:ARG:HB2	2.01	0.42
1:BA:73:C:O2'	1:BA:74:A:H8	2.03	0.42
1:BA:216:U:H4'	1:BA:464:U:H4'	2.02	0.42
11:BK:25:ALA:HA	11:BK:30:THR:HG22	2.02	0.42
13:BM:23:TYR:CD1	13:BM:69:LEU:HD23	2.55	0.42
31:CA:246:C:O2'	31:CA:385:C:H4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DH:78:VAL:HG21	35:DH:103:VAL:HG22	2.02	0.42
45:DS:16:GLU:HG3	45:DS:101:ILE:HG12	2.02	0.42
49:DW:38:LEU:HD21	49:DW:65:VAL:HG11	2.01	0.42
54:DA:1424:G:H21	63:DA:3214:PGE:H32	1.84	0.42
1:AA:932:C:H5'	7:AG:4:ARG:HE	1.84	0.42
1:AA:1048:G:H4'	14:AN:3:LYS:HE2	2.01	0.42
1:BA:1308:U:H2'	1:BA:1309:G:H8	1.85	0.42
31:CA:834:G:H1'	31:CA:2358:A:N3	2.35	0.42
31:CA:1141:U:H4'	31:CA:1142:A:O4'	2.20	0.42
39:DM:57:LEU:HA	39:DM:60:ARG:HG3	2.02	0.42
44:DR:6:ARG:HD3	54:DA:1250:G:H5''	2.02	0.42
54:DA:357:C:H2'	54:DA:358:U:C6	2.55	0.42
54:DA:2479:U:OP1	54:DA:2537:U:H1'	2.20	0.42
1:AA:49:U:O2	1:AA:362:G:H1'	2.20	0.41
1:AA:73:C:O2'	1:AA:74:A:H8	2.02	0.41
1:AA:1396:A:H3'	59:AA:1681:TAC:C43	2.48	0.41
23:C2:6:ARG:HG2	23:C2:24:THR:HB	2.01	0.41
24:C3:19:ARG:HD3	31:CA:125:A:OP2	2.20	0.41
26:C5:4:ARG:HB2	31:CA:2466:C:OP1	2.19	0.41
1:BA:567:G:H2'	1:BA:568:G:O4'	2.18	0.41
1:BA:1347:G:N2	1:BA:1373:G:H2'	2.35	0.41
1:BA:1366:C:H2'	1:BA:1367:C:C6	2.55	0.41
30:CD:155:VAL:HG11	30:CD:161:MET:CE	2.50	0.41
31:CA:2623:G:H4'	31:CA:2825:G:C8	2.55	0.41
32:CE:49:ARG:O	32:CE:74:LYS:HD2	2.20	0.41
32:CE:149:ILE:HG23	32:CE:188:MET:HG2	2.02	0.41
36:CJ:11:LEU:HD22	36:CJ:24:VAL:HG23	2.02	0.41
44:CR:113:ALA:O	44:CR:117:LEU:HD12	2.20	0.41
37:DK:58:ASN:HA	37:DK:126:ALA:O	2.20	0.41
40:DN:92:TRP:HE1	57:DN:201:MPD:HM1	1.83	0.41
42:DP:41:ALA:HB2	42:DP:48:LEU:HD21	2.01	0.41
44:DR:20:GLN:HG3	56:DR:202:PG4:C4	2.40	0.41
54:DA:527:C:H4'	54:DA:528:A:O5'	2.19	0.41
5:AE:76:LEU:HD11	5:AE:120:VAL:HG22	2.01	0.41
27:C0:9:GLN:HB3	27:C0:32:ILE:HA	2.03	0.41
1:BA:716:A:N3	11:BK:119:ASN:O	2.53	0.41
1:BA:1048:G:H4'	14:BN:3:LYS:HE2	2.02	0.41
17:BQ:46:VAL:HG11	17:BQ:61:ILE:CG2	2.50	0.41
17:BQ:47:HIS:HB2	17:BQ:67:LEU:HD13	2.01	0.41
29:CC:76:ALA:HB2	29:CC:96:TYR:CD1	2.55	0.41
31:CA:2544:G:H2'	31:CA:2545:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DC:220:VAL:HG21	54:DA:782:A:N7	2.36	0.41
36:DJ:11:LEU:HD22	36:DJ:24:VAL:HG23	2.03	0.41
45:DS:86:GLN:HG2	69:DS:318:HOH:O	2.20	0.41
54:DA:264:C:O2'	54:DA:265:A:H2'	2.20	0.41
54:DA:871:U:H2'	54:DA:872:U:C6	2.55	0.41
1:BA:268:U:H2'	1:BA:269:C:C6	2.55	0.41
19:BS:33:THR:HG22	19:BS:35:SER:H	1.86	0.41
31:CA:826:U:O2'	39:CM:53:GLY:HA3	2.19	0.41
44:CR:76:TYR:CZ	44:CR:80:ILE:HG13	2.55	0.41
51:CY:12:PRO:HB3	51:CY:30:LEU:HD23	2.02	0.41
34:DG:26:ILE:O	34:DG:79:VAL:HG11	2.20	0.41
1:AA:77:A:H2'	1:AA:78:A:C8	2.56	0.41
1:AA:307:C:C4	57:AA:1676:MPD:H12	2.52	0.41
1:AA:438:U:H5'	4:AD:120:HIS:HB3	2.03	0.41
1:AA:716:A:N3	11:AK:119:ASN:O	2.53	0.41
1:AA:1347:G:N2	1:AA:1373:G:H2'	2.35	0.41
1:BA:79:G:H22	1:BA:90:C:H42	1.67	0.41
1:BA:1402:4OC:H2'	1:BA:1403:C:O4'	2.21	0.41
3:BC:113:ALA:O	3:BC:200:VAL:HG11	2.19	0.41
5:BE:149:SER:HB2	5:BE:151:GLU:HG2	2.02	0.41
29:DC:97:LYS:HA	29:DC:97:LYS:HD3	1.72	0.41
39:CM:95:LEU:HD22	39:CM:100:ILE:HG12	2.02	0.41
35:DH:71:LYS:HB3	35:DH:108:VAL:HG22	2.02	0.41
52:DZ:46:VAL:O	52:DZ:50:VAL:HG23	2.19	0.41
54:DA:2063:C:O2	54:DA:2450:A:N1	2.53	0.41
12:AL:36:ARG:HH11	12:AL:54:ARG:NH1	2.18	0.41
31:CA:511:U:H5''	31:CA:1235:G:H4'	2.03	0.41
29:DC:154:LEU:HD13	29:DC:176:LEU:HD21	2.01	0.41
49:CW:51:GLN:HB2	49:CW:57:TYR:OH	2.21	0.41
33:DF:34:ILE:HG12	33:DF:156:ILE:HG12	2.02	0.41
34:DG:24:ILE:HG21	34:DG:72:LEU:HD21	2.02	0.41
53:DI:65:GLU:HA	53:DI:70:GLU:HG3	2.01	0.41
1:AA:649:A:H2'	1:AA:650:G:O4'	2.20	0.41
5:AE:126:LYS:HG2	5:AE:128:TYR:CZ	2.56	0.41
17:AQ:21:ILE:HD12	17:AQ:23:VAL:CG2	2.50	0.41
1:BA:269:C:H2'	1:BA:270:A:C8	2.56	0.41
1:BA:1530:G:H2'	1:BA:1531:A:C8	2.56	0.41
5:BE:57:PRO:O	5:BE:60:ILE:HG13	2.21	0.41
11:BK:43:GLY:HA3	11:BK:74:VAL:HG12	2.03	0.41
22:D1:25:VAL:HG11	46:DT:38:TYR:CB	2.51	0.41
29:CC:174:LEU:CD2	29:CC:184:VAL:HB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:264:C:O2'	31:CA:265:A:H2'	2.20	0.41
31:CA:594:U:H2'	31:CA:595:C:C6	2.55	0.41
31:CA:729:G:H2'	31:CA:1775:U:H1'	2.02	0.41
31:CA:783:A:H2	31:CA:1778:U:H4'	1.85	0.41
31:CA:1154:G:OP1	44:CR:58:ARG:HD3	2.20	0.41
39:CM:79:LEU:O	39:CM:82:LEU:HG	2.21	0.41
35:DH:3:VAL:HG12	35:DH:38:PRO:HA	2.03	0.41
42:DP:53:THR:HB	42:DP:65:THR:HG22	2.02	0.41
54:DA:1539:U:H2'	54:DA:1540:G:C8	2.55	0.41
54:DA:2698:U:H2'	54:DA:2699:C:C6	2.56	0.41
1:AA:1152:A:H2'	1:AA:1153:G:H8	1.85	0.41
1:AA:1308:U:H2'	1:AA:1309:G:H8	1.85	0.41
10:AJ:80:THR:HG22	10:AJ:82:LYS:H	1.85	0.41
1:BA:310:G:H5''	16:BP:31:ARG:HB2	2.02	0.41
1:BA:591:U:H2'	1:BA:592:G:C8	2.55	0.41
1:BA:1108:G:H5''	3:BC:176:HIS:CE1	2.56	0.41
10:BJ:80:THR:HG22	10:BJ:82:LYS:H	1.86	0.41
27:D0:8:THR:O	27:D0:55:VAL:HA	2.21	0.41
54:DA:121:G:H4'	54:DA:149:A:H5'	2.02	0.41
1:BA:629:A:H2'	1:BA:630:A:O4'	2.21	0.41
2:BB:12:ALA:HB2	2:BB:212:LEU:HD13	2.02	0.41
13:BM:80:LEU:HD22	13:BM:87:ARG:HB3	2.03	0.41
23:D2:39:PHE:HB2	23:D2:46:HIS:CE1	2.56	0.41
31:CA:563:A:H1'	31:CA:2018:G:N2	2.36	0.41
31:CA:845:A:H61	31:CA:932:U:H3	1.68	0.41
31:CA:1779:U:C5	31:CA:1784:A:N7	2.73	0.41
43:DQ:25:THR:HB	43:DQ:88:ARG:HB3	2.03	0.41
54:DA:1720:U:H2'	54:DA:1721:G:O4'	2.20	0.41
54:DA:2070:A:H2'	54:DA:2071:A:O4'	2.21	0.41
1:AA:591:U:H2'	1:AA:592:G:C8	2.55	0.41
1:AA:1402:4OC:H2'	1:AA:1403:C:O4'	2.20	0.41
2:AB:163:VAL:HG11	2:AB:173:ILE:HD11	2.03	0.41
11:AK:25:ALA:HA	11:AK:30:THR:HG22	2.03	0.41
1:BA:202:G:H21	1:BA:466:A:H61	1.67	0.41
1:BA:438:U:H5'	4:BD:120:HIS:HB3	2.02	0.41
29:CC:200:HIS:O	29:CC:203:ARG:HG2	2.21	0.41
31:CA:357:C:H2'	31:CA:358:U:C6	2.55	0.41
31:CA:388:G:N7	31:CA:390:U:H2'	2.35	0.41
31:CA:396:G:C1'	51:CY:29:PHE:HB3	2.49	0.41
31:CA:797:G:H5''	32:CE:55:SER:HB2	2.02	0.41
31:CA:2063:C:O2	31:CA:2450:A:N1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:CN:71:LYS:HB3	40:CN:93:VAL:O	2.20	0.41
32:DE:32:VAL:HG21	39:DM:6:LEU:HD13	2.03	0.41
32:DE:49:ARG:O	32:DE:74:LYS:HD2	2.21	0.41
49:DW:77:VAL:HG23	49:DW:89:ILE:HG12	2.03	0.41
54:DA:2123:G:H2'	54:DA:2124:G:H8	1.85	0.41
54:DA:2813:A:H2	54:DA:2887[B]:A:H61	1.66	0.41
57:DA:3207:MPD:H11	57:DA:3207:MPD:H4	1.99	0.41
1:AA:9:G:H5'	5:AE:108:GLY:HA3	2.03	0.41
1:AA:269:C:H2'	1:AA:270:A:C8	2.55	0.41
1:AA:677:U:H3	1:AA:713:G:H22	1.69	0.41
9:AI:19:VAL:HG11	9:AI:83:ILE:HA	2.02	0.41
20:AT:44:LYS:H	20:AT:44:LYS:HG3	1.54	0.41
4:BD:197:GLU:HA	4:BD:200:ILE:HD12	2.03	0.41
16:BP:40:ASN:O	16:BP:43:ALA:HB2	2.21	0.41
49:CW:63:ILE:CD1	49:CW:72:VAL:HG21	2.50	0.41
45:DS:21:ARG:HH21	56:DS:202:PG4:C7	2.34	0.41
46:DT:17:VAL:HB	46:DT:76:VAL:HG11	2.03	0.41
46:DT:77:ASP:HB3	54:DA:24:G:O2'	2.20	0.41
54:DA:2336:A:N3	54:DA:2385:C:H1'	2.36	0.41
1:AA:629:A:H2'	1:AA:630:A:O4'	2.21	0.40
31:CA:225:C:H2'	31:CA:226:A:O4'	2.21	0.40
31:CA:372:G:H5''	51:CY:61:LYS:HD3	2.03	0.40
31:CA:1181:U:H2'	31:CA:1182:G:C8	2.56	0.40
31:CA:1662:U:O2'	31:CA:2687:U:H5''	2.21	0.40
30:DD:167:ASN:HD21	62:DA:3198:EDO:H11	1.86	0.40
42:DP:103:VAL:HG23	69:DB:307:HOH:O	2.21	0.40
1:AA:322:C:H5	1:AA:328:C:C5	2.38	0.40
1:AA:1463:U:H2'	1:AA:1464:U:C6	2.56	0.40
1:BA:1463:U:H2'	1:BA:1464:U:C6	2.56	0.40
26:D5:2:LYS:HE2	26:D5:4:ARG:HH11	1.86	0.40
30:CD:63:PRO:HG3	31:CA:2787:C:H1'	2.02	0.40
31:CA:2698:U:H2'	31:CA:2699:C:C6	2.56	0.40
32:CE:108:ILE:HG21	32:CE:181:ILE:HD11	2.04	0.40
54:DA:78:U:H2'	54:DA:79:C:C6	2.57	0.40
54:DA:1093:G:H1'	54:DA:1099:G:N2	2.37	0.40
54:DA:1354:A:H2'	54:DA:1355:G:O4'	2.21	0.40
54:DA:2678:C:H2'	54:DA:2679:A:O4'	2.20	0.40
1:AA:244:U:O4	1:AA:906:A:H1'	2.22	0.40
1:AA:920:U:H2'	1:AA:921:U:C6	2.57	0.40
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.56	0.40
1:BA:1411:C:H2'	1:BA:1412:C:H6	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BL:33:VAL:HG22	12:BL:79:VAL:HG22	2.04	0.40
22:D1:24:ALA:HB1	46:DT:35:ILE:HG12	2.03	0.40
29:CC:13:ARG:HD3	31:CA:728:G:H4'	2.03	0.40
31:CA:1808:A:N1	51:CY:28:ARG:HD2	2.36	0.40
29:DC:199:GLU:O	29:DC:202:LEU:HB2	2.22	0.40
35:CH:71:LYS:HB3	35:CH:108:VAL:HG22	2.04	0.40
44:DR:76:TYR:CZ	44:DR:80:ILE:HG13	2.56	0.40
47:DU:33:LYS:HE2	63:DU:101:PGE:C2	2.52	0.40
47:DU:33:LYS:NZ	63:DU:101:PGE:H62	2.36	0.40
47:DU:69:ARG:HG3	47:DU:74:ILE:HG22	2.03	0.40
50:DX:11:ARG:HG2	56:DA:3193:PG4:H12	2.04	0.40
54:DA:909:A:O2'	54:DA:910:A:H5'	2.21	0.40
54:DA:2022:U:H1'	69:DA:3881:HOH:O	2.21	0.40
54:DA:2545:G:N3	54:DA:2565:A:H2	2.20	0.40
3:AC:151:VAL:HG12	3:AC:200:VAL:HG22	2.02	0.40
10:AJ:53:ILE:HG13	14:AN:85:ARG:HD2	2.04	0.40
14:AN:21:PHE:HA	14:AN:25:ALA:HB3	2.02	0.40
14:AN:46:LEU:HA	14:AN:49:GLN:HE21	1.86	0.40
16:AP:6:LEU:HB3	16:AP:17:TYR:HB3	2.02	0.40
1:BA:649:A:H2'	1:BA:650:G:O4'	2.21	0.40
1:BA:1108:G:H5''	3:BC:176:HIS:ND1	2.37	0.40
31:CA:78:U:H2'	31:CA:79:C:C6	2.57	0.40
31:CA:586:A:H5'	32:CE:84:THR:HG21	2.02	0.40
31:CA:2185:U:H2'	31:CA:2186:G:C8	2.57	0.40
31:CA:2305:U:H5''	33:CF:131:GLY:HA3	2.04	0.40
46:CT:17:VAL:HB	46:CT:76:VAL:HG11	2.03	0.40
38:DL:78:ARG:HD3	69:DL:308:HOH:O	2.21	0.40
54:DA:340:A:H2'	54:DA:341:C:O4'	2.22	0.40
63:DA:3001:PGE:H52	69:DA:5960:HOH:O	2.22	0.40
1:AA:1108:G:H5''	3:AC:176:HIS:ND1	2.37	0.40
33:DF:14:LYS:O	33:DF:18:THR:HG22	2.21	0.40
37:DK:7:LYS:HG2	54:DA:538:A:H4'	2.03	0.40
39:DM:123:ARG:HG3	39:DM:143:GLU:HG3	2.04	0.40
54:DA:364:C:H2'	54:DA:365:U:C6	2.57	0.40
54:DA:2324:U:H3'	54:DA:2325:G:C5'	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	207 (93%)	11 (5%)	4 (2%)	8	37
2	BB	222/224 (99%)	208 (94%)	10 (4%)	4 (2%)	8	37
3	AC	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	29	68
3	BC	204/206 (99%)	194 (95%)	7 (3%)	3 (2%)	10	42
4	AD	203/205 (99%)	196 (97%)	6 (3%)	1 (0%)	29	68
4	BD	203/205 (99%)	196 (97%)	6 (3%)	1 (0%)	29	68
5	AE	153/155 (99%)	145 (95%)	7 (5%)	1 (1%)	22	60
5	BE	148/155 (96%)	134 (90%)	8 (5%)	6 (4%)	3	16
6	AF	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
6	BF	98/106 (92%)	93 (95%)	1 (1%)	4 (4%)	3	16
7	AG	149/151 (99%)	134 (90%)	14 (9%)	1 (1%)	22	60
7	BG	149/151 (99%)	137 (92%)	11 (7%)	1 (1%)	22	60
8	AH	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	19	57
8	BH	127/129 (98%)	121 (95%)	4 (3%)	2 (2%)	9	40
9	AI	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
9	BI	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
10	AJ	97/99 (98%)	89 (92%)	6 (6%)	2 (2%)	7	33
10	BJ	96/99 (97%)	76 (79%)	14 (15%)	6 (6%)	1	7
11	AK	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	17	55
11	BK	115/117 (98%)	102 (89%)	12 (10%)	1 (1%)	17	55
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
12	BL	120/123 (98%)	116 (97%)	3 (2%)	1 (1%)	19	57
13	AM	112/114 (98%)	100 (89%)	9 (8%)	3 (3%)	5	26
13	BM	112/114 (98%)	99 (88%)	8 (7%)	5 (4%)	2	14
14	AN	98/100 (98%)	86 (88%)	10 (10%)	2 (2%)	7	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	BN	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	15	53
15	AO	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
15	BO	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	13	48
16	AP	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	12	45
16	BP	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	5	28
17	AQ	78/80 (98%)	71 (91%)	6 (8%)	1 (1%)	12	45
17	BQ	78/80 (98%)	67 (86%)	7 (9%)	4 (5%)	2	12
18	AR	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/79 (98%)	68 (88%)	9 (12%)	0	100	100
19	BS	77/79 (98%)	66 (86%)	10 (13%)	1 (1%)	12	45
20	AT	84/86 (98%)	81 (96%)	2 (2%)	1 (1%)	13	48
20	BT	83/86 (96%)	79 (95%)	2 (2%)	2 (2%)	6	29
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%)	47 (87%)	4 (7%)	3 (6%)	2	10
22	D1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	3	16
23	D2	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
24	C3	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	6	30
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	C4	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	9	40
25	D4	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	9	40
26	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	5	25
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	3	19
27	D0	57/58 (98%)	53 (93%)	4 (7%)	0	100	100
29	CC	269/271 (99%)	250 (93%)	15 (6%)	4 (2%)	10	42
29	DC	269/271 (99%)	250 (93%)	17 (6%)	2 (1%)	22	60
30	CD	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
30	DD	206/209 (99%)	197 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	CE	199/201 (99%)	187 (94%)	9 (4%)	3 (2%)	10	42
32	DE	199/201 (99%)	192 (96%)	6 (3%)	1 (0%)	29	68
33	CF	175/177 (99%)	164 (94%)	10 (6%)	1 (1%)	25	64
33	DF	175/177 (99%)	166 (95%)	7 (4%)	2 (1%)	14	50
34	CG	174/176 (99%)	160 (92%)	10 (6%)	4 (2%)	6	30
34	DG	174/176 (99%)	162 (93%)	11 (6%)	1 (1%)	25	64
35	CH	147/149 (99%)	128 (87%)	14 (10%)	5 (3%)	3	20
35	DH	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	11	43
36	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	4	24
36	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	4	24
37	CK	140/142 (99%)	134 (96%)	4 (3%)	2 (1%)	11	43
37	DK	140/142 (99%)	136 (97%)	3 (2%)	1 (1%)	22	60
38	CL	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	9	39
38	DL	121/123 (98%)	115 (95%)	4 (3%)	2 (2%)	9	39
39	CM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	7	33
39	DM	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	22	60
40	CN	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
40	DN	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
41	CO	118/125 (94%)	111 (94%)	5 (4%)	2 (2%)	9	39
41	DO	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
42	CP	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
42	DP	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
43	CQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	17	55
43	DQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	17	55
44	CR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
44	DR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
45	CS	101/103 (98%)	90 (89%)	8 (8%)	3 (3%)	4	24
45	DS	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	15	53
46	CT	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
46	DT	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
47	CU	91/93 (98%)	85 (93%)	5 (6%)	1 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	DU	91/93 (98%)	84 (92%)	6 (7%)	1 (1%)	14	50
48	CV	100/102 (98%)	89 (89%)	7 (7%)	4 (4%)	3	17
48	DV	100/102 (98%)	94 (94%)	4 (4%)	2 (2%)	7	34
49	CW	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
49	DW	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
50	CX	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
50	DX	75/76 (99%)	73 (97%)	2 (3%)	0	100	100
51	CY	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
51	DY	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
52	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	39
52	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
53	DI	133/135 (98%)	115 (86%)	12 (9%)	6 (4%)	2	14
All	All	11406/11629 (98%)	10673 (94%)	590 (5%)	143 (1%)	12	45

All (143) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE
3	AC	156	ARG
10	AJ	57	VAL
13	AM	5	ALA
17	AQ	82	ALA
23	C2	5	ILE
27	C0	4	THR
2	BB	126	PHE
3	BC	156	ARG
6	BF	98	GLU
10	BJ	38	GLY
10	BJ	57	VAL
10	BJ	91	ASP
13	BM	7	ILE
16	BP	80	LYS
17	BQ	82	ALA
29	CC	158	ALA
32	CE	82	GLY
32	CE	83	VAL
34	CG	119	ALA
34	CG	175	LYS

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Mol	Chain	Res	Type
34	CG	176	LYS
35	CH	10	ALA
36	CJ	19	ASN
37	CK	81	ILE
38	CL	35	VAL
39	CM	29	LYS
39	CM	69	ARG
48	CV	7	ARG
48	CV	16	GLY
35	DH	11	ASN
36	DJ	19	ASN
48	DV	52	LEU
53	DI	91	ALA
7	AG	56	LYS
13	AM	7	ILE
13	AM	105	ASN
14	AN	38	ASP
22	C1	25	VAL
22	C1	27	SER
27	C0	14	ILE
2	BB	95	ARG
3	BC	61	ALA
5	BE	51	GLY
5	BE	103	THR
6	BF	92	THR
12	BL	44	LYS
13	BM	5	ALA
13	BM	105	ASN
13	BM	114	LYS
14	BN	38	ASP
15	BO	88	ARG
19	BS	6	LYS
20	BT	5	LYS
29	CC	233	GLY
29	CC	253	LYS
29	DC	233	GLY
29	DC	253	LYS
34	CG	46	ALA
36	CJ	25	GLY
38	CL	108	ARG
47	CU	89	GLU
48	CV	17	LYS

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Mol	Chain	Res	Type
48	CV	89	ASP
34	DG	46	ALA
36	DJ	25	GLY
38	DL	108	ARG
43	DQ	105	GLY
48	DV	89	ASP
2	AB	95	ARG
4	AD	197	GLU
5	AE	162	GLU
8	AH	66	PHE
11	AK	89	PRO
23	C2	51	GLU
24	C3	45	SER
26	C5	20	ASP
2	BB	127	ASP
5	BE	110	ALA
5	BE	157	ARG
8	BH	66	PHE
10	BJ	36	VAL
10	BJ	95	GLY
11	BK	89	PRO
13	BM	4	ILE
17	BQ	17	MET
17	BQ	70	THR
20	BT	43	ASP
29	CC	197	ASN
32	CE	6	LYS
35	CH	11	ASN
39	CM	36	LYS
41	CO	118	ARG
41	CO	119	SER
32	DE	6	LYS
53	DI	70	GLU
53	DI	109	LYS
53	DI	130	PRO
2	AB	125	THR
2	AB	127	ASP
16	AP	45	GLU
22	C1	26	THR
2	BB	125	THR
4	BD	197	GLU
5	BE	24	THR

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Mol	Chain	Res	Type
6	BF	99	ALA
16	BP	44	SER
35	CH	9	VAL
36	CJ	23	PRO
37	CK	25	LEU
43	CQ	105	GLY
45	CS	43	ASN
45	CS	48	LYS
36	DJ	23	PRO
38	DL	75	SER
45	DS	44	GLY
53	DI	88	HIS
14	AN	21	PHE
20	AT	43	ASP
8	BH	67	GLN
17	BQ	18	GLU
35	CH	8	LYS
52	CZ	62	GLY
37	DK	25	LEU
39	DM	36	LYS
47	DU	89	GLU
53	DI	108	VAL
3	BC	127	ARG
6	BF	94	HIS
7	BG	56	LYS
10	BJ	93	ALA
45	CS	53	PHE
5	BE	105	ILE
35	CH	118	PRO
36	CJ	32	GLY
35	DH	118	PRO
36	DJ	32	GLY
10	AJ	33	GLY
33	CF	62	GLY
33	DF	62	GLY
25	D4	18	GLY
33	DF	176	PRO
25	C4	18	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/186 (100%)	172 (92%)	14 (8%)	13	43
2	BB	186/186 (100%)	172 (92%)	14 (8%)	13	43
3	AC	170/170 (100%)	156 (92%)	14 (8%)	11	39
3	BC	170/170 (100%)	156 (92%)	14 (8%)	11	39
4	AD	172/172 (100%)	165 (96%)	7 (4%)	30	67
4	BD	172/172 (100%)	163 (95%)	9 (5%)	23	59
5	AE	118/118 (100%)	103 (87%)	15 (13%)	4	19
5	BE	113/118 (96%)	91 (80%)	22 (20%)	1	7
6	AF	92/92 (100%)	84 (91%)	8 (9%)	10	37
6	BF	87/92 (95%)	73 (84%)	14 (16%)	2	12
7	AG	124/124 (100%)	109 (88%)	15 (12%)	5	21
7	BG	124/124 (100%)	106 (86%)	18 (14%)	3	15
8	AH	104/104 (100%)	90 (86%)	14 (14%)	4	17
8	BH	104/104 (100%)	88 (85%)	16 (15%)	2	13
9	AI	105/105 (100%)	99 (94%)	6 (6%)	20	56
9	BI	105/105 (100%)	99 (94%)	6 (6%)	20	56
10	AJ	87/87 (100%)	80 (92%)	7 (8%)	12	40
10	BJ	86/87 (99%)	76 (88%)	10 (12%)	5	23
11	AK	90/90 (100%)	90 (100%)	0	100	100
11	BK	90/90 (100%)	84 (93%)	6 (7%)	16	49
12	AL	102/102 (100%)	93 (91%)	9 (9%)	10	36
12	BL	102/102 (100%)	90 (88%)	12 (12%)	5	22
13	AM	92/92 (100%)	84 (91%)	8 (9%)	10	37
13	BM	92/92 (100%)	84 (91%)	8 (9%)	10	37
14	AN	83/83 (100%)	81 (98%)	2 (2%)	49	79
14	BN	83/83 (100%)	80 (96%)	3 (4%)	35	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	76/76 (100%)	69 (91%)	7 (9%)	9	34
15	BO	76/76 (100%)	68 (90%)	8 (10%)	7	27
16	AP	65/65 (100%)	62 (95%)	3 (5%)	27	64
16	BP	65/65 (100%)	61 (94%)	4 (6%)	18	52
17	AQ	74/74 (100%)	66 (89%)	8 (11%)	6	26
17	BQ	74/74 (100%)	63 (85%)	11 (15%)	3	14
18	AR	48/48 (100%)	47 (98%)	1 (2%)	53	82
18	BR	48/48 (100%)	48 (100%)	0	100	100
19	AS	70/70 (100%)	62 (89%)	8 (11%)	5	24
19	BS	70/70 (100%)	65 (93%)	5 (7%)	14	46
20	AT	65/65 (100%)	58 (89%)	7 (11%)	6	26
20	BT	65/65 (100%)	53 (82%)	12 (18%)	1	8
21	AU	48/48 (100%)	46 (96%)	2 (4%)	30	66
21	BU	48/48 (100%)	46 (96%)	2 (4%)	30	66
22	C1	47/47 (100%)	46 (98%)	1 (2%)	53	82
22	D1	47/47 (100%)	47 (100%)	0	100	100
23	C2	45/46 (98%)	43 (96%)	2 (4%)	28	65
23	D2	45/46 (98%)	42 (93%)	3 (7%)	16	49
24	C3	38/38 (100%)	36 (95%)	2 (5%)	22	58
24	D3	38/38 (100%)	36 (95%)	2 (5%)	22	58
25	C4	51/51 (100%)	45 (88%)	6 (12%)	5	22
25	D4	51/51 (100%)	48 (94%)	3 (6%)	19	54
26	C5	34/34 (100%)	31 (91%)	3 (9%)	10	36
26	D5	34/34 (100%)	33 (97%)	1 (3%)	42	76
27	C0	48/48 (100%)	41 (85%)	7 (15%)	3	15
27	D0	49/48 (102%)	43 (88%)	6 (12%)	5	21
29	CC	216/216 (100%)	203 (94%)	13 (6%)	19	53
29	DC	216/216 (100%)	208 (96%)	8 (4%)	34	70
30	CD	163/163 (100%)	159 (98%)	4 (2%)	47	79
30	DD	163/163 (100%)	160 (98%)	3 (2%)	59	85
32	CE	165/165 (100%)	149 (90%)	16 (10%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	DE	165/165 (100%)	159 (96%)	6 (4%)	35	70
33	CF	148/148 (100%)	134 (90%)	14 (10%)	8	32
33	DF	148/148 (100%)	134 (90%)	14 (10%)	8	32
34	CG	137/137 (100%)	134 (98%)	3 (2%)	52	81
34	DG	137/137 (100%)	133 (97%)	4 (3%)	42	76
35	CH	114/114 (100%)	102 (90%)	12 (10%)	7	27
35	DH	114/114 (100%)	105 (92%)	9 (8%)	12	41
36	CJ	104/104 (100%)	99 (95%)	5 (5%)	25	62
36	DJ	104/104 (100%)	99 (95%)	5 (5%)	25	62
37	CK	116/116 (100%)	112 (97%)	4 (3%)	37	72
37	DK	116/116 (100%)	113 (97%)	3 (3%)	46	78
38	CL	103/104 (99%)	95 (92%)	8 (8%)	12	42
38	DL	104/104 (100%)	99 (95%)	5 (5%)	25	62
39	CM	103/103 (100%)	95 (92%)	8 (8%)	12	42
39	DM	103/103 (100%)	100 (97%)	3 (3%)	42	76
40	CN	108/108 (100%)	103 (95%)	5 (5%)	27	64
40	DN	109/108 (101%)	104 (95%)	5 (5%)	27	64
41	CO	100/102 (98%)	93 (93%)	7 (7%)	15	47
41	DO	102/102 (100%)	97 (95%)	5 (5%)	25	61
42	CP	86/87 (99%)	80 (93%)	6 (7%)	15	47
42	DP	87/87 (100%)	84 (97%)	3 (3%)	37	72
43	CQ	99/99 (100%)	95 (96%)	4 (4%)	31	68
43	DQ	99/99 (100%)	98 (99%)	1 (1%)	76	91
44	CR	89/89 (100%)	85 (96%)	4 (4%)	27	64
44	DR	89/89 (100%)	85 (96%)	4 (4%)	27	64
45	CS	84/84 (100%)	77 (92%)	7 (8%)	11	39
45	DS	84/84 (100%)	82 (98%)	2 (2%)	49	79
46	CT	93/93 (100%)	87 (94%)	6 (6%)	17	50
46	DT	93/93 (100%)	89 (96%)	4 (4%)	29	66
47	CU	80/80 (100%)	71 (89%)	9 (11%)	6	24
47	DU	80/80 (100%)	77 (96%)	3 (4%)	33	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	CV	83/83 (100%)	77 (93%)	6 (7%)	14	45
48	DV	83/83 (100%)	79 (95%)	4 (5%)	25	62
49	CW	78/78 (100%)	74 (95%)	4 (5%)	24	60
49	DW	78/78 (100%)	75 (96%)	3 (4%)	33	69
50	CX	56/58 (97%)	53 (95%)	3 (5%)	22	57
50	DX	58/58 (100%)	53 (91%)	5 (9%)	10	37
51	CY	67/67 (100%)	63 (94%)	4 (6%)	19	53
51	DY	67/67 (100%)	65 (97%)	2 (3%)	41	75
52	CZ	54/54 (100%)	50 (93%)	4 (7%)	13	44
52	DZ	54/54 (100%)	53 (98%)	1 (2%)	57	84
53	DI	103/103 (100%)	96 (93%)	7 (7%)	16	48
All	All	9460/9477 (100%)	8810 (93%)	650 (7%)	15	48

All (650) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	23	TRP
2	AB	73	LYS
2	AB	93	ASN
2	AB	105	LYS
2	AB	108	ARG
2	AB	125	THR
2	AB	129	LEU
2	AB	130	THR
2	AB	135	LEU
2	AB	137	ARG
2	AB	147	SER
2	AB	161	LEU
2	AB	205	ASP
2	AB	212	LEU
3	AC	14	ILE
3	AC	21	THR
3	AC	33	LEU
3	AC	46	GLU
3	AC	55	ILE
3	AC	60	PRO
3	AC	75	ILE
3	AC	107	ARG

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Mol	Chain	Res	Type
3	AC	110	GLU
3	AC	168	TYR
3	AC	175	LEU
3	AC	178	LEU
3	AC	185	ASN
3	AC	207	ILE
4	AD	10	LYS
4	AD	17	THR
4	AD	22	LYS
4	AD	26	ARG
4	AD	28	ILE
4	AD	143	VAL
4	AD	194	ASP
5	AE	11	LEU
5	AE	14	LYS
5	AE	43	ASN
5	AE	46	VAL
5	AE	76	LEU
5	AE	78	ASN
5	AE	82	GLN
5	AE	94	VAL
5	AE	101	GLU
5	AE	106	ILE
5	AE	123	VAL
5	AE	126	LYS
5	AE	137	VAL
5	AE	148	ASN
5	AE	149	SER
6	AF	36	ILE
6	AF	39	LEU
6	AF	62	MET
6	AF	69	GLU
6	AF	71	ILE
6	AF	74	LEU
6	AF	89	VAL
6	AF	93	LYS
7	AG	18	PHE
7	AG	22	LEU
7	AG	23	LEU
7	AG	30	LEU
7	AG	36	LYS
7	AG	59	LEU

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Mol	Chain	Res	Type
7	AG	63	GLU
7	AG	76	LYS
7	AG	83	SER
7	AG	92	ARG
7	AG	95	ARG
7	AG	120	LEU
7	AG	131	LYS
7	AG	133	THR
7	AG	142	HIS
8	AH	3	MET
8	AH	13	ARG
8	AH	38	ASN
8	AH	47	GLU
8	AH	52	GLU
8	AH	54	ASP
8	AH	60	GLU
8	AH	63	LEU
8	AH	76	GLN
8	AH	90	ASP
8	AH	96	MET
8	AH	107	SER
8	AH	117	ARG
8	AH	129	VAL
9	AI	11	ARG
9	AI	61	LEU
9	AI	63	LEU
9	AI	66	THR
9	AI	96	SER
9	AI	99	ARG
10	AJ	6	ILE
10	AJ	19	ASP
10	AJ	62	ARG
10	AJ	63	ASP
10	AJ	69	THR
10	AJ	89	ARG
10	AJ	90	LEU
12	AL	24	LEU
12	AL	55	VAL
12	AL	74	LEU
12	AL	82	ILE
12	AL	86	ARG
12	AL	88	LYS

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Mol	Chain	Res	Type
12	AL	110	ARG
12	AL	115	SER
12	AL	121	ARG
13	AM	7	ILE
13	AM	13	LYS
13	AM	27	LYS
13	AM	48	LEU
13	AM	58	ASP
13	AM	63	PHE
13	AM	71	ARG
13	AM	101	ARG
14	AN	59	ARG
14	AN	80	SER
15	AO	2	SER
15	AO	24	SER
15	AO	40	GLN
15	AO	70	LEU
15	AO	84	ARG
15	AO	88	ARG
15	AO	89	ARG
16	AP	36	VAL
16	AP	48	GLU
16	AP	54	LEU
17	AQ	5	ILE
17	AQ	16	LYS
17	AQ	26	GLU
17	AQ	33	ILE
17	AQ	38	ILE
17	AQ	51	ASN
17	AQ	75	LEU
17	AQ	83	VAL
18	AR	66	SER
19	AS	5	LEU
19	AS	7	LYS
19	AS	11	ILE
19	AS	13	LEU
19	AS	27	ASP
19	AS	33	THR
19	AS	37	ARG
19	AS	56	GLN
20	AT	8	LYS
20	AT	23	SER

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Mol	Chain	Res	Type
20	AT	24	ARG
20	AT	44	LYS
20	AT	48	GLN
20	AT	66	LEU
20	AT	85	LYS
21	AU	13	ASP
21	AU	56	HIS
22	C1	10	ARG
23	C2	8	LYS
23	C2	47	VAL
24	C3	1	MET
24	C3	15	SER
25	C4	8	ARG
25	C4	13	ARG
25	C4	31	HIS
25	C4	47	LYS
25	C4	51	SER
25	C4	52	LYS
26	C5	16	ILE
26	C5	20	ASP
26	C5	26	ILE
27	C0	3	LYS
27	C0	5	ILE
27	C0	19	LYS
27	C0	36	VAL
27	C0	39	GLU
27	C0	45	ARG
27	C0	59	GLU
2	BB	23	TRP
2	BB	73	LYS
2	BB	93	ASN
2	BB	105	LYS
2	BB	108	ARG
2	BB	125	THR
2	BB	129	LEU
2	BB	130	THR
2	BB	135	LEU
2	BB	137	ARG
2	BB	147	SER
2	BB	161	LEU
2	BB	205	ASP
2	BB	212	LEU

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Mol	Chain	Res	Type
3	BC	3	GLN
3	BC	14	ILE
3	BC	21	THR
3	BC	33	LEU
3	BC	37	PHE
3	BC	38	LYS
3	BC	46	GLU
3	BC	75	ILE
3	BC	107	ARG
3	BC	110	GLU
3	BC	152	GLU
3	BC	168	TYR
3	BC	185	ASN
3	BC	207	ILE
4	BD	10	LYS
4	BD	17	THR
4	BD	22	LYS
4	BD	26	ARG
4	BD	28	ILE
4	BD	143	VAL
4	BD	173	VAL
4	BD	194	ASP
4	BD	206	LYS
5	BE	11	LEU
5	BE	14	LYS
5	BE	19	ASN
5	BE	24	THR
5	BE	43	ASN
5	BE	46	VAL
5	BE	76	LEU
5	BE	81	LEU
5	BE	82	GLN
5	BE	88	VAL
5	BE	94	VAL
5	BE	101	GLU
5	BE	103	THR
5	BE	114	VAL
5	BE	115	LEU
5	BE	123	VAL
5	BE	126	LYS
5	BE	137	VAL
5	BE	148	ASN

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Mol	Chain	Res	Type
5	BE	149	SER
5	BE	151	GLU
5	BE	159	LYS
6	BF	14	GLN
6	BF	16	GLU
6	BF	36	ILE
6	BF	39	LEU
6	BF	53	LYS
6	BF	62	MET
6	BF	68	GLN
6	BF	69	GLU
6	BF	71	ILE
6	BF	74	LEU
6	BF	79	ARG
6	BF	84	VAL
6	BF	89	VAL
6	BF	93	LYS
7	BG	4	ARG
7	BG	5	ARG
7	BG	10	ARG
7	BG	18	PHE
7	BG	23	LEU
7	BG	30	LEU
7	BG	36	LYS
7	BG	48	GLU
7	BG	50	LEU
7	BG	59	LEU
7	BG	63	GLU
7	BG	92	ARG
7	BG	95	ARG
7	BG	109	ARG
7	BG	120	LEU
7	BG	131	LYS
7	BG	133	THR
7	BG	142	HIS
8	BH	3	MET
8	BH	13	ARG
8	BH	38	ASN
8	BH	47	GLU
8	BH	51	VAL
8	BH	52	GLU
8	BH	60	GLU

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Mol	Chain	Res	Type
8	BH	76	GLN
8	BH	77	ARG
8	BH	80	ARG
8	BH	83	LEU
8	BH	90	ASP
8	BH	96	MET
8	BH	107	SER
8	BH	117	ARG
8	BH	129	VAL
9	BI	11	ARG
9	BI	61	LEU
9	BI	63	LEU
9	BI	66	THR
9	BI	96	SER
9	BI	99	ARG
10	BJ	5	ARG
10	BJ	6	ILE
10	BJ	19	ASP
10	BJ	59	LYS
10	BJ	62	ARG
10	BJ	63	ASP
10	BJ	69	THR
10	BJ	78	GLU
10	BJ	89	ARG
10	BJ	90	LEU
11	BK	18	ASP
11	BK	22	HIS
11	BK	31	ILE
11	BK	38	GLN
11	BK	72	ASP
11	BK	118	HIS
12	BL	4	VAL
12	BL	24	LEU
12	BL	44	LYS
12	BL	55	VAL
12	BL	58	THR
12	BL	74	LEU
12	BL	82	ILE
12	BL	86	ARG
12	BL	88	LYS
12	BL	110	ARG
12	BL	115	SER

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Mol	Chain	Res	Type
12	BL	121	ARG
13	BM	11	ASP
13	BM	16	VAL
13	BM	27	LYS
13	BM	30	SER
13	BM	41	GLU
13	BM	48	LEU
13	BM	54	ASP
13	BM	101	ARG
14	BN	26	GLU
14	BN	59	ARG
14	BN	80	SER
15	BO	2	SER
15	BO	17	ARG
15	BO	24	SER
15	BO	40	GLN
15	BO	64	ARG
15	BO	70	LEU
15	BO	84	ARG
15	BO	88	ARG
16	BP	19	VAL
16	BP	36	VAL
16	BP	46	LYS
16	BP	76	LYS
17	BQ	17	MET
17	BQ	20	SER
17	BQ	21	ILE
17	BQ	26	GLU
17	BQ	28	PHE
17	BQ	33	ILE
17	BQ	38	ILE
17	BQ	40	ARG
17	BQ	51	ASN
17	BQ	67	LEU
17	BQ	75	LEU
19	BS	6	LYS
19	BS	7	LYS
19	BS	11	ILE
19	BS	13	LEU
19	BS	37	ARG
20	BT	5	LYS
20	BT	12	ILE

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Mol	Chain	Res	Type
20	BT	24	ARG
20	BT	27	MET
20	BT	48	GLN
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	56	HIS
23	D2	5	ILE
23	D2	8	LYS
23	D2	47	VAL
24	D3	1	MET
24	D3	15	SER
25	D4	31	HIS
25	D4	47	LYS
25	D4	52	LYS
26	D5	16	ILE
27	D0	10	THR
27	D0	19	LYS
27	D0	25	LEU
27	D0	36	VAL
27	D0	39	GLU
27	D0	58	GLU
29	CC	97	LYS
29	CC	120	VAL
29	CC	130	LEU
29	CC	156	ARG
29	CC	157	SER
29	CC	168	ASP
29	CC	195	VAL
29	CC	202	LEU
29	CC	204	VAL
29	CC	205	LEU
29	CC	221	ARG
29	CC	236	GLU
29	CC	258	ARG
30	CD	4	LEU
30	CD	18	ASP

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Mol	Chain	Res	Type
30	CD	32	ASN
30	CD	95	SER
29	DC	70	ASN
29	DC	97	LYS
29	DC	117	GLN
29	DC	120	VAL
29	DC	130	LEU
29	DC	182	ARG
29	DC	202	LEU
29	DC	236	GLU
30	DD	18	ASP
30	DD	32	ASN
30	DD	95	SER
32	CE	7	ASP
32	CE	12	LEU
32	CE	25	GLU
32	CE	40	ARG
32	CE	44	ARG
32	CE	72	SER
32	CE	78	TRP
32	CE	83	VAL
32	CE	93	SER
32	CE	107	SER
32	CE	122	GLU
32	CE	127	GLU
32	CE	149	ILE
32	CE	152	GLU
32	CE	163	ASN
32	CE	189	THR
33	CF	35	THR
33	CF	36	LEU
33	CF	57	LEU
33	CF	72	LYS
33	CF	80	ARG
33	CF	94	GLU
33	CF	117	LEU
33	CF	123	ASP
33	CF	134	GLU
33	CF	136	ILE
33	CF	141	ILE
33	CF	149	VAL
33	CF	152	LEU

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Mol	Chain	Res	Type
33	CF	174	ASP
34	CG	11	VAL
34	CG	18	LYS
34	CG	155	GLU
35	CH	7	ASP
35	CH	15	LEU
35	CH	21	VAL
35	CH	48	GLU
35	CH	51	ARG
35	CH	53	GLU
35	CH	54	LEU
35	CH	55	GLU
35	CH	58	LEU
35	CH	89	LYS
35	CH	127	GLU
35	CH	145	ASN
36	CJ	13	VAL
36	CJ	28	LEU
36	CJ	53	LEU
36	CJ	55	ILE
36	CJ	113	LYS
37	CK	5	THR
37	CK	106	LYS
37	CK	124	VAL
37	CK	142	ILE
38	CL	35	VAL
38	CL	58	LEU
38	CL	70	ARG
38	CL	76	VAL
38	CL	80	ASP
38	CL	89	ASN
38	CL	108	ARG
38	CL	113	MET
39	CM	2	ARG
39	CM	21	ARG
39	CM	42	SER
39	CM	93	ASN
39	CM	94	THR
39	CM	100	ILE
39	CM	103	ILE
39	CM	120	VAL
40	CN	55	ARG

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Mol	Chain	Res	Type
40	CN	59	ARG
40	CN	75	GLU
40	CN	78	LEU
40	CN	132	THR
41	CO	2	ARG
41	CO	6	SER
41	CO	14	SER
41	CO	33	ILE
41	CO	71	ARG
41	CO	76	VAL
41	CO	95	THR
42	CP	18	LEU
42	CP	31	THR
42	CP	38	GLN
42	CP	48	LEU
42	CP	49	VAL
42	CP	78	VAL
43	CQ	10	GLN
43	CQ	39	ARG
43	CQ	40	LEU
43	CQ	114	LEU
44	CR	5	LYS
44	CR	9	ILE
44	CR	51	ARG
44	CR	52	GLN
45	CS	12	HIS
45	CS	18	GLN
45	CS	45	GLU
45	CS	46	GLU
45	CS	48	LYS
45	CS	51	VAL
45	CS	102	SER
46	CT	7	HIS
46	CT	69	LEU
46	CT	86	MET
46	CT	97	LEU
46	CT	108	SER
46	CT	109	ASP
47	CU	1	MET
47	CU	2	ILE
47	CU	3	ARG
47	CU	27	SER

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Mol	Chain	Res	Type
47	CU	30	ILE
47	CU	49	LYS
47	CU	69	ARG
47	CU	73	ARG
47	CU	93	LEU
48	CV	9	ASP
48	CV	28	VAL
48	CV	29	LEU
48	CV	61	LYS
48	CV	81	ASP
48	CV	98	SER
49	CW	1	MET
49	CW	7	GLU
49	CW	10	LYS
49	CW	61	LEU
50	CX	39	ARG
50	CX	40	GLN
50	CX	82	ILE
51	CY	25	THR
51	CY	35	SER
51	CY	48	THR
51	CY	71	LEU
52	CZ	18	LEU
52	CZ	38	GLN
52	CZ	40	SER
52	CZ	58	ASN
32	DE	12	LEU
32	DE	25	GLU
32	DE	107	SER
32	DE	127	GLU
32	DE	163	ASN
32	DE	189	THR
33	DF	10	ASP
33	DF	35	THR
33	DF	57	LEU
33	DF	72	LYS
33	DF	94	GLU
33	DF	117	LEU
33	DF	120	LYS
33	DF	134	GLU
33	DF	136	ILE
33	DF	141	ILE

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Mol	Chain	Res	Type
33	DF	149	VAL
33	DF	152	LEU
33	DF	158	THR
33	DF	174	ASP
34	DG	11	VAL
34	DG	18	LYS
34	DG	155	GLU
34	DG	168	VAL
35	DH	7	ASP
35	DH	15	LEU
35	DH	21	VAL
35	DH	48	GLU
35	DH	53	GLU
35	DH	54	LEU
35	DH	58	LEU
35	DH	127	GLU
35	DH	145	ASN
36	DJ	13	VAL
36	DJ	28	LEU
36	DJ	53	LEU
36	DJ	55	ILE
36	DJ	113	LYS
37	DK	106	LYS
37	DK	124	VAL
37	DK	142	ILE
38	DL	58	LEU
38	DL	70	ARG
38	DL	80	ASP
38	DL	89	ASN
38	DL	110	GLU
39	DM	2	ARG
39	DM	60	ARG
39	DM	120	VAL
40	DN	6	ARG
40	DN	75	GLU
40	DN	100	LYS
40	DN	126	ILE
40	DN	132	THR
41	DO	2	ARG
41	DO	6	SER
41	DO	14	SER
41	DO	33	ILE

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Mol	Chain	Res	Type
41	DO	76	VAL
42	DP	31	THR
42	DP	49	VAL
42	DP	78	VAL
43	DQ	40	LEU
44	DR	5	LYS
44	DR	9	ILE
44	DR	13	ARG
44	DR	51	ARG
45	DS	38	VAL
45	DS	102	SER
46	DT	1	MET
46	DT	86	MET
46	DT	108	SER
46	DT	109	ASP
47	DU	1	MET
47	DU	3	ARG
47	DU	27	SER
48	DV	28	VAL
48	DV	29	LEU
48	DV	52	LEU
48	DV	61	LYS
49	DW	7	GLU
49	DW	53	LYS
49	DW	61	LEU
50	DX	11	ARG
50	DX	39	ARG
50	DX	41[A]	ARG
50	DX	41[B]	ARG
50	DX	82	ILE
51	DY	25	THR
51	DY	71	LEU
52	DZ	38	GLN
53	DI	7	ASP
53	DI	16	SER
53	DI	31	ARG
53	DI	53	ARG
53	DI	60	LEU
53	DI	64	VAL
53	DI	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	93	ASN
2	AB	120	GLN
2	AB	146	ASN
4	AD	136	GLN
5	AE	89	HIS
6	AF	63	ASN
7	AG	97	ASN
7	AG	142	HIS
8	AH	4	GLN
10	AJ	58	ASN
16	AP	9	HIS
17	AQ	51	ASN
19	AS	57	HIS
20	AT	52	ASN
22	C1	38	HIS
2	BB	39	HIS
2	BB	93	ASN
2	BB	120	GLN
2	BB	146	ASN
3	BC	3	GLN
5	BE	70	ASN
5	BE	89	HIS
6	BF	3	HIS
7	BG	97	ASN
8	BH	4	GLN
16	BP	9	HIS
17	BQ	45	HIS
17	BQ	51	ASN
20	BT	48	GLN
20	BT	52	ASN
32	CE	115	GLN
32	CE	163	ASN
34	CG	38	ASN
36	CJ	43	ASN
45	CS	12	HIS
48	CV	74	ASN
50	CX	57	HIS
52	CZ	45	GLN
34	DG	116	GLN
36	DJ	43	ASN
41	DO	31	HIS
48	DV	54	GLN
53	DI	122	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	255 (16%)	32 (2%)
1	BA	1529/1534 (99%)	255 (16%)	36 (2%)
28	CB	117/120 (97%)	12 (10%)	1 (0%)
28	DB	119/120 (99%)	10 (8%)	0
31	CA	2892/2904 (99%)	468 (16%)	79 (2%)
54	DA	2880/2904 (99%)	397 (13%)	60 (2%)
All	All	9067/9116 (99%)	1397 (15%)	208 (2%)

All (1397) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	28	A
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	69	G
1	AA	70	U
1	AA	71	A
1	AA	72	A
1	AA	74	A
1	AA	80	A
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	94	G
1	AA	95	C

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Mol	Chain	Res	Type
1	AA	108	G
1	AA	120	A
1	AA	128	G
1	AA	130	A
1	AA	131	A
1	AA	137	U
1	AA	141	G
1	AA	142	G
1	AA	144	G
1	AA	149	A
1	AA	159	G
1	AA	163	C
1	AA	168	G
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	250	A
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	298	A
1	AA	306	A
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	346	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	382	A

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Mol	Chain	Res	Type
1	AA	384	G
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	424	G
1	AA	429	U
1	AA	430	A
1	AA	436	C
1	AA	457	G
1	AA	458	U
1	AA	466	A
1	AA	467	U
1	AA	468	A
1	AA	474	G
1	AA	479	U
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	511	C
1	AA	527	G7M
1	AA	531	U
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	564	C
1	AA	568	G
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	579	A
1	AA	615	G
1	AA	632	U
1	AA	633	G
1	AA	650	G
1	AA	653	U
1	AA	661	G

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Mol	Chain	Res	Type
1	AA	665	A
1	AA	682	G
1	AA	695	A
1	AA	702	A
1	AA	703	G
1	AA	723	U
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	814	A
1	AA	815	A
1	AA	817	C
1	AA	818	G
1	AA	821	G
1	AA	828	U
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	873	A
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	932	C
1	AA	934	C
1	AA	935	A
1	AA	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	971	G
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	987	G
1	AA	992	U
1	AA	993	G

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Mol	Chain	Res	Type
1	AA	996	A
1	AA	1004	A
1	AA	1009	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	1052	G
1	AA	1053	G
1	AA	1054	C
1	AA	1055	A
1	AA	1065	U
1	AA	1086	U
1	AA	1094	G
1	AA	1095	U
1	AA	1098	C
1	AA	1101	A
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	1143	G
1	AA	1145	A
1	AA	1146	A
1	AA	1152	A
1	AA	1159	U

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Mol	Chain	Res	Type
1	AA	1160	G
1	AA	1168	U
1	AA	1184	G
1	AA	1196	A
1	AA	1197	A
1	AA	1200	C
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1236	A
1	AA	1238	A
1	AA	1239	A
1	AA	1256	A
1	AA	1257	A
1	AA	1260	G
1	AA	1280	A
1	AA	1281	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	1320	C
1	AA	1323	G
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1379	G
1	AA	1381	U
1	AA	1397	C
1	AA	1398	A
1	AA	1429	A
1	AA	1441	A
1	AA	1446	A
1	AA	1447	A

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Mol	Chain	Res	Type
1	AA	1448	C
1	AA	1451	U
1	AA	1452	C
1	AA	1453	G
1	AA	1475	G
1	AA	1487	G
1	AA	1492	A
1	AA	1497	G
1	AA	1503	A
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1534	A
1	BA	4	U
1	BA	5	U
1	BA	6	G
1	BA	9	G
1	BA	22	G
1	BA	28	A
1	BA	32	A
1	BA	39	G
1	BA	47	C
1	BA	48	C
1	BA	50	A
1	BA	51	A
1	BA	52	C
1	BA	69	G
1	BA	70	U
1	BA	71	A
1	BA	72	A
1	BA	74	A
1	BA	80	A
1	BA	82	G
1	BA	83	C
1	BA	84	U
1	BA	85	U
1	BA	87	C
1	BA	88	U
1	BA	89	U
1	BA	90	C

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Mol	Chain	Res	Type
1	BA	94	G
1	BA	95	C
1	BA	108	G
1	BA	120	A
1	BA	130	A
1	BA	131	A
1	BA	137	U
1	BA	141	G
1	BA	142	G
1	BA	144	G
1	BA	149	A
1	BA	159	G
1	BA	163	C
1	BA	168	G
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	250	A
1	BA	251	G
1	BA	266	G
1	BA	267	C
1	BA	289	G
1	BA	298	A
1	BA	306	A
1	BA	321	A
1	BA	328	C
1	BA	329	A
1	BA	330	C
1	BA	332	G
1	BA	346	G
1	BA	352	C
1	BA	354	G
1	BA	367	U
1	BA	372	C
1	BA	373	A

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Mol	Chain	Res	Type
1	BA	382	A
1	BA	384	G
1	BA	398	U
1	BA	406	G
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	430	A
1	BA	436	C
1	BA	457	G
1	BA	458	U
1	BA	467	U
1	BA	468	A
1	BA	474	G
1	BA	481	G
1	BA	484	G
1	BA	486	U
1	BA	495	A
1	BA	511	C
1	BA	527	G7M
1	BA	528	C
1	BA	531	U
1	BA	532	A
1	BA	533	A
1	BA	547	A
1	BA	559	A
1	BA	562	U
1	BA	564	C
1	BA	568	G
1	BA	572	A
1	BA	573	A
1	BA	576	C
1	BA	577	G
1	BA	579	A
1	BA	615	G
1	BA	632	U
1	BA	633	G
1	BA	650	G

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Mol	Chain	Res	Type
1	BA	653	U
1	BA	661	G
1	BA	665	A
1	BA	682	G
1	BA	695	A
1	BA	702	A
1	BA	703	G
1	BA	723	U
1	BA	734	G
1	BA	748	G
1	BA	755	G
1	BA	777	A
1	BA	793	U
1	BA	794	A
1	BA	812	G
1	BA	814	A
1	BA	815	A
1	BA	817	C
1	BA	818	G
1	BA	821	G
1	BA	828	U
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	844	G
1	BA	845	A
1	BA	846	G
1	BA	873	A
1	BA	914	A
1	BA	926	G
1	BA	927	G
1	BA	934	C
1	BA	935	A
1	BA	960	U
1	BA	966	2MG
1	BA	969	A
1	BA	975	A
1	BA	976	G
1	BA	977	A

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Mol	Chain	Res	Type
1	BA	987	G
1	BA	992	U
1	BA	993	G
1	BA	996	A
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	1030	U
1	BA	1031	C
1	BA	1032	G
1	BA	1033	G
1	BA	1036	A
1	BA	1037	C
1	BA	1043	G
1	BA	1053	G
1	BA	1054	C
1	BA	1055	A
1	BA	1065	U
1	BA	1086	U
1	BA	1094	G
1	BA	1095	U
1	BA	1098	C
1	BA	1101	A
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	1143	G
1	BA	1145	A
1	BA	1146	A

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Mol	Chain	Res	Type
1	BA	1152	A
1	BA	1159	U
1	BA	1160	G
1	BA	1168	U
1	BA	1196	A
1	BA	1197	A
1	BA	1200	C
1	BA	1212	U
1	BA	1213	A
1	BA	1214	C
1	BA	1215	G
1	BA	1225	A
1	BA	1226	C
1	BA	1227	A
1	BA	1236	A
1	BA	1238	A
1	BA	1239	A
1	BA	1256	A
1	BA	1257	A
1	BA	1260	G
1	BA	1280	A
1	BA	1281	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	1320	C
1	BA	1323	G
1	BA	1346	A
1	BA	1353	G
1	BA	1362	A
1	BA	1363	A
1	BA	1370	G
1	BA	1379	G
1	BA	1381	U
1	BA	1397	C
1	BA	1398	A
1	BA	1419	G
1	BA	1429	A

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Mol	Chain	Res	Type
1	BA	1441	A
1	BA	1446	A
1	BA	1447	A
1	BA	1448	C
1	BA	1451	U
1	BA	1452	C
1	BA	1453	G
1	BA	1475	G
1	BA	1487	G
1	BA	1493	A
1	BA	1497	G
1	BA	1503	A
1	BA	1506	U
1	BA	1507	A
1	BA	1517	G
1	BA	1529	G
1	BA	1530	G
1	BA	1534	A
28	CB	9	G
28	CB	25	U
28	CB	35	C
28	CB	44	G
28	CB	45	A
28	CB	56	G
28	CB	57	A
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	14	A
31	CA	34	U
31	CA	39	G
31	CA	42	A
31	CA	46	G
31	CA	49	A
31	CA	58	G
31	CA	61	C
31	CA	63	A
31	CA	71	A
31	CA	74	A

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Mol	Chain	Res	Type
31	CA	75	G
31	CA	80	G
31	CA	83	A
31	CA	84	A
31	CA	101	A
31	CA	102	U
31	CA	118	A
31	CA	119	A
31	CA	120	U
31	CA	125	A
31	CA	138	U
31	CA	139	U
31	CA	140	C
31	CA	141	G
31	CA	142	A
31	CA	143	C
31	CA	165	A
31	CA	177	G
31	CA	178	G
31	CA	188	G
31	CA	196	A
31	CA	197	A
31	CA	199	A
31	CA	215	G
31	CA	216	A
31	CA	221	A
31	CA	222	A
31	CA	248	G
31	CA	264	C
31	CA	265	A
31	CA	266	G
31	CA	272	A
31	CA	276	U
31	CA	277	G
31	CA	278	A
31	CA	279	A
31	CA	285	G
31	CA	311	A
31	CA	329	G
31	CA	330	A
31	CA	343	C
31	CA	346	A

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Mol	Chain	Res	Type
31	CA	352	A
31	CA	353	C
31	CA	362	A
31	CA	370	G
31	CA	371	A
31	CA	372	G
31	CA	385	C
31	CA	386	G
31	CA	399	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	451	U
31	CA	455	C
31	CA	480	A
31	CA	481	G
31	CA	491	G
31	CA	503	A
31	CA	504	A
31	CA	505	A
31	CA	508	A
31	CA	513	A
31	CA	532	A
31	CA	543	G
31	CA	544	C
31	CA	546	U
31	CA	547	A
31	CA	549	G
31	CA	550	C
31	CA	551	G
31	CA	555	G
31	CA	556	A
31	CA	563	A
31	CA	573	U
31	CA	575	A
31	CA	586	A
31	CA	603	A
31	CA	613	A
31	CA	614	A

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Mol	Chain	Res	Type
31	CA	615	U
31	CA	622	G
31	CA	627	A
31	CA	637	A
31	CA	645	C
31	CA	647	G
31	CA	653	U
31	CA	654	A
31	CA	655	A
31	CA	670	A
31	CA	684	G
31	CA	685	A
31	CA	686	U
31	CA	695	G
31	CA	717	C
31	CA	723	C
31	CA	730	A
31	CA	740	C
31	CA	747	5MU
31	CA	775	G
31	CA	776	G
31	CA	782	A
31	CA	784	G
31	CA	785	G
31	CA	792	A
31	CA	798	G
31	CA	802	A
31	CA	805	G
31	CA	812	C
31	CA	819	A
31	CA	827	U
31	CA	828	U
31	CA	845	A
31	CA	846	U
31	CA	847	U
31	CA	858	G
31	CA	859	G
31	CA	878	A
31	CA	883	G
31	CA	896	A
31	CA	897	C
31	CA	910	A

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Mol	Chain	Res	Type
31	CA	931	U
31	CA	932	U
31	CA	941	A
31	CA	946	C
31	CA	953	G
31	CA	961	C
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	1005	C
31	CA	1012	U
31	CA	1013	C
31	CA	1022	G
31	CA	1026	G
31	CA	1033	U
31	CA	1040	A
31	CA	1046	A
31	CA	1047	G
31	CA	1057	A
31	CA	1061	U
31	CA	1062	G
31	CA	1070	A
31	CA	1073	A
31	CA	1083	U
31	CA	1088	A
31	CA	1089	A
31	CA	1090	A
31	CA	1096	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	1134	A
31	CA	1135	C

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Mol	Chain	Res	Type
31	CA	1136	G
31	CA	1142	A
31	CA	1168	G
31	CA	1169	A
31	CA	1170	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	1206	G
31	CA	1210	G
31	CA	1212	G
31	CA	1227	G
31	CA	1236	G
31	CA	1238	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	1273	U
31	CA	1300	G
31	CA	1301	A
31	CA	1313	U
31	CA	1321	A
31	CA	1329	U
31	CA	1342	A
31	CA	1344	U
31	CA	1352	U
31	CA	1365	A
31	CA	1379	U
31	CA	1380	G
31	CA	1383	A
31	CA	1395	A
31	CA	1416	G
31	CA	1417	C
31	CA	1419	A
31	CA	1420	A
31	CA	1428	C

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Mol	Chain	Res	Type
31	CA	1437	C
31	CA	1438	U
31	CA	1452	G
31	CA	1453	A
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	1523	U
31	CA	1532	A
31	CA	1534	U
31	CA	1535	A
31	CA	1536	C
31	CA	1537	G
31	CA	1565	C
31	CA	1567	G
31	CA	1568	G
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	1609	A
31	CA	1611	C
31	CA	1616	A
31	CA	1632	A
31	CA	1647	U
31	CA	1648	U
31	CA	1649	G
31	CA	1669	A
31	CA	1674	G
31	CA	1675	C
31	CA	1715	G

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Mol	Chain	Res	Type
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	1764	C
31	CA	1773	A
31	CA	1782	U
31	CA	1800	C
31	CA	1801	A
31	CA	1808	A
31	CA	1812	U
31	CA	1816	C
31	CA	1823	G
31	CA	1828	G
31	CA	1829	A
31	CA	1834	U
31	CA	1869	G
31	CA	1870	C
31	CA	1871	A
31	CA	1872	A
31	CA	1873	G
31	CA	1882	U
31	CA	1900	A
31	CA	1903	G
31	CA	1906	G
31	CA	1907	G
31	CA	1914	C
31	CA	1929	G
31	CA	1930	G
31	CA	1931	U
31	CA	1937	A
31	CA	1938	A
31	CA	1955	U
31	CA	1967	C
31	CA	1970	A
31	CA	1972	G
31	CA	1975	G
31	CA	1991	U
31	CA	1993	U
31	CA	1997	C

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Mol	Chain	Res	Type
31	CA	2006	C
31	CA	2022	U
31	CA	2023	C
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	2055	C
31	CA	2056	G
31	CA	2060	A
31	CA	2061	G
31	CA	2062	A
31	CA	2069	G7M
31	CA	2072	C
31	CA	2080	A
31	CA	2092	U
31	CA	2093	G
31	CA	2095	A
31	CA	2100	G
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	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	2146	C
31	CA	2147	A

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Mol	Chain	Res	Type
31	CA	2157	G
31	CA	2158	A
31	CA	2159	G
31	CA	2162	G
31	CA	2164	C
31	CA	2165	C
31	CA	2171	A
31	CA	2172	U
31	CA	2173	A
31	CA	2174	C
31	CA	2183	A
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	2259	U
31	CA	2268	A
31	CA	2278	A
31	CA	2280	G
31	CA	2283	C
31	CA	2287	A
31	CA	2305	U
31	CA	2311	A
31	CA	2322	A
31	CA	2325	G
31	CA	2326	C
31	CA	2327	A
31	CA	2331	G
31	CA	2333	A
31	CA	2334	U
31	CA	2335	A
31	CA	2345	G
31	CA	2347	C
31	CA	2350	C
31	CA	2354	C
31	CA	2361	G
31	CA	2383	G

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Mol	Chain	Res	Type
31	CA	2385	C
31	CA	2402	U
31	CA	2403	C
31	CA	2406	A
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	2441	U
31	CA	2448	A
31	CA	2465	C
31	CA	2469	A
31	CA	2474	U
31	CA	2476	A
31	CA	2484	G
31	CA	2491	U
31	CA	2502	G
31	CA	2505	G
31	CA	2518	A
31	CA	2529	G
31	CA	2535	G
31	CA	2547	A
31	CA	2554	U
31	CA	2556	C
31	CA	2566	A
31	CA	2567	G
31	CA	2573	C
31	CA	2578	G
31	CA	2579	C
31	CA	2582	G
31	CA	2585	U
31	CA	2586	U
31	CA	2592	G
31	CA	2603	G
31	CA	2609	U
31	CA	2613	U
31	CA	2623	G
31	CA	2629	U
31	CA	2630	G
31	CA	2646	C

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Mol	Chain	Res	Type
31	CA	2661	G
31	CA	2663	G
31	CA	2681	C
31	CA	2682	A
31	CA	2689	U
31	CA	2690	U
31	CA	2714	G
31	CA	2716	C
31	CA	2718	G
31	CA	2720	U
31	CA	2726	A
31	CA	2744	G
31	CA	2748	A
31	CA	2765	A
31	CA	2769	U
31	CA	2778	A
31	CA	2779	U
31	CA	2780	G
31	CA	2791	G
31	CA	2794	C
31	CA	2799	A
31	CA	2818	U
31	CA	2820	A
31	CA	2821	A
31	CA	2825	G
31	CA	2833	U
31	CA	2835	A
31	CA	2836	U
31	CA	2861	U
31	CA	2865	U
31	CA	2867	G
31	CA	2880	C
31	CA	2883	A
31	CA	2884	U
31	CA	2886	A
31	CA	2903	U
28	DB	25	U
28	DB	35	C
28	DB	44	G
28	DB	45	A
28	DB	56	G
28	DB	57	A

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Mol	Chain	Res	Type
28	DB	88	C
28	DB	89	U
28	DB	90	C
28	DB	109	A
54	DA	10	A
54	DA	12	U
54	DA	14	A
54	DA	15	G
54	DA	34	U
54	DA	39	G
54	DA	42	A
54	DA	46	G
54	DA	58	G
54	DA	61	C
54	DA	63	A
54	DA	71	A
54	DA	74	A
54	DA	75	G
54	DA	84	A
54	DA	101	A
54	DA	102	U
54	DA	118	A
54	DA	119	A
54	DA	120	U
54	DA	125	A
54	DA	138	U
54	DA	139	U
54	DA	140	C
54	DA	141	G
54	DA	142	A
54	DA	143	C
54	DA	165	A
54	DA	196	A
54	DA	197	A
54	DA	199	A
54	DA	200	U
54	DA	215	G
54	DA	216	A
54	DA	221	A
54	DA	222	A
54	DA	248	G
54	DA	264	C

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Mol	Chain	Res	Type
54	DA	265	A
54	DA	266	G
54	DA	272	A
54	DA	276	U
54	DA	277	G
54	DA	278	A
54	DA	279	A
54	DA	285	G
54	DA	302	C
54	DA	311	A
54	DA	329	G
54	DA	330	A
54	DA	343	C
54	DA	352	A
54	DA	353	C
54	DA	362	A
54	DA	370	G
54	DA	372	G
54	DA	385	C
54	DA	386	G
54	DA	399	U
54	DA	411	G
54	DA	412	A
54	DA	420	C
54	DA	424	G
54	DA	451	U
54	DA	480	A
54	DA	481	G
54	DA	491	G
54	DA	504	A
54	DA	505	A
54	DA	508	A
54	DA	513	A
54	DA	528	A
54	DA	532	A
54	DA	533	G
54	DA	543	G
54	DA	544	C
54	DA	546	U
54	DA	547	A
54	DA	548	G
54	DA	549	G

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Mol	Chain	Res	Type
54	DA	550	C
54	DA	551	G
54	DA	563	A
54	DA	573	U
54	DA	575	A
54	DA	586	A
54	DA	603	A
54	DA	613	A
54	DA	614	A
54	DA	615	U
54	DA	627	A
54	DA	637	A
54	DA	645	C
54	DA	647	G
54	DA	653	U
54	DA	654	A
54	DA	655	A
54	DA	686	U
54	DA	717	C
54	DA	723	C
54	DA	730	A
54	DA	747	5MU
54	DA	764	A
54	DA	765	C
54	DA	775	G
54	DA	776	G
54	DA	782	A
54	DA	784	G
54	DA	785	G
54	DA	790	U
54	DA	805	G
54	DA	812	C
54	DA	827	U
54	DA	828	U
54	DA	858	G
54	DA	859	G
54	DA	878	A
54	DA	883	G
54	DA	885	C
54	DA	896	A
54	DA	897	C
54	DA	910	A

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Mol	Chain	Res	Type
54	DA	931	U
54	DA	932	U
54	DA	933	A
54	DA	946	C
54	DA	953	G
54	DA	961	C
54	DA	974	G
54	DA	983	A
54	DA	985	C
54	DA	996	A
54	DA	1012	U
54	DA	1013	C
54	DA	1022	G
54	DA	1026	G
54	DA	1033	U
54	DA	1040	A
54	DA	1047	G
54	DA	1057	A
54	DA	1061	U
54	DA	1062	G
54	DA	1068	G
54	DA	1070	A
54	DA	1073	A
54	DA	1083	U
54	DA	1088	A
54	DA	1089	A
54	DA	1090	A
54	DA	1096	A
54	DA	1097	U
54	DA	1112	G
54	DA	1119	U
54	DA	1128	G
54	DA	1129	A
54	DA	1132	U
54	DA	1133	A
54	DA	1134	A
54	DA	1135	C
54	DA	1136	G
54	DA	1142	A
54	DA	1155	A
54	DA	1168	G
54	DA	1171	G

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Mol	Chain	Res	Type
54	DA	1172	C
54	DA	1176	U
54	DA	1177	G
54	DA	1180	U
54	DA	1206	G
54	DA	1212	G
54	DA	1238	G
54	DA	1253	A
54	DA	1256	G
54	DA	1271	G
54	DA	1272	A
54	DA	1273	U
54	DA	1300	G
54	DA	1301	A
54	DA	1321	A
54	DA	1329	U
54	DA	1342	A
54	DA	1352	U
54	DA	1365	A
54	DA	1379	U
54	DA	1383	A
54	DA	1416	G
54	DA	1417	C
54	DA	1427	A
54	DA	1428	C
54	DA	1435	G
54	DA	1452	G
54	DA	1453	A
54	DA	1460	U
54	DA	1478	G
54	DA	1482	G
54	DA	1490	A
54	DA	1491	G
54	DA	1493	C
54	DA	1494	A
54	DA	1497	U
54	DA	1504	A
54	DA	1508	A
54	DA	1509	A
54	DA	1510	G
54	DA	1515	A
54	DA	1523	U

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Mol	Chain	Res	Type
54	DA	1532	A
54	DA	1534	U
54	DA	1535	A
54	DA	1536	C
54	DA	1537	G
54	DA	1569	A
54	DA	1578	U
54	DA	1583	A
54	DA	1585	C
54	DA	1607	C
54	DA	1608	A
54	DA	1609	A
54	DA	1616	A
54	DA	1647	U
54	DA	1648	U
54	DA	1649	G
54	DA	1674	G
54	DA	1715	G
54	DA	1729	U
54	DA	1730	C
54	DA	1738	G
54	DA	1744	A
54	DA	1754	A
54	DA	1764	C
54	DA	1773	A
54	DA	1782	U
54	DA	1800	C
54	DA	1801	A
54	DA	1808	A
54	DA	1812	U
54	DA	1816	C
54	DA	1829	A
54	DA	1869	G
54	DA	1870	C
54	DA	1871	A
54	DA	1872	A
54	DA	1873	G
54	DA	1906	G
54	DA	1907	G
54	DA	1913	A
54	DA	1914	C
54	DA	1929	G

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Mol	Chain	Res	Type
54	DA	1930	G
54	DA	1931	U
54	DA	1937	A
54	DA	1938	A
54	DA	1955	U
54	DA	1965	C
54	DA	1967	C
54	DA	1970	A
54	DA	1972	G
54	DA	1991	U
54	DA	1993	U
54	DA	1997	C
54	DA	2023	C
54	DA	2031	A
54	DA	2033	A
54	DA	2043	C
54	DA	2055	C
54	DA	2056	G
54	DA	2060	A
54	DA	2061	G
54	DA	2062	A
54	DA	2069	G7M
54	DA	2093	G
54	DA	2097	A
54	DA	2100	G
54	DA	2105	U
54	DA	2111	U
54	DA	2112	G
54	DA	2113	U
54	DA	2116	G
54	DA	2117	A
54	DA	2118	U
54	DA	2119	A
54	DA	2120	G
54	DA	2123	G
54	DA	2125	G
54	DA	2126	A
54	DA	2128	G
54	DA	2131	U
54	DA	2132	U
54	DA	2133	G
54	DA	2134	A

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Mol	Chain	Res	Type
54	DA	2135	A
54	DA	2145	C
54	DA	2146	C
54	DA	2148	G
54	DA	2158	A
54	DA	2159	G
54	DA	2160	C
54	DA	2161	C
54	DA	2162	G
54	DA	2163	A
54	DA	2164	C
54	DA	2165	C
54	DA	2167	U
54	DA	2168	G
54	DA	2169	A
54	DA	2170	A
54	DA	2171	A
54	DA	2172	U
54	DA	2173	A
54	DA	2178	C
54	DA	2179	C
54	DA	2181	U
54	DA	2183	A
54	DA	2185	U
54	DA	2186	G
54	DA	2190	G
54	DA	2198	A
54	DA	2203	U
54	DA	2204	G
54	DA	2211	A
54	DA	2225	A
54	DA	2238	G
54	DA	2239	G
54	DA	2268	A
54	DA	2278	A
54	DA	2280	G
54	DA	2283	C
54	DA	2286	G
54	DA	2287	A
54	DA	2305	U
54	DA	2308	G
54	DA	2312	U

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Mol	Chain	Res	Type
54	DA	2322	A
54	DA	2324	U
54	DA	2325	G
54	DA	2327	A
54	DA	2331	G
54	DA	2335	A
54	DA	2345	G
54	DA	2347	C
54	DA	2383	G
54	DA	2385	C
54	DA	2402	U
54	DA	2406	A
54	DA	2407	A
54	DA	2424	C
54	DA	2425	A
54	DA	2435	A
54	DA	2441	U
54	DA	2448	A
54	DA	2465	C
54	DA	2474	U
54	DA	2476	A
54	DA	2484	G
54	DA	2491	U
54	DA	2502	G
54	DA	2505	G
54	DA	2518	A
54	DA	2529	G
54	DA	2535	G
54	DA	2547	A
54	DA	2556	C
54	DA	2566	A
54	DA	2567	G
54	DA	2573	C
54	DA	2585	U
54	DA	2586	U
54	DA	2603	G
54	DA	2609	U
54	DA	2613	U
54	DA	2629	U
54	DA	2630	G
54	DA	2661	G
54	DA	2663	G

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Mol	Chain	Res	Type
54	DA	2689	U
54	DA	2690	U
54	DA	2714	G
54	DA	2716	C
54	DA	2726	A
54	DA	2744	G
54	DA	2748	A
54	DA	2765	A
54	DA	2778	A
54	DA	2791	G
54	DA	2798	U
54	DA	2799	A
54	DA	2818	U
54	DA	2820	A
54	DA	2821	A
54	DA	2825	G
54	DA	2833	U
54	DA	2835	A
54	DA	2836	U
54	DA	2867	G
54	DA	2880	C
54	DA	2883	A
54	DA	2903	U

All (208) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	30	U
1	AA	70	U
1	AA	88	U
1	AA	89	U
1	AA	209	U
1	AA	305	G
1	AA	367	U
1	AA	413	G
1	AA	422	C
1	AA	429	U
1	AA	576	C
1	AA	653	U
1	AA	702	A
1	AA	733	G

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Mol	Chain	Res	Type
1	AA	793	U
1	AA	841	C
1	AA	884	U
1	AA	992	U
1	AA	1086	U
1	AA	1094	G
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1225	A
1	AA	1281	C
1	AA	1299	A
1	AA	1301	U
1	AA	1397	C
1	AA	1447	A
1	AA	1452	C
1	BA	5	U
1	BA	70	U
1	BA	86	G
1	BA	89	U
1	BA	209	U
1	BA	305	G
1	BA	367	U
1	BA	422	C
1	BA	429	U
1	BA	559	A
1	BA	560	A
1	BA	561	U
1	BA	576	C
1	BA	653	U
1	BA	702	A
1	BA	733	G
1	BA	793	U
1	BA	842	U
1	BA	844	G
1	BA	884	U
1	BA	992	U
1	BA	1008	U
1	BA	1086	U
1	BA	1137	C
1	BA	1139	G

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Mol	Chain	Res	Type
1	BA	1140	C
1	BA	1141	C
1	BA	1225	A
1	BA	1281	C
1	BA	1299	A
1	BA	1301	U
1	BA	1362	A
1	BA	1363	A
1	BA	1397	C
1	BA	1447	A
1	BA	1452	C
28	CB	89	U
31	CA	33	C
31	CA	83	A
31	CA	138	U
31	CA	141	G
31	CA	177	G
31	CA	196	A
31	CA	199	A
31	CA	221	A
31	CA	271	G
31	CA	278	A
31	CA	310	A
31	CA	371	A
31	CA	403	U
31	CA	404	A
31	CA	411	G
31	CA	503	A
31	CA	527	C
31	CA	555	G
31	CA	620	G
31	CA	764	A
31	CA	775	G
31	CA	784	G
31	CA	827	U
31	CA	846	U
31	CA	973	A
31	CA	984	A
31	CA	1045	C
31	CA	1046	A
31	CA	1061	U
31	CA	1069	A

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Mol	Chain	Res	Type
31	CA	1070	A
31	CA	1088	A
31	CA	1089	A
31	CA	1128	G
31	CA	1132	U
31	CA	1133	A
31	CA	1253	A
31	CA	1286	A
31	CA	1300	G
31	CA	1320	C
31	CA	1329	U
31	CA	1379	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	1567	G
31	CA	1607	C
31	CA	1609	A
31	CA	1647	U
31	CA	1870	C
31	CA	1871	A
31	CA	1900	A
31	CA	1929	G
31	CA	1970	A
31	CA	2035	G
31	CA	2095	A
31	CA	2119	A
31	CA	2126	A
31	CA	2146	C
31	CA	2157	G
31	CA	2164	C
31	CA	2172	U
31	CA	2225	A
31	CA	2282	G
31	CA	2324	U
31	CA	2326	C
31	CA	2423	U
31	CA	2425	A
31	CA	2581	G

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Mol	Chain	Res	Type
31	CA	2680	U
31	CA	2681	C
31	CA	2778	A
31	CA	2779	U
31	CA	2820	A
31	CA	2849	U
31	CA	2873	A
54	DA	138	U
54	DA	141	G
54	DA	196	A
54	DA	199	A
54	DA	271	G
54	DA	278	A
54	DA	310	A
54	DA	370	G
54	DA	371	A
54	DA	403	U
54	DA	503	A
54	DA	620	G
54	DA	764	A
54	DA	784	G
54	DA	984	A
54	DA	1061	U
54	DA	1069	A
54	DA	1070	A
54	DA	1087	G
54	DA	1089	A
54	DA	1128	G
54	DA	1133	A
54	DA	1141	U
54	DA	1142	A
54	DA	1171	G
54	DA	1175	A
54	DA	1253	A
54	DA	1286	A
54	DA	1300	G
54	DA	1301	A
54	DA	1320	C
54	DA	1490	A
54	DA	1497	U
54	DA	1508	A
54	DA	1509	A

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Mol	Chain	Res	Type
54	DA	1535	A
54	DA	1607	C
54	DA	1609	A
54	DA	1647	U
54	DA	1870	C
54	DA	1871	A
54	DA	2062	A
54	DA	2097	A
54	DA	2119	A
54	DA	2127	G
54	DA	2146	C
54	DA	2157	G
54	DA	2158	A
54	DA	2164	C
54	DA	2172	U
54	DA	2286	G
54	DA	2311	A
54	DA	2324	U
54	DA	2406	A
54	DA	2423	U
54	DA	2585	U
54	DA	2779	U
54	DA	2798	U
54	DA	2820	A
54	DA	2873	A

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

77 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
54	G7M	DA	2069	54	20,26,27	0.77	1 (5%)	17,39,42	0.71	0
54	2MG	DA	1835	54	18,26,27	1.01	2 (11%)	16,38,41	0.56	0
30	MEQ	CD	150	30	7,8,10	0.43	0	4,9,12	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	4D4	CN	81	40	9,11,12	2.09	2 (22%)	8,13,15	2.37	2 (25%)
31	5MU	CA	747	31	19,22,23	0.37	0	28,32,35	0.31	0
1	PSU	AA	516	1,55	18,21,22	0.41	0	22,30,33	0.48	0
1	UR3	BA	1498	1	19,22,23	0.44	0	26,32,35	0.34	0
1	2MG	AA	1207	1	18,26,27	0.86	0	16,38,41	0.54	0
31	PSU	CA	1917	31	18,21,22	0.33	0	22,30,33	0.51	0
54	2MG	DA	2445	54	18,26,27	1.17	2 (11%)	16,38,41	0.75	0
1	2MG	AA	1516	1	18,26,27	0.87	1 (5%)	16,38,41	0.57	0
31	PSU	CA	2580	31	18,21,22	0.49	0	22,30,33	0.62	0
1	5MC	BA	1407	1	18,22,23	0.56	0	26,32,35	0.47	0
54	6MZ	DA	1618	54	18,25,26	0.95	1 (5%)	16,36,39	0.67	0
54	PSU	DA	1917	54	18,21,22	0.49	0	22,30,33	0.56	0
12	D2T	BL	89	12	7,9,10	1.09	1 (14%)	6,11,13	1.22	0
54	PSU	DA	2604	54	18,21,22	1.02	2 (11%)	22,30,33	0.66	0
31	6MZ	CA	2030	31	18,25,26	0.92	0	16,36,39	0.88	1 (6%)
54	3TD	DA	1915	54	18,22,23	0.43	0	22,32,35	0.50	0
1	MA6	BA	1519	1	19,26,27	0.87	0	18,38,41	1.29	1 (5%)
12	D2T	AL	89	12	7,9,10	1.44	2 (28%)	6,11,13	1.28	0
1	5MC	AA	967	1	18,22,23	0.34	0	26,32,35	0.38	0
31	2MG	CA	2445	31	18,26,27	0.94	0	16,38,41	0.65	0
54	6MZ	DA	2030	54	18,25,26	1.29	2 (11%)	16,36,39	1.13	3 (18%)
30	MEQ	DD	150[B]	30	8,9,10	1.52	1 (12%)	5,10,12	0.84	0
31	2MA	CA	2503	31	17,25,26	0.81	0	17,37,40	0.48	0
1	MA6	AA	1518	1	19,26,27	0.88	0	18,38,41	1.21	1 (5%)
31	3TD	CA	1915	31	18,22,23	0.47	0	22,32,35	0.49	0
54	PSU	DA	2457	54	18,21,22	0.54	0	22,30,33	0.46	0
54	PSU	DA	2605	54	18,21,22	0.69	0	22,30,33	0.65	0
31	OMC	CA	2498	31,55	19,22,23	0.46	0	26,31,34	0.48	0
54	OMG	DA	2251	54	18,26,27	1.04	2 (11%)	19,38,41	0.57	0
54	PSU	DA	2504	54	18,21,22	0.49	0	22,30,33	0.43	0
1	G7M	BA	527	1	20,26,27	0.66	0	17,39,42	0.58	0
54	2MA	DA	2503	54,55	17,25,26	0.93	2 (11%)	17,37,40	0.45	0
54	1MG	DA	745	54	18,26,27	1.08	1 (5%)	19,39,42	0.50	0
40	4D4	DN	81[A]	-	9,11,12	2.12	2 (22%)	8,13,15	2.51	2 (25%)
31	PSU	CA	1911	31	18,21,22	0.29	0	22,30,33	0.39	0
31	5MC	CA	1962	31	18,22,23	0.35	0	26,32,35	0.41	0
1	4OC	BA	1402	1	20,23,24	0.40	0	26,32,35	0.44	0
54	5MU	DA	1939	54	19,22,23	0.68	0	28,32,35	0.46	0
31	PSU	CA	2457	31	18,21,22	0.71	1 (5%)	22,30,33	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PSU	CA	2605	31	18,21,22	0.41	0	22,30,33	0.60	0
31	PSU	CA	2604	31	18,21,22	1.77	3 (16%)	22,30,33	1.37	3 (13%)
31	G7M	CA	2069	31	20,26,27	0.62	0	17,39,42	0.59	0
31	1MG	CA	745	31	18,26,27	0.76	1 (5%)	19,39,42	0.45	0
31	PSU	CA	746	31,55	18,21,22	0.60	1 (5%)	22,30,33	0.38	0
40	4D4	DN	81[B]	-	9,11,12	1.53	1 (11%)	8,13,15	2.60	2 (25%)
1	4OC	AA	1402	1	20,23,24	0.37	0	26,32,35	0.43	0
31	2MG	CA	1835	31	18,26,27	0.99	1 (5%)	16,38,41	0.46	0
31	OMU	CA	2552	31	19,22,23	0.34	0	26,31,34	0.28	0
1	5MC	AA	1407	1	18,22,23	0.59	0	26,32,35	0.49	0
1	2MG	BA	1516	1	18,26,27	0.81	0	16,38,41	0.51	0
1	2MG	BA	966	1	18,26,27	0.81	0	16,38,41	0.56	0
31	5MU	CA	1939	31	19,22,23	0.56	0	28,32,35	0.37	0
1	UR3	AA	1498	1	19,22,23	0.72	1 (5%)	26,32,35	0.42	0
54	5MC	DA	1962	54	18,22,23	0.78	1 (5%)	26,32,35	0.47	0
31	PSU	CA	955	31	18,21,22	0.37	0	22,30,33	0.53	0
54	OMU	DA	2552	54	19,22,23	0.61	0	26,31,34	0.29	0
1	5MC	BA	967	1	18,22,23	0.30	0	26,32,35	0.38	0
1	MA6	AA	1519	1	19,26,27	0.89	0	18,38,41	1.37	1 (5%)
1	2MG	BA	1207	1	18,26,27	0.78	0	16,38,41	0.52	0
54	H2U	DA	2449	54	18,21,22	0.57	0	21,30,33	0.55	0
54	PSU	DA	955	54	18,21,22	0.57	0	22,30,33	0.64	0
54	OMC	DA	2498	54,55	19,22,23	0.57	0	26,31,34	0.53	0
1	2MG	AA	966	1	18,26,27	0.77	0	16,38,41	0.51	0
54	PSU	DA	746	54,55	18,21,22	1.02	2 (11%)	22,30,33	0.32	0
31	6MZ	CA	1618	31	18,25,26	0.92	0	16,36,39	0.89	2 (12%)
31	OMG	CA	2251	31	18,26,27	0.79	0	19,38,41	0.66	0
1	MA6	BA	1518	1	19,26,27	0.82	0	18,38,41	1.19	1 (5%)
54	5MU	DA	747	54	19,22,23	0.44	0	28,32,35	0.38	0
31	PSU	CA	2504	31	18,21,22	0.43	0	22,30,33	0.44	0
54	PSU	DA	1911	54	18,21,22	0.33	0	22,30,33	0.38	0
1	PSU	BA	516	1	18,21,22	0.46	0	22,30,33	0.46	0
1	G7M	AA	527	1	20,26,27	0.81	0	17,39,42	0.90	1 (5%)
30	MEQ	DD	150[A]	30	8,9,10	0.47	0	5,10,12	0.50	0
54	PSU	DA	2580	54	18,21,22	0.88	2 (11%)	22,30,33	0.74	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	G7M	DA	2069	54	-	1/3/25/26	0/3/3/3
54	2MG	DA	1835	54	-	2/5/27/28	0/3/3/3
30	MEQ	CD	150	30	-	3/6/7/11	-
40	4D4	CN	81	40	-	1/11/12/14	-
31	5MU	CA	747	31	-	1/7/25/26	0/2/2/2
1	PSU	AA	516	1,55	-	0/7/25/26	0/2/2/2
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
54	2MG	DA	2445	54	-	2/5/27/28	0/3/3/3
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
54	6MZ	DA	1618	54	-	0/5/27/28	0/3/3/3
54	PSU	DA	1917	54	-	0/7/25/26	0/2/2/2
12	D2T	BL	89	12	-	2/7/12/14	-
54	PSU	DA	2604	54	-	0/7/25/26	0/2/2/2
31	6MZ	CA	2030	31	-	1/5/27/28	0/3/3/3
54	3TD	DA	1915	54	-	0/7/25/26	0/2/2/2
1	MA6	BA	1519	1	-	2/7/29/30	0/3/3/3
12	D2T	AL	89	12	-	1/7/12/14	-
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3
54	6MZ	DA	2030	54	-	1/5/27/28	0/3/3/3
30	MEQ	DD	150[B]	30	-	3/8/9/11	-
31	2MA	CA	2503	31	-	1/3/25/26	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
54	PSU	DA	2457	54	-	0/7/25/26	0/2/2/2
54	PSU	DA	2605	54	-	0/7/25/26	0/2/2/2
31	OMC	CA	2498	31,55	-	0/9/27/28	0/2/2/2
54	OMG	DA	2251	54	-	0/5/27/28	0/3/3/3
54	PSU	DA	2504	54	-	0/7/25/26	0/2/2/2
1	G7M	BA	527	1	-	2/3/25/26	0/3/3/3
54	2MA	DA	2503	54,55	-	1/3/25/26	0/3/3/3
54	1MG	DA	745	54	-	0/3/25/26	0/3/3/3
40	4D4	DN	81[A]	-	-	2/11/12/14	-
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
31	5MC	CA	1962	31	-	0/7/25/26	0/2/2/2
1	4OC	BA	1402	1	-	0/9/29/30	0/2/2/2
54	5MU	DA	1939	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2604	31	-	0/7/25/26	0/2/2/2
31	G7M	CA	2069	31	-	1/3/25/26	0/3/3/3
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
31	PSU	CA	746	31,55	-	1/7/25/26	0/2/2/2
40	4D4	DN	81[B]	-	-	6/11/12/14	-
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
31	2MG	CA	1835	31	-	2/5/27/28	0/3/3/3
31	OMU	CA	2552	31	-	0/9/27/28	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
1	2MG	BA	966	1	-	0/5/27/28	0/3/3/3
31	5MU	CA	1939	31	-	0/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
54	5MC	DA	1962	54	-	2/7/25/26	0/2/2/2
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
54	OMU	DA	2552	54	-	0/9/27/28	0/2/2/2
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	2/7/29/30	0/3/3/3
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
54	H2U	DA	2449	54	-	1/7/38/39	0/2/2/2
54	PSU	DA	955	54	-	0/7/25/26	0/2/2/2
54	OMC	DA	2498	54,55	-	0/9/27/28	0/2/2/2
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
54	PSU	DA	746	54,55	-	2/7/25/26	0/2/2/2
31	6MZ	CA	1618	31	-	1/5/27/28	0/3/3/3
31	OMG	CA	2251	31	-	0/5/27/28	0/3/3/3
1	MA6	BA	1518	1	-	0/7/29/30	0/3/3/3
54	5MU	DA	747	54	-	2/7/25/26	0/2/2/2
31	PSU	CA	2504	31	-	0/7/25/26	0/2/2/2
54	PSU	DA	1911	54	-	0/7/25/26	0/2/2/2
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3
30	MEQ	DD	150[A]	30	-	4/8/9/11	-
54	PSU	DA	2580	54	-	0/7/25/26	0/2/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2604	PSU	C2-N1	5.87	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	CN	81	4D4	CZ-NE	5.79	1.44	1.33
40	DN	81[A]	4D4	CZ-NE	5.79	1.44	1.33
30	DD	150[B]	MEQ	CB-CA	4.13	1.59	1.53
40	DN	81[B]	4D4	CZ-NE	3.98	1.41	1.33
54	DA	2030	6MZ	C2'-C1'	-3.20	1.48	1.53
54	DA	2251	OMG	C5-C6	-3.12	1.41	1.47
54	DA	746	PSU	O4'-C1'	-3.10	1.39	1.43
54	DA	1962	5MC	O5'-C5'	-2.93	1.37	1.44
12	AL	89	D2T	CB-SB	2.81	1.85	1.82
54	DA	745	1MG	O3'-C3'	-2.71	1.36	1.43
54	DA	2030	6MZ	O4'-C1'	-2.67	1.37	1.41
31	CA	2604	PSU	C6-C5	2.65	1.38	1.35
54	DA	2604	PSU	O3'-C3'	-2.52	1.37	1.43
12	BL	89	D2T	CB-CG	2.50	1.56	1.52
54	DA	746	PSU	C2'-C1'	-2.46	1.50	1.53
54	DA	2069	G7M	O5'-C5'	-2.32	1.39	1.44
54	DA	2445	2MG	C2'-C1'	-2.31	1.50	1.53
40	DN	81[A]	4D4	CZ-NH1	2.29	1.44	1.34
54	DA	1835	2MG	C5-C4	-2.25	1.37	1.43
54	DA	2445	2MG	O3'-C3'	-2.25	1.37	1.43
54	DA	2580	PSU	O4'-C1'	-2.19	1.40	1.43
54	DA	2604	PSU	O5'-C5'	-2.16	1.39	1.44
31	CA	2604	PSU	O5'-C5'	-2.13	1.39	1.44
1	AA	1516	2MG	C5-C4	-2.12	1.37	1.43
54	DA	1618	6MZ	C8-N7	-2.10	1.30	1.34
31	CA	1835	2MG	C8-N7	-2.10	1.31	1.35
31	CA	2457	PSU	O5'-C5'	-2.10	1.39	1.44
54	DA	1835	2MG	C8-N7	-2.09	1.31	1.35
54	DA	2503	2MA	C8-N7	-2.06	1.31	1.35
12	AL	89	D2T	CB-CG	2.05	1.55	1.52
54	DA	2251	OMG	C8-N7	-2.04	1.31	1.35
1	AA	1498	UR3	O3'-C3'	2.03	1.47	1.43
31	CA	745	1MG	C8-N7	-2.03	1.31	1.35
54	DA	2503	2MA	C5-C4	-2.03	1.37	1.43
40	CN	81	4D4	CZ-NH1	2.02	1.43	1.34
54	DA	2580	PSU	O5'-C5'	-2.01	1.39	1.44
31	CA	746	PSU	O4'-C1'	-2.00	1.41	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	DN	81[B]	4D4	NE-CZ-NH2	5.93	131.13	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	DN	81[A]	4D4	NE-CZ-NH2	5.75	130.81	120.70
40	CN	81	4D4	NE-CZ-NH2	5.60	130.54	120.70
1	AA	1519	MA6	N1-C6-N6	-4.81	111.99	117.06
1	BA	1519	MA6	N1-C6-N6	-4.44	112.39	117.06
31	CA	2604	PSU	C6-C5-C4	4.06	121.04	118.20
1	AA	1518	MA6	N1-C6-N6	-4.04	112.81	117.06
1	BA	1518	MA6	N1-C6-N6	-4.03	112.81	117.06
40	DN	81[B]	4D4	NH1-CZ-NE	-3.98	110.01	119.19
40	DN	81[A]	4D4	NH1-CZ-NE	-3.26	111.68	119.19
31	CA	2604	PSU	C6-N1-C2	-3.15	119.47	122.68
40	CN	81	4D4	NH1-CZ-NE	-2.83	112.67	119.19
54	DA	2030	6MZ	C2-N1-C6	2.51	118.74	116.59
1	AA	527	G7M	O4'-C1'-C2'	-2.42	103.39	106.93
54	DA	2030	6MZ	O4'-C1'-C2'	-2.29	103.57	106.93
31	CA	2604	PSU	O2-C2-N1	2.29	125.31	122.79
31	CA	1618	6MZ	C2-N1-C6	2.27	118.53	116.59
31	CA	2030	6MZ	C9-N6-C6	2.06	124.65	122.87
54	DA	2580	PSU	O4'-C1'-C2'	2.06	108.05	105.14
31	CA	1618	6MZ	O4'-C1'-C2'	-2.03	103.97	106.93
54	DA	2030	6MZ	C9-N6-C6	2.00	124.59	122.87

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	O4'-C4'-C5'-O5'
1	AA	527	G7M	C3'-C4'-C5'-O5'
1	BA	527	G7M	O4'-C4'-C5'-O5'
1	BA	527	G7M	C3'-C4'-C5'-O5'
40	DN	81[B]	4D4	N-CA-CB-CG
40	DN	81[B]	4D4	CA-CB-CG-CD
54	DA	746	PSU	C2'-C1'-C5-C4
30	CD	150	MEQ	C-CA-CB-CG
30	DD	150[A]	MEQ	C-CA-CB-CG
30	DD	150[B]	MEQ	N-CA-CB-CG
1	AA	1519	MA6	O4'-C4'-C5'-O5'
1	BA	1519	MA6	O4'-C4'-C5'-O5'
30	CD	150	MEQ	CA-CB-CG-CD
30	DD	150[B]	MEQ	CA-CB-CG-CD
30	DD	150[A]	MEQ	OE1-CD-CG-CB
40	DN	81[B]	4D4	OB-CB-CG-CD
30	DD	150[A]	MEQ	NE2-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
30	DD	150[B]	MEQ	C-CA-CB-CG
1	AA	1519	MA6	C3'-C4'-C5'-O5'
54	DA	747	5MU	C3'-C4'-C5'-O5'
1	BA	1519	MA6	C3'-C4'-C5'-O5'
31	CA	747	5MU	C3'-C4'-C5'-O5'
40	DN	81[B]	4D4	C-CA-CB-OB
12	AL	89	D2T	CG-CB-SB-CB1
12	BL	89	D2T	CG-CB-SB-CB1
54	DA	2445	2MG	C3'-C4'-C5'-O5'
30	CD	150	MEQ	N-CA-CB-CG
30	DD	150[A]	MEQ	N-CA-CB-CG
54	DA	2030	6MZ	O4'-C4'-C5'-O5'
40	DN	81[A]	4D4	CG-CD-NE-CZ
31	CA	1835	2MG	O4'-C4'-C5'-O5'
54	DA	2449	H2U	C4'-C5'-O5'-P
54	DA	1962	5MC	C2'-C1'-N1-C6
31	CA	1835	2MG	C3'-C4'-C5'-O5'
31	CA	2030	6MZ	O4'-C4'-C5'-O5'
12	BL	89	D2T	SB-CB-CG-OD2
54	DA	1835	2MG	C3'-C4'-C5'-O5'
54	DA	1962	5MC	O4'-C1'-N1-C6
54	DA	1835	2MG	O4'-C4'-C5'-O5'
54	DA	2445	2MG	O4'-C4'-C5'-O5'
31	CA	746	PSU	O4'-C1'-C5-C6
54	DA	746	PSU	O4'-C1'-C5-C6
31	CA	2069	G7M	O4'-C4'-C5'-O5'
54	DA	2069	G7M	O4'-C4'-C5'-O5'
40	DN	81[B]	4D4	C-CA-CB-CG
40	DN	81[B]	4D4	N-CA-CB-OB
31	CA	2503	2MA	O4'-C4'-C5'-O5'
54	DA	747	5MU	O4'-C4'-C5'-O5'
54	DA	2503	2MA	O4'-C4'-C5'-O5'
40	CN	81	4D4	O-C-CA-CB
40	DN	81[A]	4D4	O-C-CA-CB
31	CA	1618	6MZ	C4'-C5'-O5'-P

There are no ring outliers.

18 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	CA	747	5MU	1	0
31	CA	2580	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	CA	2030	6MZ	3	0
1	BA	1519	MA6	2	0
1	AA	967	5MC	1	0
54	DA	2030	6MZ	1	0
30	DD	150[B]	MEQ	2	0
31	CA	2503	2MA	1	0
1	AA	1518	MA6	2	0
31	CA	1915	3TD	1	0
54	DA	2251	OMG	1	0
1	BA	1402	4OC	1	0
1	AA	1402	4OC	1	0
1	AA	1519	MA6	2	0
54	DA	2498	OMC	1	0
1	BA	1518	MA6	2	0
54	DA	747	5MU	1	0
30	DD	150[A]	MEQ	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 559 ligands modelled in this entry, 475 are monoatomic - leaving 84 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	$\# Z > 2$
61	PEG	DA	3218	-	6,6,6	0.25	0	5,5,5	0.09	0
57	MPD	AA	1676	-	7,7,7	0.79	0	9,10,10	0.71	0
57	MPD	DE	302	-	7,7,7	0.95	1 (14%)	9,10,10	0.54	0
61	PEG	DA	3226	-	6,6,6	0.45	0	5,5,5	0.19	0
57	MPD	DT	201	-	7,7,7	0.53	0	9,10,10	0.22	0
57	MPD	DT	202	-	7,7,7	0.82	0	9,10,10	0.39	0
62	EDO	D1	101	-	3,3,3	0.74	0	2,2,2	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	PGE	D1	102	-	9,9,9	0.24	0	8,8,8	0.22	0
59	TAC	BA	1643	55	33,35,35	0.42	0	42,58,58	0.80	2 (4%)
64	SPD	DA	3183	-	9,9,9	0.11	0	8,8,8	0.14	0
57	MPD	DA	3192	-	7,7,7	0.43	0	9,10,10	0.67	0
56	PG4	DA	3193	-	12,12,12	0.40	0	11,11,11	0.34	0
58	PUT	DA	3219	-	5,5,5	0.21	0	4,4,4	0.13	0
57	MPD	DE	301	-	7,7,7	0.82	0	9,10,10	0.52	0
63	PGE	DA	3217	-	9,9,9	0.19	0	8,8,8	0.26	0
64	SPD	DA	3224	-	9,9,9	0.24	0	8,8,8	0.45	0
65	1PE	DA	3185	-	15,15,15	0.20	0	14,14,14	0.36	0
62	EDO	DB	201	-	3,3,3	0.70	0	2,2,2	0.15	0
66	ACY	DA	3196	-	3,3,3	2.33	1 (33%)	3,3,3	2.24	2 (66%)
64	SPD	DA	3187	-	9,9,9	0.20	0	8,8,8	0.31	0
57	MPD	AA	1671	-	7,7,7	0.69	0	9,10,10	0.51	0
62	EDO	DA	3209	-	3,3,3	0.66	0	2,2,2	0.27	0
63	PGE	DA	3001	-	9,9,9	0.31	0	8,8,8	0.32	0
62	EDO	DA	3194	-	3,3,3	0.97	0	2,2,2	0.18	0
56	PG4	DQ	202	-	12,12,12	0.21	0	11,11,11	0.16	0
61	PEG	DQ	201	-	6,6,6	0.18	0	5,5,5	0.17	0
62	EDO	DA	3215	-	3,3,3	0.79	0	2,2,2	0.15	0
58	PUT	DA	3213	-	5,5,5	0.21	0	4,4,4	0.23	0
62	EDO	DB	211	-	3,3,3	0.67	0	2,2,2	0.19	0
66	ACY	DA	3191	-	3,3,3	0.93	0	3,3,3	1.07	0
61	PEG	DA	3227	-	6,6,6	0.26	0	5,5,5	0.18	0
58	PUT	DA	3212	-	5,5,5	0.26	0	4,4,4	0.03	0
67	GUN	DA	3211	-	7,12,12	0.40	0	8,17,17	0.64	0
63	PGE	DA	3214	-	9,9,9	0.30	0	8,8,8	0.41	0
58	PUT	DA	3223	-	5,5,5	0.24	0	4,4,4	0.16	0
59	TAC	AA	1680	55	33,35,35	0.51	0	42,58,58	0.75	1 (2%)
65	1PE	DA	3202	-	15,15,15	0.36	0	14,14,14	0.36	0
58	PUT	DA	3222	-	5,5,5	0.52	0	4,4,4	0.70	0
61	PEG	DP	201	-	6,6,6	0.30	0	5,5,5	0.17	0
58	PUT	DA	3221	-	5,5,5	0.22	0	4,4,4	0.15	0
61	PEG	D3	101	-	6,6,6	0.28	0	5,5,5	0.30	0
57	MPD	DA	3190	-	7,7,7	0.36	0	9,10,10	0.41	0
57	MPD	DN	201	-	7,7,7	0.96	1 (14%)	9,10,10	0.53	0
57	MPD	DA	3210	-	7,7,7	0.81	0	9,10,10	0.31	0
56	PG4	DA	3216	-	12,12,12	0.18	0	11,11,11	0.23	0
58	PUT	AA	1673	-	5,5,5	0.14	0	4,4,4	0.11	0
56	PG4	AA	1670	-	12,12,12	0.34	0	11,11,11	0.41	0
62	EDO	DA	3198	-	3,3,3	0.61	0	2,2,2	0.38	0
58	PUT	DA	3189	-	5,5,5	0.26	0	4,4,4	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
64	SPD	DA	3206	-	9,9,9	0.25	0	8,8,8	0.23	0
57	MPD	DS	203	-	7,7,7	0.28	0	9,10,10	0.36	0
63	PGE	DU	101	-	9,9,9	0.21	0	8,8,8	0.13	0
62	EDO	DB	212	-	3,3,3	0.79	0	2,2,2	0.17	0
63	PGE	DA	3225	-	9,9,9	0.17	0	8,8,8	0.16	0
61	PEG	D1	103	-	6,6,6	0.37	0	5,5,5	0.20	0
63	PGE	DS	201	-	9,9,9	0.40	0	8,8,8	0.31	0
58	PUT	DA	3184	-	5,5,5	0.44	0	4,4,4	0.26	0
58	PUT	DA	3188	-	5,5,5	0.25	0	4,4,4	0.12	0
61	PEG	DL	201	-	6,6,6	0.10	0	5,5,5	0.14	0
58	PUT	AA	1674	-	5,5,5	0.17	0	4,4,4	0.13	0
57	MPD	DA	3207	-	7,7,7	0.84	0	9,10,10	0.48	0
58	PUT	DA	3205	-	5,5,5	0.21	0	4,4,4	0.20	0
62	EDO	DA	3003	-	3,3,3	0.62	0	2,2,2	0.22	0
62	EDO	DA	3197	-	3,3,3	0.78	0	2,2,2	0.07	0
62	EDO	DA	3002	-	3,3,3	0.62	0	2,2,2	0.35	0
57	MPD	DK	201	-	7,7,7	0.53	0	9,10,10	0.28	0
63	PGE	DA	3203	-	9,9,9	0.31	0	8,8,8	0.27	0
56	PG4	BA	1642	-	12,12,12	0.23	0	11,11,11	0.17	0
58	PUT	AA	1672	-	5,5,5	0.26	0	4,4,4	0.28	0
66	ACY	DA	3201	-	3,3,3	0.65	0	3,3,3	1.10	0
61	PEG	DA	3200	-	6,6,6	0.38	0	5,5,5	0.23	0
68	TRS	DA	3220	-	7,7,7	0.28	0	9,9,9	0.29	0
58	PUT	DA	3195	-	5,5,5	0.39	0	4,4,4	0.60	0
62	EDO	DA	3208	-	3,3,3	0.66	0	2,2,2	0.24	0
61	PEG	AL	201	-	6,6,6	0.32	0	5,5,5	0.17	0
59	TAC	BA	1644	55	33,35,35	0.53	0	42,58,58	0.80	1 (2%)
58	PUT	AA	1675	-	5,5,5	0.19	0	4,4,4	0.09	0
57	MPD	DA	3204	-	7,7,7	0.84	0	9,10,10	0.67	0
59	TAC	AA	1681	55	33,35,35	0.53	0	42,58,58	0.81	2 (4%)
58	PUT	DM	201	-	5,5,5	0.14	0	4,4,4	0.09	0
61	PEG	DA	3199	-	6,6,6	0.22	0	5,5,5	0.16	0
63	PGE	DA	3186	-	9,9,9	0.38	0	8,8,8	0.44	0
56	PG4	DR	202	-	12,12,12	0.29	0	11,11,11	0.38	0
56	PG4	DS	202	-	12,12,12	0.41	0	11,11,11	0.34	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
61	PEG	DA	3218	-	-	1/4/4/4	-
57	MPD	AA	1676	-	-	0/5/5/5	-
57	MPD	DE	302	-	-	3/5/5/5	-
61	PEG	DA	3226	-	-	3/4/4/4	-
57	MPD	DT	201	-	-	3/5/5/5	-
57	MPD	DT	202	-	-	2/5/5/5	-
62	EDO	D1	101	-	-	0/1/1/1	-
63	PGE	D1	102	-	-	5/7/7/7	-
59	TAC	BA	1643	55	-	8/8/74/74	0/4/4/4
64	SPD	DA	3183	-	-	1/7/7/7	-
57	MPD	DA	3192	-	-	2/5/5/5	-
56	PG4	DA	3193	-	-	6/10/10/10	-
58	PUT	DA	3219	-	-	0/3/3/3	-
57	MPD	DE	301	-	-	2/5/5/5	-
63	PGE	DA	3217	-	-	2/7/7/7	-
64	SPD	DA	3224	-	-	3/7/7/7	-
65	1PE	DA	3185	-	-	5/13/13/13	-
62	EDO	DB	201	-	-	0/1/1/1	-
64	SPD	DA	3187	-	-	2/7/7/7	-
57	MPD	AA	1671	-	-	1/5/5/5	-
62	EDO	DA	3209	-	-	0/1/1/1	-
63	PGE	DA	3001	-	-	4/7/7/7	-
62	EDO	DA	3194	-	-	0/1/1/1	-
56	PG4	DQ	202	-	-	3/10/10/10	-
61	PEG	DQ	201	-	-	1/4/4/4	-
62	EDO	DA	3215	-	-	0/1/1/1	-
58	PUT	DA	3213	-	-	0/3/3/3	-
62	EDO	DB	211	-	-	0/1/1/1	-
61	PEG	DA	3227	-	-	0/4/4/4	-
58	PUT	DA	3212	-	-	1/3/3/3	-
67	GUN	DA	3211	-	-	-	0/2/2/2
63	PGE	DA	3214	-	-	3/7/7/7	-
58	PUT	DA	3223	-	-	1/3/3/3	-
59	TAC	AA	1680	55	-	1/8/74/74	0/4/4/4
65	1PE	DA	3202	-	-	7/13/13/13	-
58	PUT	DA	3222	-	-	0/3/3/3	-
61	PEG	DP	201	-	-	3/4/4/4	-
58	PUT	DA	3221	-	-	0/3/3/3	-
61	PEG	D3	101	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	MPD	DA	3190	-	-	1/5/5/5	-
57	MPD	DN	201	-	-	2/5/5/5	-
57	MPD	DA	3210	-	-	0/5/5/5	-
56	PG4	DA	3216	-	-	4/10/10/10	-
58	PUT	AA	1673	-	-	0/3/3/3	-
56	PG4	AA	1670	-	-	4/10/10/10	-
62	EDO	DA	3198	-	-	0/1/1/1	-
58	PUT	DA	3189	-	-	0/3/3/3	-
64	SPD	DA	3206	-	-	2/7/7/7	-
57	MPD	DS	203	-	-	0/5/5/5	-
63	PGE	DU	101	-	-	3/7/7/7	-
62	EDO	DB	212	-	-	1/1/1/1	-
63	PGE	DA	3225	-	-	5/7/7/7	-
61	PEG	D1	103	-	-	1/4/4/4	-
63	PGE	DS	201	-	-	3/7/7/7	-
58	PUT	DA	3184	-	-	0/3/3/3	-
58	PUT	DA	3188	-	-	0/3/3/3	-
61	PEG	DL	201	-	-	1/4/4/4	-
58	PUT	AA	1674	-	-	0/3/3/3	-
57	MPD	DA	3207	-	-	3/5/5/5	-
58	PUT	DA	3205	-	-	0/3/3/3	-
62	EDO	DA	3003	-	-	1/1/1/1	-
62	EDO	DA	3197	-	-	1/1/1/1	-
62	EDO	DA	3002	-	-	1/1/1/1	-
57	MPD	DK	201	-	-	2/5/5/5	-
63	PGE	DA	3203	-	-	4/7/7/7	-
56	PG4	BA	1642	-	-	0/10/10/10	-
58	PUT	AA	1672	-	-	0/3/3/3	-
61	PEG	DA	3200	-	-	2/4/4/4	-
68	TRS	DA	3220	-	-	0/9/9/9	-
58	PUT	DA	3195	-	-	0/3/3/3	-
62	EDO	DA	3208	-	-	1/1/1/1	-
61	PEG	AL	201	-	-	2/4/4/4	-
59	TAC	BA	1644	55	-	6/8/74/74	0/4/4/4
58	PUT	AA	1675	-	-	1/3/3/3	-
57	MPD	DA	3204	-	-	2/5/5/5	-
59	TAC	AA	1681	55	-	6/8/74/74	0/4/4/4
58	PUT	DM	201	-	-	0/3/3/3	-
61	PEG	DA	3199	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PGE	DA	3186	-	-	2/7/7/7	-
56	PG4	DR	202	-	-	5/10/10/10	-
56	PG4	DS	202	-	-	4/10/10/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	DA	3196	ACY	O-C	3.87	1.40	1.22
57	DE	302	MPD	C3-C2	2.22	1.59	1.53
57	DN	201	MPD	C3-C2	2.04	1.59	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BA	1644	TAC	O3-C3-C2	-3.00	117.69	122.96
66	DA	3196	ACY	OXT-C-CH3	2.82	126.81	115.18
66	DA	3196	ACY	O-C-CH3	-2.65	112.00	122.33
59	AA	1681	TAC	O3-C3-C2	-2.64	118.32	122.96
59	BA	1643	TAC	O3-C3-C2	-2.16	119.16	122.96
59	AA	1681	TAC	C42-N4-C4	2.16	119.17	114.09
59	BA	1643	TAC	C11-C1B-C12	2.10	120.46	118.80
59	AA	1680	TAC	O3-C3-C2	-2.07	119.32	122.96

There are no chirality outliers.

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	DT	201	MPD	O2-C2-C3-C4
59	AA	1681	TAC	C1-C2-C21-O21
59	AA	1681	TAC	C3-C2-C21-O21
59	AA	1681	TAC	C3-C2-C21-N21
59	AA	1681	TAC	C41-C4-N4-C42
59	BA	1643	TAC	C1-C2-C21-O21
59	BA	1643	TAC	C1-C2-C21-N21
59	BA	1643	TAC	C3-C4-N4-C42
59	BA	1643	TAC	C3-C4-N4-C43
59	BA	1643	TAC	C41-C4-N4-C42
59	BA	1644	TAC	C1-C2-C21-O21
59	BA	1644	TAC	C1-C2-C21-N21
59	BA	1644	TAC	C3-C4-N4-C43

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Mol	Chain	Res	Type	Atoms
59	BA	1644	TAC	C41-C4-N4-C42
65	DA	3202	1PE	OH4-C13-C23-OH3
65	DA	3202	1PE	OH5-C14-C24-OH4
63	DA	3186	PGE	O3-C5-C6-O4
56	DR	202	PG4	O2-C3-C4-O3
63	DU	101	PGE	O1-C1-C2-O2
63	DU	101	PGE	O3-C5-C6-O4
63	DA	3203	PGE	O3-C5-C6-O4
63	DA	3203	PGE	O2-C3-C4-O3
64	DA	3224	SPD	C4-C5-N6-C7
56	DQ	202	PG4	O1-C1-C2-O2
56	DS	202	PG4	O1-C1-C2-O2
63	DA	3001	PGE	O3-C5-C6-O4
63	DA	3214	PGE	O3-C5-C6-O4
63	DA	3186	PGE	O1-C1-C2-O2
62	DA	3197	EDO	O1-C1-C2-O2
64	DA	3183	SPD	C2-C3-C4-C5
64	DA	3206	SPD	C8-C7-N6-C5
63	DA	3225	PGE	O2-C3-C4-O3
56	DS	202	PG4	O4-C7-C8-O5
61	D1	103	PEG	O2-C3-C4-O4
61	DA	3226	PEG	O1-C1-C2-O2
65	DA	3202	1PE	OH2-C12-C22-OH3
58	DA	3223	PUT	C1-C2-C3-C4
63	DA	3225	PGE	O3-C5-C6-O4
58	AA	1675	PUT	C1-C2-C3-C4
56	DA	3193	PG4	O3-C5-C6-O4
64	DA	3187	SPD	C2-C3-C4-C5
56	DQ	202	PG4	O2-C3-C4-O3
61	DP	201	PEG	O1-C1-C2-O2
57	AA	1671	MPD	O2-C2-C3-C4
64	DA	3206	SPD	C4-C5-N6-C7
65	DA	3185	1PE	C24-C14-OH5-C25
61	DA	3200	PEG	C1-C2-O2-C3
61	DP	201	PEG	C4-C3-O2-C2
63	DA	3203	PGE	C3-C4-O3-C5
56	DA	3216	PG4	C3-C4-O3-C5
56	DA	3216	PG4	C1-C2-O2-C3
61	DA	3226	PEG	C4-C3-O2-C2
65	DA	3202	1PE	C12-C22-OH3-C23
56	DR	202	PG4	C4-C3-O2-C2
61	DA	3199	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
63	DA	3203	PGE	C4-C3-O2-C2
56	DA	3193	PG4	C6-C5-O3-C4
63	D1	102	PGE	C4-C3-O2-C2
56	DS	202	PG4	C5-C6-O4-C7
56	DA	3193	PG4	C4-C3-O2-C2
61	DA	3218	PEG	C1-C2-O2-C3
61	DA	3226	PEG	C1-C2-O2-C3
63	DA	3001	PGE	C3-C4-O3-C5
65	DA	3185	1PE	C12-C22-OH3-C23
65	DA	3185	1PE	C13-C23-OH3-C22
61	D3	101	PEG	C1-C2-O2-C3
56	DA	3193	PG4	O1-C1-C2-O2
63	DA	3225	PGE	C1-C2-O2-C3
56	DR	202	PG4	C6-C5-O3-C4
61	DA	3200	PEG	C4-C3-O2-C2
57	DE	301	MPD	C2-C3-C4-C5
57	DN	201	MPD	C2-C3-C4-C5
57	DT	202	MPD	C2-C3-C4-C5
57	DA	3190	MPD	C2-C3-C4-C5
57	DA	3204	MPD	C2-C3-C4-C5
57	DA	3207	MPD	C2-C3-C4-C5
59	AA	1680	TAC	C3-C4-N4-C43
59	AA	1681	TAC	C3-C4-N4-C43
59	BA	1643	TAC	C41-C4-N4-C43
63	DU	101	PGE	C6-C5-O3-C4
63	D1	102	PGE	C3-C4-O3-C5
59	BA	1644	TAC	C3-C2-C21-N21
63	D1	102	PGE	O1-C1-C2-O2
63	DA	3217	PGE	C1-C2-O2-C3
59	BA	1644	TAC	C3-C2-C21-O21
64	DA	3224	SPD	C8-C7-N6-C5
63	DA	3214	PGE	C4-C3-O2-C2
57	DE	302	MPD	C2-C3-C4-O4
57	DA	3192	MPD	C2-C3-C4-O4
65	DA	3202	1PE	OH7-C16-C26-OH6
57	DT	201	MPD	C1-C2-C3-C4
57	DT	201	MPD	CM-C2-C3-C4
57	DA	3207	MPD	C1-C2-C3-C4
59	AA	1681	TAC	C1-C2-C21-N21
61	AL	201	PEG	C4-C3-O2-C2
65	DA	3185	1PE	C16-C26-OH6-C15
56	AA	1670	PG4	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
56	AA	1670	PG4	O1-C1-C2-O2
65	DA	3202	1PE	C23-C13-OH4-C24
61	AL	201	PEG	C1-C2-O2-C3
58	DA	3212	PUT	C1-C2-C3-C4
56	DS	202	PG4	C1-C2-O2-C3
63	DS	201	PGE	C6-C5-O3-C4
63	DA	3001	PGE	C4-C3-O2-C2
63	DA	3217	PGE	C4-C3-O2-C2
63	DA	3001	PGE	C1-C2-O2-C3
63	D1	102	PGE	O2-C3-C4-O3
61	DP	201	PEG	C1-C2-O2-C3
64	DA	3224	SPD	C7-C8-C9-N10
61	DQ	201	PEG	C1-C2-O2-C3
56	DA	3193	PG4	C3-C4-O3-C5
64	DA	3187	SPD	N6-C7-C8-C9
56	DA	3216	PG4	O1-C1-C2-O2
63	DA	3225	PGE	C3-C4-O3-C5
61	DL	201	PEG	O1-C1-C2-O2
56	DA	3216	PG4	O4-C7-C8-O5
62	DA	3002	EDO	O1-C1-C2-O2
63	DA	3214	PGE	O2-C3-C4-O3
63	D1	102	PGE	C1-C2-O2-C3
57	DE	302	MPD	O2-C2-C3-C4
57	DA	3207	MPD	O2-C2-C3-C4
63	DA	3225	PGE	O1-C1-C2-O2
63	DS	201	PGE	C1-C2-O2-C3
56	AA	1670	PG4	C1-C2-O2-C3
62	DA	3003	EDO	O1-C1-C2-O2
62	DA	3208	EDO	O1-C1-C2-O2
65	DA	3185	1PE	OH4-C13-C23-OH3
56	DA	3193	PG4	O2-C3-C4-O3
56	AA	1670	PG4	C8-C7-O4-C6
57	DE	302	MPD	C2-C3-C4-C5
57	DK	201	MPD	C2-C3-C4-C5
57	DA	3192	MPD	C2-C3-C4-C5
56	DR	202	PG4	O3-C5-C6-O4
65	DA	3202	1PE	C14-C24-OH4-C13
59	BA	1643	TAC	C3-C2-C21-N21
61	D3	101	PEG	O1-C1-C2-O2
56	DQ	202	PG4	C5-C6-O4-C7
62	DB	212	EDO	O1-C1-C2-O2
59	BA	1643	TAC	C3-C2-C21-O21

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Mol	Chain	Res	Type	Atoms
57	DE	301	MPD	C2-C3-C4-O4
57	DK	201	MPD	C2-C3-C4-O4
57	DN	201	MPD	C2-C3-C4-O4
57	DT	202	MPD	C2-C3-C4-O4
57	DA	3204	MPD	C2-C3-C4-O4
56	DR	202	PG4	C8-C7-O4-C6
63	DS	201	PGE	O2-C3-C4-O3

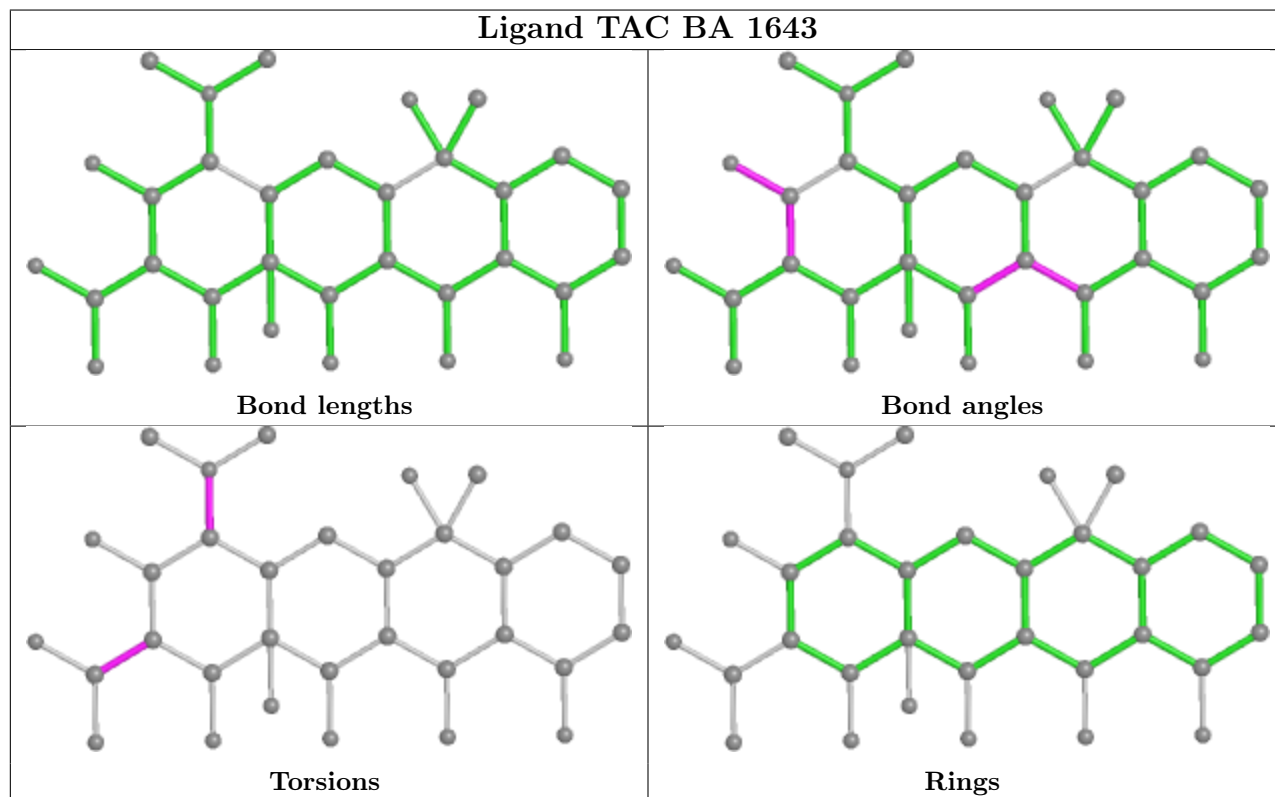
There are no ring outliers.

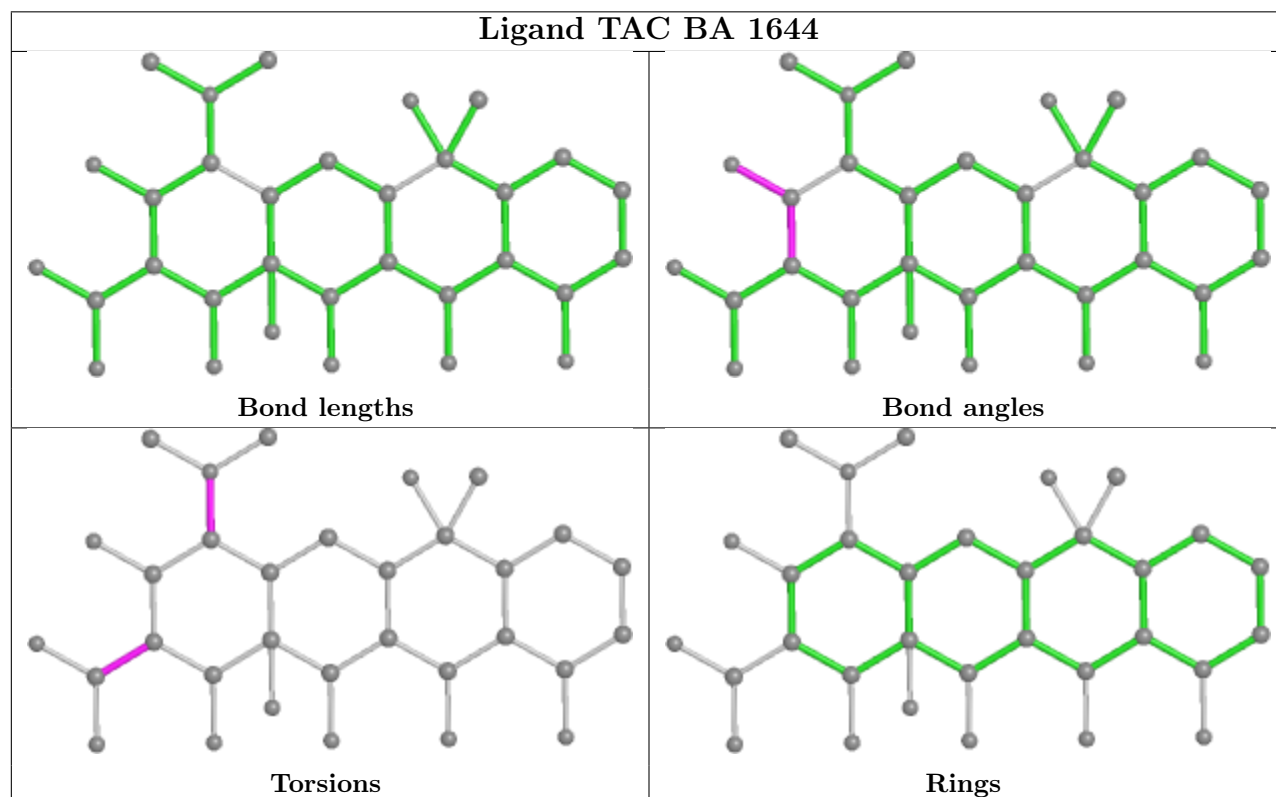
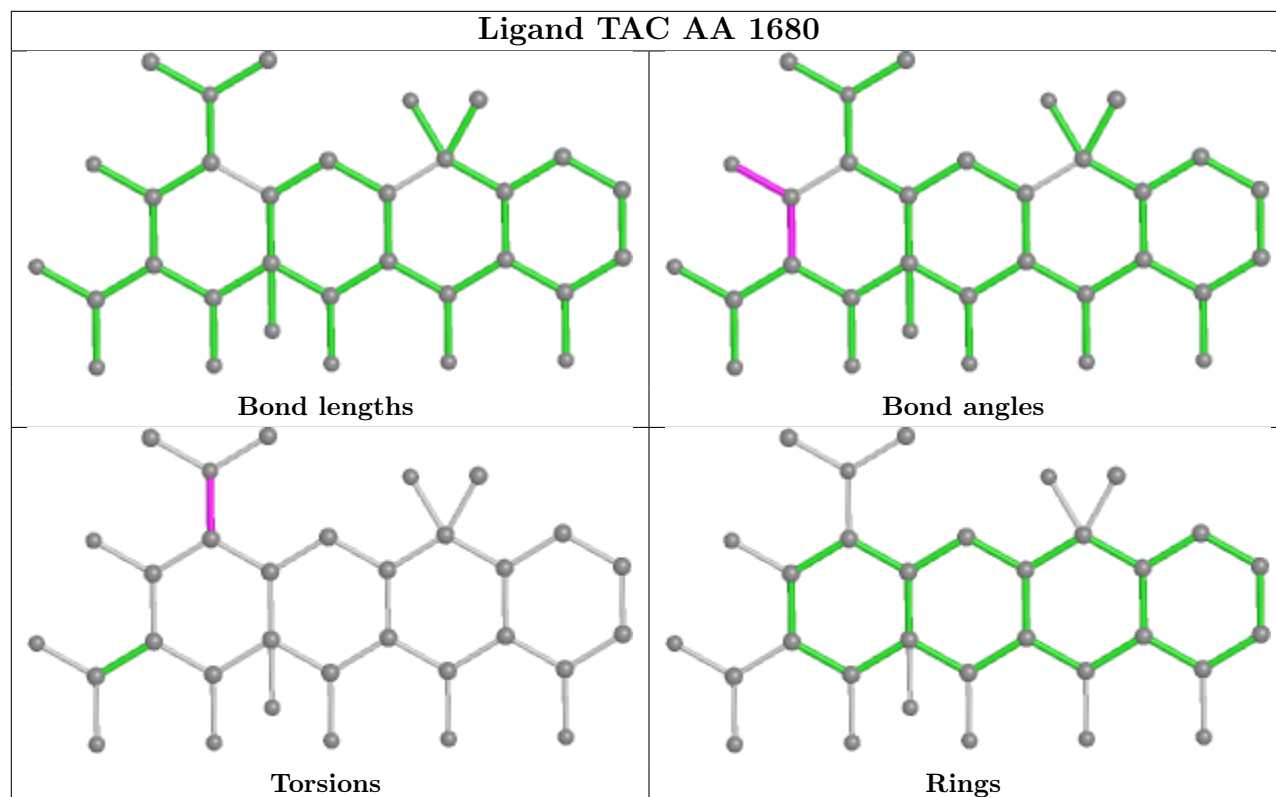
27 monomers are involved in 46 short contacts:

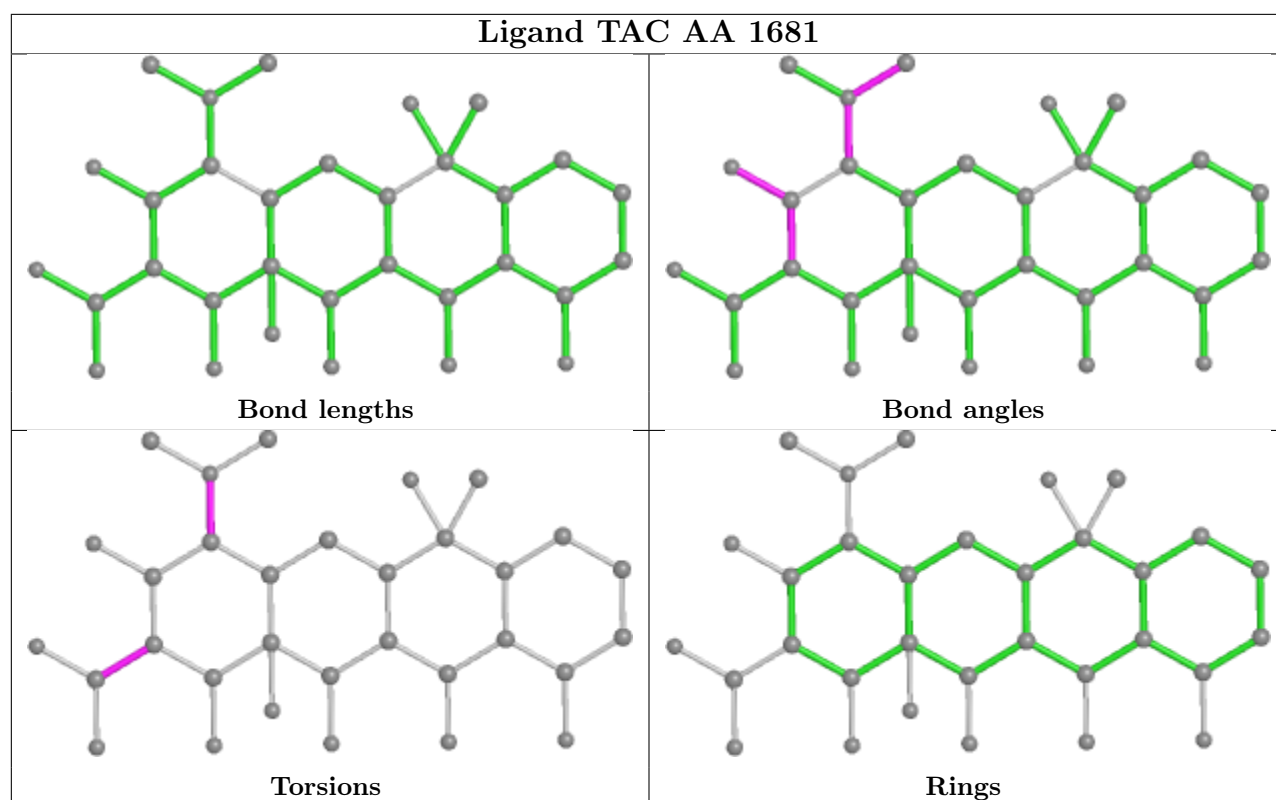
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	1676	MPD	3	0
63	D1	102	PGE	2	0
57	DA	3192	MPD	1	0
56	DA	3193	PG4	2	0
64	DA	3224	SPD	2	0
63	DA	3001	PGE	1	0
63	DA	3214	PGE	1	0
65	DA	3202	1PE	1	0
58	DA	3222	PUT	3	0
61	DP	201	PEG	1	0
57	DN	201	MPD	1	0
56	DA	3216	PG4	1	0
56	AA	1670	PG4	1	0
62	DA	3198	EDO	1	0
58	DA	3189	PUT	1	0
63	DU	101	PGE	3	0
63	DA	3225	PGE	2	0
61	D1	103	PEG	1	0
63	DS	201	PGE	1	0
57	DA	3207	MPD	1	0
56	BA	1642	PG4	1	0
68	DA	3220	TRS	1	0
58	DA	3195	PUT	3	0
57	DA	3204	MPD	1	0
59	AA	1681	TAC	2	0
56	DR	202	PG4	5	0
56	DS	202	PG4	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.06	29 (1%) 66 37	37, 86, 227, 287	0
1	BA	1522/1534 (99%)	0.47	166 (10%) 5 2	58, 109, 255, 271	0
2	AB	224/224 (100%)	0.63	28 (12%) 3 1	65, 117, 185, 228	0
2	BB	224/224 (100%)	0.89	36 (16%) 1 0	89, 139, 197, 228	0
3	AC	206/206 (100%)	-0.11	2 (0%) 82 59	67, 98, 127, 149	0
3	BC	206/206 (100%)	0.98	40 (19%) 1 0	90, 138, 170, 184	0
4	AD	205/205 (100%)	-0.31	0 100 100	63, 92, 129, 160	0
4	BD	205/205 (100%)	-0.45	0 100 100	53, 77, 106, 132	0
5	AE	155/155 (100%)	-0.10	0 100 100	54, 75, 108, 159	0
5	BE	150/155 (96%)	0.07	2 (1%) 77 51	61, 92, 129, 201	0
6	AF	106/106 (100%)	0.00	1 (0%) 84 63	63, 93, 120, 134	0
6	BF	100/106 (94%)	0.43	2 (2%) 65 36	77, 117, 140, 153	0
7	AG	151/151 (100%)	0.88	30 (19%) 1 0	95, 136, 160, 174	0
7	BG	151/151 (100%)	2.32	77 (50%) 0 0	136, 196, 213, 220	0
8	AH	129/129 (100%)	-0.09	1 (0%) 86 65	59, 82, 107, 122	0
8	BH	129/129 (100%)	0.03	4 (3%) 49 21	85, 110, 137, 152	0
9	AI	127/127 (100%)	1.11	27 (21%) 0 0	74, 135, 164, 171	0
9	BI	127/127 (100%)	1.89	49 (38%) 0 0	133, 164, 201, 210	0
10	AJ	99/99 (100%)	0.62	11 (11%) 5 1	83, 118, 141, 147	0
10	BJ	98/99 (98%)	3.08	59 (60%) 0 0	134, 168, 189, 195	0
11	AK	117/117 (100%)	0.24	5 (4%) 35 13	44, 100, 129, 139	0
11	BK	117/117 (100%)	0.23	3 (2%) 56 27	59, 104, 132, 163	0
12	AL	122/123 (99%)	-0.28	1 (0%) 86 65	43, 60, 92, 130	0
12	BL	122/123 (99%)	0.32	4 (3%) 46 20	65, 86, 114, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	1.42	34 (29%) 0 0	108, 130, 165, 171	0
13	BM	114/114 (100%)	3.36	87 (76%) 0 0	195, 230, 238, 247	0
14	AN	100/100 (100%)	1.02	17 (17%) 1 0	77, 117, 178, 184	0
14	BN	100/100 (100%)	2.56	52 (52%) 0 0	124, 178, 216, 222	0
15	AO	88/88 (100%)	-0.07	1 (1%) 80 56	54, 84, 107, 129	0
15	BO	88/88 (100%)	0.45	6 (6%) 17 5	75, 109, 133, 153	0
16	AP	82/82 (100%)	0.40	3 (3%) 41 17	55, 75, 121, 140	0
16	BP	82/82 (100%)	1.17	19 (23%) 0 0	81, 98, 148, 155	0
17	AQ	80/80 (100%)	0.02	2 (2%) 57 29	58, 78, 113, 129	0
17	BQ	80/80 (100%)	1.11	17 (21%) 0 0	83, 120, 145, 157	0
18	AR	55/55 (100%)	0.14	1 (1%) 68 40	63, 89, 130, 153	0
18	BR	55/55 (100%)	0.26	3 (5%) 25 9	65, 86, 129, 168	0
19	AS	79/79 (100%)	0.83	11 (13%) 2 1	114, 135, 155, 163	0
19	BS	79/79 (100%)	3.80	60 (75%) 0 0	210, 226, 239, 245	0
20	AT	86/86 (100%)	0.01	0 100 100	54, 77, 108, 129	0
20	BT	85/86 (98%)	1.29	22 (25%) 0 0	93, 119, 147, 159	0
21	AU	56/56 (100%)	0.26	2 (3%) 42 17	66, 107, 153, 165	0
21	BU	56/56 (100%)	0.30	1 (1%) 68 40	63, 95, 134, 143	0
22	C1	56/56 (100%)	1.10	12 (21%) 0 0	78, 133, 163, 173	0
22	D1	56/56 (100%)	-0.56	0 100 100	18, 37, 65, 104	0
23	C2	50/51 (98%)	3.00	34 (68%) 0 0	131, 157, 168, 196	0
23	D2	51/51 (100%)	-0.00	0 100 100	46, 60, 87, 104	0
24	C3	46/46 (100%)	1.49	13 (28%) 0 0	90, 117, 130, 138	0
24	D3	46/46 (100%)	-0.38	0 100 100	23, 31, 48, 112	0
25	C4	64/64 (100%)	0.89	9 (14%) 2 1	96, 120, 140, 154	0
25	D4	64/64 (100%)	-0.46	0 100 100	23, 35, 48, 61	0
26	C5	38/38 (100%)	1.23	9 (23%) 0 0	91, 114, 127, 138	0
26	D5	38/38 (100%)	-0.33	0 100 100	30, 44, 62, 80	0
27	C0	58/58 (100%)	0.80	9 (15%) 2 1	90, 111, 135, 139	0
27	D0	58/58 (100%)	-0.52	0 100 100	21, 30, 53, 80	0
28	CB	118/120 (98%)	0.65	9 (7%) 13 4	102, 170, 229, 238	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	120/120 (100%)	-0.35	0 100 100	29, 53, 95, 122	0
29	CC	271/271 (100%)	0.36	16 (5%) 22 7	71, 94, 116, 128	0
29	DC	271/271 (100%)	-0.47	0 100 100	22, 49, 76, 92	0
30	CD	208/209 (99%)	0.91	31 (14%) 2 1	73, 111, 141, 155	0
30	DD	208/209 (99%)	-0.51	0 100 100	13, 34, 66, 93	0
31	CA	2875/2904 (99%)	0.61	261 (9%) 9 3	61, 127, 244, 289	0
32	CE	201/201 (100%)	1.30	46 (22%) 0 0	85, 153, 183, 194	0
32	DE	201/201 (100%)	-0.40	1 (0%) 91 75	19, 50, 96, 132	0
33	CF	177/177 (100%)	3.04	112 (63%) 0 0	193, 211, 219, 227	0
33	DF	177/177 (100%)	-0.17	1 (0%) 89 72	44, 75, 117, 142	0
34	CG	176/176 (100%)	1.95	77 (43%) 0 0	130, 159, 185, 198	0
34	DG	176/176 (100%)	-0.16	1 (0%) 89 72	38, 66, 97, 123	0
35	CH	149/149 (100%)	1.37	38 (25%) 0 0	79, 144, 170, 184	0
35	DH	149/149 (100%)	0.85	27 (18%) 1 0	55, 142, 179, 198	0
36	CJ	134/134 (100%)	6.11	120 (89%) 0 0	235, 251, 263, 270	0
36	DJ	134/134 (100%)	3.49	83 (61%) 0 0	200, 227, 240, 245	0
37	CK	142/142 (100%)	0.34	4 (2%) 53 25	84, 101, 127, 139	0
37	DK	142/142 (100%)	-0.57	0 100 100	18, 30, 57, 82	0
38	CL	122/123 (99%)	0.29	6 (4%) 29 11	73, 101, 135, 154	0
38	DL	123/123 (100%)	-0.52	0 100 100	20, 38, 66, 94	0
39	CM	144/144 (100%)	2.01	55 (38%) 0 0	88, 144, 181, 214	0
39	DM	144/144 (100%)	-0.53	0 100 100	10, 45, 79, 102	0
40	CN	135/136 (99%)	0.34	6 (4%) 34 13	71, 104, 130, 165	0
40	DN	135/136 (99%)	-0.64	0 100 100	21, 34, 63, 95	0
41	CO	120/125 (96%)	1.28	28 (23%) 0 0	94, 117, 139, 180	0
41	DO	125/125 (100%)	-0.48	0 100 100	16, 32, 66, 128	0
42	CP	116/117 (99%)	1.91	47 (40%) 0 0	133, 156, 174, 184	0
42	DP	117/117 (100%)	-0.36	0 100 100	34, 52, 82, 94	0
43	CQ	114/114 (100%)	1.18	24 (21%) 1 0	98, 114, 134, 148	0
43	DQ	114/114 (100%)	-0.49	0 100 100	26, 43, 75, 116	0
44	CR	117/117 (100%)	0.95	19 (16%) 1 0	81, 103, 125, 141	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DR	117/117 (100%)	-0.46	1 (0%) 84 63	14, 25, 43, 75	0
45	CS	103/103 (100%)	1.66	33 (32%) 0 0	101, 121, 157, 167	0
45	DS	103/103 (100%)	-0.53	0 100 100	15, 39, 68, 94	0
46	CT	110/110 (100%)	0.85	14 (12%) 3 1	98, 120, 152, 162	0
46	DT	110/110 (100%)	-0.59	0 100 100	15, 28, 56, 111	0
47	CU	93/93 (100%)	1.60	30 (32%) 0 0	124, 146, 173, 182	0
47	DU	93/93 (100%)	-0.01	2 (2%) 62 33	27, 52, 110, 129	0
48	CV	102/102 (100%)	2.59	58 (56%) 0 0	124, 156, 188, 199	0
48	DV	102/102 (100%)	-0.25	2 (1%) 65 36	36, 56, 101, 131	0
49	CW	94/94 (100%)	1.45	30 (31%) 0 0	111, 134, 151, 161	0
49	DW	94/94 (100%)	-0.52	0 100 100	32, 48, 80, 91	0
50	CX	75/76 (98%)	1.42	23 (30%) 0 0	86, 118, 132, 172	0
50	DX	76/76 (100%)	-0.52	1 (1%) 77 51	25, 36, 62, 104	0
51	CY	77/77 (100%)	0.44	3 (3%) 39 15	78, 113, 143, 160	0
51	DY	77/77 (100%)	-0.42	0 100 100	24, 50, 85, 112	0
52	CZ	62/62 (100%)	2.37	32 (51%) 0 0	123, 162, 179, 190	0
52	DZ	62/62 (100%)	-0.03	1 (1%) 72 44	41, 67, 104, 131	0
53	DI	135/135 (100%)	1.23	30 (22%) 0 0	75, 153, 204, 213	1 (0%)
54	DA	2873/2904 (98%)	-0.09	88 (3%) 49 21	16, 39, 206, 298	0
All	All	20632/20745 (99%)	0.49	2361 (11%) 5 1	10, 100, 227, 298	1 (0%)

All (2361) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	CJ	13	VAL	22.9
36	DJ	54	PRO	22.9
36	CJ	54	PRO	20.6
36	CJ	14	ALA	17.1
36	CJ	87	LYS	16.7
36	CJ	76	ALA	16.4
36	CJ	69	PHE	16.1
36	CJ	23	PRO	15.2
36	CJ	12	GLN	13.1
9	BI	128	SER	12.9
36	CJ	55	ILE	12.5

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Mol	Chain	Res	Type	RSRZ
36	CJ	17	MET	12.5
31	CA	2172	U	12.3
36	DJ	135	SER	12.1
36	CJ	53	LEU	11.9
36	DJ	53	LEU	11.9
36	CJ	21	SER	11.5
10	BJ	74	VAL	11.4
10	BJ	75	ASP	11.3
31	CA	1067	A	11.1
54	DA	2120	G	11.0
36	CJ	56	PRO	10.9
36	CJ	20	PRO	10.9
36	DJ	67	PHE	10.7
36	DJ	79	LEU	10.6
31	CA	1068	G	10.4
36	CJ	57	VAL	10.3
36	CJ	59	ILE	10.2
45	CS	50	GLY	10.1
36	CJ	51	LYS	10.1
19	BS	48	THR	10.0
54	DA	2111	U	10.0
36	DJ	94	ASN	9.9
36	DJ	96	ASP	9.9
36	CJ	11	LEU	9.9
1	AA	1030	U	9.8
36	CJ	42	PHE	9.7
36	CJ	75	PRO	9.7
36	CJ	82	LYS	9.5
36	DJ	80	LEU	9.5
36	DJ	24	VAL	9.4
54	DA	2110	G	9.4
53	DI	131	THR	9.3
23	C2	52	ALA	9.3
14	AN	23	LYS	9.2
19	BS	66	MET	9.2
14	AN	21	PHE	9.1
36	CJ	47	ASP	9.0
9	BI	31	ASN	9.0
39	CM	81	ASP	9.0
10	BJ	76	ILE	9.0
36	CJ	22	PRO	8.9
31	CA	2174	C	8.9

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Mol	Chain	Res	Type	RSRZ
36	CJ	46	THR	8.8
10	BJ	8	ILE	8.7
31	CA	2402	U	8.7
36	CJ	89	GLY	8.7
36	CJ	80	LEU	8.7
33	CF	128	TYR	8.6
20	BT	4	ILE	8.6
36	CJ	86	ILE	8.6
1	BA	1302	C	8.6
9	BI	67	VAL	8.6
36	DJ	23	PRO	8.4
9	BI	126	GLN	8.4
19	BS	39	THR	8.4
36	CJ	120	ALA	8.4
36	CJ	60	THR	8.4
36	CJ	68	THR	8.4
36	CJ	126	THR	8.3
7	BG	62	PHE	8.3
19	BS	38	SER	8.3
36	CJ	132	THR	8.3
33	CF	154	ILE	8.3
54	DA	2163	A	8.3
39	CM	82	LEU	8.2
1	BA	983	A	8.2
36	CJ	52	GLY	8.2
36	CJ	138	LEU	8.1
33	CF	106	ILE	8.1
36	CJ	88	SER	8.1
14	BN	60	GLN	8.0
36	DJ	20	PRO	8.0
1	BA	1242	G	8.0
13	BM	23	TYR	8.0
10	BJ	73	LEU	8.0
36	CJ	78	VAL	8.0
19	BS	12	ASP	7.9
14	BN	54	ASP	7.9
36	CJ	83	ALA	7.9
31	CA	1087	G	7.9
36	CJ	121	ASP	7.9
54	DA	2124	G	7.9
10	BJ	41	PRO	7.9
31	CA	2110	G	7.9

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Mol	Chain	Res	Type	RSRZ
52	CZ	45	GLN	7.9
33	CF	153	ASP	7.8
54	DA	2125	G	7.8
33	CF	85	ILE	7.8
36	DJ	55	ILE	7.8
31	CA	2126	A	7.7
36	CJ	61	VAL	7.7
36	CJ	71	THR	7.7
13	BM	45	ILE	7.7
36	CJ	77	ALA	7.7
36	CJ	38	PHE	7.7
13	BM	10	PRO	7.7
34	CG	32	GLU	7.6
33	CF	156	ILE	7.6
54	DA	2127	G	7.6
19	BS	60	VAL	7.6
36	DJ	13	VAL	7.6
9	BI	16	ALA	7.6
33	CF	117	LEU	7.5
48	CV	87	PHE	7.5
36	CJ	9	VAL	7.5
19	BS	14	HIS	7.5
48	CV	80	ALA	7.5
31	CA	2125	G	7.4
19	BS	74	PHE	7.4
7	BG	42	ILE	7.3
36	CJ	139	VAL	7.3
39	CM	114	GLY	7.3
36	CJ	24	VAL	7.3
31	CA	2173	A	7.2
36	CJ	129	ILE	7.2
14	BN	35	ASN	7.2
10	BJ	90	LEU	7.1
23	C2	24	THR	7.1
13	BM	39	ILE	7.1
19	BS	49	ILE	7.1
36	CJ	99	GLY	7.1
31	CA	1066	U	7.1
13	BM	105	ASN	7.0
10	BJ	26	VAL	7.0
14	BN	21	PHE	7.0
13	BM	84	GLY	7.0

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Mol	Chain	Res	Type	RSRZ
33	CF	132	VAL	7.0
1	BA	211	G	7.0
33	CF	155	THR	6.9
33	CF	176	PRO	6.9
48	CV	20	GLY	6.9
31	CA	1084	A	6.9
14	BN	36	ALA	6.9
54	DA	884	U	6.9
36	CJ	50	GLU	6.9
45	CS	27	ILE	6.9
36	CJ	79	LEU	6.9
48	CV	89	ASP	6.9
31	CA	1104	C	6.9
33	CF	113	ASP	6.8
7	BG	151	PHE	6.8
48	CV	36	VAL	6.8
10	BJ	39	PRO	6.8
19	BS	29	LYS	6.8
48	CV	3	ALA	6.8
19	BS	63	THR	6.8
1	BA	82	G	6.8
18	BR	20	GLU	6.8
14	BN	49	GLN	6.7
54	DA	1172	C	6.7
13	BM	40	ALA	6.7
1	AA	86	G	6.7
31	CA	1537	G	6.7
36	CJ	15	ALA	6.7
40	CN	136	MET	6.7
34	CG	103	ILE	6.7
14	BN	17	ALA	6.6
50	CX	54	GLY	6.6
36	CJ	73	THR	6.6
36	CJ	96	ASP	6.6
36	CJ	90	SER	6.6
33	CF	95	ARG	6.6
43	CQ	85	SER	6.6
10	BJ	38	GLY	6.6
7	BG	116	MET	6.6
9	AI	130	ARG	6.6
9	BI	130	ARG	6.6
36	CJ	119	GLY	6.6

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Mol	Chain	Res	Type	RSRZ
36	DJ	76	ALA	6.6
31	CA	1085	A	6.5
31	CA	1103	A	6.5
1	AA	844	G	6.5
1	BA	209	U	6.5
19	BS	28	LYS	6.5
13	BM	47	GLU	6.5
33	CF	97	TRP	6.5
39	CM	144	GLU	6.5
1	BA	1030	U	6.5
52	CZ	15	ASN	6.5
7	BG	52	GLN	6.5
1	BA	1241	G	6.5
33	CF	144	ASP	6.5
19	BS	32	ARG	6.5
13	BM	48	LEU	6.5
34	CG	33	LEU	6.5
19	BS	41	PHE	6.5
33	CF	136	ILE	6.4
36	CJ	131	GLY	6.4
36	DJ	138	LEU	6.4
14	BN	43	ASN	6.4
10	BJ	91	ASP	6.4
13	BM	96	PRO	6.4
36	DJ	114	ALA	6.4
7	BG	43	VAL	6.4
9	BI	17	ALA	6.4
13	BM	64	VAL	6.3
1	AA	87	C	6.3
53	DI	128	THR	6.3
14	BN	40	ASP	6.3
36	DJ	12	GLN	6.3
9	AI	20	PHE	6.3
23	C2	47	VAL	6.3
36	DJ	38	PHE	6.3
36	DJ	137	GLY	6.3
10	BJ	7	ARG	6.2
48	CV	31	SER	6.2
2	AB	123	ASP	6.2
33	CF	92	ARG	6.2
10	BJ	35	GLN	6.2
31	CA	1057	A	6.1

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Mol	Chain	Res	Type	RSRZ
1	BA	1243	C	6.1
54	DA	2123	G	6.1
10	BJ	6	ILE	6.1
33	CF	96	MET	6.1
19	BS	37	ARG	6.1
10	BJ	37	ARG	6.1
54	DA	2174	C	6.1
19	BS	61	PHE	6.1
36	DJ	87	LYS	6.1
36	DJ	42	PHE	6.0
13	BM	22	ILE	6.0
36	CJ	45	LYS	6.0
36	DJ	36	MET	6.0
36	DJ	88	SER	6.0
54	DA	2121	G	6.0
39	CM	101	ILE	6.0
7	AG	62	PHE	6.0
36	CJ	19	ASN	6.0
31	CA	1175	A	6.0
34	CG	2	SER	6.0
34	CG	105	LEU	6.0
52	CZ	17	GLU	6.0
17	BQ	70	THR	6.0
10	BJ	102	LEU	6.0
54	DA	885	C	6.0
31	CA	331	C	5.9
36	CJ	74	PRO	5.9
52	CZ	40	SER	5.9
36	CJ	84	ALA	5.9
1	BA	1016	A	5.9
54	DA	892	A	5.9
36	CJ	18	ALA	5.9
36	DJ	21	SER	5.9
33	CF	23	ASN	5.9
14	BN	50	THR	5.9
50	CX	52	GLY	5.9
20	BT	36	TYR	5.9
1	AA	1032	G	5.9
7	BG	39	ALA	5.9
39	CM	8	PRO	5.9
48	CV	88	GLU	5.9
36	CJ	44	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
31	CA	1065	U	5.9
23	C2	37	LYS	5.9
36	DJ	68	THR	5.9
14	BN	52	PRO	5.8
1	BA	1032	G	5.8
10	BJ	40	ILE	5.8
36	CJ	28	LEU	5.8
33	CF	175	PHE	5.8
36	DJ	133	ALA	5.8
1	AA	1031	C	5.8
48	CV	13	VAL	5.8
13	BM	46	SER	5.8
31	CA	1105	U	5.8
10	BJ	25	ILE	5.8
10	BJ	77	VAL	5.8
36	CJ	118	THR	5.8
45	CS	32	THR	5.8
1	BA	1024	G	5.8
33	CF	116	GLY	5.8
7	BG	41	SER	5.8
52	CZ	49	ASP	5.8
34	CG	40	ALA	5.7
33	CF	147	ASP	5.7
1	BA	1017	U	5.7
12	AL	124	ALA	5.7
48	CV	32	GLY	5.7
33	CF	112	ARG	5.7
33	CF	65	PRO	5.7
7	BG	45	SER	5.7
13	BM	95	LEU	5.7
36	DJ	19	ASN	5.7
54	DA	1729	U	5.7
54	DA	2118	U	5.7
13	AM	33	ILE	5.7
48	CV	33	LYS	5.7
36	CJ	116	ASP	5.6
33	CF	40	VAL	5.6
13	BM	83	LEU	5.6
14	BN	55	SER	5.6
32	CE	104	ALA	5.6
1	BA	1296	C	5.6
14	BN	58	SER	5.6

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Mol	Chain	Res	Type	RSRZ
54	DA	1731	G	5.6
49	CW	94	ALA	5.6
31	CA	2127	G	5.6
33	CF	157	THR	5.6
14	BN	45	VAL	5.5
31	CA	877	A	5.5
1	BA	1240	U	5.5
54	DA	2175	C	5.5
7	BG	75	VAL	5.5
26	C5	38	GLY	5.5
9	AI	21	ILE	5.5
19	BS	76	PRO	5.5
36	CJ	43	ASN	5.5
7	BG	65	ALA	5.5
23	C2	31	PRO	5.5
36	DJ	132	THR	5.5
31	CA	1086	A	5.5
19	BS	13	LEU	5.4
39	CM	92	LEU	5.4
7	BG	148	ASN	5.4
7	BG	8	GLY	5.4
7	BG	91	VAL	5.4
33	CF	93	GLY	5.4
31	CA	2120	G	5.4
36	CJ	62	TYR	5.4
9	AI	90	TYR	5.4
19	BS	42	PRO	5.4
36	DJ	22	PRO	5.4
54	DA	1065	U	5.4
1	BA	1020	G	5.4
13	BM	31	LYS	5.4
9	BI	38	TYR	5.4
33	CF	135	GLN	5.4
10	BJ	27	GLU	5.4
31	CA	1095	A	5.4
36	CJ	122	ILE	5.4
19	BS	65	GLU	5.4
36	CJ	98	VAL	5.3
36	CJ	67	PHE	5.3
53	DI	96	PHE	5.3
54	DA	2116	G	5.3
33	CF	102	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
10	BJ	87	LEU	5.3
33	CF	130	MET	5.3
53	DI	130	PRO	5.3
13	BM	33	ILE	5.3
13	BM	56	LEU	5.3
33	CF	35	THR	5.3
33	CF	131	GLY	5.3
19	BS	31	LEU	5.3
36	CJ	8	TYR	5.3
36	CJ	33	VAL	5.3
13	BM	104	THR	5.3
36	CJ	94	ASN	5.3
31	CA	1083	U	5.3
13	AM	30	SER	5.2
45	CS	63	VAL	5.2
36	DJ	69	PHE	5.2
48	CV	98	SER	5.2
19	BS	30	PRO	5.2
3	BC	192	THR	5.2
47	CU	43	ILE	5.2
34	CG	102	VAL	5.2
13	BM	85	CYS	5.2
37	CK	142	ILE	5.2
53	DI	121	SER	5.2
54	DA	2172	U	5.2
53	DI	134	GLU	5.2
39	CM	78	ARG	5.2
31	CA	878	A	5.2
19	BS	11	ILE	5.2
7	BG	150	ALA	5.2
31	CA	2123	G	5.2
33	CF	31	VAL	5.2
39	CM	10	GLU	5.2
9	BI	68	LYS	5.2
33	CF	60	ILE	5.2
35	CH	11	ASN	5.1
43	CQ	111	LYS	5.1
39	CM	80	SER	5.1
9	BI	127	PHE	5.1
14	BN	53	ARG	5.1
33	CF	152	LEU	5.1
42	CP	64	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
33	CF	34	ILE	5.1
13	AM	13	LYS	5.1
13	BM	19	LEU	5.1
23	C2	35	GLU	5.1
14	BN	51	LEU	5.1
45	CS	96	VAL	5.1
10	BJ	21	ALA	5.1
31	CA	931	U	5.1
23	C2	21	TYR	5.1
12	BL	124	ALA	5.1
33	CF	170	LEU	5.1
10	BJ	72	ARG	5.1
31	CA	75	G	5.1
31	CA	2171	A	5.1
54	DA	883	G	5.1
31	CA	1536	C	5.1
15	BO	17	ARG	5.0
52	CZ	32	ALA	5.0
31	CA	2119	A	5.0
23	C2	36	LEU	5.0
14	BN	48	LEU	5.0
31	CA	2163	A	5.0
14	BN	20	TYR	5.0
49	CW	6	ALA	5.0
14	BN	37	SER	5.0
33	CF	36	LEU	5.0
36	DJ	78	VAL	5.0
1	BA	1218	C	5.0
7	BG	49	THR	5.0
54	DA	896	A	5.0
31	CA	2161	C	5.0
36	CJ	85	GLY	5.0
9	BI	32	GLN	5.0
54	DA	2167	U	5.0
7	BG	134	ALA	4.9
9	BI	5	GLN	4.9
19	BS	5	LEU	4.9
48	CV	79	LYS	4.9
23	C2	18	GLY	4.9
48	CV	29	LEU	4.9
13	AM	43	VAL	4.9
14	BN	31	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
33	CF	151	GLY	4.9
14	BN	27	LEU	4.9
36	CJ	123	GLU	4.9
32	CE	143	LEU	4.9
13	BM	30	SER	4.9
7	BG	71	PRO	4.9
31	CA	2128	G	4.9
31	CA	546	U	4.9
10	BJ	22	THR	4.9
34	CG	52	PHE	4.9
43	CQ	115	ASN	4.9
32	CE	119	ILE	4.9
33	CF	86	GLY	4.9
13	BM	61	ALA	4.9
7	BG	4	ARG	4.9
33	CF	143	TYR	4.9
48	CV	35	ILE	4.9
1	BA	949	A	4.9
16	BP	57	ILE	4.8
16	AP	47	GLU	4.8
36	CJ	26	PRO	4.8
1	BA	1026	G	4.8
13	BM	41	GLU	4.8
33	CF	107	ALA	4.8
36	CJ	48	SER	4.8
13	BM	38	GLY	4.8
54	DA	138	U	4.8
42	CP	40	ILE	4.8
7	BG	37	SER	4.8
13	BM	32	ALA	4.8
52	CZ	63	ALA	4.8
39	CM	126	ARG	4.8
42	CP	29	HIS	4.8
48	CV	5	ILE	4.8
41	CO	63	ARG	4.8
21	AU	2	PRO	4.8
31	CA	896	A	4.8
31	CA	318	C	4.8
13	BM	29	ARG	4.8
9	BI	44	ALA	4.8
44	CR	118	ALA	4.8
2	BB	123	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
36	CJ	70	VAL	4.8
33	CF	173	PHE	4.8
39	CM	77	ILE	4.7
19	BS	43	ASN	4.7
31	CA	1179	G	4.7
29	CC	27	GLY	4.7
33	CF	28	VAL	4.7
52	CZ	33	ALA	4.7
36	CJ	113	LYS	4.7
9	AI	5	GLN	4.7
31	CA	846	U	4.7
13	BM	55	THR	4.7
31	CA	879	G	4.7
13	BM	65	VAL	4.7
36	DJ	110	ALA	4.7
54	DA	882	G	4.7
32	CE	172	ALA	4.7
36	DJ	40	LYS	4.7
31	CA	1535	A	4.7
14	BN	39	GLU	4.7
32	CE	164	LEU	4.7
34	CG	111	HIS	4.7
42	CP	63	LYS	4.7
23	C2	53	LYS	4.7
39	CM	89	VAL	4.7
13	AM	5	ALA	4.7
13	AM	24	GLY	4.7
7	BG	48	GLU	4.7
9	AI	22	LYS	4.7
17	BQ	78	VAL	4.7
10	BJ	86	ALA	4.7
36	CJ	135	SER	4.6
42	CP	52	SER	4.6
42	CP	41	ALA	4.6
45	CS	49	ILE	4.6
54	DA	2126	A	4.6
39	CM	120	VAL	4.6
31	CA	2124	G	4.6
33	CF	25	VAL	4.6
3	BC	196	ILE	4.6
44	CR	73	GLY	4.6
33	CF	122	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	BA	1028	C	4.6
48	CV	81	ASP	4.6
3	BC	71	ALA	4.6
36	CJ	58	VAL	4.6
19	BS	24	GLU	4.6
7	AG	4	ARG	4.6
13	BM	34	LEU	4.6
19	BS	27	ASP	4.6
13	BM	11	ASP	4.5
1	BA	954	G	4.5
48	CV	19	LYS	4.5
1	BA	1031	C	4.5
13	BM	5	ALA	4.5
42	CP	117	PHE	4.5
47	CU	83	ALA	4.5
33	CF	32	GLU	4.5
35	CH	78	VAL	4.5
41	CO	119	SER	4.5
26	C5	1	MET	4.5
41	CO	28	LEU	4.5
42	CP	38	GLN	4.5
9	BI	40	GLY	4.5
39	CM	100	ILE	4.5
1	BA	844	G	4.5
33	CF	105	THR	4.5
14	BN	47	LYS	4.5
31	CA	1090	A	4.5
36	CJ	32	GLY	4.5
53	DI	136	ILE	4.5
1	BA	1025	U	4.5
19	BS	23	VAL	4.5
31	CA	81	G	4.5
36	CJ	41	ALA	4.5
7	BG	35	LYS	4.5
7	BG	133	THR	4.5
36	DJ	66	SER	4.5
36	DJ	134	ARG	4.5
52	CZ	42	LEU	4.5
54	DA	2109	U	4.5
31	CA	329	G	4.5
10	BJ	42	LEU	4.4
36	CJ	133	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
42	CP	24	THR	4.4
50	CX	63	ALA	4.4
33	CF	37	ASN	4.4
54	DA	2147	A	4.4
13	AM	32	ALA	4.4
14	AN	31	ILE	4.4
36	CJ	95	LYS	4.4
13	BM	2	ALA	4.4
14	BN	41	ARG	4.4
48	CV	78	GLY	4.4
43	CQ	12	GLN	4.4
36	CJ	130	GLU	4.4
14	BN	13	ARG	4.4
13	BM	12	HIS	4.4
19	BS	69	HIS	4.4
9	BI	14	SER	4.4
52	CZ	22	LEU	4.4
54	DA	1068	G	4.4
32	CE	183	PHE	4.4
41	CO	120	GLU	4.4
31	CA	549	G	4.4
2	BB	82	ASP	4.4
10	BJ	19	ASP	4.4
16	BP	17	TYR	4.3
19	BS	51	VAL	4.3
36	CJ	136	MET	4.3
36	CJ	27	ALA	4.3
52	CZ	31	GLN	4.3
36	DJ	49	ILE	4.3
49	CW	27	PRO	4.3
1	BA	1126	U	4.3
54	DA	2166	U	4.3
36	DJ	131	GLY	4.3
26	C5	32	LYS	4.3
31	CA	2121	G	4.3
49	CW	48	MET	4.3
2	BB	135	LEU	4.3
7	BG	72	THR	4.3
33	CF	129	SER	4.3
10	BJ	101	SER	4.3
3	BC	206	GLU	4.3
10	BJ	80	THR	4.3

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Mol	Chain	Res	Type	RSRZ
32	CE	33	VAL	4.3
10	AJ	35	GLN	4.3
10	AJ	75	ASP	4.3
1	BA	1314	C	4.3
19	BS	71	LEU	4.3
14	BN	30	ILE	4.3
30	CD	10	GLY	4.3
9	AI	128	SER	4.3
7	BG	144	MET	4.3
1	BA	213	G	4.3
31	CA	1731	G	4.3
34	CG	104	ASN	4.3
13	BM	24	GLY	4.3
45	CS	20	VAL	4.3
1	BA	1022	A	4.2
7	AG	58	GLU	4.2
31	CA	2164	C	4.2
48	CV	30	SER	4.2
36	CJ	125	MET	4.2
52	CZ	41	HIS	4.2
39	CM	115	GLU	4.2
31	CA	1047	G	4.2
54	DA	881	G	4.2
39	CM	142	ILE	4.2
54	DA	1077	A	4.2
7	BG	5	ARG	4.2
14	BN	33	ASP	4.2
1	BA	1247	U	4.2
9	AI	32	GLN	4.2
7	AG	8	GLY	4.2
1	BA	953	G	4.2
10	BJ	10	LEU	4.2
33	CF	137	ILE	4.2
43	CQ	110	ILE	4.2
19	BS	33	THR	4.2
32	CE	197	GLU	4.2
1	BA	1321	U	4.2
20	BT	3	ASN	4.2
34	CG	27	LYS	4.2
36	CJ	25	GLY	4.2
13	BM	36	ALA	4.2
23	C2	46	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	BA	208	U	4.2
3	BC	53	SER	4.2
45	CS	26	ASP	4.2
36	DJ	28	LEU	4.2
36	DJ	25	GLY	4.2
36	DJ	52	GLY	4.2
1	BA	1245	C	4.1
31	CA	1211	C	4.1
54	DA	1067	A	4.1
39	CM	108	ALA	4.1
31	CA	2116	G	4.1
13	BM	25	VAL	4.1
34	CG	26	ILE	4.1
54	DA	893	C	4.1
13	AM	64	VAL	4.1
39	CM	130	GLY	4.1
1	AA	1020	G	4.1
13	BM	13	LYS	4.1
31	CA	613	A	4.1
47	CU	8	LEU	4.1
31	CA	1064	C	4.1
31	CA	2170	A	4.1
7	BG	54	SER	4.1
1	BA	1235	U	4.1
50	CX	53	CYS	4.1
13	BM	6	GLY	4.1
9	BI	39	PHE	4.1
13	BM	35	ALA	4.1
31	CA	1106	G	4.1
32	CE	201	ALA	4.1
31	CA	1048	A	4.1
14	BN	16	LEU	4.1
31	CA	2797	U	4.1
33	CF	76	GLY	4.1
13	BM	4	ILE	4.1
31	CA	2802	G	4.1
36	DJ	97	LYS	4.1
54	DA	2176	A	4.1
39	CM	79	LEU	4.1
31	CA	344	A	4.1
9	AI	6	TYR	4.1
31	CA	138	U	4.1

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Mol	Chain	Res	Type	RSRZ
34	CG	83	PHE	4.1
53	DI	124	ASP	4.1
16	BP	52	LEU	4.1
9	AI	129	LYS	4.0
10	BJ	99	GLN	4.0
42	CP	36	TYR	4.0
1	BA	985	C	4.0
1	BA	1244	G	4.0
2	BB	34	ALA	4.0
13	BM	58	ASP	4.0
14	BN	4	GLN	4.0
39	CM	90	VAL	4.0
43	CQ	27	GLU	4.0
3	BC	159	GLY	4.0
1	BA	1305	G	4.0
16	BP	60	TRP	4.0
31	CA	1046	A	4.0
31	CA	2666	C	4.0
35	CH	72	ILE	4.0
36	DJ	93	PRO	4.0
10	BJ	36	VAL	4.0
36	CJ	117	MET	4.0
1	BA	942	G	4.0
36	CJ	31	GLN	4.0
31	CA	12	U	4.0
48	CV	28	VAL	4.0
36	DJ	11	LEU	4.0
33	CF	139	PRO	4.0
13	BM	70	ARG	4.0
31	CA	1078	U	4.0
36	DJ	99	GLY	4.0
54	DA	2146	C	4.0
43	CQ	84	ILE	4.0
54	DA	1847	A	4.0
9	AI	89	GLU	4.0
33	CF	174	ASP	4.0
36	DJ	85	GLY	4.0
42	CP	65	THR	4.0
42	CP	92	PHE	4.0
34	CG	17	VAL	4.0
47	CU	55	VAL	4.0
53	DI	38	MET	4.0

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Mol	Chain	Res	Type	RSRZ
52	CZ	24	GLU	4.0
24	C3	35	ARG	4.0
3	BC	193	TYR	3.9
31	CA	183	C	3.9
54	DA	2115	G	3.9
48	CV	95	PHE	3.9
32	CE	144	GLU	3.9
33	CF	94	GLU	3.9
45	CS	31	GLU	3.9
7	BG	137	LYS	3.9
47	DU	1	MET	3.9
54	DA	2178	C	3.9
10	BJ	89	ARG	3.9
10	BJ	94	ALA	3.9
19	BS	68	GLY	3.9
14	BN	6	MET	3.9
33	CF	111	ILE	3.9
7	BG	66	LEU	3.9
7	AG	54	SER	3.9
1	BA	85	U	3.9
1	BA	955	U	3.9
31	CA	1107	G	3.9
47	CU	57	VAL	3.9
44	CR	71	GLN	3.9
36	DJ	48	SER	3.9
36	DJ	59	ILE	3.9
39	CM	70	LYS	3.9
15	BO	89	ARG	3.9
31	CA	1049	C	3.9
48	CV	50	PRO	3.9
13	BM	60	VAL	3.9
31	CA	1530	G	3.9
54	DA	879	G	3.9
23	C2	39	PHE	3.9
36	CJ	97	LYS	3.9
31	CA	2162	G	3.9
31	CA	2665	A	3.9
54	DA	1062	G	3.9
13	AM	25	VAL	3.9
48	DV	56	GLY	3.9
7	AG	109	ARG	3.9
1	BA	1125	U	3.9

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Mol	Chain	Res	Type	RSRZ
14	AN	18	ASP	3.9
23	C2	45	GLN	3.9
10	BJ	24	GLU	3.9
7	BG	69	VAL	3.9
35	CH	61	VAL	3.9
44	CR	74	ILE	3.9
31	CA	1094	U	3.9
14	AN	25	ALA	3.9
24	C3	32	ALA	3.9
1	AA	1286	U	3.8
49	CW	67	GLY	3.8
31	CA	2169	A	3.8
1	BA	842	U	3.8
31	CA	880	G	3.8
45	CS	24	LYS	3.8
10	BJ	34	ALA	3.8
41	CO	76	VAL	3.8
2	AB	46	THR	3.8
47	CU	60	THR	3.8
49	CW	29	ILE	3.8
7	BG	46	ALA	3.8
30	CD	4	LEU	3.8
3	BC	197	GLY	3.8
42	CP	93	ASP	3.8
31	CA	876	C	3.8
7	BG	15	ASP	3.8
7	BG	38	THR	3.8
7	BG	88	PRO	3.8
1	BA	4	U	3.8
15	AO	17	ARG	3.8
9	BI	92	GLU	3.8
3	BC	76	VAL	3.8
13	BM	37	ALA	3.8
24	C3	1	MET	3.8
39	CM	132	ARG	3.8
7	BG	129	GLU	3.8
9	BI	64	TYR	3.8
35	DH	137	GLU	3.8
33	CF	67	ILE	3.8
1	BA	1034	G	3.8
6	BF	39	LEU	3.8
39	CM	85	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
47	CU	72	GLN	3.8
23	C2	23	THR	3.8
47	CU	15	HIS	3.8
9	AI	19	VAL	3.8
14	BN	22	ALA	3.8
2	AB	4	VAL	3.8
31	CA	1870	C	3.8
34	CG	43	VAL	3.8
35	CH	136	SER	3.8
14	BN	28	LYS	3.7
33	CF	62	GLY	3.7
36	CJ	81	LYS	3.7
13	BM	113	ARG	3.7
7	AG	7	ILE	3.7
23	C2	48	ILE	3.7
52	CZ	37	LEU	3.7
13	BM	97	VAL	3.7
41	CO	116	VAL	3.7
31	CA	2667	C	3.7
53	DI	104	ALA	3.7
33	CF	141	ILE	3.7
48	CV	4	LYS	3.7
14	BN	32	SER	3.7
47	CU	1	MET	3.7
14	BN	2	ALA	3.7
16	BP	42	ILE	3.7
9	BI	66	THR	3.7
7	BG	16	PRO	3.7
16	BP	56	ARG	3.7
31	CA	1045	C	3.7
31	CA	1547	C	3.7
41	CO	26	GLY	3.7
10	BJ	28	THR	3.7
10	BJ	100	ILE	3.7
13	BM	52	GLN	3.7
42	CP	30	ARG	3.7
54	DA	1089	A	3.7
9	BI	117	GLY	3.7
2	BB	67	ILE	3.7
9	BI	20	PHE	3.7
33	CF	138	PHE	3.7
49	CW	42	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
53	DI	135	ALA	3.7
10	BJ	20	GLN	3.7
34	CG	112	PRO	3.7
10	BJ	9	ARG	3.7
46	CT	84	ARG	3.7
33	CF	99	PHE	3.7
48	CV	39	ILE	3.7
19	AS	56	GLN	3.7
36	DJ	60	THR	3.7
54	DA	1064	C	3.7
2	AB	225	ARG	3.7
54	DA	2162	G	3.7
30	CD	26	VAL	3.7
1	BA	1219	A	3.7
9	BI	15	SER	3.7
32	CE	200	LEU	3.7
48	CV	51	ALA	3.7
7	BG	109	ARG	3.7
48	CV	18	ASP	3.7
13	BM	63	PHE	3.7
36	CJ	35	ILE	3.7
7	AG	5	ARG	3.7
42	CP	67	ASN	3.7
32	CE	17	THR	3.6
52	CZ	6	LEU	3.6
7	BG	73	VAL	3.6
48	CV	25	VAL	3.6
53	DI	132	TYR	3.6
14	AN	24	ARG	3.6
39	CM	91	ASP	3.6
54	DA	2168	G	3.6
17	BQ	45	HIS	3.6
16	AP	82	ALA	3.6
34	CG	56	ASP	3.6
49	CW	45	ASP	3.6
52	CZ	29	ARG	3.6
35	CH	140	ALA	3.6
39	CM	133	ALA	3.6
31	CA	895	U	3.6
39	CM	117	THR	3.6
34	CG	108	GLY	3.6
9	BI	41	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
32	CE	12	LEU	3.6
13	AM	7	ILE	3.6
1	BA	984	C	3.6
47	CU	69	ARG	3.6
10	BJ	81	GLU	3.6
19	BS	15	LEU	3.6
30	CD	186	LEU	3.6
31	CA	1044	C	3.6
13	AM	44	LYS	3.6
14	BN	18	ASP	3.6
1	AA	121	U	3.6
14	BN	9	ARG	3.6
2	BB	33	GLY	3.6
19	BS	21	LYS	3.6
7	BG	106	GLU	3.6
19	BS	75	ALA	3.6
34	CG	121	ILE	3.6
34	CG	169	VAL	3.6
43	CQ	9	GLU	3.6
54	DA	1078	U	3.6
20	BT	48	GLN	3.6
2	BB	35	ARG	3.6
31	CA	1171	G	3.6
31	CA	1524	G	3.6
34	CG	62	TRP	3.6
3	BC	179	ARG	3.6
20	BT	49	LYS	3.6
34	CG	106	SER	3.6
9	BI	125	PRO	3.6
42	CP	66	GLY	3.6
31	CA	1167	C	3.5
17	BQ	17	MET	3.5
36	DJ	98	VAL	3.5
32	CE	118	LEU	3.5
17	BQ	83	VAL	3.5
23	C2	43	VAL	3.5
41	CO	62	ASN	3.5
1	AA	81	A	3.5
3	BC	79	LYS	3.5
7	BG	113	ASP	3.5
22	C1	46	ASP	3.5
33	CF	56	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
50	CX	59	LEU	3.5
3	BC	80	LYS	3.5
27	C0	56	LYS	3.5
36	DJ	51	LYS	3.5
7	BG	141	VAL	3.5
42	CP	46	GLU	3.5
47	CU	10	VAL	3.5
20	BT	46	ALA	3.5
36	DJ	89	GLY	3.5
1	BA	1018	G	3.5
32	CE	23	PHE	3.5
54	DA	546	U	3.5
54	DA	2132	U	3.5
31	CA	2178	C	3.5
1	BA	958	A	3.5
1	BA	1201	A	3.5
17	BQ	53	CYS	3.5
35	CH	76	GLU	3.5
1	BA	94	G	3.5
34	CG	148	LEU	3.5
19	BS	22	ALA	3.5
52	DZ	63	ALA	3.5
50	CX	85	GLU	3.5
54	DA	2122	U	3.5
16	BP	53	ASP	3.5
36	DJ	37	GLU	3.5
1	BA	1145	A	3.5
13	BM	54	ASP	3.5
36	DJ	100	LYS	3.5
7	BG	87	VAL	3.5
48	CV	40	ASN	3.5
7	BG	103	TRP	3.5
47	CU	16	VAL	3.5
52	CZ	18	LEU	3.5
1	BA	1221	G	3.5
16	BP	81	ALA	3.5
35	CH	74	ALA	3.5
42	CP	20	GLU	3.4
13	BM	74	SER	3.4
31	CA	1077	A	3.4
36	DJ	46	THR	3.4
30	CD	6	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
43	CQ	91	ALA	3.4
52	CZ	36	GLN	3.4
7	BG	111	ARG	3.4
34	CG	9	VAL	3.4
10	BJ	32	THR	3.4
45	CS	35	PHE	3.4
13	BM	42	ASP	3.4
1	BA	121	U	3.4
13	BM	49	SER	3.4
13	BM	109	ARG	3.4
31	CA	513	A	3.4
48	CV	2	ALA	3.4
50	CX	57	HIS	3.4
34	CG	24	ILE	3.4
16	BP	80	LYS	3.4
31	CA	1548	A	3.4
33	CF	142	ASP	3.4
34	CG	166	ASP	3.4
1	BA	1304	G	3.4
31	CA	2168	G	3.4
36	DJ	83	ALA	3.4
39	CM	131	ALA	3.4
7	BG	6	VAL	3.4
13	AM	19	LEU	3.4
36	DJ	106	LEU	3.4
48	CV	83	VAL	3.4
36	CJ	29	GLY	3.4
9	BI	4	ASN	3.4
20	BT	79	LEU	3.4
44	DR	118	ALA	3.4
34	CG	80	THR	3.4
45	CS	7	SER	3.4
13	BM	77	ILE	3.4
35	CH	132	PHE	3.4
48	CV	26	LYS	3.4
10	BJ	82	LYS	3.4
17	AQ	53	CYS	3.4
19	BS	18	LYS	3.4
13	BM	9	ILE	3.4
50	CX	83	GLU	3.4
19	BS	70	LYS	3.4
33	CF	172	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
34	CG	172	LYS	3.4
42	CP	103	VAL	3.4
30	CD	25	THR	3.4
1	BA	1275	A	3.4
3	BC	156	ARG	3.4
31	CA	345	A	3.4
50	CX	55	ARG	3.4
14	BN	42	TRP	3.4
35	CH	142	VAL	3.4
2	BB	89	GLN	3.4
13	BM	50	GLU	3.4
41	CO	56	LYS	3.4
38	CL	48	PRO	3.3
41	CO	29	VAL	3.3
1	BA	80	A	3.3
13	AM	36	ALA	3.3
10	AJ	76	ILE	3.3
35	CH	107	GLY	3.3
36	CJ	16	GLY	3.3
39	CM	102	GLY	3.3
19	AS	39	THR	3.3
31	CA	1734	G	3.3
54	DA	277	G	3.3
2	BB	37	LYS	3.3
31	CA	101	A	3.3
50	CX	25	ARG	3.3
1	BA	1001	C	3.3
1	BA	1222	G	3.3
1	BA	250	A	3.3
1	BA	1021	A	3.3
36	DJ	43	ASN	3.3
1	BA	90	C	3.3
7	AG	50	LEU	3.3
7	AG	59	LEU	3.3
54	DA	2106	U	3.3
31	CA	882	G	3.3
1	BA	1274	A	3.3
53	DI	2	ALA	3.3
7	AG	52	GLN	3.3
34	CG	45	HIS	3.3
1	BA	81	A	3.3
1	BA	1019	A	3.3

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Mol	Chain	Res	Type	RSRZ
54	DA	1087	G	3.3
2	AB	135	LEU	3.3
48	CV	52	LEU	3.3
2	AB	14	VAL	3.3
31	CA	2175	C	3.3
1	BA	1307	U	3.3
31	CA	2111	U	3.3
36	DJ	27	ALA	3.3
13	AM	115	PRO	3.3
1	BA	1015	G	3.3
31	CA	1407	G	3.3
53	DI	133	GLU	3.3
23	C2	50	LYS	3.3
31	CA	431	U	3.3
31	CA	2181	U	3.3
46	CT	101	SER	3.3
52	CZ	14	LEU	3.3
32	CE	199	MET	3.3
33	CF	26	MET	3.3
46	CT	94	ASP	3.3
7	BG	152	ALA	3.3
49	CW	89	ILE	3.3
13	BM	94	GLY	3.3
50	CX	61	ALA	3.3
31	CA	214	G	3.3
1	BA	1303	C	3.3
13	BM	28	THR	3.3
48	CV	15	THR	3.3
32	DE	7	ASP	3.3
1	BA	1534	A	3.3
1	BA	79	G	3.3
31	CA	881	G	3.3
32	CE	10	SER	3.3
54	DA	2141	G	3.3
1	BA	948	C	3.3
1	BA	1271	A	3.2
19	BS	59	PRO	3.2
31	CA	332	A	3.2
31	CA	1069	A	3.2
1	AA	88	U	3.2
52	CZ	59	GLU	3.2
3	BC	155	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
7	BG	145	ALA	3.2
33	CF	110	ARG	3.2
1	BA	1236	A	3.2
39	CM	20	GLY	3.2
39	CM	124	GLY	3.2
35	CH	15	LEU	3.2
3	BC	195	VAL	3.2
11	AK	18	ASP	3.2
36	CJ	127	ARG	3.2
31	CA	1056	G	3.2
19	BS	40	ILE	3.2
1	BA	843	U	3.2
16	BP	39	PHE	3.2
7	BG	58	GLU	3.2
54	DA	1072	C	3.2
35	CH	133	GLN	3.2
1	BA	1033	G	3.2
2	BB	12	ALA	3.2
1	BA	1000	A	3.2
1	BA	1035	A	3.2
31	CA	892	A	3.2
23	C2	16	GLY	3.2
1	BA	1317	C	3.2
31	CA	1531	C	3.2
36	DJ	14	ALA	3.2
46	CT	5	ALA	3.2
31	CA	2107	G	3.2
52	CZ	5	GLU	3.2
33	CF	39	GLY	3.2
36	CJ	36	MET	3.2
36	CJ	49	ILE	3.2
42	CP	87	ILE	3.2
43	CQ	8	LEU	3.2
23	C2	49	TYR	3.2
45	CS	62	GLU	3.2
48	DV	53	ASN	3.2
31	CA	2180	U	3.2
36	DJ	84	ALA	3.2
33	CF	80	ARG	3.2
36	CJ	34	ASN	3.2
42	CP	62	LEU	3.2
42	CP	69	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	AA	1025	U	3.2
29	CC	30	PHE	3.2
31	CA	1061	U	3.2
31	CA	2118	U	3.2
34	CG	7	ALA	3.2
39	CM	127	VAL	3.2
35	DH	87	GLU	3.2
54	DA	880	G	3.2
54	DA	2171	A	3.2
23	C2	25	LYS	3.2
54	DA	2165	C	3.2
27	C0	2	ALA	3.2
14	BN	10	GLU	3.2
31	CA	2109	U	3.2
1	BA	1248	A	3.2
3	BC	126	ARG	3.2
9	AI	17	ALA	3.2
19	BS	50	ALA	3.2
34	CG	84	THR	3.2
31	CA	184	C	3.2
9	BI	21	ILE	3.2
23	C2	38	LYS	3.2
34	CG	25	THR	3.2
54	DA	1175	A	3.2
31	CA	1082	U	3.1
48	CV	12	ILE	3.1
30	CD	1	MET	3.1
41	CO	24	MET	3.1
11	AK	81	ASN	3.1
13	AM	11	ASP	3.1
42	CP	115	LEU	3.1
19	AS	55	ARG	3.1
31	CA	1111	A	3.1
31	CA	228	C	3.1
54	DA	2180	U	3.1
7	AG	106	GLU	3.1
33	CF	27	GLN	3.1
42	CP	107	ALA	3.1
44	CR	99	ALA	3.1
7	AG	57	SER	3.1
2	BB	21	ARG	3.1
2	BB	201	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
7	AG	42	ILE	3.1
42	CP	58	ILE	3.1
44	CR	106	PHE	3.1
1	AA	1019	A	3.1
31	CA	330	A	3.1
33	CF	149	VAL	3.1
1	BA	83	C	3.1
1	BA	632	U	3.1
31	CA	893	C	3.1
34	CG	8	PRO	3.1
34	CG	54	PRO	3.1
42	CP	108	ASP	3.1
10	BJ	98	VAL	3.1
36	DJ	33	VAL	3.1
1	BA	1005	A	3.1
31	CA	1468	U	3.1
31	CA	1729	U	3.1
42	CP	99	TYR	3.1
1	BA	1217	C	3.1
54	DA	2164	C	3.1
32	CE	140	ASP	3.1
2	AB	136	MET	3.1
9	BI	58	VAL	3.1
34	CG	132	VAL	3.1
39	CM	113	ALA	3.1
45	CS	28	ALA	3.1
45	CS	25	LEU	3.1
1	BA	1038	C	3.1
13	BM	43	VAL	3.1
30	CD	43	ASP	3.1
41	CO	59	SER	3.1
39	CM	121	THR	3.1
47	CU	47	VAL	3.1
31	CA	1059	G	3.1
31	CA	1546	G	3.1
50	CX	60	PHE	3.1
3	BC	170	GLU	3.1
36	CJ	140	VAL	3.1
46	CT	97	LEU	3.1
31	CA	1529	G	3.1
34	CG	141	ILE	3.1
48	CV	84	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
2	BB	14	VAL	3.1
10	AJ	74	VAL	3.1
1	BA	950	U	3.1
14	AN	55	SER	3.1
29	CC	242	LYS	3.1
35	CH	35	LYS	3.1
35	DH	63	ALA	3.1
30	CD	30	GLU	3.1
39	CM	122	VAL	3.1
22	C1	57	LYS	3.1
1	AA	4	U	3.1
49	CW	5	ASN	3.1
9	BI	124	ARG	3.1
34	CG	157	TYR	3.1
32	CE	24	ASN	3.1
34	CG	20	ASN	3.1
1	BA	84	U	3.1
24	C3	33	ARG	3.1
42	CP	33	ARG	3.1
9	BI	129	LYS	3.0
17	BQ	50	ASN	3.0
19	BS	64	ASP	3.0
22	C1	27	SER	3.0
17	BQ	23	VAL	3.0
7	BG	53	ARG	3.0
14	BN	61	ARG	3.0
26	C5	10	LEU	3.0
31	CA	1873	G	3.0
36	CJ	72	LYS	3.0
9	BI	48	VAL	3.0
13	BM	108	THR	3.0
54	DA	1066	U	3.0
42	CP	26	LEU	3.0
39	CM	75	ALA	3.0
31	CA	1093	G	3.0
45	CS	37	GLU	3.0
44	CR	113	ALA	3.0
10	AJ	6	ILE	3.0
23	C2	40	ASP	3.0
44	CR	117	LEU	3.0
49	CW	57	TYR	3.0
14	AN	47	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
19	BS	47	LEU	3.0
2	AB	27	MET	3.0
2	AB	42	ASN	3.0
25	C4	28	ASN	3.0
33	CF	29	PRO	3.0
33	CF	69	LYS	3.0
34	CG	162	VAL	3.0
19	BS	56	GLN	3.0
50	CX	32	LEU	3.0
13	AM	57	ARG	3.0
7	BG	60	GLU	3.0
12	BL	70	GLU	3.0
47	CU	71	GLY	3.0
1	BA	89	U	3.0
14	BN	46	LEU	3.0
51	CY	20	HIS	3.0
36	DJ	34	ASN	3.0
38	CL	110	GLU	3.0
9	BI	81	HIS	3.0
48	CV	6	ARG	3.0
54	DA	2177	C	3.0
33	CF	75	ALA	3.0
36	CJ	137	GLY	3.0
8	AH	121	LEU	3.0
18	BR	74	HIS	3.0
29	CC	5	LYS	3.0
31	CA	2150	C	3.0
39	CM	106	GLU	3.0
20	BT	38	ALA	3.0
31	CA	1089	A	3.0
48	CV	69	ASN	3.0
36	DJ	95	LYS	3.0
54	DA	2128	G	3.0
49	CW	63	ILE	3.0
54	DA	1061	U	3.0
42	CP	54	VAL	3.0
1	BA	203	G	2.9
9	BI	69	GLY	2.9
17	BQ	21	ILE	2.9
31	CA	1071	G	2.9
2	AB	210	VAL	2.9
13	BM	16	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
23	C2	34	LEU	2.9
42	CP	39	VAL	2.9
45	CS	22	LEU	2.9
35	DH	86	ASP	2.9
1	BA	1004	A	2.9
48	CV	86	ARG	2.9
2	BB	40	ILE	2.9
2	BB	213	TYR	2.9
1	BA	1023	U	2.9
1	BA	1048	G	2.9
31	CA	1534	U	2.9
34	CG	31	GLY	2.9
3	BC	50	ALA	2.9
31	CA	2860	A	2.9
1	BA	1002	G	2.9
10	BJ	95	GLY	2.9
31	CA	289	G	2.9
49	CW	34	LYS	2.9
19	BS	52	HIS	2.9
33	CF	91	LEU	2.9
34	CG	126	PRO	2.9
7	AG	53	ARG	2.9
31	CA	213	A	2.9
13	BM	103	LYS	2.9
31	CA	1217	U	2.9
7	BG	89	VAL	2.9
33	CF	8	TYR	2.9
36	DJ	71	THR	2.9
2	AB	9	MET	2.9
1	BA	1049	U	2.9
11	BK	84	VAL	2.9
45	CS	18	GLN	2.9
31	CA	1060	U	2.9
44	CR	81	ASN	2.9
31	CA	2801	G	2.9
36	DJ	17	MET	2.9
39	CM	1	MET	2.9
9	BI	37	GLN	2.9
13	BM	93	ARG	2.9
23	C2	12	VAL	2.9
1	BA	977	A	2.9
31	CA	311	A	2.9

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Mol	Chain	Res	Type	RSRZ
49	CW	10	LYS	2.9
9	AI	63	LEU	2.9
22	C1	15	MET	2.9
43	CQ	86	VAL	2.9
46	CT	82	MET	2.9
10	BJ	85	ASP	2.9
31	CA	1172	C	2.9
34	CG	94	TYR	2.9
1	BA	981	U	2.9
33	CF	30	ARG	2.9
36	CJ	10	LYS	2.9
2	BB	32	PHE	2.9
35	DH	98	ASP	2.9
36	CJ	124	ALA	2.9
1	BA	1014	A	2.9
17	BQ	44	LEU	2.9
32	CE	171	ASP	2.9
19	BS	4	SER	2.9
42	CP	82	ALA	2.9
25	C4	36	LYS	2.9
19	BS	46	GLY	2.9
2	AB	49	MET	2.8
1	BA	999	C	2.8
20	BT	87	ALA	2.8
23	C2	15	ALA	2.8
42	CP	53	THR	2.8
1	BA	1003	G	2.8
13	BM	14	HIS	2.8
54	DA	1063	G	2.8
7	BG	79	ARG	2.8
21	AU	9	ASN	2.8
1	BA	219	U	2.8
9	BI	90	TYR	2.8
27	C0	8	THR	2.8
3	BC	127	ARG	2.8
16	BP	41	PRO	2.8
24	C3	28	ARG	2.8
31	CA	626	A	2.8
35	CH	47	PHE	2.8
31	CA	312	G	2.8
45	CS	92	TRP	2.8
32	CE	8	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
35	DH	66	ASN	2.8
42	CP	51	ALA	2.8
19	BS	67	VAL	2.8
36	CJ	101	ILE	2.8
36	DJ	92	LYS	2.8
41	CO	52	ILE	2.8
36	CJ	110	ALA	2.8
42	CP	37	ALA	2.8
54	DA	2119	A	2.8
14	AN	27	LEU	2.8
33	CF	4	LEU	2.8
33	CF	126	GLY	2.8
1	BA	989	U	2.8
35	CH	108	VAL	2.8
35	CH	130	VAL	2.8
9	AI	62	ASP	2.8
31	CA	1075	C	2.8
45	CS	66	HIS	2.8
5	BE	91	GLY	2.8
5	BE	159	LYS	2.8
34	CG	86	LYS	2.8
3	BC	106	VAL	2.8
49	CW	65	VAL	2.8
1	BA	957	U	2.8
32	CE	127	GLU	2.8
1	BA	1209	C	2.8
25	C4	61	CYS	2.8
12	BL	108	LYS	2.8
41	CO	79	LEU	2.8
50	CX	62	LYS	2.8
22	C1	34	SER	2.8
2	AB	30	PHE	2.8
1	BA	1362	A	2.8
30	CD	39	ASP	2.8
13	AM	35	ALA	2.8
39	CM	84	LYS	2.8
29	CC	233	GLY	2.8
33	CF	166	GLY	2.8
7	AG	69	VAL	2.8
30	CD	180	VAL	2.8
36	DJ	39	CYS	2.8
36	CJ	128	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	AB	6	MET	2.8
36	DJ	50	GLU	2.8
36	DJ	103	ARG	2.8
14	AN	22	ALA	2.8
14	BN	15	ALA	2.8
15	BO	19	ALA	2.8
31	CA	1143	A	2.8
31	CA	1466	U	2.8
35	DH	142	VAL	2.8
7	BG	17	LYS	2.8
19	BS	3	ARG	2.8
31	CA	1543	G	2.8
33	CF	165	GLU	2.8
52	CZ	47	ARG	2.8
9	BI	43	THR	2.8
32	CE	173	THR	2.8
13	AM	48	LEU	2.8
1	BA	1029	U	2.8
14	BN	11	VAL	2.8
22	C1	3	VAL	2.8
40	CN	80	VAL	2.8
54	DA	2117	A	2.8
22	C1	11	SER	2.8
6	AF	61	LEU	2.8
34	CG	51	THR	2.8
39	CM	118	THR	2.8
46	CT	43	ALA	2.8
7	BG	18	PHE	2.8
31	CA	317	G	2.8
31	CA	1210	G	2.8
47	CU	37	ASP	2.8
13	AM	39	ILE	2.8
48	CV	82	ARG	2.8
1	BA	218	U	2.8
33	CF	38	MET	2.8
24	C3	42	LEU	2.8
1	BA	1027	C	2.8
2	AB	131	LYS	2.8
7	AG	26	PHE	2.8
9	BI	33	ARG	2.8
10	BJ	83	THR	2.8
30	CD	8	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
33	CF	18	THR	2.8
36	DJ	9	VAL	2.8
9	AI	59	GLU	2.7
1	AA	82	G	2.7
1	BA	1276	G	2.7
31	CA	1238	G	2.7
47	CU	24	MET	2.7
54	DA	1094	U	2.7
54	DA	2133	G	2.7
7	BG	112	GLY	2.7
20	BT	76	LYS	2.7
31	CA	2660	A	2.7
33	CF	61	SER	2.7
34	CG	30	ASN	2.7
33	CF	158	THR	2.7
48	CV	77	THR	2.7
36	CJ	64	ASP	2.7
31	CA	1606	C	2.7
35	CH	58	LEU	2.7
1	AA	1026	G	2.7
42	CP	78	VAL	2.7
9	BI	30	ILE	2.7
23	C2	32	GLU	2.7
14	BN	38	ASP	2.7
10	BJ	71	LEU	2.7
54	DA	897	C	2.7
7	AG	65	ALA	2.7
1	BA	951	G	2.7
7	AG	110	LYS	2.7
10	BJ	30	LYS	2.7
32	CE	150	THR	2.7
54	DA	1088	A	2.7
32	CE	103	GLY	2.7
35	CH	144	VAL	2.7
35	DH	67	ALA	2.7
41	CO	114	GLU	2.7
27	C0	9	GLN	2.7
3	BC	43	LEU	2.7
1	BA	959	A	2.7
13	BM	51	GLY	2.7
31	CA	88	G	2.7
33	CF	100	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
48	CV	85	PHE	2.7
19	BS	6	LYS	2.7
35	CH	60	GLU	2.7
1	AA	84	U	2.7
1	BA	979	C	2.7
49	CW	91	PHE	2.7
9	BI	122	ARG	2.7
14	BN	25	ALA	2.7
13	BM	17	ILE	2.7
31	CA	1322	A	2.7
31	CA	117	G	2.7
31	CA	2862	G	2.7
34	CG	110	SER	2.7
54	DA	2105	U	2.7
9	BI	10	GLY	2.7
17	BQ	54	GLY	2.7
2	BB	119	THR	2.7
12	BL	109	ASP	2.7
14	BN	44	ALA	2.7
35	DH	74	ALA	2.7
3	BC	111	LEU	2.7
3	BC	124	LEU	2.7
1	BA	1280	A	2.7
31	CA	2287	A	2.7
41	CO	118	ARG	2.7
45	CS	12	HIS	2.7
48	CV	48	PRO	2.7
1	AA	1024	G	2.7
1	BA	847	G	2.7
2	BB	187	VAL	2.7
31	CA	2803	G	2.7
31	CA	1518	C	2.7
49	CW	69	GLU	2.7
44	CR	90	ILE	2.7
2	BB	131	LYS	2.7
1	BA	1287	A	2.7
13	AM	16	VAL	2.7
34	CG	161	GLY	2.7
14	BN	8	ALA	2.7
31	CA	1098	A	2.7
31	CA	1321	A	2.7
7	BG	130	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
33	CF	43	ALA	2.7
49	CW	16	ALA	2.7
36	DJ	116	ASP	2.7
49	CW	66	ASP	2.7
53	DI	103	ASN	2.7
28	CB	23	G	2.7
31	CA	1533	C	2.7
16	AP	45	GLU	2.7
24	C3	30	VAL	2.7
49	CW	7	GLU	2.7
9	AI	7	TYR	2.7
32	CE	128	ALA	2.7
39	CM	135	ILE	2.7
2	BB	57	LEU	2.7
7	AG	49	THR	2.7
53	DI	129	LEU	2.7
1	BA	1230	C	2.7
32	CE	124	PHE	2.7
11	AK	19	GLY	2.7
31	CA	1444	G	2.7
32	CE	193	VAL	2.7
35	CH	13	GLY	2.7
10	BJ	78	GLU	2.7
23	C2	7	GLU	2.7
20	BT	47	ALA	2.7
9	AI	127	PHE	2.6
1	AA	1441	A	2.6
1	BA	1123	U	2.6
50	CX	58	THR	2.6
31	CA	103	A	2.6
34	CG	10	VAL	2.6
36	CJ	91	GLY	2.6
1	BA	1320	C	2.6
13	AM	62	LYS	2.6
36	CJ	63	ALA	2.6
7	BG	59	LEU	2.6
24	C3	31	LEU	2.6
53	DI	84	TYR	2.6
24	C3	18	PHE	2.6
41	CO	84	GLY	2.6
45	CS	88	GLY	2.6
13	AM	45	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
54	DA	654	A	2.6
1	BA	207	C	2.6
1	BA	1273	C	2.6
36	DJ	128	SER	2.6
2	BB	210	VAL	2.6
3	BC	181	ASP	2.6
26	C5	20	ASP	2.6
23	C2	29	THR	2.6
31	CA	1863	G	2.6
31	CA	2627	G	2.6
1	BA	982	U	2.6
31	CA	1108	U	2.6
30	CD	201	LEU	2.6
31	CA	1525	A	2.6
3	BC	172	ARG	2.6
13	BM	99	GLY	2.6
8	BH	54	ASP	2.6
47	CU	56	GLU	2.6
31	CA	2891	U	2.6
47	CU	35	ALA	2.6
7	BG	77	SER	2.6
19	BS	58	VAL	2.6
48	CV	90	GLY	2.6
49	CW	35	GLU	2.6
52	CZ	8	GLU	2.6
28	CB	49	C	2.6
31	CA	2165	C	2.6
37	CK	141	ASP	2.6
52	CZ	25	GLN	2.6
2	BB	130	THR	2.6
3	AC	189	ALA	2.6
10	BJ	29	ALA	2.6
14	BN	3	LYS	2.6
34	CG	171	THR	2.6
36	DJ	115	ALA	2.6
23	C2	6	ARG	2.6
2	BB	80	VAL	2.6
54	DA	1059	G	2.6
9	BI	61	LEU	2.6
31	CA	1532	A	2.6
32	CE	191	ASP	2.6
39	CM	134	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
9	AI	9	THR	2.6
33	CF	177	PHE	2.6
35	DH	127	GLU	2.6
48	CV	93	VAL	2.6
13	AM	17	ILE	2.6
33	CF	103	LEU	2.6
1	BA	102	G	2.6
13	BM	79	ARG	2.6
18	BR	51	TYR	2.6
31	CA	2877	G	2.6
35	CH	65	ALA	2.6
31	CA	2108	A	2.6
28	CB	19	C	2.6
29	CC	241	GLY	2.6
30	CD	166	GLY	2.6
33	CF	33	LYS	2.6
34	CG	50	LEU	2.6
34	CG	131	ILE	2.6
14	AN	37	SER	2.6
20	BT	50	ALA	2.6
41	CO	77	ALA	2.6
40	CN	88	ASN	2.6
9	BI	9	THR	2.6
13	BM	44	LYS	2.6
17	BQ	46	VAL	2.6
31	CA	1169	A	2.6
34	CG	152	ARG	2.6
31	CA	1406	U	2.6
31	CA	2122	U	2.6
32	CE	11	ALA	2.6
33	CF	114	PHE	2.6
35	CH	67	ALA	2.6
44	CR	68	ALA	2.6
32	CE	198	GLU	2.6
3	BC	109	PRO	2.6
7	BG	68	ASN	2.6
35	DH	95	GLY	2.6
54	DA	1098	A	2.6
33	CF	83	TYR	2.6
36	DJ	104	ALA	2.6
54	DA	1870	C	2.6
16	BP	10	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
19	AS	25	SER	2.6
19	BS	81	ARG	2.6
32	CE	88	ARG	2.6
48	CV	49	VAL	2.6
10	AJ	73	LEU	2.6
32	CE	47	LYS	2.5
13	BM	59	GLU	2.5
1	BA	1039	G	2.5
1	BA	1270	G	2.5
13	BM	3	ARG	2.5
45	CS	14	VAL	2.5
54	DA	2108	A	2.5
35	CH	143	ILE	2.5
46	CT	103	ILE	2.5
34	CG	6	LYS	2.5
39	CM	74	THR	2.5
47	CU	68	LYS	2.5
52	CZ	4	LYS	2.5
35	DH	105	ALA	2.5
1	AA	1492	A	2.5
1	BA	962	C	2.5
45	CS	95	ASP	2.5
31	CA	215	G	2.5
43	CQ	22	PRO	2.5
48	CV	72	ILE	2.5
54	DA	1093	G	2.5
2	BB	206	ALA	2.5
13	AM	40	ALA	2.5
13	BM	57	ARG	2.5
34	CG	69	ARG	2.5
36	CJ	134	ARG	2.5
44	CR	89	GLU	2.5
32	CE	147	LEU	2.5
13	AM	58	ASP	2.5
19	BS	10	PHE	2.5
21	BU	9	ASN	2.5
31	CA	898	C	2.5
31	CA	1073	A	2.5
49	CW	37	PRO	2.5
33	CF	101	GLU	2.5
41	CO	61	ALA	2.5
47	DU	92	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
7	BG	132	GLY	2.5
45	CS	30	GLY	2.5
27	C0	48	ILE	2.5
35	DH	94	ILE	2.5
29	CC	272	SER	2.5
35	CH	70	GLU	2.5
49	CW	41	GLU	2.5
33	CF	12	VAL	2.5
33	CF	59	ALA	2.5
34	CG	151	TYR	2.5
1	AA	959	A	2.5
35	DH	11	ASN	2.5
1	AA	1015	G	2.5
13	BM	53	ILE	2.5
31	CA	2410	G	2.5
50	CX	26	PHE	2.5
9	AI	64	TYR	2.5
31	CA	1542	U	2.5
35	DH	107	GLY	2.5
54	DA	613	A	2.5
49	CW	11	GLU	2.5
3	BC	78	GLY	2.5
35	CH	27	ARG	2.5
35	CH	79	THR	2.5
2	BB	9	MET	2.5
42	CP	35	ILE	2.5
1	BA	1036	A	2.5
1	BA	1132	C	2.5
7	AG	66	LEU	2.5
14	BN	59	ARG	2.5
50	CX	51	VAL	2.5
23	C2	9	ILE	2.5
31	CA	405	U	2.5
31	CA	545	U	2.5
34	CG	109	PHE	2.5
39	CM	107	PHE	2.5
47	CU	59	ASN	2.5
6	BF	97	THR	2.5
7	BG	70	ARG	2.5
1	AA	1022	A	2.5
31	CA	316	C	2.5
33	CF	121	SER	2.5

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Mol	Chain	Res	Type	RSRZ
44	CR	37	GLN	2.5
19	BS	79	THR	2.5
33	CF	115	ARG	2.5
1	AA	1127	G	2.5
1	BA	1124	G	2.5
10	BJ	23	ALA	2.5
10	BJ	33	GLY	2.5
25	C4	37	ALA	2.5
28	CB	51	G	2.5
54	DA	1071	G	2.5
2	BB	88	ASP	2.5
8	BH	2	SER	2.5
13	BM	21	SER	2.5
14	BN	5	SER	2.5
10	AJ	5	ARG	2.5
10	BJ	88	MET	2.5
24	C3	22	MET	2.5
10	AJ	36	VAL	2.5
43	CQ	59	PHE	2.5
29	CC	79	GLU	2.5
31	CA	1168	G	2.5
41	CO	113	ILE	2.5
31	CA	74	A	2.4
33	CF	120	LYS	2.4
36	CJ	92	LYS	2.4
36	DJ	10	LYS	2.4
50	CX	34	GLY	2.4
1	BA	1364	U	2.4
30	CD	41	ALA	2.4
32	CE	131	THR	2.4
13	BM	101	ARG	2.4
39	CM	73	ILE	2.4
47	CU	76	ARG	2.4
7	BG	90	GLU	2.4
3	BC	108	LYS	2.4
23	C2	30	LYS	2.4
44	CR	29	SER	2.4
48	CV	92	LYS	2.4
1	BA	1322	C	2.4
31	CA	45	G	2.4
31	CA	548	G	2.4
34	CG	136	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	BA	978	A	2.4
31	CA	646	U	2.4
44	CR	30	ARG	2.4
52	CZ	48	ARG	2.4
48	CV	37	GLU	2.4
9	AI	55	VAL	2.4
47	CU	87	LEU	2.4
34	CG	35	ARG	2.4
34	CG	68	ALA	2.4
36	CJ	115	ALA	2.4
1	BA	980	C	2.4
13	AM	4	ILE	2.4
15	BO	25	THR	2.4
31	CA	343	C	2.4
31	CA	2904	U	2.4
32	CE	175	ILE	2.4
36	CJ	30	GLN	2.4
36	DJ	117	MET	2.4
19	AS	67	VAL	2.4
9	AI	18	ARG	2.4
10	BJ	31	ARG	2.4
34	CG	67	THR	2.4
1	BA	210	C	2.4
7	AG	6	VAL	2.4
7	BG	120	LEU	2.4
31	CA	1058	U	2.4
31	CA	2177	C	2.4
41	CO	83	LEU	2.4
1	BA	202	G	2.4
9	BI	91	ASP	2.4
31	CA	1528	A	2.4
38	CL	89	ASN	2.4
2	AB	221	VAL	2.4
50	CX	33	ALA	2.4
10	AJ	37	ARG	2.4
48	CV	14	LEU	2.4
48	CV	27	ASN	2.4
53	DI	72	LEU	2.4
24	C3	7	PRO	2.4
33	CF	64	LYS	2.4
33	CF	84	PRO	2.4
34	CG	175	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
7	BG	74	GLU	2.4
31	CA	894	U	2.4
39	CM	76	GLU	2.4
17	BQ	20	SER	2.4
41	CO	27	SER	2.4
3	BC	198	VAL	2.4
11	AK	82	LEU	2.4
19	BS	62	VAL	2.4
34	CG	116	GLN	2.4
36	DJ	107	GLN	2.4
29	CC	239	ASN	2.4
52	CZ	35	GLY	2.4
35	CH	77	THR	2.4
7	BG	83	SER	2.4
19	BS	35	SER	2.4
31	CA	897	C	2.4
35	DH	108	VAL	2.4
19	AS	74	PHE	2.4
54	DA	2114	A	2.4
2	AB	12	ALA	2.4
20	BT	75	HIS	2.4
13	BM	68	ASP	2.4
28	CB	24	G	2.4
31	CA	1215	G	2.4
45	CS	101	ILE	2.4
31	CA	1864	U	2.4
35	CH	110	VAL	2.4
33	CF	42	GLU	2.4
20	BT	34	LYS	2.4
31	CA	2117	A	2.4
46	CT	85	ILE	2.4
19	AS	27	ASP	2.4
50	CX	56	ASP	2.4
31	CA	1112	G	2.4
1	AA	1027	C	2.4
7	AG	79	ARG	2.3
9	BI	11	ARG	2.3
34	CG	21	GLY	2.3
11	BK	64	GLN	2.3
48	CV	43	LYS	2.3
1	BA	1006	G	2.3
20	BT	45	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
31	CA	2892	G	2.3
53	DI	120	ALA	2.3
7	AG	151	PHE	2.3
50	CX	78	LYS	2.3
1	BA	532	A	2.3
31	CA	900	A	2.3
30	CD	97	SER	2.3
13	BM	98	ARG	2.3
13	BM	115	PRO	2.3
36	CJ	93	PRO	2.3
38	CL	33	ALA	2.3
39	CM	6	LEU	2.3
40	CN	72	PRO	2.3
41	CO	94	TYR	2.3
47	CU	74	ILE	2.3
1	BA	1312	G	2.3
2	BB	36	ASN	2.3
14	AN	54	ASP	2.3
41	CO	117	ASP	2.3
16	BP	51	ARG	2.3
33	CF	119	ALA	2.3
2	BB	16	PHE	2.3
3	BC	2	GLY	2.3
7	BG	131	LYS	2.3
16	BP	20	VAL	2.3
31	CA	1174	U	2.3
19	BS	44	MET	2.3
53	DI	29	ASP	2.3
53	DI	36	ASP	2.3
1	BA	1297	G	2.3
13	BM	71	ARG	2.3
14	BN	24	ARG	2.3
3	BC	75	ILE	2.3
9	BI	7	TYR	2.3
31	CA	1868	C	2.3
31	CA	2159	G	2.3
31	CA	2630	G	2.3
36	DJ	8	TYR	2.3
9	AI	27	LYS	2.3
31	CA	2800	A	2.3
16	BP	45	GLU	2.3
26	C5	33	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
32	CE	101	TYR	2.3
35	CH	12	LEU	2.3
41	CO	68	ALA	2.3
14	AN	11	VAL	2.3
25	C4	2	PRO	2.3
31	CA	2286	G	2.3
9	BI	119	ARG	2.3
30	CD	74	GLU	2.3
34	CG	75	MET	2.3
34	CG	167	GLU	2.3
17	BQ	73	TRP	2.3
34	CG	58	TYR	2.3
35	CH	6	LEU	2.3
7	AG	45	SER	2.3
9	BI	51	PRO	2.3
9	BI	123	ARG	2.3
28	CB	27	C	2.3
31	CA	1454	C	2.3
1	BA	1013	G	2.3
1	BA	1144	G	2.3
1	BA	101	A	2.3
1	BA	1441	A	2.3
33	CF	22	TYR	2.3
33	CF	54	ALA	2.3
35	DH	64	ALA	2.3
33	CF	47	LYS	2.3
22	C1	55	ILE	2.3
26	C5	35	GLN	2.3
42	CP	104	GLN	2.3
32	CE	161	ALA	2.3
34	CG	5	ALA	2.3
1	BA	1041	G	2.3
1	BA	1253	G	2.3
1	BA	1323	G	2.3
31	CA	2405	G	2.3
36	DJ	47	ASP	2.3
41	CO	93	GLY	2.3
44	CR	26	GLY	2.3
45	CS	55	ASP	2.3
31	CA	899	A	2.3
47	CU	36	LYS	2.3
40	CN	69	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
19	BS	25	SER	2.3
34	CG	101	ASN	2.3
39	CM	13	LYS	2.3
42	CP	22	GLY	2.3
7	AG	48	GLU	2.3
36	CJ	37	GLU	2.3
7	BG	47	LEU	2.3
31	CA	44	A	2.3
31	CA	2525	G	2.3
31	CA	2895	G	2.3
10	AJ	25	ILE	2.3
42	CP	25	ARG	2.3
8	BH	130	ALA	2.3
26	C5	2	LYS	2.3
2	AB	44	GLU	2.3
17	BQ	42	THR	2.3
31	CA	328	U	2.3
31	CA	2628	C	2.3
7	BG	143	ARG	2.3
33	DF	176	PRO	2.3
49	CW	1	MET	2.3
32	CE	30	GLN	2.3
43	CQ	43	PHE	2.3
1	BA	1246	A	2.3
34	CG	174	ALA	2.3
49	CW	64	VAL	2.3
1	BA	1220	G	2.2
54	DA	2107	G	2.2
1	AA	85	U	2.2
45	CS	94	THR	2.2
47	CU	77	ARG	2.2
50	CX	64	ASP	2.2
1	BA	1281	C	2.2
13	BM	112	PRO	2.2
31	CA	335	C	2.2
31	CA	2129	C	2.2
31	CA	2300	C	2.2
23	C2	13	SER	2.2
33	CF	55	ALA	2.2
1	BA	275	G	2.2
13	BM	81	MET	2.2
31	CA	327	G	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	356	G	2.2
43	CQ	5	ILE	2.2
13	AM	99	GLY	2.2
14	AN	60	GLN	2.2
16	BP	47	GLU	2.2
33	CF	11	GLU	2.2
36	CJ	104	ALA	2.2
1	BA	196	A	2.2
30	CD	103	ASP	2.2
30	CD	200	ASP	2.2
42	CP	27	VAL	2.2
43	CQ	17	VAL	2.2
1	BA	976	G	2.2
13	AM	26	GLY	2.2
22	C1	5	GLN	2.2
31	CA	291	G	2.2
39	CM	140	GLY	2.2
44	CR	21	ALA	2.2
49	CW	33	GLY	2.2
54	DA	141	G	2.2
2	AB	15	HIS	2.2
2	AB	64	LYS	2.2
46	CT	6	LYS	2.2
31	CA	885	C	2.2
34	CG	117	LEU	2.2
13	BM	75	MET	2.2
2	BB	164	ILE	2.2
3	BC	120	ILE	2.2
13	BM	66	GLU	2.2
30	CD	42	ASN	2.2
1	BA	974	A	2.2
33	CF	98	GLU	2.2
35	CH	137	GLU	2.2
35	DH	77	THR	2.2
44	CR	33	ARG	2.2
35	DH	89	LYS	2.2
1	BA	945	G	2.2
16	BP	35	ARG	2.2
32	CE	120	VAL	2.2
44	CR	98	ILE	2.2
47	CU	73	ARG	2.2
53	DI	55	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
20	BT	5	LYS	2.2
29	CC	18	LYS	2.2
29	CC	180	GLU	2.2
33	CF	164	GLU	2.2
24	C3	36	ALA	2.2
34	CG	96	ALA	2.2
52	CZ	58	ASN	2.2
19	AS	57	HIS	2.2
46	CT	86	MET	2.2
48	CV	21	LYS	2.2
1	BA	222	C	2.2
33	CF	134	GLU	2.2
31	CA	1862	G	2.2
31	CA	1875	G	2.2
2	BB	129	LEU	2.2
39	CM	4	ASN	2.2
53	DI	3	LEU	2.2
2	AB	74	ARG	2.2
1	BA	1148	U	2.2
1	BA	1286	U	2.2
14	BN	12	LYS	2.2
30	CD	90	PHE	2.2
2	AB	5	SER	2.2
3	BC	51	SER	2.2
31	CA	1213	A	2.2
31	CA	1522	A	2.2
31	CA	1872	A	2.2
30	CD	76	GLY	2.2
39	CM	143	GLU	2.2
43	CQ	11	GLU	2.2
3	BC	146	ALA	2.2
30	CD	209	ALA	2.2
1	BA	1237	C	2.2
29	CC	251	GLN	2.2
42	CP	32	PRO	2.2
49	CW	12	GLN	2.2
11	BK	110	ILE	2.2
31	CA	2305	U	2.2
9	BI	6	TYR	2.2
43	CQ	19	SER	2.2
2	AB	117	LEU	2.2
41	CO	46	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
43	CQ	97	LEU	2.2
9	AI	125	PRO	2.2
14	AN	28	LYS	2.2
17	BQ	69	LYS	2.2
13	AM	8	ASN	2.2
35	DH	124	THR	2.2
19	BS	20	GLU	2.2
29	CC	3	VAL	2.2
35	CH	135	HIS	2.2
35	DH	70	GLU	2.2
1	BA	1331	G	2.2
31	CA	476	G	2.2
10	BJ	92	LEU	2.2
13	AM	15	ALA	2.2
13	AM	23	TYR	2.2
28	CB	32	U	2.2
32	CE	21	ARG	2.2
33	CF	24	SER	2.2
36	DJ	45	LYS	2.2
31	CA	216	A	2.2
18	AR	20	GLU	2.2
30	CD	44	GLY	2.2
33	CF	5	HIS	2.2
30	CD	184	ARG	2.2
7	BG	108	ALA	2.2
7	BG	115	SER	2.2
10	BJ	12	ALA	2.2
34	CG	74	SER	2.2
1	BA	1356	G	2.2
20	BT	82	GLN	2.2
31	CA	1216	G	2.2
46	CT	95	ARG	2.2
52	CZ	2	LYS	2.2
1	AA	984	C	2.1
39	CM	15	ALA	2.1
9	AI	126	GLN	2.1
30	CD	9	VAL	2.1
35	CH	21	VAL	2.1
35	DH	99	ILE	2.1
3	BC	204	LYS	2.1
25	C4	43	HIS	2.1
32	CE	13	THR	2.1

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Mol	Chain	Res	Type	RSRZ
33	CF	49	LEU	2.1
34	CG	127	THR	2.1
7	AG	61	ALA	2.1
20	BT	72	ALA	2.1
45	CS	103	ALA	2.1
53	DI	106	PHE	2.1
1	AA	1302	C	2.1
3	AC	103	ILE	2.1
15	BO	26	GLU	2.1
30	CD	56	LYS	2.1
34	CG	42	GLU	2.1
2	AB	124	GLY	2.1
27	C0	24	LEU	2.1
3	BC	104	ALA	2.1
46	CT	100	THR	2.1
48	CV	99	ASN	2.1
1	BA	946	A	2.1
28	CB	56	G	2.1
54	DA	2169	A	2.1
2	AB	47	VAL	2.1
29	CC	19	VAL	2.1
27	C0	29	LEU	2.1
35	CH	75	LEU	2.1
2	AB	37	LYS	2.1
3	BC	203	PHE	2.1
10	BJ	16	ARG	2.1
13	AM	29	ARG	2.1
52	CZ	54	LYS	2.1
7	BG	9	GLN	2.1
39	CM	38	GLN	2.1
1	BA	201	G	2.1
13	BM	80	LEU	2.1
22	C1	18	SER	2.1
31	CA	2657	A	2.1
1	BA	1341	U	2.1
7	AG	140	ASP	2.1
13	BM	86	TYR	2.1
25	C4	14	PHE	2.1
30	CD	179	ARG	2.1
31	CA	288	U	2.1
31	CA	334	C	2.1
31	CA	336	C	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	1320	C	2.1
10	AJ	8	ILE	2.1
17	BQ	61	ILE	2.1
20	BT	35	VAL	2.1
23	C2	42	VAL	2.1
9	AI	88	MET	2.1
39	CM	7	SER	2.1
42	CP	109	ALA	2.1
1	BA	972	C	2.1
2	BB	217	VAL	2.1
37	CK	93	ILE	2.1
43	CQ	7	GLN	2.1
23	C2	44	ARG	2.1
35	CH	68	ARG	2.1
48	CV	94	ARG	2.1
32	CE	7	ASP	2.1
32	CE	168	ASP	2.1
35	DH	65	ALA	2.1
41	CO	66	ALA	2.1
48	CV	75	ALA	2.1
2	BB	186	ILE	2.1
16	BP	9	HIS	2.1
31	CA	2602	A	2.1
35	CH	103	VAL	2.1
31	CA	2796	U	2.1
31	CA	2799	A	2.1
1	BA	251	G	2.1
1	BA	987	G	2.1
2	AB	36	ASN	2.1
14	AN	16	LEU	2.1
20	BT	60	ARG	2.1
34	CG	44	LYS	2.1
31	CA	1874	C	2.1
20	BT	63	ALA	2.1
36	CJ	39	CYS	2.1
36	DJ	44	ALA	2.1
25	C4	54	ASP	2.1
29	CC	245	VAL	2.1
47	CU	67	VAL	2.1
19	AS	71	LEU	2.1
29	CC	127	GLY	2.1
34	CG	22	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
13	AM	63	PHE	2.1
16	BP	16	PHE	2.1
1	BA	86	G	2.1
31	CA	185	G	2.1
32	CE	122	GLU	2.1
43	CQ	95	ALA	2.1
48	CV	60	GLU	2.1
2	BB	64	LYS	2.1
19	AS	49	ILE	2.1
45	CS	59	ILE	2.1
47	CU	70	HIS	2.1
7	AG	56	LYS	2.1
31	CA	1088	A	2.1
42	CP	42	PRO	2.1
51	CY	78	TYR	2.1
33	CF	150	ARG	2.1
53	DI	92	ALA	2.1
53	DI	105	LYS	2.1
11	AK	110	ILE	2.1
27	C0	7	ILE	2.1
45	CS	15	SER	2.1
54	DA	2161	C	2.1
31	CA	776	G	2.1
31	CA	1869	G	2.1
2	BB	69	PHE	2.1
1	BA	92	U	2.1
2	BB	139	ARG	2.1
3	BC	107	ARG	2.1
50	CX	68	LYS	2.1
53	DI	94	ARG	2.1
35	DH	56	ALA	2.1
45	CS	52	PRO	2.1
48	CV	76	ALA	2.1
7	BG	7	ILE	2.1
2	AB	65	GLY	2.1
42	CP	75	GLY	2.1
1	AA	1037	C	2.1
1	BA	998	C	2.1
31	CA	1958	C	2.1
20	BT	8	LYS	2.0
22	C1	53	LYS	2.0
24	C3	37	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
35	CH	109	GLU	2.0
7	AG	133	THR	2.0
22	C1	6	ASN	2.0
49	CW	28	ALA	2.0
7	BG	50	LEU	2.0
9	AI	28	ILE	2.0
30	CD	146	ILE	2.0
31	CA	150	U	2.0
32	CE	157	LEU	2.0
35	DH	72	ILE	2.0
10	BJ	11	LYS	2.0
13	AM	114	LYS	2.0
15	BO	15	PHE	2.0
28	CB	50	A	2.0
31	CA	514	A	2.0
31	CA	2835	A	2.0
39	CM	141	LYS	2.0
43	CQ	29	LYS	2.0
38	CL	56	ASP	2.0
7	BG	63	GLU	2.0
17	AQ	83	VAL	2.0
37	CK	21	THR	2.0
52	CZ	56	LEU	2.0
53	DI	119	PRO	2.0
13	BM	62	LYS	2.0
25	C4	41	LYS	2.0
31	CA	1212	G	2.0
31	CA	2106	U	2.0
31	CA	2629	U	2.0
31	CA	2857	G	2.0
34	DG	177	LYS	2.0
42	CP	88	LYS	2.0
46	CT	49	LYS	2.0
14	BN	63	ARG	2.0
42	CP	97	PHE	2.0
3	BC	39	VAL	2.0
31	CA	508	A	2.0
3	BC	144	LEU	2.0
7	BG	107	ALA	2.0
14	AN	15	ALA	2.0
35	DH	138	VAL	2.0
7	BG	82	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
8	BH	55	THR	2.0
26	C5	13	ASN	2.0
36	DJ	73	THR	2.0
50	DX	10	THR	2.0
31	CA	930	G	2.0
43	CQ	24	ASP	2.0
35	DH	141	LYS	2.0
36	DJ	124	ALA	2.0
9	BI	18	ARG	2.0
40	CN	73	ILE	2.0
47	CU	61	LEU	2.0
52	CZ	21	LEU	2.0
31	CA	734	A	2.0
34	CG	82	GLY	2.0
1	BA	307	C	2.0
31	CA	357	C	2.0
7	BG	123	GLU	2.0
27	C0	39	GLU	2.0
31	CA	1460	U	2.0
31	CA	1467	U	2.0
31	CA	1865	U	2.0
30	CD	203	VAL	2.0
36	CJ	100	LYS	2.0
38	CL	14	SER	2.0
49	CW	43	ASP	2.0
51	CY	34	HIS	2.0
19	AS	22	ALA	2.0
43	CQ	4	ILE	2.0
2	BB	162	PHE	2.0
31	CA	488	G	2.0
31	CA	1042	G	2.0
31	CA	2409	G	2.0
53	DI	32	GLY	2.0
54	DA	283	G	2.0
54	DA	1090	A	2.0
31	CA	1043	C	2.0
47	CU	33	LYS	2.0
53	DI	101	LYS	2.0
30	CD	24	VAL	2.0
45	CS	38	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	5MC	BA	967	21/22	0.82	0.31	148,154,156,157	0
1	2MG	BA	966	24/25	0.84	0.34	149,153,160,161	0
1	2MG	BA	1207	24/25	0.84	0.21	158,159,162,165	0
31	PSU	CA	1917	20/21	0.87	0.19	118,126,134,134	0
31	3TD	CA	1915	21/22	0.88	0.18	146,150,155,155	0
1	PSU	BA	516	20/21	0.89	0.16	91,96,99,102	0
30	MEQ	CD	150	9/11	0.89	0.25	81,87,117,120	0
31	2MA	CA	2503	23/24	0.90	0.21	90,96,102,102	0
31	6MZ	CA	2030	23/24	0.92	0.20	78,86,97,99	0
1	2MG	AA	1207	24/25	0.92	0.13	113,117,120,122	0
31	PSU	CA	2504	20/21	0.92	0.20	78,86,90,91	0
31	PSU	CA	1911	20/21	0.92	0.18	111,128,131,132	0
31	PSU	CA	955	20/21	0.93	0.17	84,89,90,90	0
31	G7M	CA	2069	24/25	0.93	0.20	78,83,88,88	0
1	5MC	BA	1407	21/22	0.93	0.17	81,95,99,100	0
12	D2T	BL	89	10/11	0.93	0.26	81,86,96,96	0
40	4D4	CN	81	12/13	0.93	0.27	83,89,102,103	0
31	PSU	CA	746	20/21	0.93	0.15	93,99,101,102	0
31	6MZ	CA	1618	23/24	0.94	0.23	98,107,108,109	0
31	5MU	CA	747	21/22	0.94	0.17	93,100,102,105	0
31	OMU	CA	2552	21/22	0.94	0.34	78,81,85,89	0
31	PSU	CA	2580	20/21	0.94	0.19	77,86,88,89	0
12	D2T	AL	89	10/11	0.94	0.20	47,53,67,70	0
54	3TD	DA	1915	21/22	0.94	0.20	86,90,102,103	0
31	2MG	CA	2445	24/25	0.94	0.25	66,75,80,83	0
31	PSU	CA	2457	20/21	0.95	0.16	79,83,85,85	0
31	1MG	CA	745	24/25	0.95	0.21	85,87,90,93	0
1	2MG	AA	966	24/25	0.95	0.15	78,87,97,97	0
1	2MG	BA	1516	24/25	0.95	0.15	61,67,78,80	0
1	MA6	BA	1518	24/25	0.95	0.20	67,74,79,79	0
1	5MC	AA	967	21/22	0.95	0.16	76,93,96,97	0
31	OMG	CA	2251	24/25	0.95	0.24	67,73,75,77	0
31	2MG	CA	1835	24/25	0.95	0.16	60,73,76,78	0
1	4OC	BA	1402	22/23	0.96	0.15	74,79,81,82	0
1	G7M	BA	527	24/25	0.96	0.16	80,85,91,93	0
31	PSU	CA	2605	20/21	0.96	0.16	74,75,78,80	0
31	OMC	CA	2498	21/22	0.96	0.18	77,80,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MA6	BA	1519	24/25	0.96	0.21	68,73,77,78	0
54	PSU	DA	1917	20/21	0.96	0.15	63,73,79,79	0
1	UR3	BA	1498	21/22	0.96	0.13	78,80,84,84	0
1	2MG	AA	1516	24/25	0.97	0.15	44,49,52,53	0
1	MA6	AA	1519	24/25	0.97	0.18	46,48,50,54	0
54	2MG	DA	1835	24/25	0.97	0.18	31,42,47,48	0
54	PSU	DA	1911	20/21	0.97	0.17	67,74,75,75	0
1	UR3	AA	1498	21/22	0.97	0.14	51,53,57,59	0
31	5MU	CA	1939	21/22	0.97	0.14	69,74,80,82	0
31	5MC	CA	1962	21/22	0.97	0.22	67,72,76,76	0
31	PSU	CA	2604	20/21	0.97	0.14	65,71,84,84	0
40	4D4	DN	81[B]	12/13	0.98	0.21	11,21,28,29	9
1	G7M	AA	527	24/25	0.98	0.14	53,59,62,65	0
1	PSU	AA	516	20/21	0.98	0.13	68,72,78,78	0
1	MA6	AA	1518	24/25	0.98	0.17	44,46,50,53	0
1	4OC	AA	1402	22/23	0.98	0.16	48,55,61,62	0
54	5MC	DA	1962	21/22	0.98	0.18	28,37,39,42	0
1	5MC	AA	1407	21/22	0.98	0.14	43,47,52,53	0
30	MEQ	DD	150[A]	10/11	0.98	0.21	11,18,25,27	10
30	MEQ	DD	150[B]	10/11	0.98	0.21	19,28,34,35	10
40	4D4	DN	81[A]	12/13	0.98	0.21	26,33,49,50	9
54	5MU	DA	1939	21/22	0.99	0.18	25,30,36,40	0
54	6MZ	DA	1618	23/24	0.99	0.16	17,24,27,28	0
54	6MZ	DA	2030	23/24	0.99	0.18	15,20,26,28	0
54	G7M	DA	2069	24/25	0.99	0.16	20,28,31,33	0
54	OMG	DA	2251	24/25	0.99	0.17	21,25,34,42	0
54	2MG	DA	2445	24/25	0.99	0.18	16,22,24,25	0
54	H2U	DA	2449	20/21	0.99	0.17	19,22,24,26	0
54	PSU	DA	2457	20/21	0.99	0.17	22,25,26,29	0
54	OMC	DA	2498	21/22	0.99	0.18	18,21,24,27	0
54	2MA	DA	2503	23/24	0.99	0.18	15,28,32,41	0
54	PSU	DA	2504	20/21	0.99	0.17	31,33,36,38	0
54	OMU	DA	2552	21/22	0.99	0.17	22,26,30,35	0
54	PSU	DA	2580	20/21	0.99	0.17	17,21,28,29	0
54	PSU	DA	2604	20/21	0.99	0.16	32,36,47,47	0
54	PSU	DA	2605	20/21	0.99	0.16	26,34,37,38	0
54	1MG	DA	745	24/25	0.99	0.18	16,22,28,30	0
54	PSU	DA	746	20/21	0.99	0.17	18,23,26,30	0
54	5MU	DA	747	21/22	0.99	0.18	20,25,31,38	0
54	PSU	DA	955	20/21	0.99	0.19	20,23,26,26	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	CA	3154	1/1	-0.24	1.38	136,136,136,136	0
55	MG	AA	1617	1/1	0.09	0.29	147,147,147,147	0
55	MG	CA	3060	1/1	0.20	0.45	234,234,234,234	0
55	MG	BA	1637	1/1	0.23	1.04	86,86,86,86	0
55	MG	CA	3001	1/1	0.25	0.27	296,296,296,296	0
55	MG	AA	1626	1/1	0.36	1.72	113,113,113,113	0
55	MG	BA	1639	1/1	0.39	0.49	93,93,93,93	0
55	MG	AA	1622	1/1	0.45	1.00	116,116,116,116	0
55	MG	CA	3075	1/1	0.45	2.17	221,221,221,221	0
55	MG	CA	3005	1/1	0.45	0.72	239,239,239,239	0
55	MG	CA	3131	1/1	0.48	0.59	83,83,83,83	0
55	MG	CA	3034	1/1	0.49	0.16	244,244,244,244	0
55	MG	DA	3170	1/1	0.53	0.43	90,90,90,90	0
55	MG	CA	3003	1/1	0.54	1.52	270,270,270,270	0
55	MG	AA	1616	1/1	0.55	0.50	87,87,87,87	0
55	MG	CA	3061	1/1	0.55	0.07	225,225,225,225	0
55	MG	CA	3139	1/1	0.56	0.37	83,83,83,83	0
55	MG	CA	3135	1/1	0.58	0.57	107,107,107,107	0
61	PEG	DQ	201	7/7	0.58	0.98	104,108,109,109	0
55	MG	CA	3123	1/1	0.60	0.62	115,115,115,115	0
55	MG	DA	3163	1/1	0.60	0.34	84,84,84,84	0
57	MPD	AA	1676	8/8	0.62	0.68	102,115,118,121	0
55	MG	DA	3133	1/1	0.62	0.23	78,78,78,78	0
55	MG	CA	3156	1/1	0.63	0.17	218,218,218,218	0
55	MG	CA	3008	1/1	0.63	0.10	147,147,147,147	0
55	MG	BA	1638	1/1	0.64	0.65	107,107,107,107	0
55	MG	AA	1678	1/1	0.64	0.22	76,76,76,76	0
55	MG	AA	1624	1/1	0.64	0.49	93,93,93,93	0
55	MG	CA	3134	1/1	0.65	0.46	126,126,126,126	0
55	MG	CA	3038	1/1	0.65	0.14	258,258,258,258	0
55	MG	BA	1641	1/1	0.66	0.28	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	CA	3133	1/1	0.66	0.50	83,83,83,83	0
55	MG	DA	3137	1/1	0.67	0.30	80,80,80,80	0
55	MG	CA	3014	1/1	0.68	0.16	200,200,200,200	0
55	MG	CA	3093	1/1	0.69	0.14	84,84,84,84	0
55	MG	CA	3028	1/1	0.70	0.23	274,274,274,274	0
58	PUT	AA	1672	6/6	0.70	0.50	90,93,95,95	0
58	PUT	AA	1674	6/6	0.70	0.72	128,131,132,133	0
55	MG	DA	3144	1/1	0.70	1.10	107,107,107,107	0
55	MG	DA	3130	1/1	0.71	0.39	99,99,99,99	0
55	MG	CA	3047	1/1	0.71	0.18	238,238,238,238	0
55	MG	CA	3007	1/1	0.72	0.40	214,214,214,214	0
55	MG	CB	203	1/1	0.73	0.09	133,133,133,133	0
55	MG	CA	3115	1/1	0.73	0.23	72,72,72,72	0
55	MG	BA	1604	1/1	0.73	0.18	187,187,187,187	0
58	PUT	DA	3195	6/6	0.73	0.60	76,81,86,87	0
55	MG	CA	3077	1/1	0.73	0.59	232,232,232,232	0
61	PEG	D1	103	7/7	0.74	0.46	76,77,78,78	0
59	TAC	BA	1644	32/32	0.74	0.45	139,152,159,159	0
55	MG	CA	3122	1/1	0.75	0.57	106,106,106,106	0
61	PEG	D3	101	7/7	0.75	1.12	83,89,94,95	0
55	MG	BA	1612	1/1	0.75	0.28	159,159,159,159	0
63	PGE	D1	102	10/10	0.75	0.65	107,117,119,119	0
55	MG	AA	1658	1/1	0.76	0.13	101,101,101,101	0
58	PUT	AA	1675	6/6	0.76	0.47	106,107,108,109	0
64	SPD	DA	3206	10/10	0.76	0.32	86,93,96,96	0
55	MG	DA	3152	1/1	0.77	0.30	94,94,94,94	0
55	MG	CA	3113	1/1	0.77	0.57	79,79,79,79	0
55	MG	AA	1603	1/1	0.77	0.36	81,81,81,81	0
55	MG	CA	3094	1/1	0.77	0.23	126,126,126,126	0
57	MPD	DE	301	8/8	0.77	0.82	123,126,129,129	0
55	MG	AA	1628	1/1	0.78	0.23	110,110,110,110	0
55	MG	AA	1621	1/1	0.78	0.61	97,97,97,97	0
55	MG	CA	3110	1/1	0.78	0.24	102,102,102,102	0
66	ACY	DA	3196	4/4	0.78	0.31	72,76,77,77	0
55	MG	CA	3129	1/1	0.79	0.20	89,89,89,89	0
57	MPD	DT	201	8/8	0.79	0.37	84,87,99,100	0
63	PGE	DA	3001	10/10	0.79	0.58	75,85,99,101	0
55	MG	CA	3151	1/1	0.79	0.29	81,81,81,81	0
61	PEG	DP	201	7/7	0.79	0.82	90,91,93,95	0
57	MPD	DN	201	8/8	0.80	0.46	84,91,101,101	0
55	MG	AA	1661	1/1	0.80	0.20	139,139,139,139	0
57	MPD	DT	202	8/8	0.80	0.35	105,107,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	AA	1627	1/1	0.80	0.22	72,72,72,72	0
55	MG	DA	3062	1/1	0.80	0.10	211,211,211,211	0
55	MG	CA	3128	1/1	0.80	0.44	82,82,82,82	0
55	MG	BA	1624	1/1	0.80	0.29	249,249,249,249	0
55	MG	CA	3116	1/1	0.80	0.45	75,75,75,75	0
55	MG	CA	3119	1/1	0.81	0.35	86,86,86,86	0
55	MG	CA	3046	1/1	0.81	0.12	117,117,117,117	0
57	MPD	DA	3204	8/8	0.81	0.43	117,118,124,125	0
55	MG	BA	1630	1/1	0.81	0.10	160,160,160,160	0
55	MG	BA	1603	1/1	0.81	0.50	279,279,279,279	0
55	MG	BA	1629	1/1	0.81	0.37	184,184,184,184	0
55	MG	CA	3130	1/1	0.81	0.29	76,76,76,76	0
55	MG	DA	3138	1/1	0.81	0.52	38,38,38,38	1
55	MG	CA	3039	1/1	0.82	0.59	158,158,158,158	0
55	MG	DA	3166	1/1	0.82	0.65	88,88,88,88	0
55	MG	CA	3052	1/1	0.82	0.07	71,71,71,71	0
63	PGE	DS	201	10/10	0.82	0.39	65,78,83,83	0
55	MG	DA	3179	1/1	0.82	0.36	101,101,101,101	0
56	PG4	DR	202	13/13	0.82	0.37	97,109,121,121	0
55	MG	AA	1654	1/1	0.82	0.35	259,259,259,259	0
55	MG	CA	3111	1/1	0.83	0.24	76,76,76,76	0
55	MG	CA	3124	1/1	0.83	0.20	124,124,124,124	0
55	MG	DA	3172	1/1	0.83	0.29	81,81,81,81	0
55	MG	AA	1601	1/1	0.83	0.87	76,76,76,76	0
61	PEG	DA	3200	7/7	0.83	0.68	65,68,77,77	0
61	PEG	DA	3226	7/7	0.83	0.29	57,62,74,75	0
55	MG	BA	1647	1/1	0.83	0.11	86,86,86,86	0
55	MG	CA	3054	1/1	0.83	0.12	118,118,118,118	0
55	MG	CA	3019	1/1	0.83	0.18	58,58,58,58	0
58	PUT	DA	3222	6/6	0.83	0.33	41,43,47,47	0
55	MG	CA	3002	1/1	0.83	0.19	258,258,258,258	0
68	TRS	DA	3220	8/8	0.83	0.54	94,100,107,109	0
55	MG	AA	1612	1/1	0.84	0.34	57,57,57,57	0
55	MG	CA	3009	1/1	0.84	0.23	240,240,240,240	0
62	EDO	DA	3209	4/4	0.84	0.43	93,94,95,95	0
55	MG	CA	3043	1/1	0.84	0.08	86,86,86,86	0
61	PEG	AL	201	7/7	0.84	0.22	79,79,85,86	0
55	MG	CA	3114	1/1	0.84	0.31	57,57,57,57	0
55	MG	CA	3068	1/1	0.84	0.24	205,205,205,205	0
55	MG	CA	3104	1/1	0.84	0.21	254,254,254,254	0
57	MPD	DK	201	8/8	0.84	0.32	96,98,100,100	0
55	MG	BA	1606	1/1	0.85	0.18	251,251,251,251	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3131	1/1	0.85	0.22	63,63,63,63	0
55	MG	CA	3071	1/1	0.85	0.09	152,152,152,152	0
57	MPD	DA	3210	8/8	0.85	0.34	87,89,92,94	0
55	MG	CA	3150	1/1	0.85	0.54	74,74,74,74	0
61	PEG	DA	3218	7/7	0.85	0.33	99,105,110,112	0
55	MG	AA	1618	1/1	0.85	1.19	86,86,86,86	0
56	PG4	DA	3193	13/13	0.85	0.72	65,77,93,94	0
55	MG	CA	3076	1/1	0.85	0.18	132,132,132,132	0
58	PUT	DA	3212	6/6	0.85	0.28	54,63,66,70	0
58	PUT	DA	3221	6/6	0.85	0.40	113,116,117,118	0
55	MG	CA	3035	1/1	0.85	0.23	89,89,89,89	0
55	MG	CA	3066	1/1	0.85	0.12	110,110,110,110	0
55	MG	DA	3165	1/1	0.85	0.19	47,47,47,47	0
55	MG	CA	3013	1/1	0.86	0.15	99,99,99,99	0
55	MG	CA	3125	1/1	0.86	0.25	98,98,98,98	0
58	PUT	DA	3205	6/6	0.86	0.33	77,82,89,91	0
55	MG	DA	3167	1/1	0.86	0.35	90,90,90,90	0
58	PUT	DA	3213	6/6	0.86	0.50	83,85,91,93	0
62	EDO	DA	3003	4/4	0.86	0.31	89,89,89,89	0
55	MG	DA	3134	1/1	0.86	0.28	95,95,95,95	0
55	MG	CA	3056	1/1	0.86	0.36	78,78,78,78	0
59	TAC	BA	1643	32/32	0.86	0.16	146,150,152,152	0
55	MG	AA	1615	1/1	0.86	0.48	84,84,84,84	0
55	MG	DB	208	1/1	0.86	0.79	77,77,77,77	0
55	MG	CA	3138	1/1	0.86	0.11	84,84,84,84	0
55	MG	CA	3070	1/1	0.86	0.09	87,87,87,87	0
55	MG	CA	3012	1/1	0.87	0.12	84,84,84,84	0
62	EDO	D1	101	4/4	0.87	0.24	56,57,60,60	0
55	MG	DA	3146	1/1	0.87	0.24	70,70,70,70	0
55	MG	AA	1605	1/1	0.87	0.52	80,80,80,80	0
55	MG	DA	3182	1/1	0.87	0.28	52,52,52,52	0
55	MG	CA	3146	1/1	0.87	0.16	164,164,164,164	0
55	MG	CA	3149	1/1	0.87	0.42	63,63,63,63	0
61	PEG	DA	3199	7/7	0.87	0.41	79,84,92,93	0
55	MG	AA	1614	1/1	0.87	0.10	79,79,79,79	0
55	MG	DA	3121	1/1	0.87	0.16	70,70,70,70	0
55	MG	DA	3171	1/1	0.88	0.54	74,74,74,74	0
55	MG	BA	1609	1/1	0.88	0.16	168,168,168,168	0
55	MG	AA	1664	1/1	0.88	0.18	199,199,199,199	0
55	MG	AA	1623	1/1	0.88	0.27	62,62,62,62	0
56	PG4	AA	1670	13/13	0.88	0.25	64,79,91,92	0
55	MG	CA	3067	1/1	0.88	0.46	277,277,277,277	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	BA	1646	1/1	0.88	0.36	141,141,141,141	0
55	MG	AA	1619	1/1	0.88	0.31	93,93,93,93	0
62	EDO	DA	3194	4/4	0.88	0.24	61,63,64,65	0
55	MG	AA	1606	1/1	0.88	0.23	83,83,83,83	0
57	MPD	DE	302	8/8	0.88	0.57	71,76,83,85	0
55	MG	CA	3140	1/1	0.88	0.22	75,75,75,75	0
55	MG	CA	3074	1/1	0.88	0.09	101,101,101,101	0
55	MG	DA	3132	1/1	0.88	0.15	54,54,54,54	0
55	MG	DA	3168	1/1	0.88	0.48	106,106,106,106	0
67	GUN	DA	3211	11/11	0.88	0.36	82,84,86,86	0
55	MG	AA	1608	1/1	0.88	0.41	78,78,78,78	0
55	MG	CA	3048	1/1	0.89	0.13	91,91,91,91	0
57	MPD	DA	3207	8/8	0.89	0.32	86,86,88,89	0
55	MG	CA	3062	1/1	0.89	0.11	190,190,190,190	0
55	MG	CA	3141	1/1	0.89	0.28	66,66,66,66	0
58	PUT	AA	1673	6/6	0.89	0.29	92,93,93,94	0
55	MG	DA	3154	1/1	0.89	0.34	62,62,62,62	0
55	MG	DA	3129	1/1	0.89	0.16	67,67,67,67	0
58	PUT	DA	3184	6/6	0.89	0.29	53,55,60,60	0
56	PG4	DA	3216	13/13	0.89	0.27	77,89,96,96	0
62	EDO	DB	211	4/4	0.89	0.31	88,88,90,90	0
55	MG	BA	1623	1/1	0.89	0.57	254,254,254,254	0
55	MG	AA	1657	1/1	0.89	0.20	105,105,105,105	0
55	MG	CA	3112	1/1	0.89	0.17	62,62,62,62	0
58	PUT	DA	3219	6/6	0.89	0.29	63,64,65,66	0
55	MG	AA	1655	1/1	0.89	0.14	151,151,151,151	0
55	MG	CA	3011	1/1	0.89	0.16	70,70,70,70	0
55	MG	CA	3126	1/1	0.89	0.13	85,85,85,85	0
55	MG	DB	207	1/1	0.89	0.57	80,80,80,80	0
60	ZN	C5	101	1/1	0.89	0.05	149,149,149,149	0
57	MPD	DA	3192	8/8	0.89	0.43	69,77,79,80	0
55	MG	AA	1609	1/1	0.90	0.20	88,88,88,88	0
55	MG	DA	3160	1/1	0.90	0.68	81,81,81,81	0
55	MG	DA	3161	1/1	0.90	0.28	62,62,62,62	0
55	MG	DA	3123	1/1	0.90	0.31	81,81,81,81	0
61	PEG	DA	3227	7/7	0.90	0.32	75,79,86,87	0
55	MG	AA	1634	1/1	0.90	0.18	144,144,144,144	0
55	MG	AA	1602	1/1	0.90	0.19	75,75,75,75	0
55	MG	CA	3105	1/1	0.90	0.60	260,260,260,260	0
55	MG	AA	1613	1/1	0.90	0.82	59,59,59,59	0
62	EDO	DA	3198	4/4	0.90	0.28	76,79,79,79	0
55	MG	BA	1627	1/1	0.90	0.30	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
62	EDO	DA	3215	4/4	0.90	0.24	67,71,74,74	0
55	MG	CA	3155	1/1	0.90	0.22	152,152,152,152	0
55	MG	CA	3136	1/1	0.90	0.23	87,87,87,87	0
55	MG	CA	3078	1/1	0.90	0.06	153,153,153,153	0
55	MG	CA	3080	1/1	0.90	0.24	119,119,119,119	0
65	1PE	DA	3202	16/16	0.90	0.36	55,64,72,72	0
55	MG	DB	210	1/1	0.90	0.43	76,76,76,76	0
55	MG	CA	3090	1/1	0.90	0.40	170,170,170,170	0
55	MG	DA	3153	1/1	0.90	0.23	53,53,53,53	0
55	MG	BA	1602	1/1	0.91	0.06	84,84,84,84	0
55	MG	CA	3085	1/1	0.91	0.08	69,69,69,69	0
55	MG	AA	1625	1/1	0.91	0.38	68,68,68,68	0
55	MG	BA	1625	1/1	0.91	0.24	251,251,251,251	0
55	MG	CA	3117	1/1	0.91	0.43	69,69,69,69	0
56	PG4	DS	202	13/13	0.91	0.30	52,54,63,64	0
55	MG	CA	3118	1/1	0.91	0.30	64,64,64,64	0
62	EDO	DA	3002	4/4	0.91	0.59	71,74,79,82	0
55	MG	AA	1630	1/1	0.91	0.15	105,105,105,105	0
55	MG	DA	3156	1/1	0.91	0.35	72,72,72,72	0
55	MG	DA	3158	1/1	0.91	0.37	63,63,63,63	0
62	EDO	DA	3208	4/4	0.91	0.25	69,71,72,72	0
55	MG	CA	3137	1/1	0.91	0.29	123,123,123,123	0
55	MG	CA	3057	1/1	0.91	0.10	106,106,106,106	0
55	MG	BA	1640	1/1	0.91	0.22	94,94,94,94	0
55	MG	CA	3106	1/1	0.91	0.18	75,75,75,75	0
55	MG	BA	1617	1/1	0.91	0.12	105,105,105,105	0
63	PGE	DA	3203	10/10	0.91	0.31	68,72,76,76	0
63	PGE	DA	3225	10/10	0.91	0.29	73,81,92,92	0
57	MPD	DA	3190	8/8	0.91	0.30	78,82,85,89	0
55	MG	CA	3145	1/1	0.91	0.23	62,62,62,62	0
66	ACY	DA	3191	4/4	0.91	0.28	80,82,82,82	0
55	MG	CA	3004	1/1	0.91	0.07	106,106,106,106	0
55	MG	CA	3127	1/1	0.91	0.09	65,65,65,65	0
55	MG	BA	1645	1/1	0.91	0.12	94,94,94,94	0
55	MG	CA	3029	1/1	0.92	0.27	114,114,114,114	0
58	PUT	DA	3189	6/6	0.92	0.32	40,44,47,47	0
55	MG	CA	3032	1/1	0.92	0.54	244,244,244,244	0
55	MG	DA	3124	1/1	0.92	0.24	76,76,76,76	0
55	MG	DA	3128	1/1	0.92	0.98	62,62,62,62	0
55	MG	CA	3006	1/1	0.92	0.10	143,143,143,143	0
55	MG	BA	1634	1/1	0.92	0.09	129,129,129,129	0
55	MG	CA	3153	1/1	0.92	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	BA	1635	1/1	0.92	0.07	113,113,113,113	0
59	TAC	AA	1681	32/32	0.92	0.21	94,106,109,110	0
55	MG	AA	1620	1/1	0.92	0.27	63,63,63,63	0
55	MG	CA	3109	1/1	0.92	0.24	62,62,62,62	0
55	MG	DB	206	1/1	0.92	0.58	64,64,64,64	0
63	PGE	DU	101	10/10	0.92	0.41	79,84,91,92	0
55	MG	CA	3069	1/1	0.92	0.23	110,110,110,110	0
55	MG	DA	3141	1/1	0.92	0.23	40,40,40,40	0
55	MG	AA	1660	1/1	0.92	0.27	281,281,281,281	0
61	PEG	DL	201	7/7	0.92	0.25	66,69,70,71	0
55	MG	CA	3144	1/1	0.92	0.07	63,63,63,63	0
55	MG	CA	3132	1/1	0.92	0.47	97,97,97,97	0
56	PG4	BA	1642	13/13	0.92	0.42	84,86,94,96	0
56	PG4	DQ	202	13/13	0.92	0.20	53,59,69,71	0
55	MG	DA	3111	1/1	0.92	0.29	292,292,292,292	0
55	MG	CA	3120	1/1	0.93	0.15	137,137,137,137	0
55	MG	DA	3162	1/1	0.93	0.12	57,57,57,57	0
55	MG	CA	3023	1/1	0.93	0.15	159,159,159,159	0
55	MG	BA	1628	1/1	0.93	0.12	92,92,92,92	0
55	MG	CA	3099	1/1	0.93	0.22	156,156,156,156	0
55	MG	CA	3102	1/1	0.93	0.10	104,104,104,104	0
55	MG	CA	3147	1/1	0.93	0.39	51,51,51,51	1
55	MG	AA	1610	1/1	0.93	0.44	95,95,95,95	0
55	MG	CA	3031	1/1	0.93	0.07	73,73,73,73	0
55	MG	BA	1608	1/1	0.93	0.08	86,86,86,86	0
55	MG	DA	3176	1/1	0.93	0.32	97,97,97,97	0
55	MG	BA	1631	1/1	0.93	0.06	45,45,45,45	0
58	PUT	DA	3188	6/6	0.93	0.22	43,50,50,51	0
55	MG	DA	3180	1/1	0.93	1.60	95,95,95,95	0
55	MG	BA	1632	1/1	0.93	0.11	78,78,78,78	0
55	MG	CA	3037	1/1	0.93	0.30	146,146,146,146	0
55	MG	CA	3017	1/1	0.93	0.07	75,75,75,75	0
55	MG	AA	1677	1/1	0.93	0.15	138,138,138,138	0
55	MG	DA	3147	1/1	0.93	0.16	104,104,104,104	0
55	MG	DA	3148	1/1	0.93	0.20	62,62,62,62	0
55	MG	CA	3063	1/1	0.93	0.16	118,118,118,118	0
59	TAC	AA	1680	32/32	0.93	0.19	70,81,96,96	0
63	PGE	DA	3214	10/10	0.93	0.36	56,58,66,66	0
63	PGE	DA	3217	10/10	0.93	0.34	67,71,76,76	0
55	MG	CA	3083	1/1	0.93	0.13	203,203,203,203	0
64	SPD	DA	3183	10/10	0.93	0.43	60,70,74,75	0
57	MPD	AA	1671	8/8	0.93	0.45	83,86,89,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
64	SPD	DA	3224	10/10	0.93	0.23	30,40,57,60	0
55	MG	CA	3065	1/1	0.93	0.11	72,72,72,72	0
55	MG	CA	3089	1/1	0.93	0.18	54,54,54,54	0
55	MG	CA	3022	1/1	0.93	0.83	206,206,206,206	0
55	MG	DA	3159	1/1	0.93	0.10	76,76,76,76	0
55	MG	CA	3092	1/1	0.93	0.06	125,125,125,125	0
55	MG	CA	3152	1/1	0.94	0.44	145,145,145,145	0
55	MG	DA	3149	1/1	0.94	0.11	47,47,47,47	0
55	MG	DA	3173	1/1	0.94	0.45	100,100,100,100	0
55	MG	DA	3174	1/1	0.94	0.27	70,70,70,70	0
55	MG	DA	3175	1/1	0.94	0.21	68,68,68,68	0
55	MG	AA	1636	1/1	0.94	0.26	113,113,113,113	0
55	MG	CA	3030	1/1	0.94	0.06	64,64,64,64	0
55	MG	BA	1607	1/1	0.94	0.46	203,203,203,203	0
55	MG	DA	3181	1/1	0.94	0.31	70,70,70,70	0
55	MG	CB	202	1/1	0.94	0.12	113,113,113,113	0
55	MG	CA	3143	1/1	0.94	0.14	67,67,67,67	0
55	MG	AA	1611	1/1	0.94	0.15	94,94,94,94	0
55	MG	AA	1665	1/1	0.94	0.36	136,136,136,136	0
55	MG	DA	3136	1/1	0.94	0.20	43,43,43,43	0
55	MG	CA	3021	1/1	0.94	0.82	261,261,261,261	0
55	MG	AA	1604	1/1	0.94	0.29	50,50,50,50	0
55	MG	CA	3072	1/1	0.94	0.54	249,249,249,249	0
65	1PE	DA	3185	16/16	0.94	0.18	37,52,80,82	0
55	MG	DA	3143	1/1	0.94	0.18	50,50,50,50	0
55	MG	DA	3120	1/1	0.94	0.34	81,81,81,81	0
62	EDO	DB	201	4/4	0.94	0.19	72,75,76,76	0
55	MG	CA	3010	1/1	0.94	0.34	245,245,245,245	0
55	MG	BA	1614	1/1	0.94	0.15	137,137,137,137	0
55	MG	CA	3108	1/1	0.95	0.21	73,73,73,73	0
55	MG	DA	3126	1/1	0.95	0.28	57,57,57,57	0
55	MG	DA	3127	1/1	0.95	0.37	71,71,71,71	0
55	MG	CA	3036	1/1	0.95	0.14	133,133,133,133	0
55	MG	CA	3148	1/1	0.95	0.60	46,46,46,46	1
55	MG	AA	1667	1/1	0.95	0.10	41,41,41,41	0
55	MG	CA	3025	1/1	0.95	0.08	87,87,87,87	0
55	MG	CA	3026	1/1	0.95	0.34	111,111,111,111	0
62	EDO	DB	212	4/4	0.95	0.24	70,72,73,73	0
55	MG	CA	3084	1/1	0.95	0.26	167,167,167,167	0
55	MG	CA	3027	1/1	0.95	0.14	68,68,68,68	0
55	MG	CA	3045	1/1	0.95	0.11	107,107,107,107	0
62	EDO	DA	3197	4/4	0.95	0.22	51,51,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1626	1/1	0.95	0.10	85,85,85,85	0
55	MG	DA	3178	1/1	0.95	0.21	69,69,69,69	0
55	MG	AA	1632	1/1	0.95	0.04	65,65,65,65	0
55	MG	DR	201	1/1	0.95	0.34	32,32,32,32	0
55	MG	DA	3142	1/1	0.95	0.38	84,84,84,84	0
55	MG	BA	1636	1/1	0.95	0.45	91,91,91,91	0
55	MG	BA	1616	1/1	0.95	0.17	162,162,162,162	0
55	MG	CA	3053	1/1	0.95	0.15	81,81,81,81	0
63	PGE	DA	3186	10/10	0.95	0.16	33,40,41,41	0
55	MG	AA	1641	1/1	0.95	0.07	65,65,65,65	0
58	PUT	DA	3223	6/6	0.95	0.20	54,55,62,64	0
55	MG	DA	3007	1/1	0.95	0.06	88,88,88,88	0
55	MG	DA	3008	1/1	0.95	0.09	87,87,87,87	0
55	MG	DA	3012	1/1	0.95	0.22	153,153,153,153	0
55	MG	DA	3026	1/1	0.95	0.09	92,92,92,92	0
55	MG	DA	3030	1/1	0.95	0.19	42,42,42,42	0
55	MG	DA	3037	1/1	0.95	0.24	22,22,22,22	0
55	MG	AA	1644	1/1	0.95	0.17	87,87,87,87	0
55	MG	CA	3142	1/1	0.95	0.10	71,71,71,71	0
55	MG	AA	1649	1/1	0.95	0.07	57,57,57,57	0
66	ACY	DA	3201	4/4	0.95	0.21	66,68,68,69	0
55	MG	CA	3058	1/1	0.95	0.22	138,138,138,138	0
55	MG	CA	3107	1/1	0.95	0.37	65,65,65,65	0
55	MG	AA	1651	1/1	0.96	0.09	69,69,69,69	0
55	MG	CA	3049	1/1	0.96	0.12	57,57,57,57	0
55	MG	DA	3164	1/1	0.96	0.29	59,59,59,59	0
55	MG	CA	3016	1/1	0.96	0.50	164,164,164,164	0
55	MG	AA	1666	1/1	0.96	0.05	47,47,47,47	0
55	MG	CA	3033	1/1	0.96	0.11	91,91,91,91	0
55	MG	CA	3055	1/1	0.96	0.07	135,135,135,135	0
55	MG	BA	1619	1/1	0.96	0.19	79,79,79,79	0
55	MG	AA	1659	1/1	0.96	0.07	74,74,74,74	0
55	MG	BA	1633	1/1	0.96	0.13	241,241,241,241	0
55	MG	DR	203	1/1	0.96	0.12	140,140,140,140	0
55	MG	DB	202	1/1	0.96	0.09	52,52,52,52	0
55	MG	DA	3135	1/1	0.96	0.04	78,78,78,78	0
55	MG	DB	204	1/1	0.96	0.06	37,37,37,37	0
55	MG	DA	3177	1/1	0.96	0.17	67,67,67,67	0
55	MG	CA	3079	1/1	0.96	0.10	116,116,116,116	0
55	MG	AA	1607	1/1	0.96	0.48	70,70,70,70	0
55	MG	DA	3140	1/1	0.96	0.20	68,68,68,68	0
55	MG	CA	3082	1/1	0.96	0.25	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3024	1/1	0.96	0.12	81,81,81,81	0
55	MG	CB	201	1/1	0.96	0.06	159,159,159,159	0
55	MG	AA	1647	1/1	0.96	0.09	149,149,149,149	0
55	MG	CA	3064	1/1	0.96	0.28	260,260,260,260	0
55	MG	CA	3044	1/1	0.96	0.09	59,59,59,59	0
55	MG	CA	3091	1/1	0.96	0.09	80,80,80,80	0
55	MG	BA	1610	1/1	0.96	0.04	93,93,93,93	0
55	MG	DA	3044	1/1	0.96	0.10	70,70,70,70	0
55	MG	AA	1663	1/1	0.96	0.09	94,94,94,94	0
55	MG	DA	3065	1/1	0.96	0.15	19,19,19,19	0
55	MG	DA	3092	1/1	0.96	0.10	21,21,21,21	0
55	MG	DA	3097	1/1	0.96	0.07	26,26,26,26	0
55	MG	AA	1631	1/1	0.96	0.08	47,47,47,47	0
55	MG	CA	3097	1/1	0.96	0.08	83,83,83,83	0
55	MG	CA	3098	1/1	0.96	0.07	78,78,78,78	0
55	MG	BA	1648	1/1	0.97	0.35	68,68,68,68	0
55	MG	CA	3088	1/1	0.97	0.08	67,67,67,67	0
55	MG	DA	3033	1/1	0.97	0.16	26,26,26,26	0
55	MG	CA	3100	1/1	0.97	0.17	73,73,73,73	0
55	MG	DA	3043	1/1	0.97	0.14	32,32,32,32	0
55	MG	DA	3169	1/1	0.97	0.27	66,66,66,66	0
55	MG	DD	301	1/1	0.97	0.18	40,40,40,40	0
55	MG	DA	3047	1/1	0.97	0.12	58,58,58,58	0
55	MG	DA	3049	1/1	0.97	0.10	39,39,39,39	0
55	MG	DA	3052	1/1	0.97	0.10	70,70,70,70	0
58	PUT	DM	201	6/6	0.97	0.17	40,48,52,56	0
55	MG	AA	1645	1/1	0.97	0.07	46,46,46,46	0
55	MG	DA	3139	1/1	0.97	0.10	55,55,55,55	0
55	MG	CA	3103	1/1	0.97	0.11	90,90,90,90	0
55	MG	DA	3074	1/1	0.97	0.04	47,47,47,47	0
55	MG	DA	3083	1/1	0.97	0.05	45,45,45,45	0
55	MG	AA	1642	1/1	0.97	0.21	89,89,89,89	0
55	MG	DA	3094	1/1	0.97	0.15	20,20,20,20	0
55	MG	DA	3095	1/1	0.97	0.12	74,74,74,74	0
55	MG	BA	1605	1/1	0.97	0.07	146,146,146,146	0
55	MG	DA	3098	1/1	0.97	0.10	87,87,87,87	0
55	MG	AA	1640	1/1	0.97	0.09	52,52,52,52	0
55	MG	DA	3151	1/1	0.97	0.25	30,30,30,30	0
55	MG	DA	3116	1/1	0.97	0.13	34,34,34,34	0
55	MG	DA	3117	1/1	0.97	0.20	62,62,62,62	0
55	MG	CA	3073	1/1	0.97	0.33	229,229,229,229	0
64	SPD	DA	3187	10/10	0.97	0.20	30,41,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	ZN	AB	301	1/1	0.97	0.12	150,150,150,150	0
55	MG	DA	3155	1/1	0.97	0.19	60,60,60,60	0
55	MG	CA	3121	1/1	0.97	0.14	65,65,65,65	0
55	MG	DA	3122	1/1	0.97	0.45	46,46,46,46	0
55	MG	DB	209	1/1	0.97	0.23	65,65,65,65	0
55	MG	CA	3051	1/1	0.97	0.10	73,73,73,73	0
55	MG	CA	3095	1/1	0.97	0.07	69,69,69,69	0
55	MG	CA	3096	1/1	0.97	0.05	64,64,64,64	0
55	MG	AA	1650	1/1	0.97	0.07	79,79,79,79	0
55	MG	DA	3090	1/1	0.98	0.14	30,30,30,30	0
55	MG	CA	3086	1/1	0.98	0.08	59,59,59,59	0
55	MG	CA	3042	1/1	0.98	0.10	82,82,82,82	0
55	MG	BA	1621	1/1	0.98	0.22	36,36,36,36	0
55	MG	AA	1633	1/1	0.98	0.23	128,128,128,128	0
55	MG	AA	1638	1/1	0.98	0.07	86,86,86,86	0
55	MG	DA	3100	1/1	0.98	0.15	26,26,26,26	0
55	MG	DA	3101	1/1	0.98	0.09	45,45,45,45	0
55	MG	DA	3105	1/1	0.98	0.19	31,31,31,31	0
55	MG	DA	3107	1/1	0.98	0.14	35,35,35,35	0
55	MG	AA	1652	1/1	0.98	0.25	21,21,21,21	0
55	MG	DA	3113	1/1	0.98	0.09	52,52,52,52	0
55	MG	AA	1669	1/1	0.98	0.14	172,172,172,172	0
55	MG	AA	1653	1/1	0.98	0.07	61,61,61,61	0
55	MG	DA	3118	1/1	0.98	0.08	36,36,36,36	0
55	MG	DA	3006	1/1	0.98	0.06	75,75,75,75	0
55	MG	AA	1648	1/1	0.98	0.08	60,60,60,60	0
55	MG	CA	3050	1/1	0.98	0.09	54,54,54,54	0
55	MG	AA	1679	1/1	0.98	0.21	62,62,62,62	0
55	MG	DA	3015	1/1	0.98	0.11	40,40,40,40	0
55	MG	DA	3125	1/1	0.98	0.19	58,58,58,58	0
55	MG	DA	3016	1/1	0.98	0.09	43,43,43,43	0
55	MG	DA	3021	1/1	0.98	0.13	27,27,27,27	0
55	MG	DA	3230	1/1	0.98	0.07	48,48,48,48	0
55	MG	BA	1601	1/1	0.98	0.25	130,130,130,130	0
55	MG	DA	3027	1/1	0.98	0.13	33,33,33,33	0
55	MG	DA	3028	1/1	0.98	0.12	56,56,56,56	0
55	MG	BA	1615	1/1	0.98	0.06	65,65,65,65	0
55	MG	DA	3031	1/1	0.98	0.17	27,27,27,27	0
55	MG	AA	1662	1/1	0.98	0.15	73,73,73,73	0
55	MG	CA	3101	1/1	0.98	0.09	97,97,97,97	0
55	MG	CA	3015	1/1	0.98	0.18	57,57,57,57	0
55	MG	AA	1629	1/1	0.98	0.10	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	BA	1618	1/1	0.98	0.07	69,69,69,69	0
55	MG	CA	3018	1/1	0.98	0.18	90,90,90,90	0
55	MG	CA	3081	1/1	0.98	0.06	84,84,84,84	0
55	MG	DA	3053	1/1	0.98	0.11	44,44,44,44	0
57	MPD	DS	203	8/8	0.98	0.20	47,50,57,58	0
55	MG	DA	3054	1/1	0.98	0.10	70,70,70,70	0
55	MG	AA	1656	1/1	0.98	0.13	140,140,140,140	0
55	MG	DA	3063	1/1	0.98	0.07	85,85,85,85	0
55	MG	CA	3020	1/1	0.98	0.13	86,86,86,86	0
55	MG	DA	3070	1/1	0.98	0.07	62,62,62,62	0
55	MG	DA	3072	1/1	0.98	0.19	55,55,55,55	0
55	MG	BA	1620	1/1	0.98	0.09	113,113,113,113	0
55	MG	DA	3078	1/1	0.98	0.07	52,52,52,52	0
55	MG	DA	3079	1/1	0.98	0.16	124,124,124,124	0
55	MG	DA	3080	1/1	0.98	0.14	149,149,149,149	0
55	MG	DA	3081	1/1	0.98	0.09	45,45,45,45	0
55	MG	DA	3082	1/1	0.98	0.12	72,72,72,72	0
55	MG	CA	3040	1/1	0.98	0.07	83,83,83,83	0
55	MG	DA	3085	1/1	0.98	0.12	50,50,50,50	0
55	MG	DA	3157	1/1	0.98	0.14	54,54,54,54	0
55	MG	DA	3087	1/1	0.98	0.14	34,34,34,34	0
55	MG	DA	3089	1/1	0.98	0.18	23,23,23,23	0
55	MG	DM	202	1/1	0.99	0.04	34,34,34,34	0
55	MG	DA	3055	1/1	0.99	0.21	24,24,24,24	0
55	MG	DA	3056	1/1	0.99	0.17	42,42,42,42	0
55	MG	DA	3057	1/1	0.99	0.08	13,13,13,13	0
55	MG	DA	3059	1/1	0.99	0.08	23,23,23,23	0
55	MG	DA	3061	1/1	0.99	0.14	30,30,30,30	0
55	MG	DA	3013	1/1	0.99	0.19	19,19,19,19	0
55	MG	DA	3014	1/1	0.99	0.15	14,14,14,14	0
55	MG	DA	3064	1/1	0.99	0.11	49,49,49,49	0
55	MG	AA	1637	1/1	0.99	0.07	53,53,53,53	0
55	MG	DA	3066	1/1	0.99	0.17	40,40,40,40	0
55	MG	DA	3067	1/1	0.99	0.06	36,36,36,36	0
55	MG	DA	3068	1/1	0.99	0.16	35,35,35,35	0
55	MG	DA	3069	1/1	0.99	0.15	46,46,46,46	0
55	MG	CA	3087	1/1	0.99	0.05	59,59,59,59	0
55	MG	DA	3071	1/1	0.99	0.10	34,34,34,34	0
55	MG	DA	3018	1/1	0.99	0.08	43,43,43,43	0
55	MG	DA	3019	1/1	0.99	0.28	8,8,8,8	0
55	MG	DA	3145	1/1	0.99	0.11	78,78,78,78	0
55	MG	DA	3075	1/1	0.99	0.15	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	DA	3076	1/1	0.99	0.13	23,23,23,23	0
55	MG	DA	3077	1/1	0.99	0.07	30,30,30,30	0
55	MG	BA	1611	1/1	0.99	0.10	56,56,56,56	0
55	MG	DA	3150	1/1	0.99	0.10	50,50,50,50	0
55	MG	DA	3022	1/1	0.99	0.15	21,21,21,21	0
55	MG	DA	3023	1/1	0.99	0.18	20,20,20,20	0
55	MG	DA	3024	1/1	0.99	0.18	36,36,36,36	0
55	MG	DA	3025	1/1	0.99	0.10	31,31,31,31	0
55	MG	AA	1635	1/1	0.99	0.08	104,104,104,104	0
55	MG	DA	3084	1/1	0.99	0.11	35,35,35,35	0
55	MG	DB	205	1/1	0.99	0.13	46,46,46,46	0
55	MG	BA	1613	1/1	0.99	0.16	79,79,79,79	0
55	MG	DA	3088	1/1	0.99	0.10	42,42,42,42	0
55	MG	DA	3029	1/1	0.99	0.18	29,29,29,29	0
55	MG	BA	1622	1/1	0.99	0.07	99,99,99,99	0
55	MG	DA	3091	1/1	0.99	0.16	17,17,17,17	0
55	MG	AA	1646	1/1	0.99	0.06	49,49,49,49	0
55	MG	DA	3093	1/1	0.99	0.18	23,23,23,23	0
55	MG	DA	3032	1/1	0.99	0.18	23,23,23,23	0
55	MG	CA	3059	1/1	0.99	0.09	74,74,74,74	0
55	MG	DA	3096	1/1	0.99	0.12	36,36,36,36	0
55	MG	DA	3034	1/1	0.99	0.13	16,16,16,16	0
55	MG	DA	3035	1/1	0.99	0.20	32,32,32,32	0
55	MG	DA	3099	1/1	0.99	0.14	23,23,23,23	0
55	MG	DA	3036	1/1	0.99	0.19	25,25,25,25	0
55	MG	AA	1639	1/1	0.99	0.08	89,89,89,89	0
55	MG	DA	3102	1/1	0.99	0.09	30,30,30,30	0
55	MG	DA	3103	1/1	0.99	0.12	35,35,35,35	0
55	MG	DA	3104	1/1	0.99	0.19	34,34,34,34	0
55	MG	DA	3038	1/1	0.99	0.09	19,19,19,19	0
55	MG	DA	3106	1/1	0.99	0.17	41,41,41,41	0
55	MG	DA	3040	1/1	0.99	0.08	36,36,36,36	0
55	MG	DA	3108	1/1	0.99	0.09	30,30,30,30	0
55	MG	DA	3110	1/1	0.99	0.16	35,35,35,35	0
55	MG	DA	3041	1/1	0.99	0.20	11,11,11,11	0
55	MG	DA	3112	1/1	0.99	0.18	24,24,24,24	0
55	MG	DA	3228	1/1	0.99	0.16	36,36,36,36	0
55	MG	DA	3229	1/1	0.99	0.07	36,36,36,36	0
55	MG	DA	3042	1/1	0.99	0.10	29,29,29,29	0
55	MG	DA	3231	1/1	0.99	0.24	36,36,36,36	0
55	MG	DA	3114	1/1	0.99	0.12	39,39,39,39	0
55	MG	DA	3115	1/1	0.99	0.16	37,37,37,37	0

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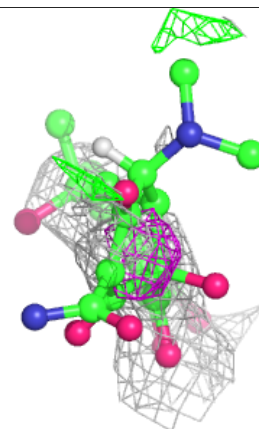
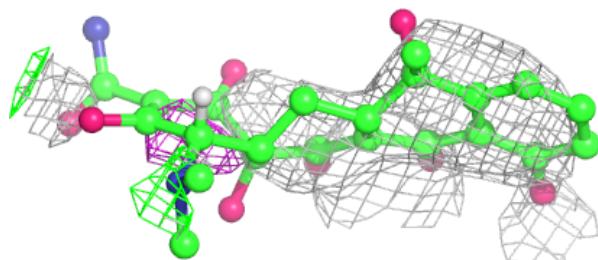
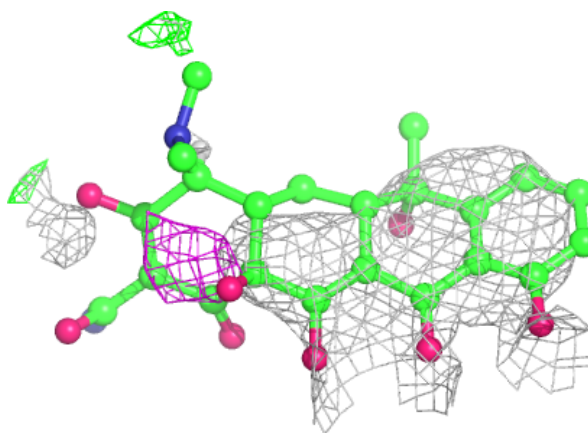
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3004	1/1	0.99	0.09	60,60,60,60	0
55	MG	DA	3005	1/1	0.99	0.12	60,60,60,60	0
55	MG	DA	3045	1/1	0.99	0.05	49,49,49,49	0
55	MG	DA	3119	1/1	0.99	0.31	69,69,69,69	0
55	MG	AA	1668	1/1	0.99	0.13	59,59,59,59	0
55	MG	DA	3048	1/1	0.99	0.13	26,26,26,26	0
55	MG	CA	3041	1/1	0.99	0.05	50,50,50,50	0
55	MG	DA	3050	1/1	0.99	0.13	18,18,18,18	0
55	MG	DA	3051	1/1	0.99	0.09	14,14,14,14	0
55	MG	AA	1643	1/1	0.99	0.12	53,53,53,53	0
55	MG	DA	3009	1/1	0.99	0.12	23,23,23,23	0
55	MG	DA	3039	1/1	1.00	0.13	23,23,23,23	0
55	MG	DA	3046	1/1	1.00	0.13	31,31,31,31	0
55	MG	DB	203	1/1	1.00	0.10	30,30,30,30	0
55	MG	DA	3073	1/1	1.00	0.13	31,31,31,31	0
55	MG	DA	3020	1/1	1.00	0.05	45,45,45,45	0
55	MG	DA	3010	1/1	1.00	0.11	17,17,17,17	0
55	MG	DA	3086	1/1	1.00	0.11	29,29,29,29	0
55	MG	DA	3109	1/1	1.00	0.16	23,23,23,23	0
60	ZN	D5	101	1/1	1.00	0.12	55,55,55,55	0
55	MG	DA	3017	1/1	1.00	0.14	20,20,20,20	0
55	MG	DA	3058	1/1	1.00	0.09	32,32,32,32	0
55	MG	DA	3011	1/1	1.00	0.08	33,33,33,33	0
55	MG	DA	3060	1/1	1.00	0.14	21,21,21,21	0

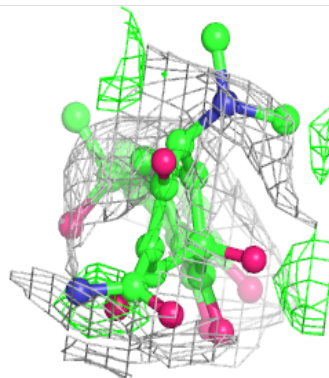
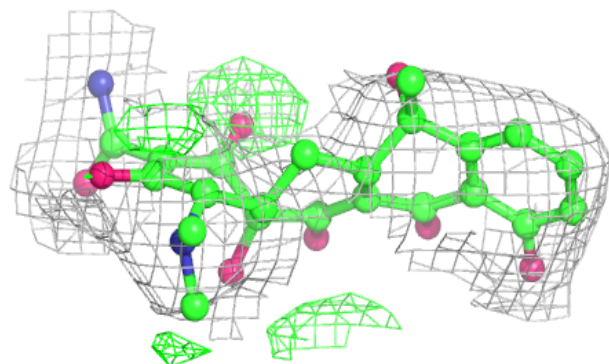
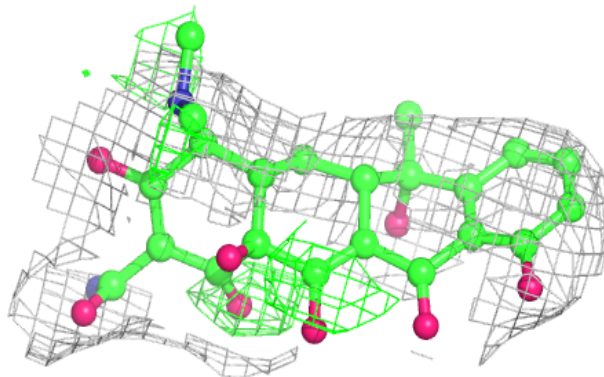
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TAC BA 1644:

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

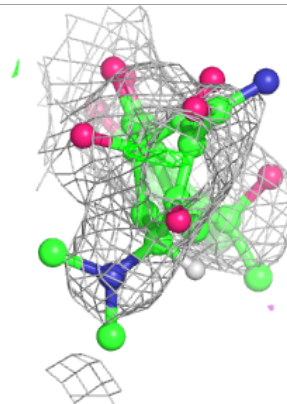
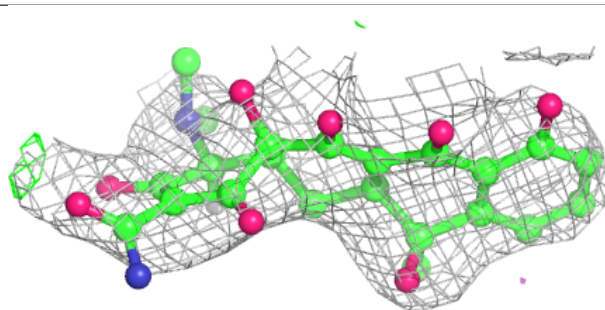
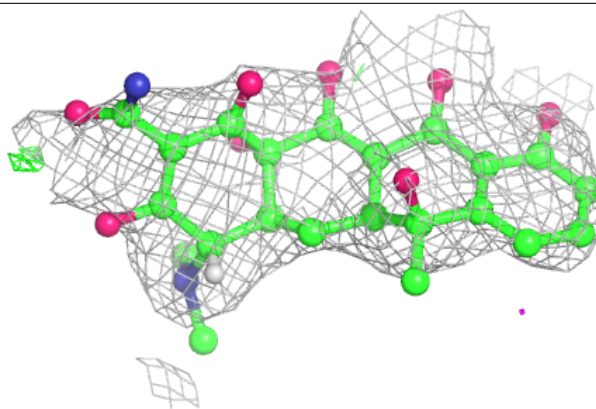
**Electron density around TAC BA 1643:**

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

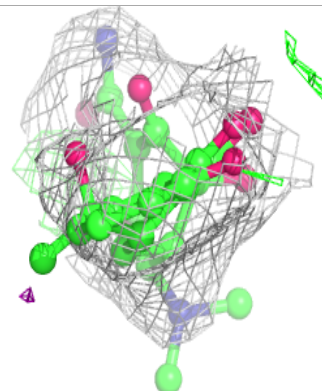
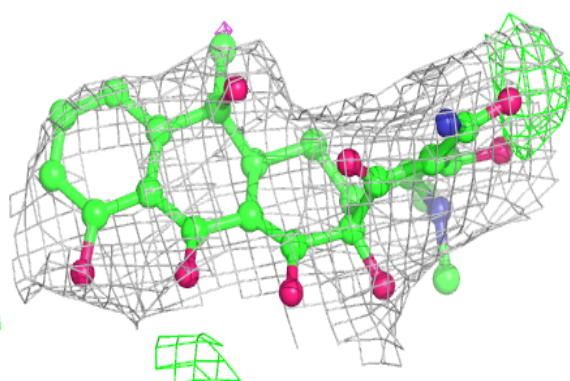
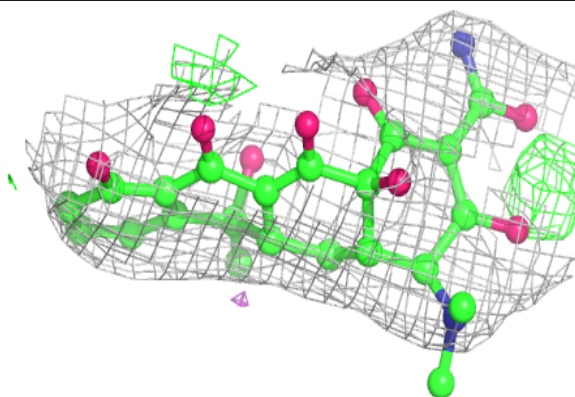


Electron density around TAC AA 1681:

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

**Electron density around TAC AA 1680:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.