



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 12:34 PM EDT

PDB ID : 5J8A / pdb_00005j8a
Title : Structure of the E coli 70S ribosome with the U1052G mutation in 16S rRNA bound to tigecycline
Authors : Cocozaki, A.; Ferguson, A.
Deposited on : 2016-04-07
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

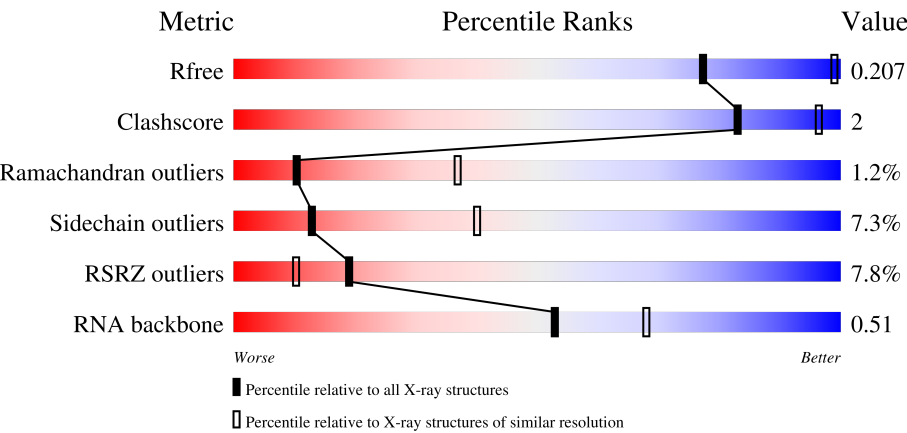
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	5% 76% 21% .
1	BA	1534	6% 75% 23% .
2	AB	224	4% 85% 12% .
2	BB	224	7% 86% 12% .

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	BC	206	
4	AD	205	
4	BD	205	
5	AE	155	
5	BE	155	
6	AF	106	
6	BF	106	
7	AG	151	
7	BG	151	
8	AH	129	
8	BH	129	
9	AI	127	
9	BI	127	
10	AJ	99	
10	BJ	99	
11	AK	117	
11	BK	117	
12	AL	123	
12	BL	123	
13	AM	114	
13	BM	114	
14	AN	100	
14	BN	100	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	BO	88	95% ..
16	AP	82	6% 80% 20%
16	BP	82	13% 74% 23% .
17	AQ	80	2% 79% 19% .
17	BQ	80	5% 64% 31% ..
18	AR	55	4% 84% 15% .
18	BR	55	7% 87% 13%
19	AS	79	23% 81% 18% .
19	BS	79	19% 84% 13% ..
20	AT	86	2% 92% 7% .
20	BT	86	20% 74% 15% 8% ..
21	AU	56	7% 80% 20%
21	BU	56	9% 82% 18%
22	C1	56	30% 84% 12% .
22	D1	56	82% 16% .
23	C2	51	33% 63% 33% ..
23	D2	51	2% 71% 25% .
24	C3	46	57% 85% 13% .
24	D3	46	2% 91% 9%
25	C4	64	77% 94% 6%
25	D4	64	95% 5%
26	C5	38	32% 71% 29%
26	D5	38	87% 13%
27	C0	58	29% 74% 22% .
27	D0	58	3% 93% 5% .

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Mol	Chain	Length	Quality of chain
28	CB	120	9% 83% 13% • •
28	DB	120	91% 8% •
29	CC	272	14% 82% 14% •
29	DC	272	2% 89% 9% •
30	CD	209	11% 89% 11%
31	CA	2904	9% 75% 22% •
32	DD	209	90% 9% •
33	CE	201	17% 85% 12% •
33	DE	201	89% 10%
34	CF	178	3% 73% 24% • •
34	DF	178	76% 21% • •
35	CG	176	2% 86% 13% •
35	DG	176	3% 89% 11%
36	CH	149	2% 78% 20% •
36	DH	149	3% 78% 22%
37	CJ	135	22% 84% 13% • •
37	DJ	135	24% 85% 13% • •
38	CK	142	8% 89% 11% •
38	DK	142	89% 10% •
39	CL	123	7% 83% 13% • • •
39	DL	123	85% 13% •
40	CM	144	23% 78% 19% •
40	DM	144	90% 9% •
41	CN	136	9% 82% 18% •
41	DN	136	89% 11%

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Mol	Chain	Length	Quality of chain
42	CO	125	
42	DO	125	
43	CP	117	
43	DP	117	
44	CQ	114	
44	DQ	114	
45	CR	117	
45	DR	117	
46	CS	103	
46	DS	103	
47	CT	110	
47	DT	110	
48	CU	93	
48	DU	93	
49	CV	103	
49	DV	103	
50	CW	94	
50	DW	94	
51	CX	83	
51	DX	83	
52	CY	77	
52	DY	77	
53	CZ	62	
53	DZ	62	
54	DI	135	

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Mol	Chain	Length	Quality of chain
55	DA	2904	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	1640	-	-	-	X
56	MG	CA	3021	-	-	-	X
56	MG	CA	3122	-	-	-	X
56	MG	CA	3147	-	-	-	X
56	MG	CA	3148	-	-	-	X
59	PUT	AA	1672	-	-	-	X
67	ACY	DA	3196	-	X	-	-

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 295207 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0	0
			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 675819282
BA	1052	G	U	engineered mutation	GB 675819282

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

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	BC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
15	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	BQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			456	288	86	82			
18	BR	55	Total	C	N	O	0	0	0
			456	288	86	82			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	BS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
33	DE	201	Total	C	N	O	S	0	0	0
			1551	974	283	289	5			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	CU	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
48	DU	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

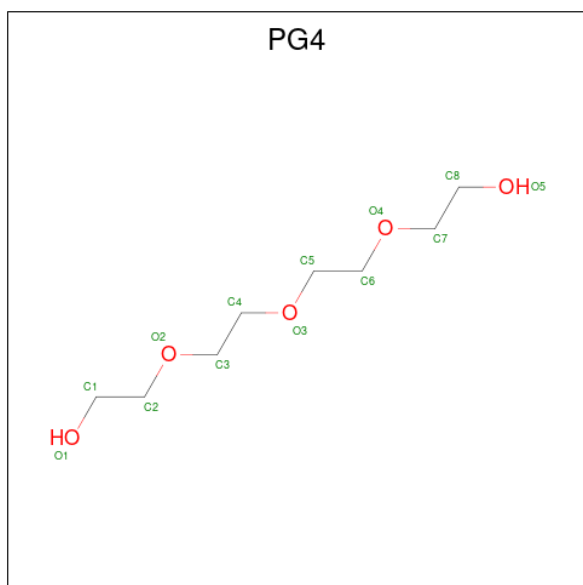
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	72	Total	Mg	0	0
			72	72		
56	BA	45	Total	Mg	0	0
			45	45		
56	CB	3	Total	Mg	0	0
			3	3		
56	CA	156	Total	Mg	0	0
			156	156		
56	DD	1	Total	Mg	0	0
			1	1		
56	DM	1	Total	Mg	0	0
			1	1		
56	DR	1	Total	Mg	0	0
			1	1		

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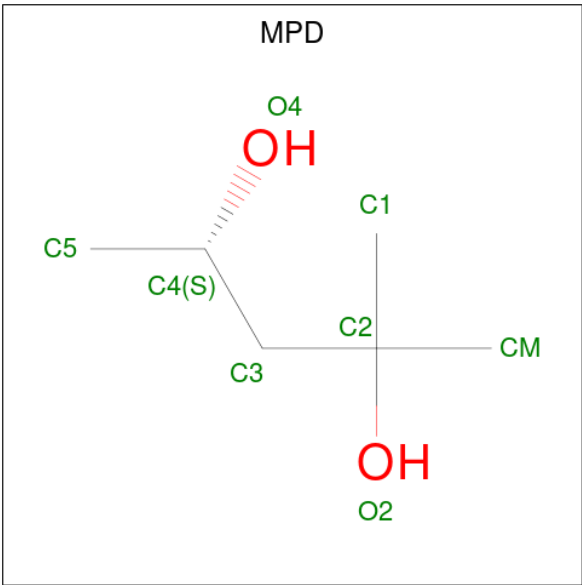
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DB	9	Total	Mg	0	0
			9	9		
56	DA	184	Total	Mg	0	0
			184	184		

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



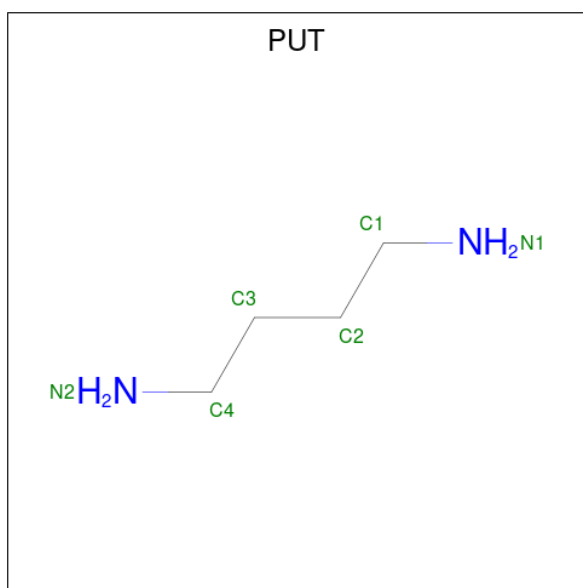
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			13	8	5		
57	BA	1	Total	C	O	0	0
			13	8	5		
57	DQ	1	Total	C	O	0	0
			13	8	5		
57	DR	1	Total	C	O	0	0
			13	8	5		
57	DS	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		

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



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

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



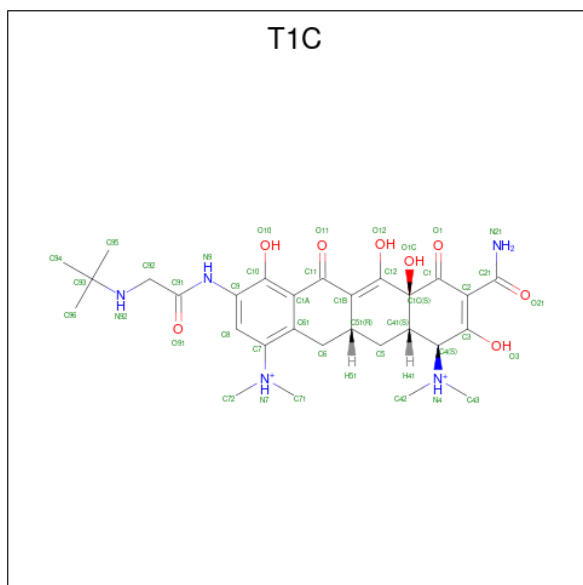
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6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

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

- Molecule 60 is TIGECYCLINE (CCD ID: T1C) (formula: $C_{29}H_{41}N_5O_8$).

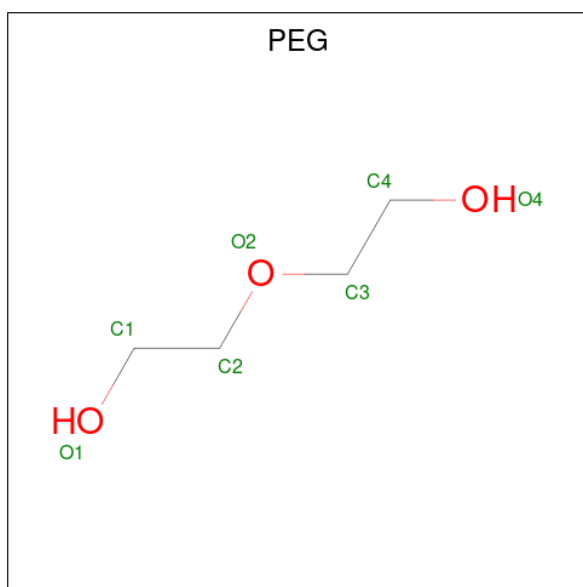


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
60	AA	1	Total	C	N	O	0	0
			42	29	5	8		
60	BA	1	Total	C	N	O	0	0
			42	29	5	8		

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

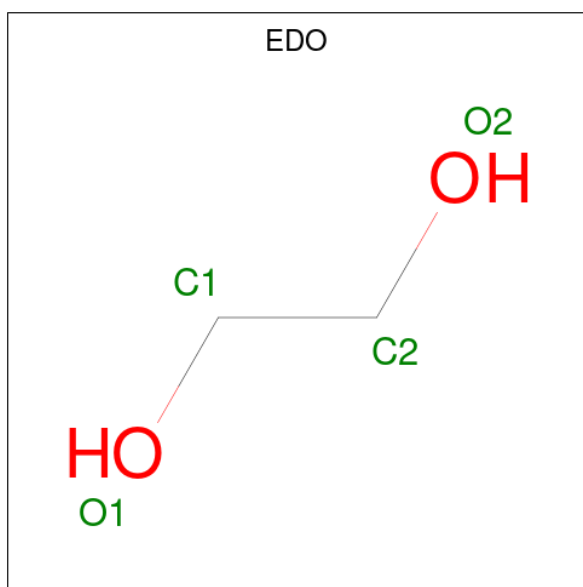
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AB	1	Total	Zn	0	0
			1	1		
61	C5	1	Total	Zn	0	0
			1	1		
61	D5	1	Total	Zn	0	0
			1	1		

- Molecule 62 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



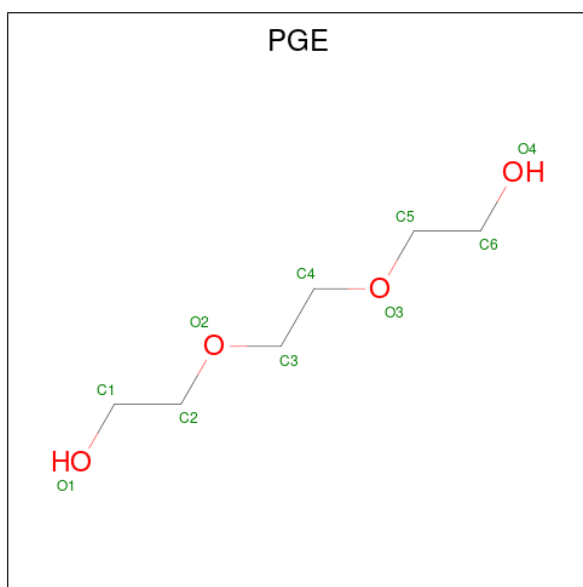
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	AL	1	Total	C	O	0	0
			7	4	3		
62	D1	1	Total	C	O	0	0
			7	4	3		
62	D3	1	Total	C	O	0	0
			7	4	3		
62	DL	1	Total	C	O	0	0
			7	4	3		
62	DP	1	Total	C	O	0	0
			7	4	3		
62	DQ	1	Total	C	O	0	0
			7	4	3		
62	DA	1	Total	C	O	0	0
			7	4	3		
62	DA	1	Total	C	O	0	0
			7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

- Molecule 63 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



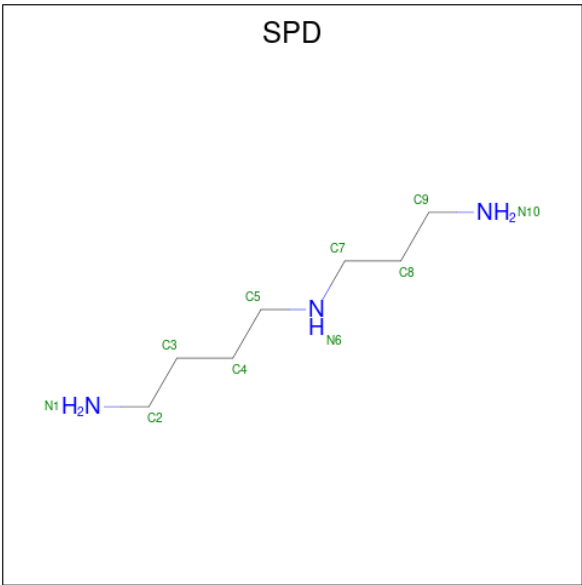
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			4	2	2		
63	DB	1	Total	C	O	0	0
			4	2	2		
63	DB	1	Total	C	O	0	0
			4	2	2		
63	DB	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4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

- Molecule 64 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



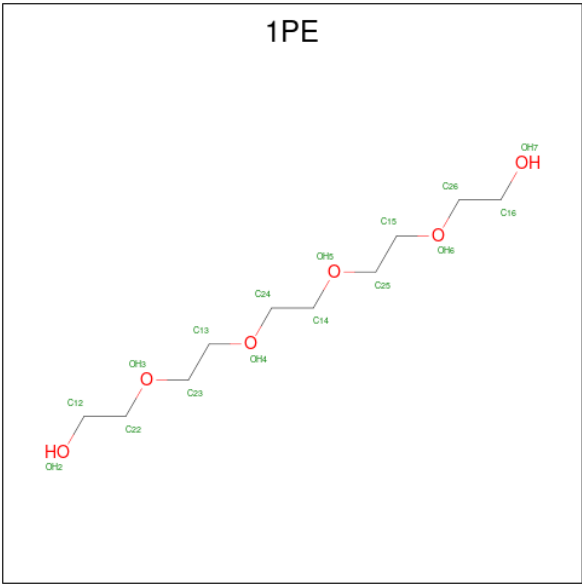
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	D1	1	Total	C	O	0	0
			10	6	4		
64	D3	1	Total	C	O	0	0
			10	6	4		
64	DS	1	Total	C	O	0	0
			10	6	4		
64	DU	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		

- Molecule 65 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



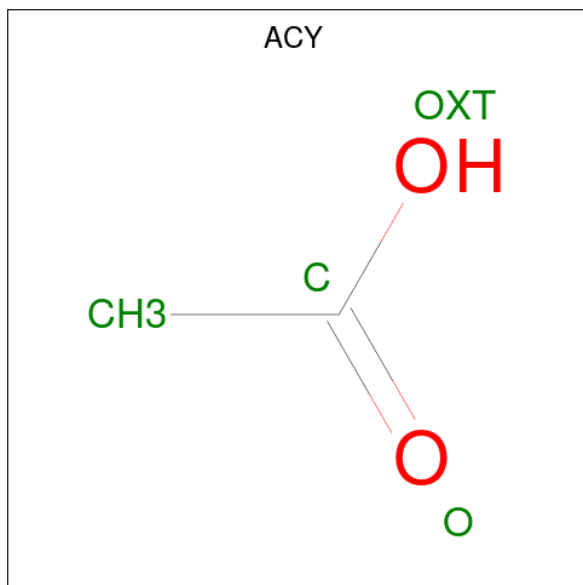
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
65	DA	1	Total	C	N	0	0
			10	7	3		
65	DA	1	Total	C	N	0	0
			10	7	3		
65	DA	1	Total	C	N	0	0
			10	7	3		
65	DA	1	Total	C	N	0	0
			10	7	3		

- Molecule 66 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



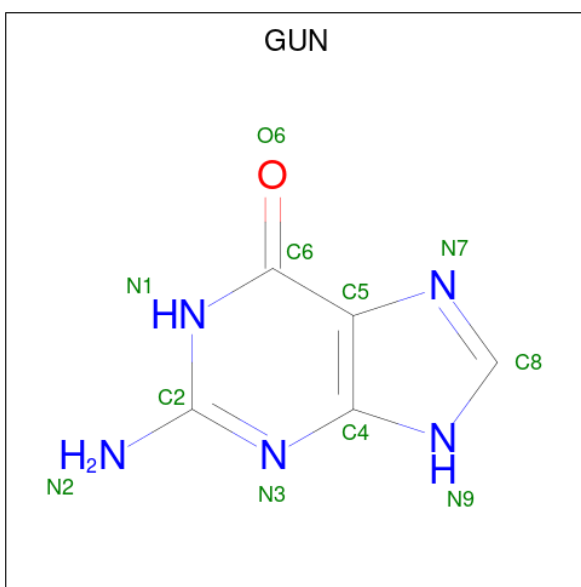
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			16	10	6		
66	DA	1	Total	C	O	0	0
			16	10	6		

- Molecule 67 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



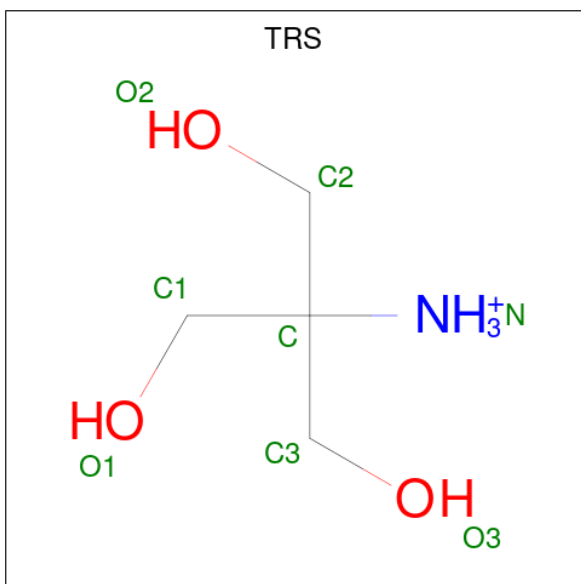
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
67	DA	1	Total	C	O	0	0
			4	2	2		
67	DA	1	Total	C	O	0	0
			4	2	2		
67	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 68 is GUANINE (CCD ID: GUN) (formula: $C_5H_5N_5O$).



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

- Molecule 69 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



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

- Molecule 70 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
70	AA	500	Total 500	O 500	0	0
70	AC	5	Total 5	O 5	0	0
70	AD	2	Total 2	O 2	0	0
70	AE	4	Total 4	O 4	0	0
70	AF	1	Total 1	O 1	0	0
70	AG	1	Total 1	O 1	0	0
70	AH	1	Total 1	O 1	0	0
70	AJ	2	Total 2	O 2	0	0
70	AK	6	Total 6	O 6	0	0
70	AL	10	Total 10	O 10	0	0
70	AM	4	Total 4	O 4	0	0
70	AN	7	Total 7	O 7	0	0
70	AO	2	Total 2	O 2	0	0
70	AP	2	Total 2	O 2	0	0
70	AR	1	Total 1	O 1	0	0
70	AT	3	Total 3	O 3	0	0
70	AU	2	Total 2	O 2	0	0
70	C3	3	Total 3	O 3	0	0
70	C4	1	Total 1	O 1	0	0
70	BA	288	Total 288	O 288	0	0
70	BD	12	Total 12	O 12	0	0
70	BE	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
70	BF	2	Total	O	0	0
			2	2		
70	BK	2	Total	O	0	0
			2	2		
70	BL	2	Total	O	0	0
			2	2		
70	BN	2	Total	O	0	0
			2	2		
70	BO	1	Total	O	0	0
			1	1		
70	BP	3	Total	O	0	0
			3	3		
70	BT	4	Total	O	0	0
			4	4		
70	BU	1	Total	O	0	0
			1	1		
70	D1	45	Total	O	0	0
			45	45		
70	D2	7	Total	O	0	0
			7	7		
70	D3	23	Total	O	0	0
			23	23		
70	D4	39	Total	O	0	0
			39	39		
70	D5	12	Total	O	0	0
			12	12		
70	D0	21	Total	O	0	0
			21	21		
70	CB	13	Total	O	0	0
			13	13		
70	CC	12	Total	O	0	0
			12	12		
70	CD	6	Total	O	0	0
			6	6		
70	CA	692	Total	O	0	0
			692	692		
70	DC	104	Total	O	0	0
			104	104		
70	DD	92	Total	O	0	0
			92	92		
70	CE	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
70	CL	1	Total	O	0	0
			1	1		
70	CM	4	Total	O	0	0
			4	4		
70	CO	1	Total	O	0	0
			1	1		
70	CU	3	Total	O	0	0
			3	3		
70	CV	1	Total	O	0	0
			1	1		
70	CW	1	Total	O	0	0
			1	1		
70	CY	1	Total	O	0	0
			1	1		
70	DE	60	Total	O	0	0
			60	60		
70	DF	15	Total	O	0	0
			15	15		
70	DG	6	Total	O	0	0
			6	6		
70	DH	2	Total	O	0	0
			2	2		
70	DK	64	Total	O	0	0
			64	64		
70	DL	51	Total	O	0	0
			51	51		
70	DM	64	Total	O	0	0
			64	64		
70	DN	73	Total	O	0	0
			73	73		
70	DO	46	Total	O	0	0
			46	46		
70	DP	40	Total	O	0	0
			40	40		
70	DQ	32	Total	O	0	0
			32	32		
70	DR	63	Total	O	0	0
			63	63		
70	DS	44	Total	O	0	0
			44	44		
70	DT	69	Total	O	0	0
			69	69		

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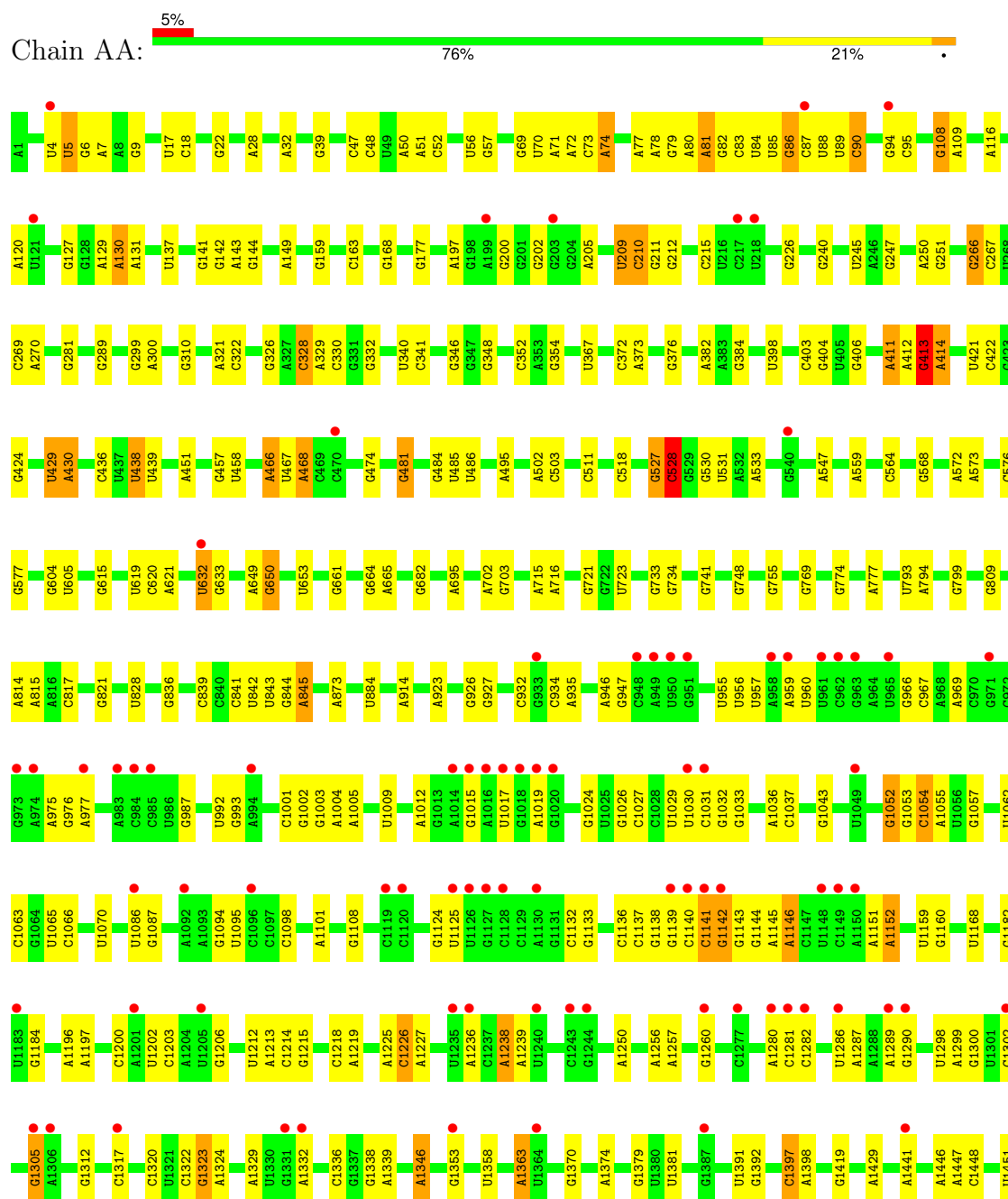
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
70	DU	21	Total 21	O 21	0	0
70	DV	20	Total 20	O 20	0	0
70	DW	31	Total 31	O 31	0	0
70	DX	26	Total 26	O 26	0	0
70	DY	11	Total 11	O 11	0	0
70	DZ	7	Total 7	O 7	0	0
70	DB	213	Total 213	O 213	0	0
70	DA	4829	Total 4829	O 4829	0	0

3 Residue-property plots

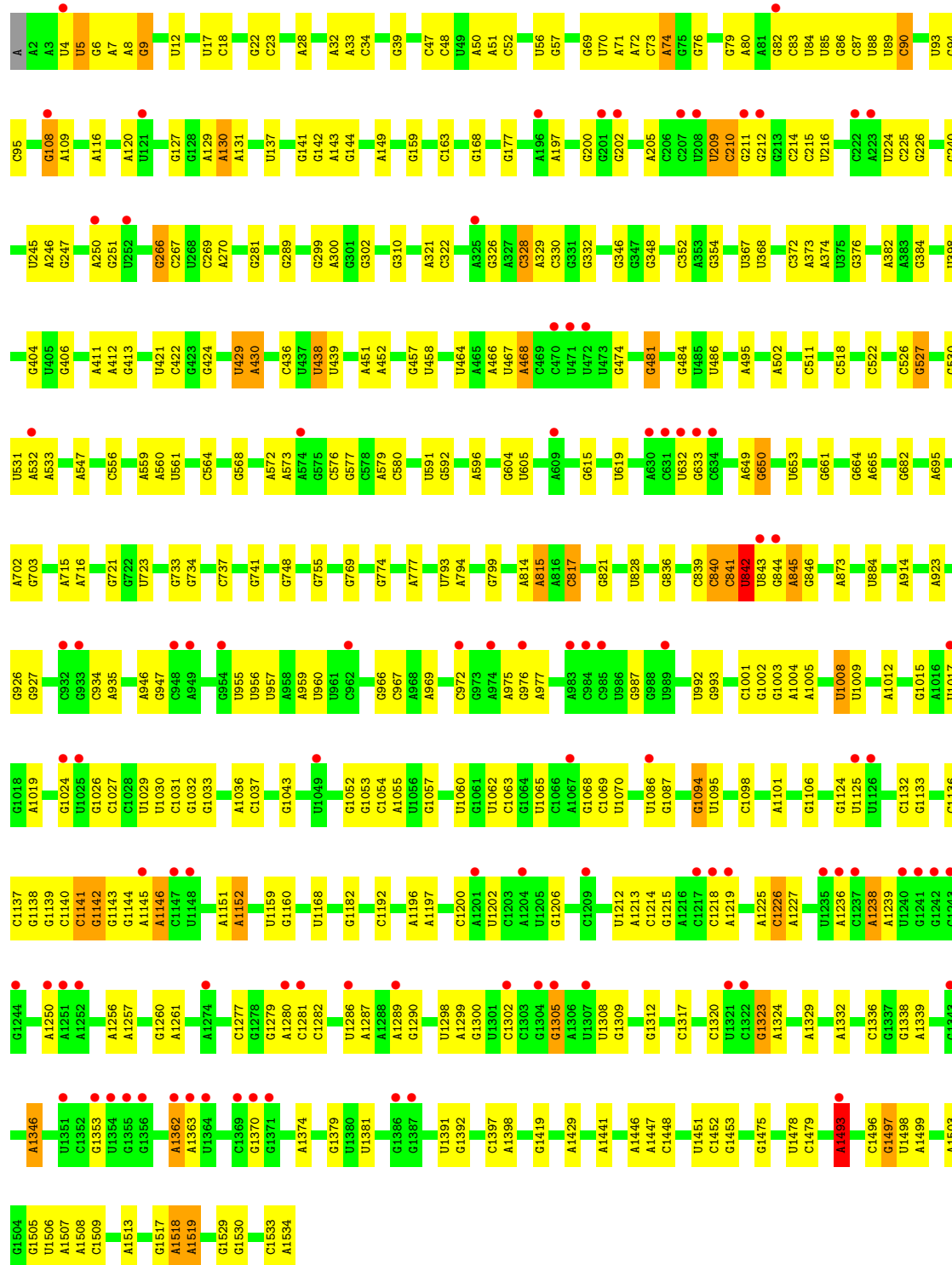
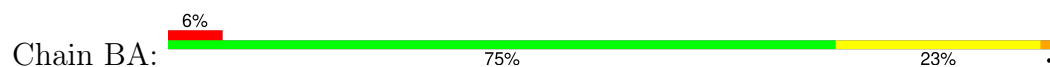
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

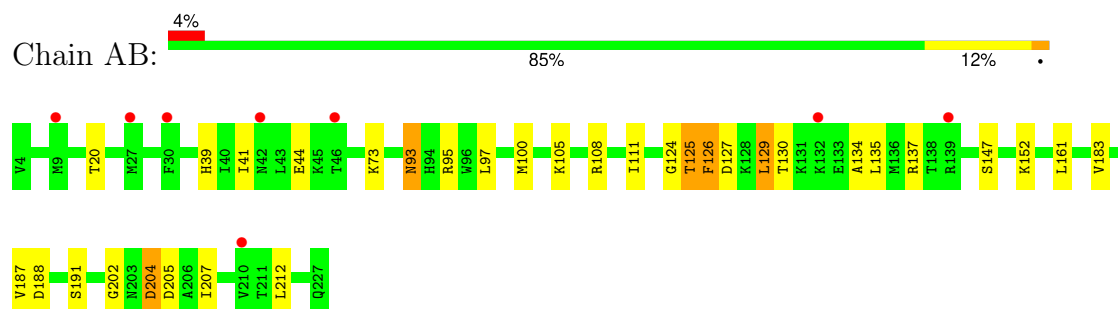




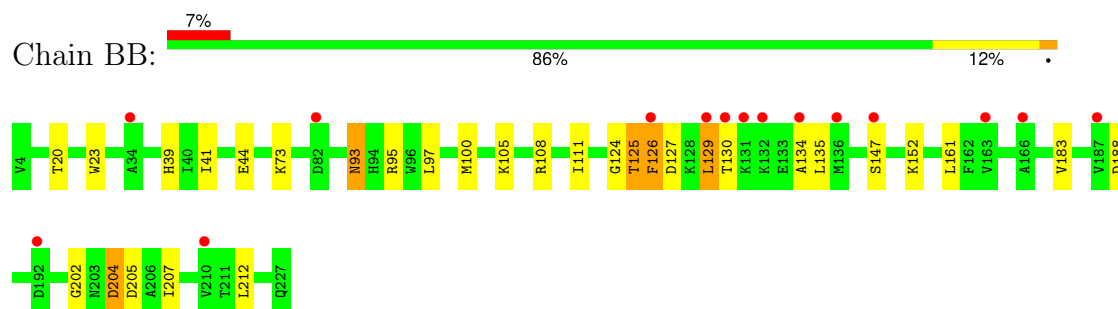
• Molecule 1: 16S rRNA



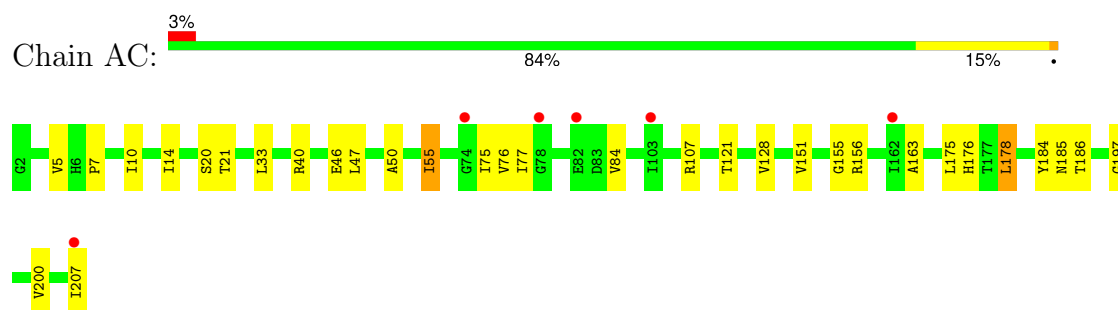
- Molecule 2: 30S ribosomal protein S2



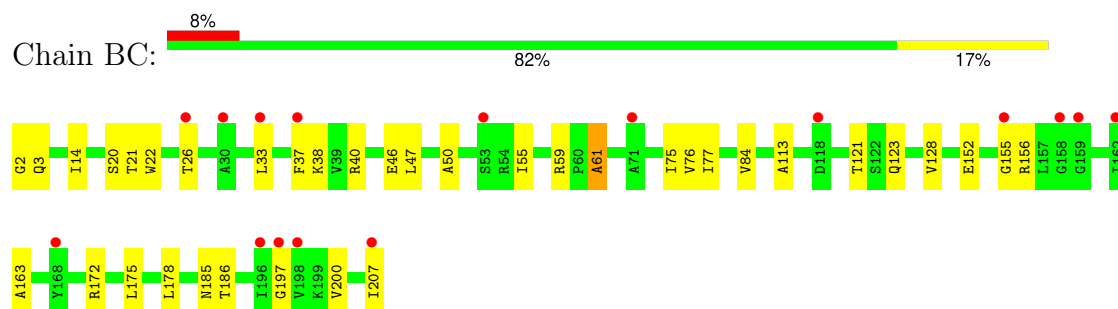
- Molecule 2: 30S ribosomal protein S2



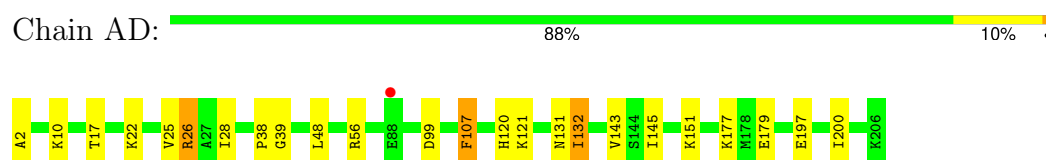
- Molecule 3: 30S ribosomal protein S3



- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4



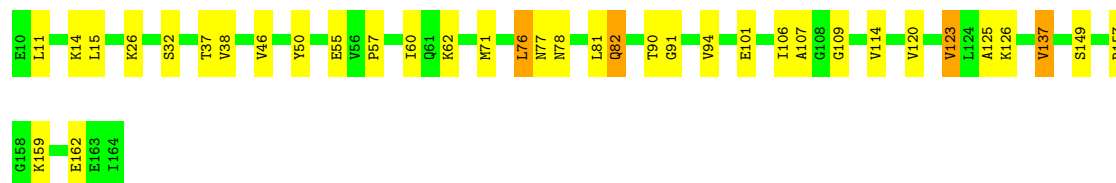
- Molecule 4: 30S ribosomal protein S4

Chain BD:  85% 13%



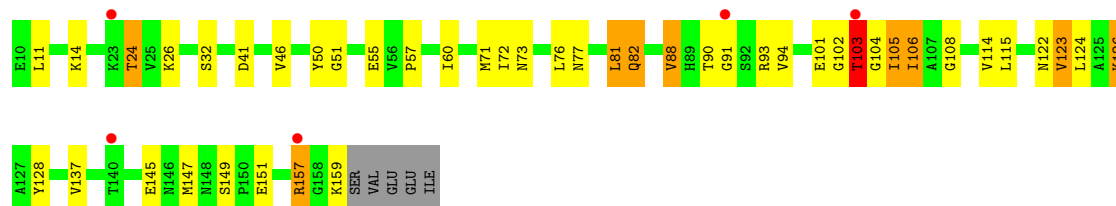
- Molecule 5: 30S ribosomal protein S5

Chain AE:  77% 21%



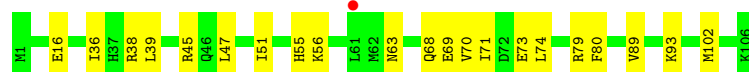
- Molecule 5: 30S ribosomal protein S5

Chain BE:  3% 68% 23% 6%



- Molecule 6: 30S ribosomal protein S6

Chain AF:  80% 20%



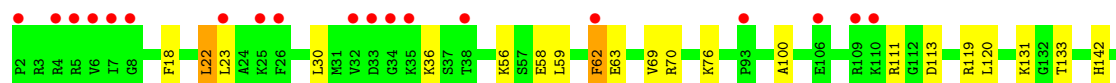
- Molecule 6: 30S ribosomal protein S6

Chain BF:  3% 70% 23% 6%



- Molecule 7: 30S ribosomal protein S7

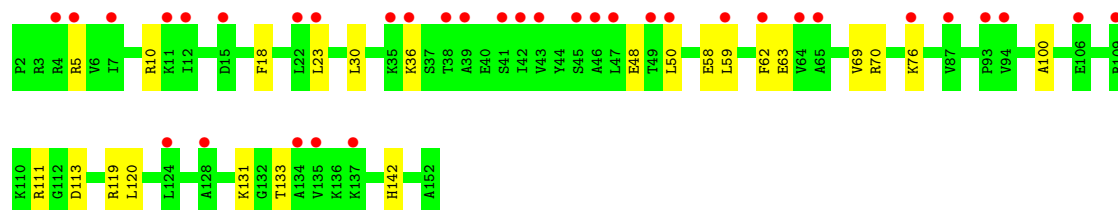
Chain AG:  13% 85% 13%





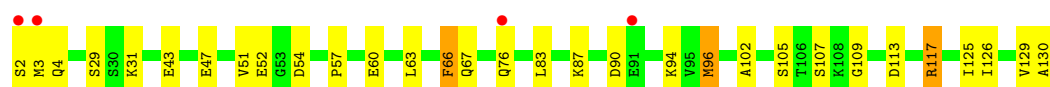
- Molecule 7: 30S ribosomal protein S7

Chain BG: 23% 85% 15%



- Molecule 8: 30S ribosomal protein S8

Chain AH: 3% 76% 22%



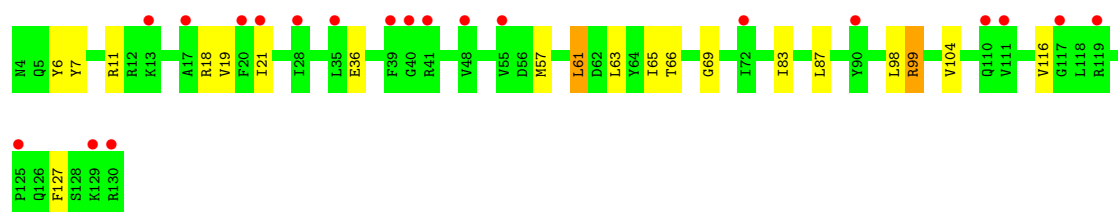
- Molecule 8: 30S ribosomal protein S8

Chain BH: 5% 77% 22%



- Molecule 9: 30S ribosomal protein S9

Chain AI: 16% 84% 14%

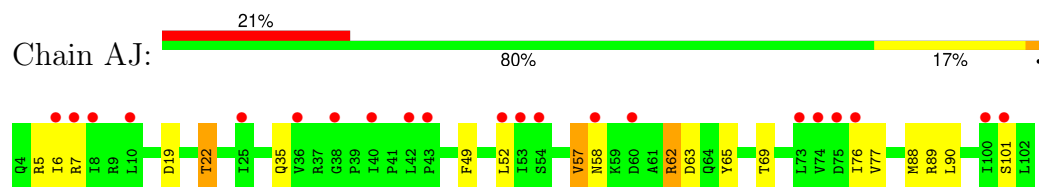


- Molecule 9: 30S ribosomal protein S9

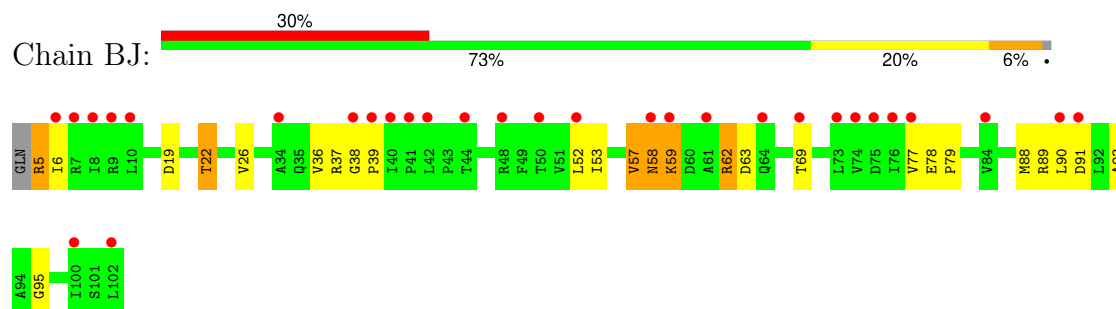
Chain BI: 21% 83% 16%



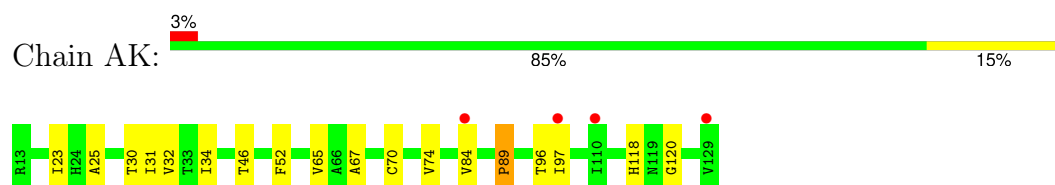
- Molecule 10: 30S ribosomal protein S10



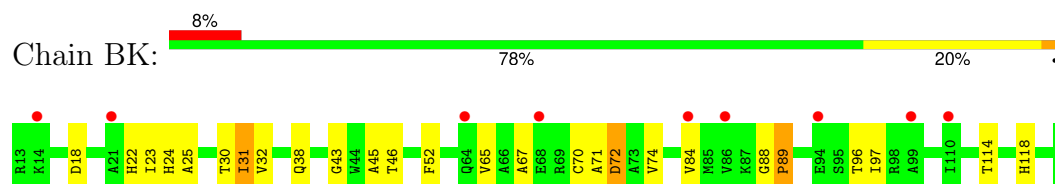
- Molecule 10: 30S ribosomal protein S10



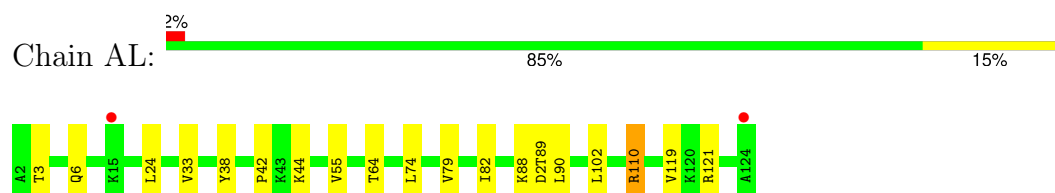
- Molecule 11: 30S ribosomal protein S11



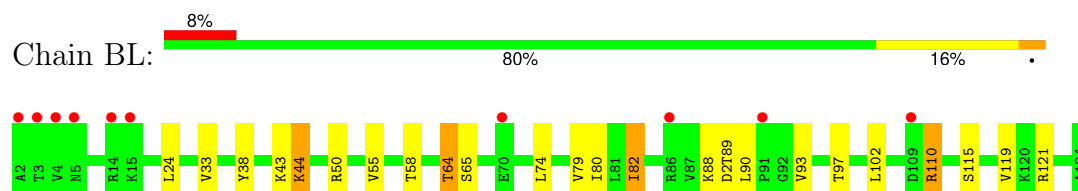
- Molecule 11: 30S ribosomal protein S11



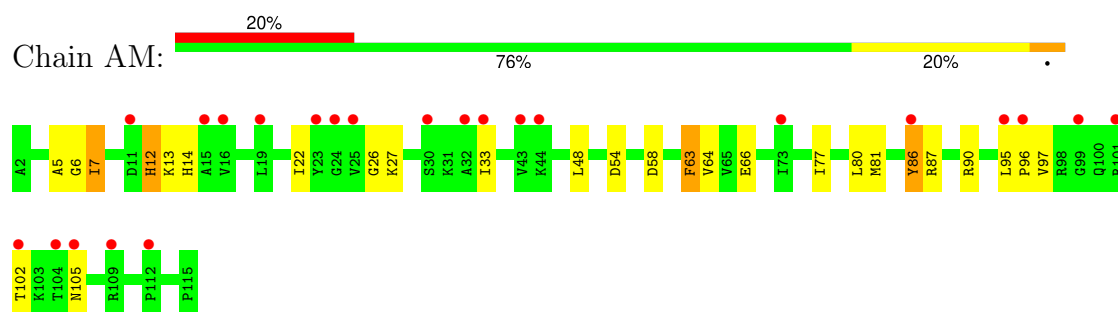
- Molecule 12: 30S ribosomal protein S12



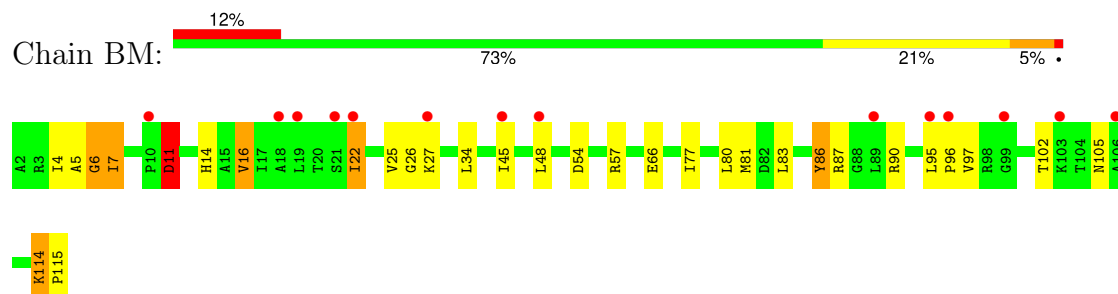
- Molecule 12: 30S ribosomal protein S12



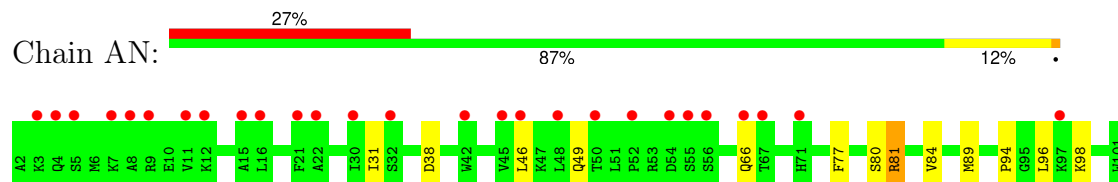
- Molecule 13: 30S ribosomal protein S13



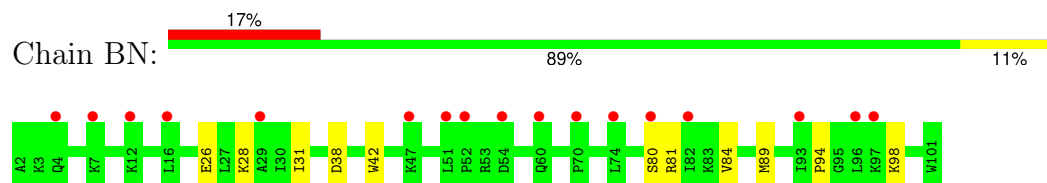
- Molecule 13: 30S ribosomal protein S13



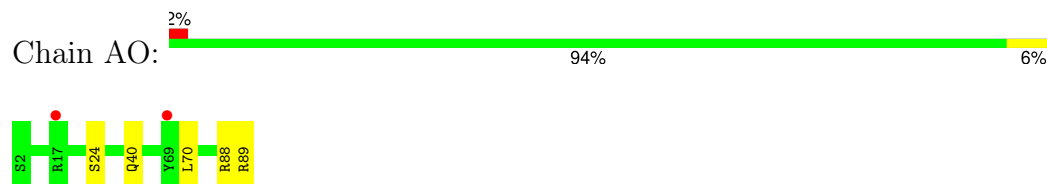
- Molecule 14: 30S ribosomal protein S14



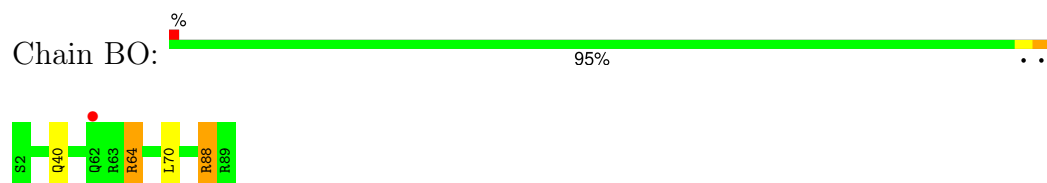
- Molecule 14: 30S ribosomal protein S14



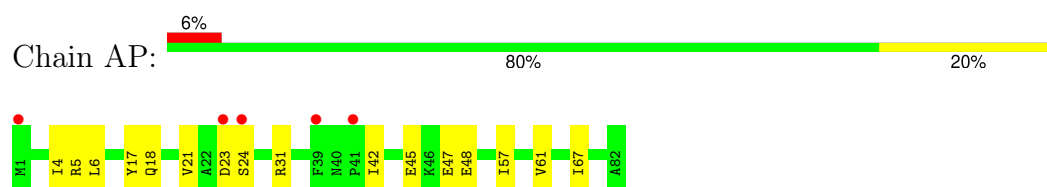
- Molecule 15: 30S ribosomal protein S15



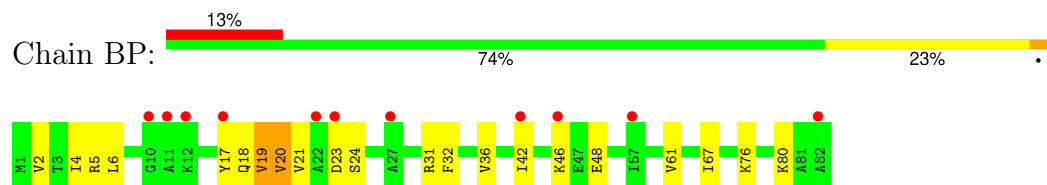
- Molecule 15: 30S ribosomal protein S15



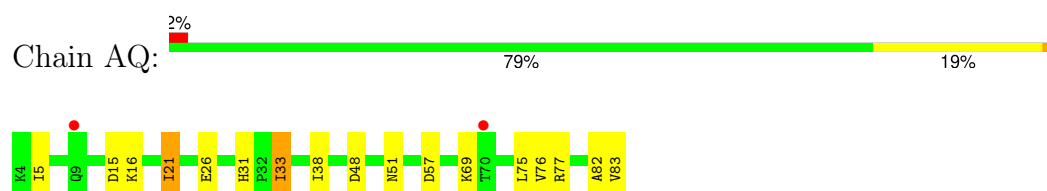
- Molecule 16: 30S ribosomal protein S16



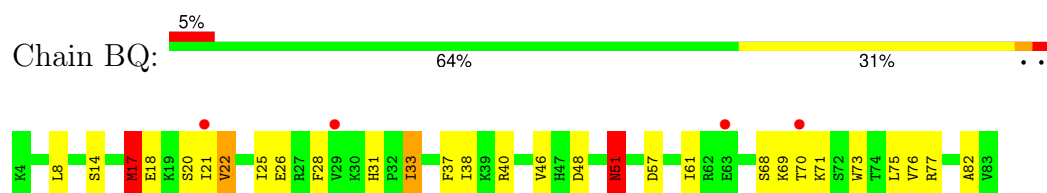
- Molecule 16: 30S ribosomal protein S16



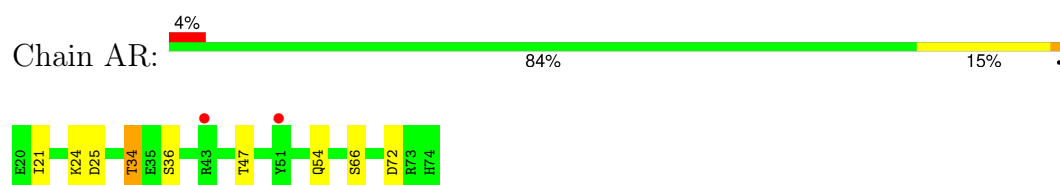
- Molecule 17: 30S ribosomal protein S17



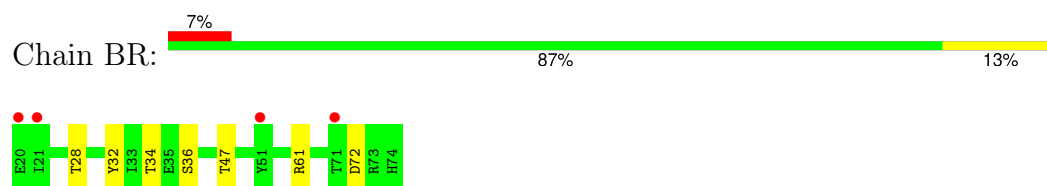
- Molecule 17: 30S ribosomal protein S17



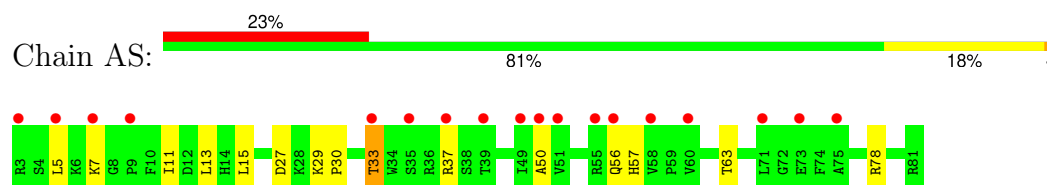
- Molecule 18: 30S ribosomal protein S18



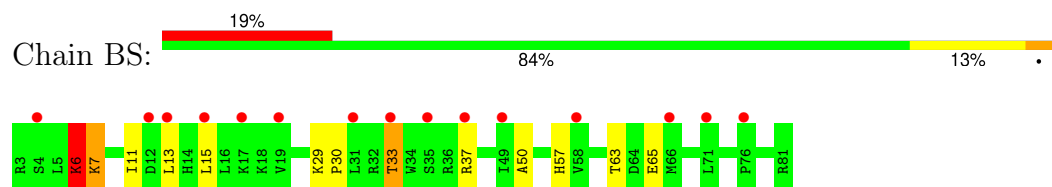
- Molecule 18: 30S ribosomal protein S18



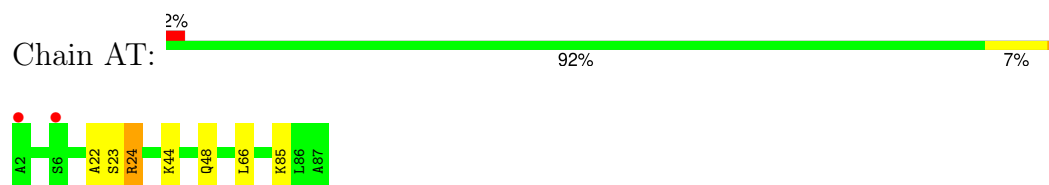
- Molecule 19: 30S ribosomal protein S19



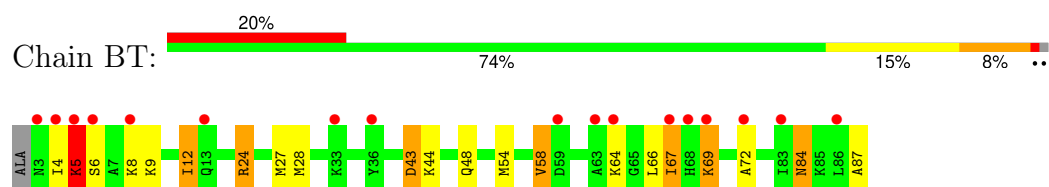
● Molecule 19: 30S ribosomal protein S19



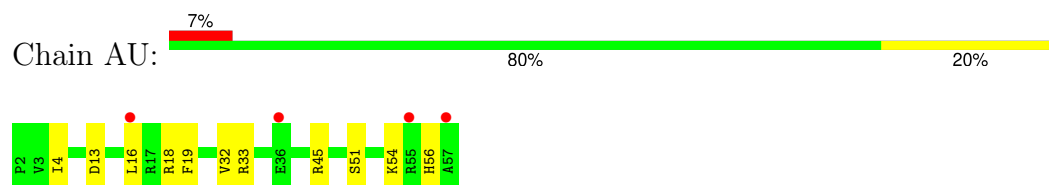
● Molecule 20: 30S ribosomal protein S20



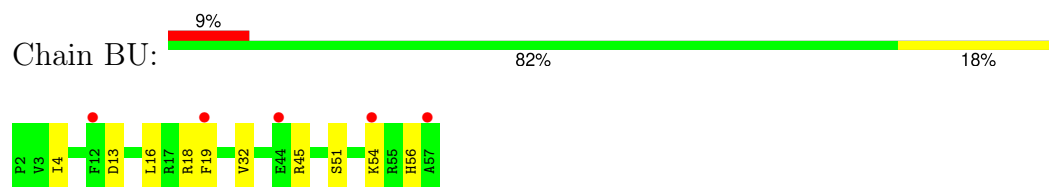
● Molecule 20: 30S ribosomal protein S20



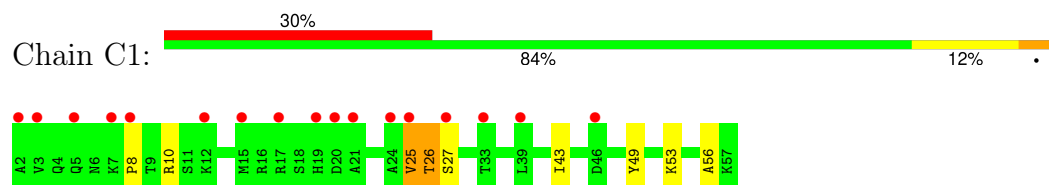
● Molecule 21: 30S ribosomal protein S21



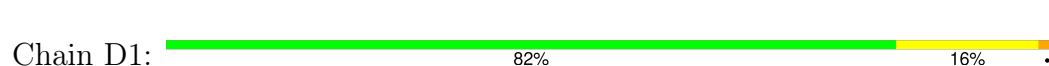
● Molecule 21: 30S ribosomal protein S21

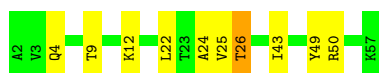


● Molecule 22: 50S ribosomal protein L32



● Molecule 22: 50S ribosomal protein L32

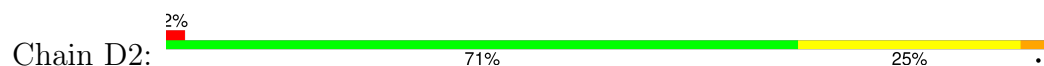




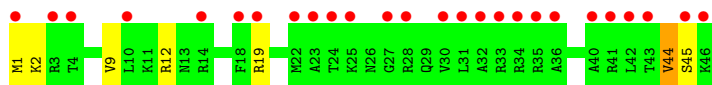
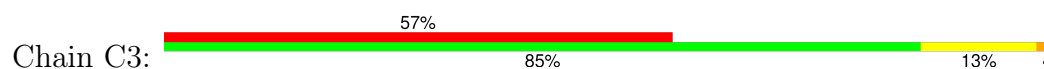
- Molecule 23: 50S ribosomal protein L33



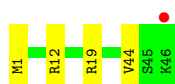
- Molecule 23: 50S ribosomal protein L33



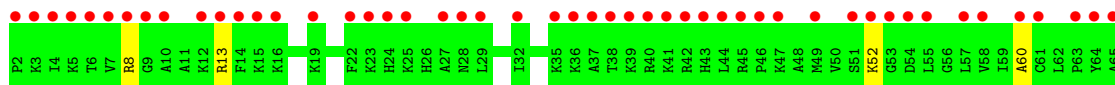
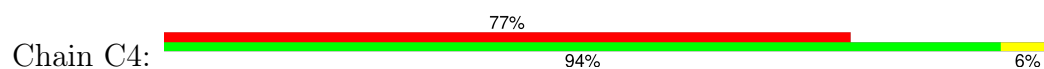
- Molecule 24: 50S ribosomal protein L34



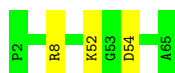
- Molecule 24: 50S ribosomal protein L34



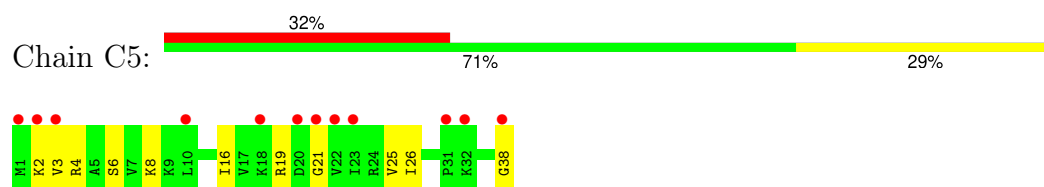
- Molecule 25: 50S ribosomal protein L35



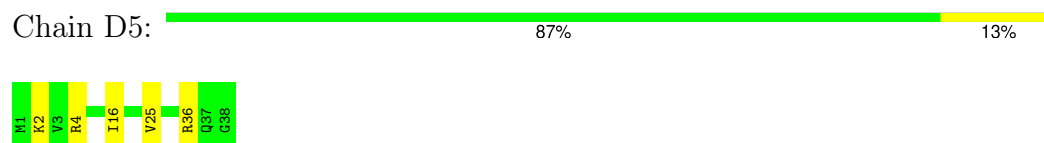
- Molecule 25: 50S ribosomal protein L35



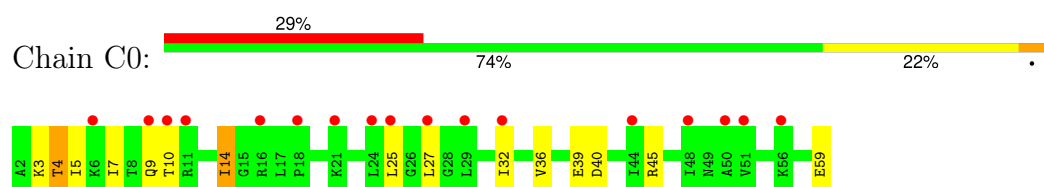
- Molecule 26: 50S ribosomal protein L36



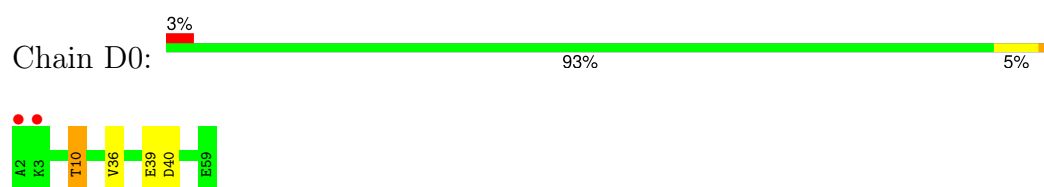
- Molecule 26: 50S ribosomal protein L36



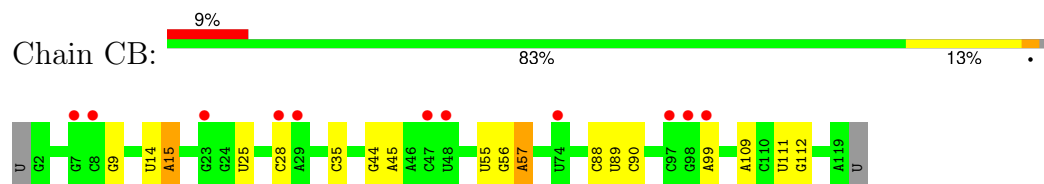
- Molecule 27: 50S ribosomal protein L30



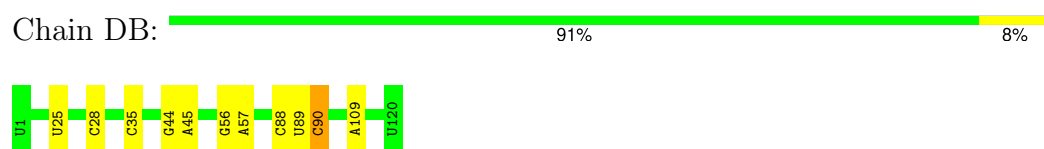
- Molecule 27: 50S ribosomal protein L30



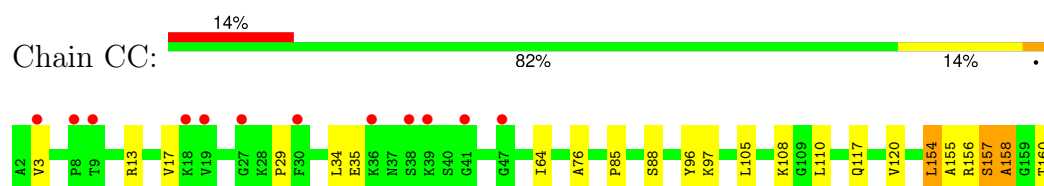
- Molecule 28: 5S rRNA

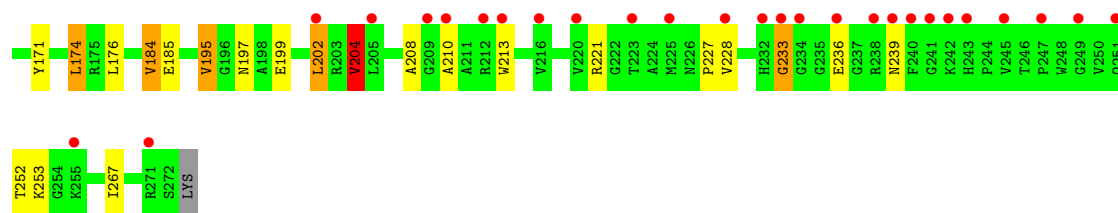


- Molecule 28: 5S rRNA

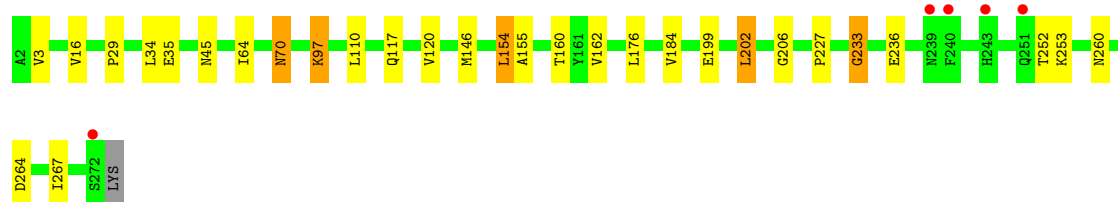
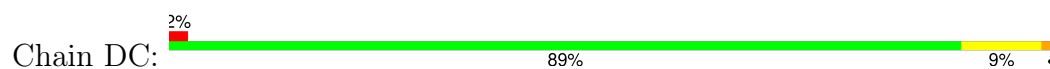


- Molecule 29: 50S ribosomal protein L2

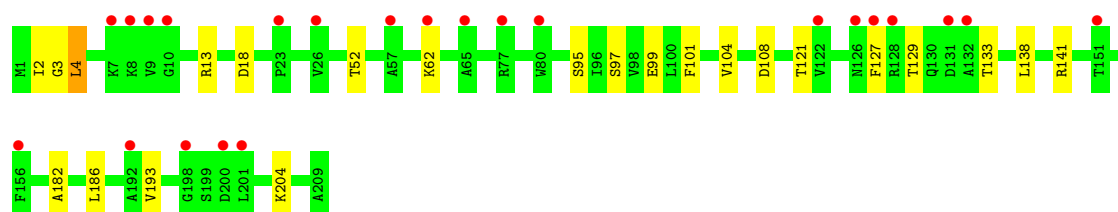
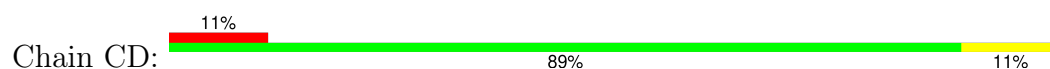




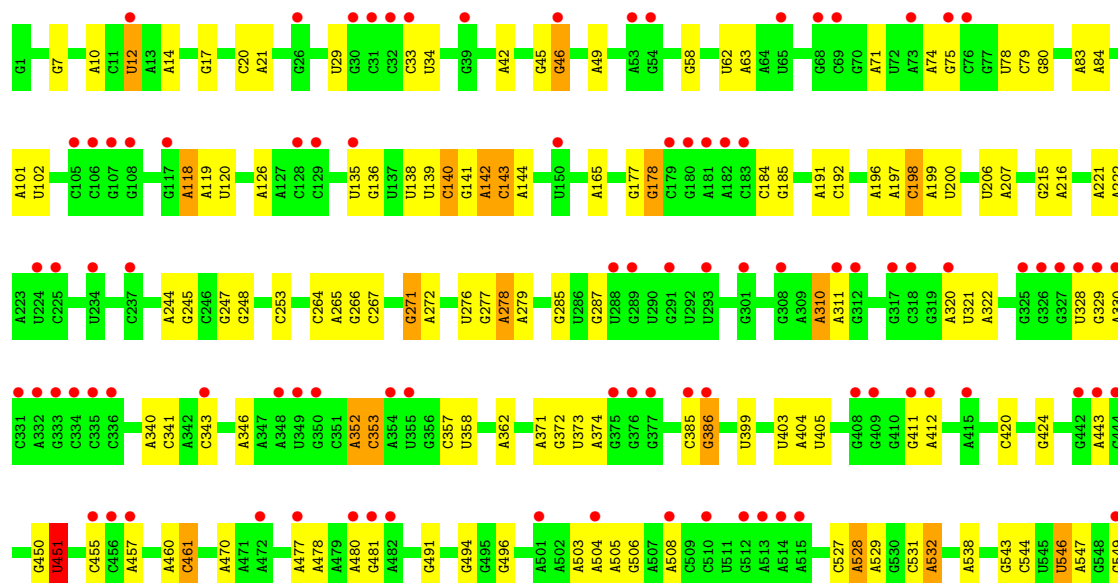
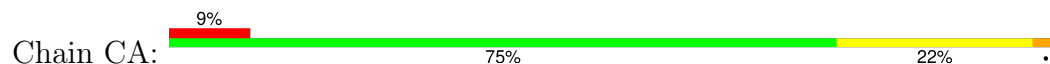
• Molecule 29: 50S ribosomal protein L2

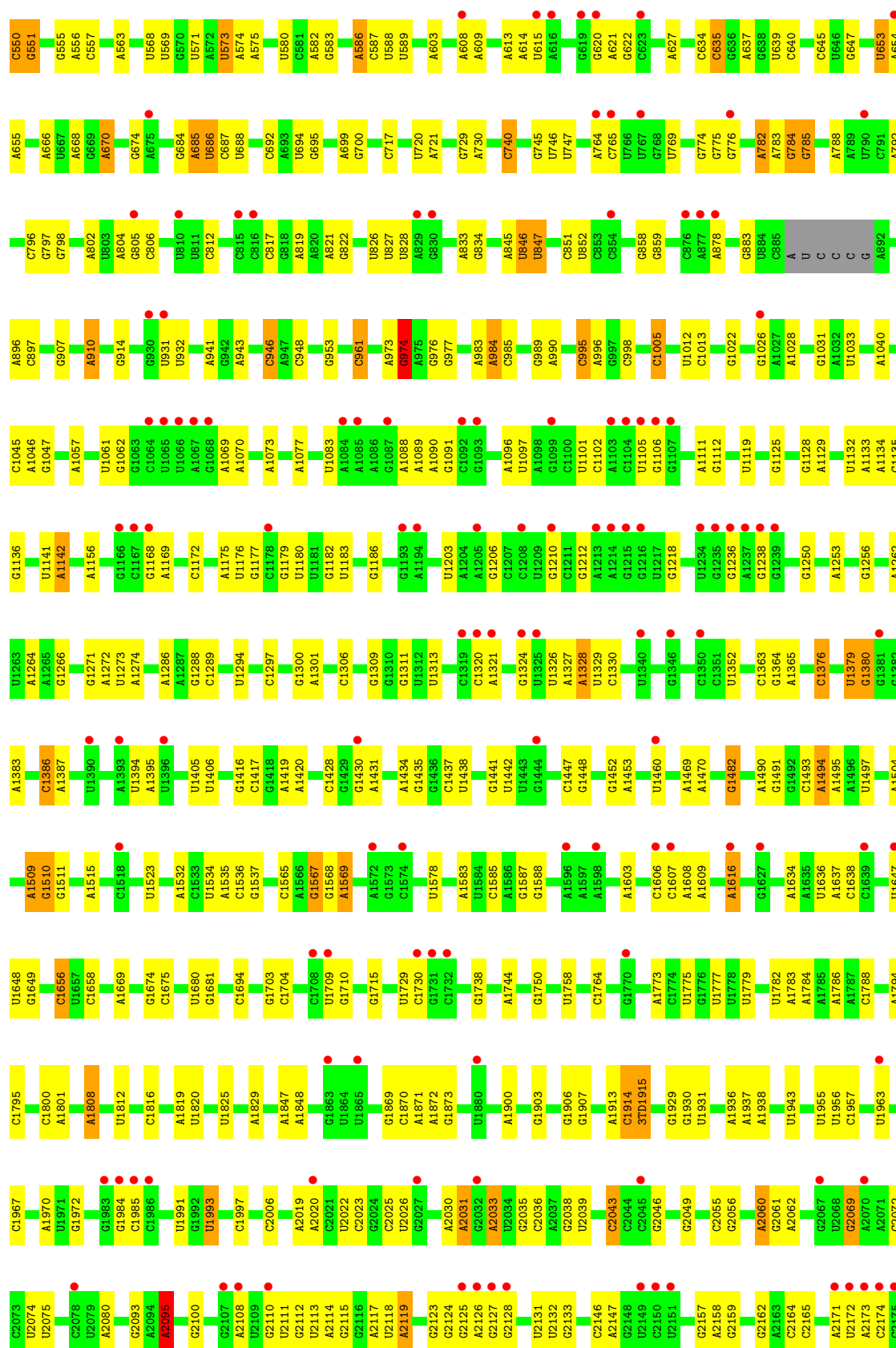


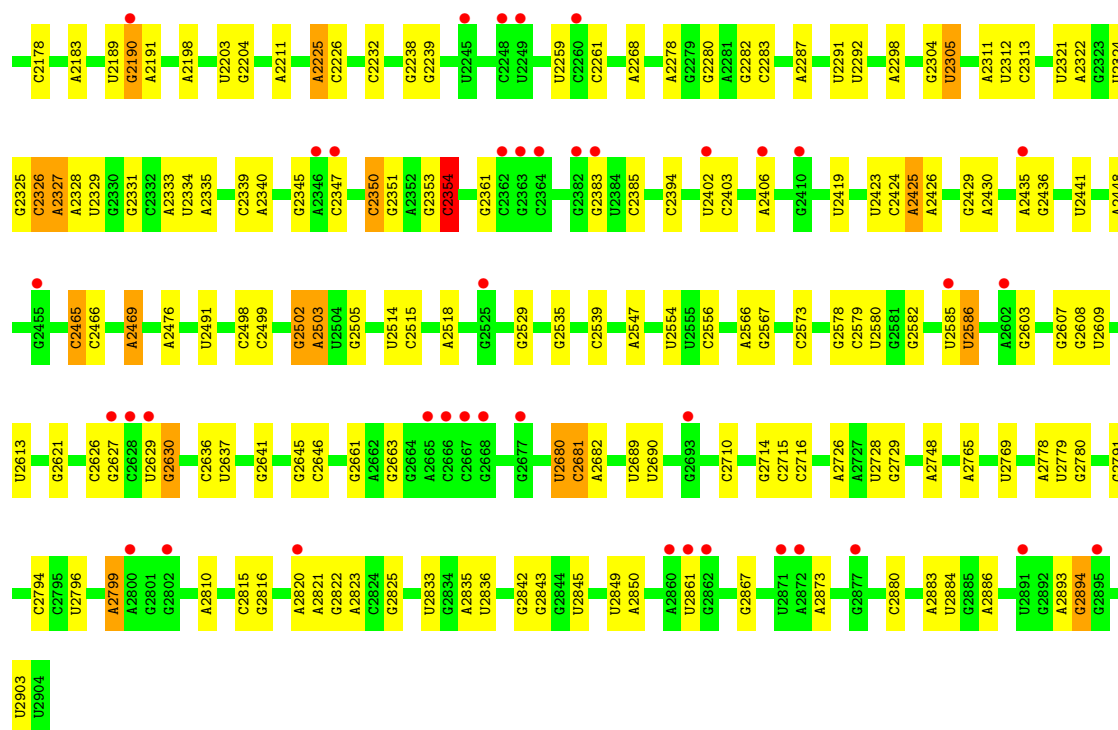
• Molecule 30: 50S ribosomal protein L3



• Molecule 31: 23S rRNA







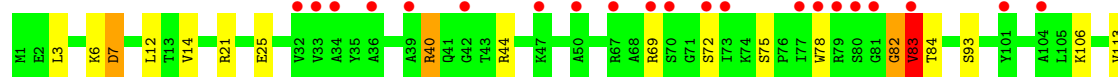
• Molecule 32: 50S ribosomal protein L3

Chain DD: 90% 9% .



• Molecule 33: 50S ribosomal protein L4

Chain CE: 17% 85% 12% .

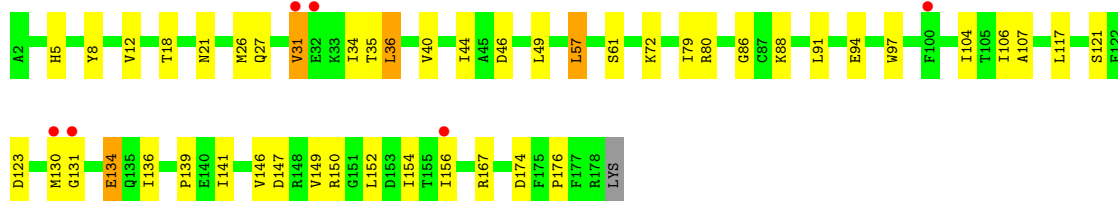


• Molecule 33: 50S ribosomal protein L4

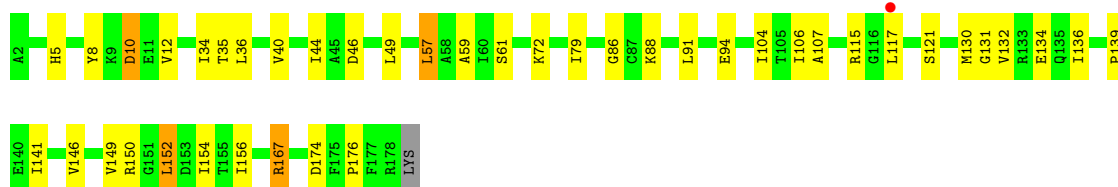
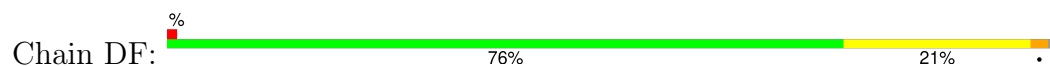
Chain DE: 89% 10% .



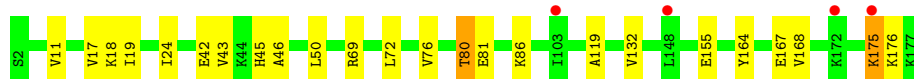
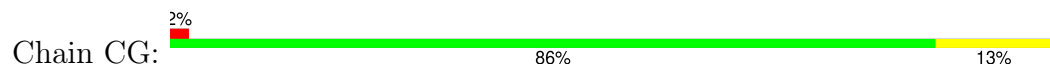
• Molecule 34: 50S ribosomal protein L5



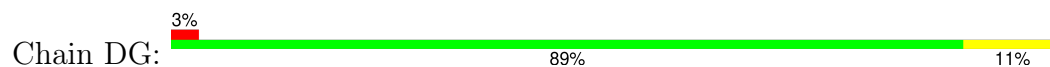
- Molecule 34: 50S ribosomal protein L5



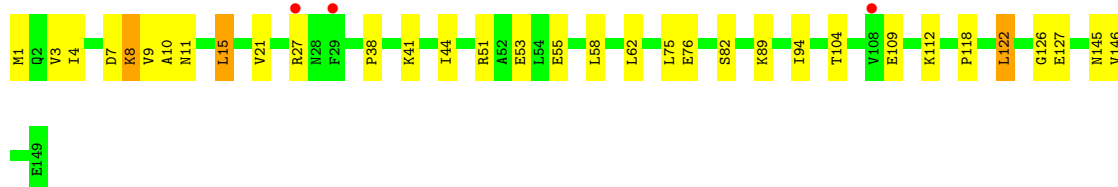
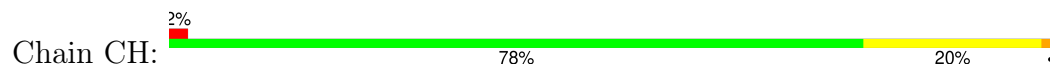
- Molecule 35: 50S ribosomal protein L6



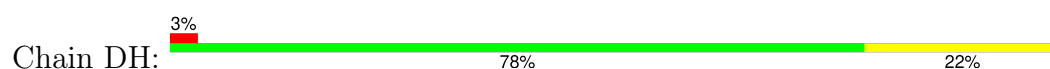
- Molecule 35: 50S ribosomal protein L6

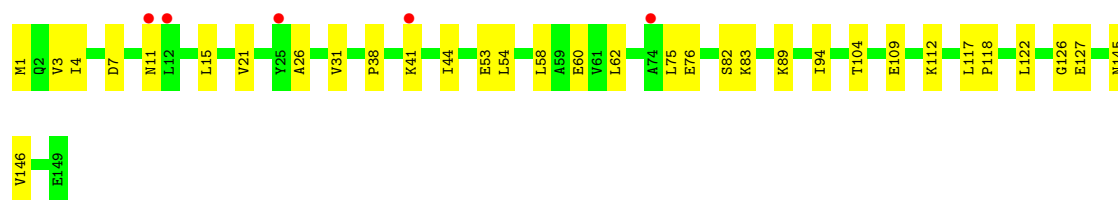


- Molecule 36: 50S ribosomal protein L9



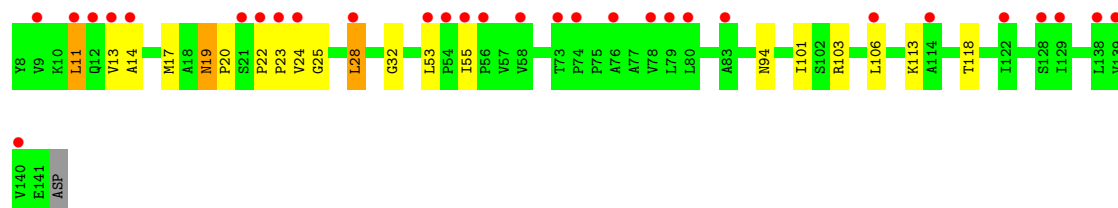
- Molecule 36: 50S ribosomal protein L9





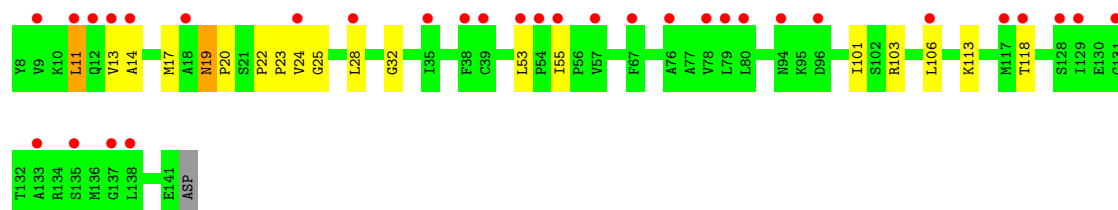
- Molecule 37: 50S ribosomal protein L11

Chain CJ: 22% 84% 13% ..



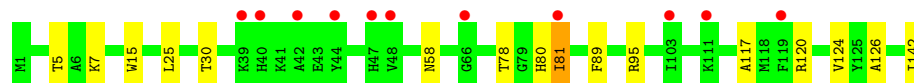
- Molecule 37: 50S ribosomal protein L11

Chain DJ: 24% 85% 13% ..



- Molecule 38: 50S ribosomal protein L13

Chain CK: 8% 89% 11% .



- Molecule 38: 50S ribosomal protein L13

Chain DK: 89% 10% .



- Molecule 39: 50S ribosomal protein L14

Chain CL: 7% 83% 13% ...



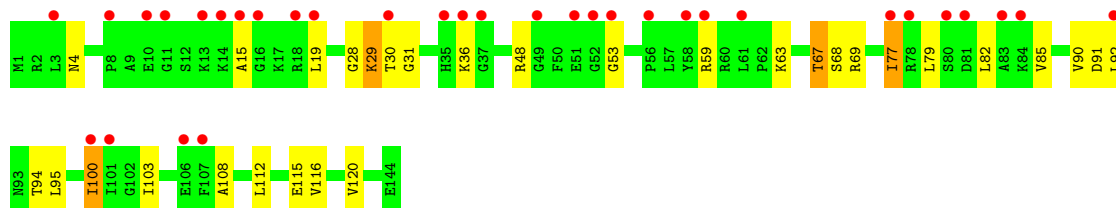
- Molecule 39: 50S ribosomal protein L14

Chain DL:  85% 13% .

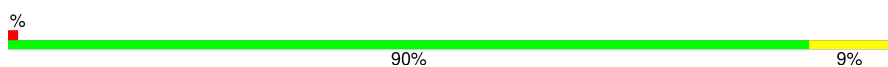


- Molecule 40: 50S ribosomal protein L15

Chain CM:  23% 78% 19% .



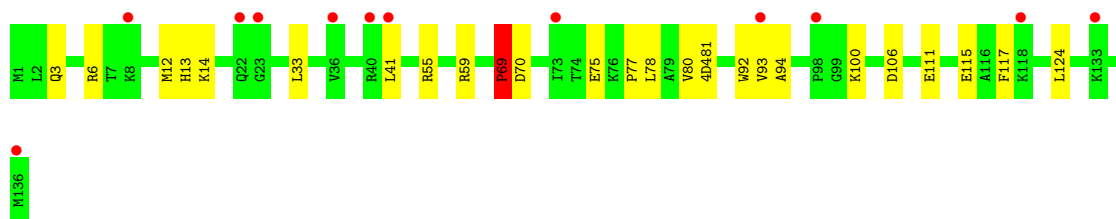
- Molecule 40: 50S ribosomal protein L15

Chain DM:  90% 9% .



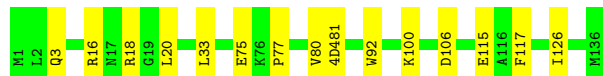
- Molecule 41: 50S ribosomal protein L16

Chain CN:  9% 82% 18% .



- Molecule 41: 50S ribosomal protein L16

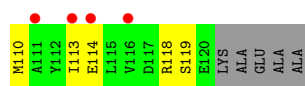
Chain DN:  89% 11% .



- Molecule 42: 50S ribosomal protein L17

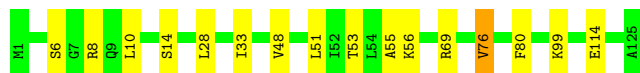
Chain CO:  27% 80% 13% .





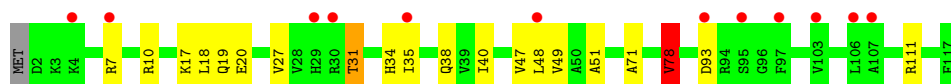
- Molecule 42: 50S ribosomal protein L17

Chain DO: 87% 12% .



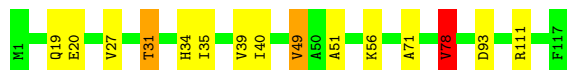
- Molecule 43: 50S ribosomal protein L18

Chain CP: 10% 82% 15% ...



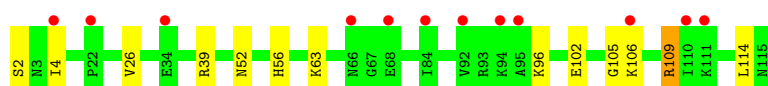
- Molecule 43: 50S ribosomal protein L18

Chain DP: 87% 10% ..



- Molecule 44: 50S ribosomal protein L19

Chain CQ: 11% 89% 11% .



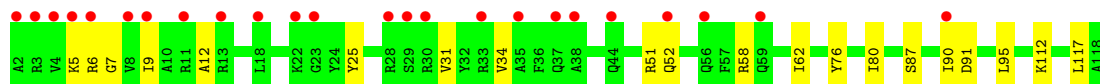
- Molecule 44: 50S ribosomal protein L19

Chain DQ: % 86% 12% .



- Molecule 45: 50S ribosomal protein L20

Chain CR: 21% 83% 17%



- Molecule 45: 50S ribosomal protein L20

Chain DR:  85% 14%

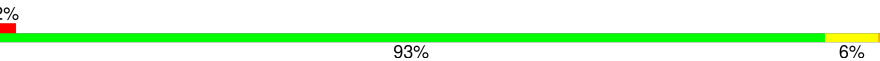


- Molecule 46: 50S ribosomal protein L21

Chain CS:  18% 83% 14%



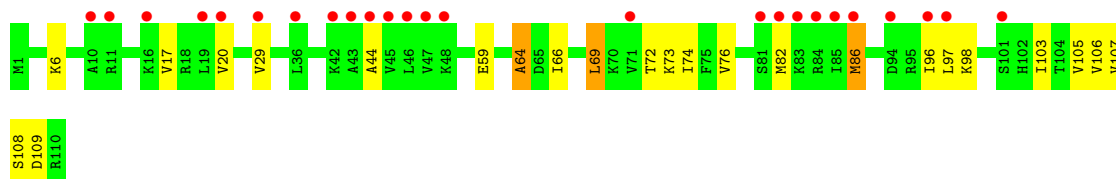
- Molecule 46: 50S ribosomal protein L21

Chain DS:  2% 93% 6%



- Molecule 47: 50S ribosomal protein L22

Chain CT:  23% 78% 19%



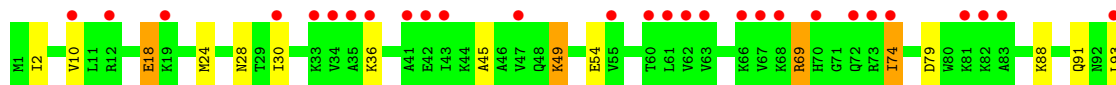
- Molecule 47: 50S ribosomal protein L22

Chain DT:  84% 16%



- Molecule 48: 50S ribosomal protein L23

Chain CU:  30% 83% 13%

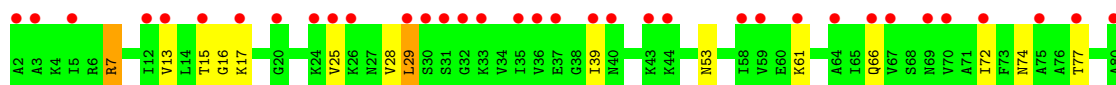
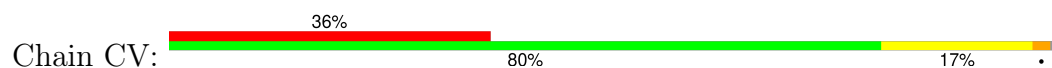


- Molecule 48: 50S ribosomal protein L23

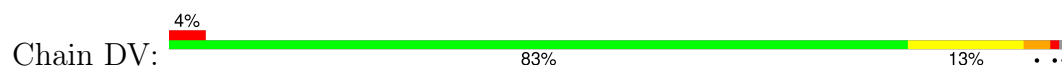
Chain DU:  4% 85% 15%



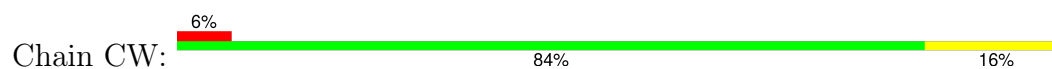
- Molecule 49: 50S ribosomal protein L24



- Molecule 49: 50S ribosomal protein L24



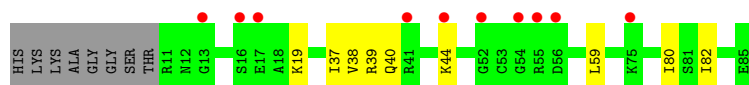
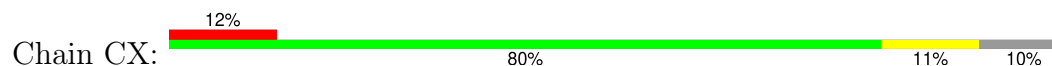
- Molecule 50: 50S ribosomal protein L25



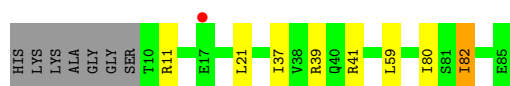
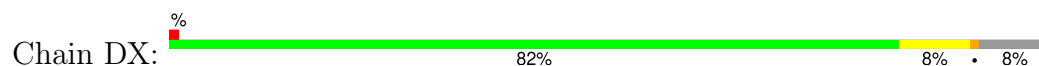
- Molecule 50: 50S ribosomal protein L25



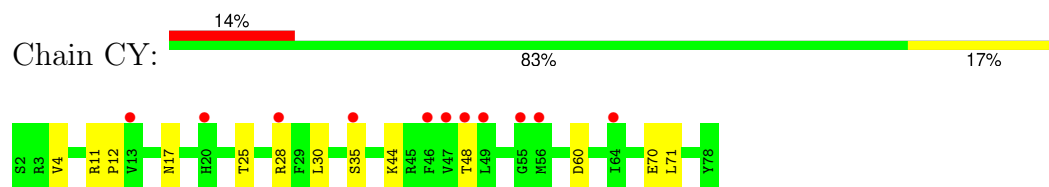
- Molecule 51: 50S ribosomal protein L27



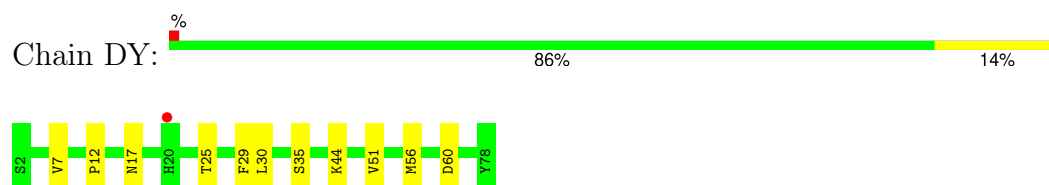
- Molecule 51: 50S ribosomal protein L27



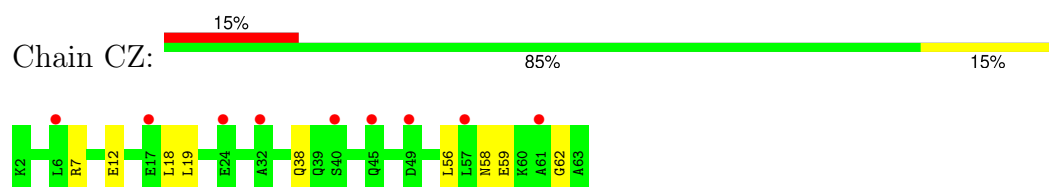
- Molecule 52: 50S ribosomal protein L28



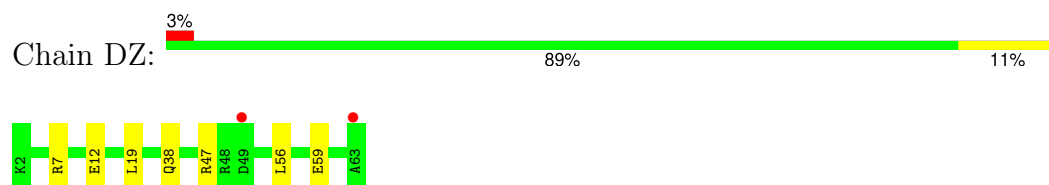
- Molecule 52: 50S ribosomal protein L28



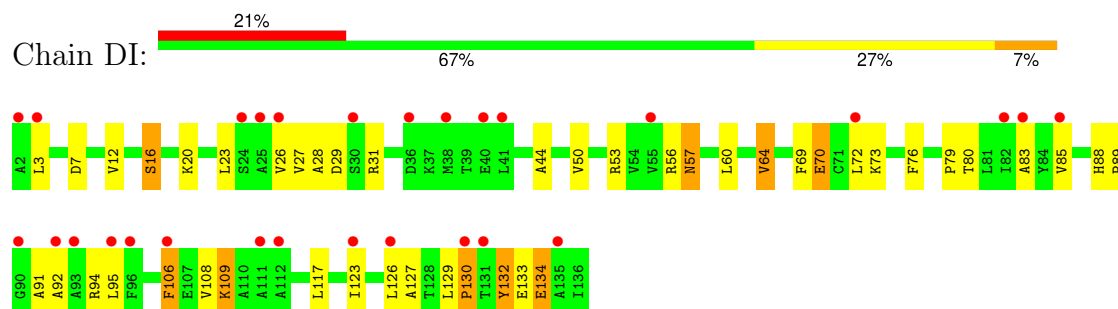
- Molecule 53: 50S ribosomal protein L29



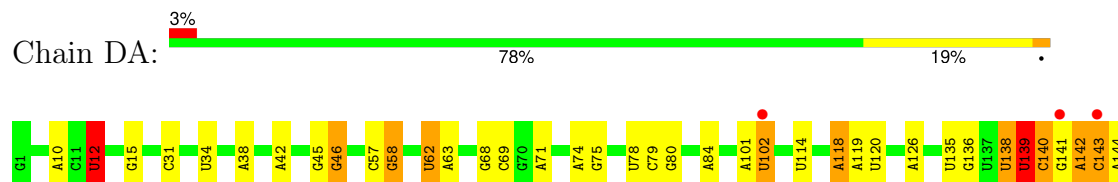
- Molecule 53: 50S ribosomal protein L29

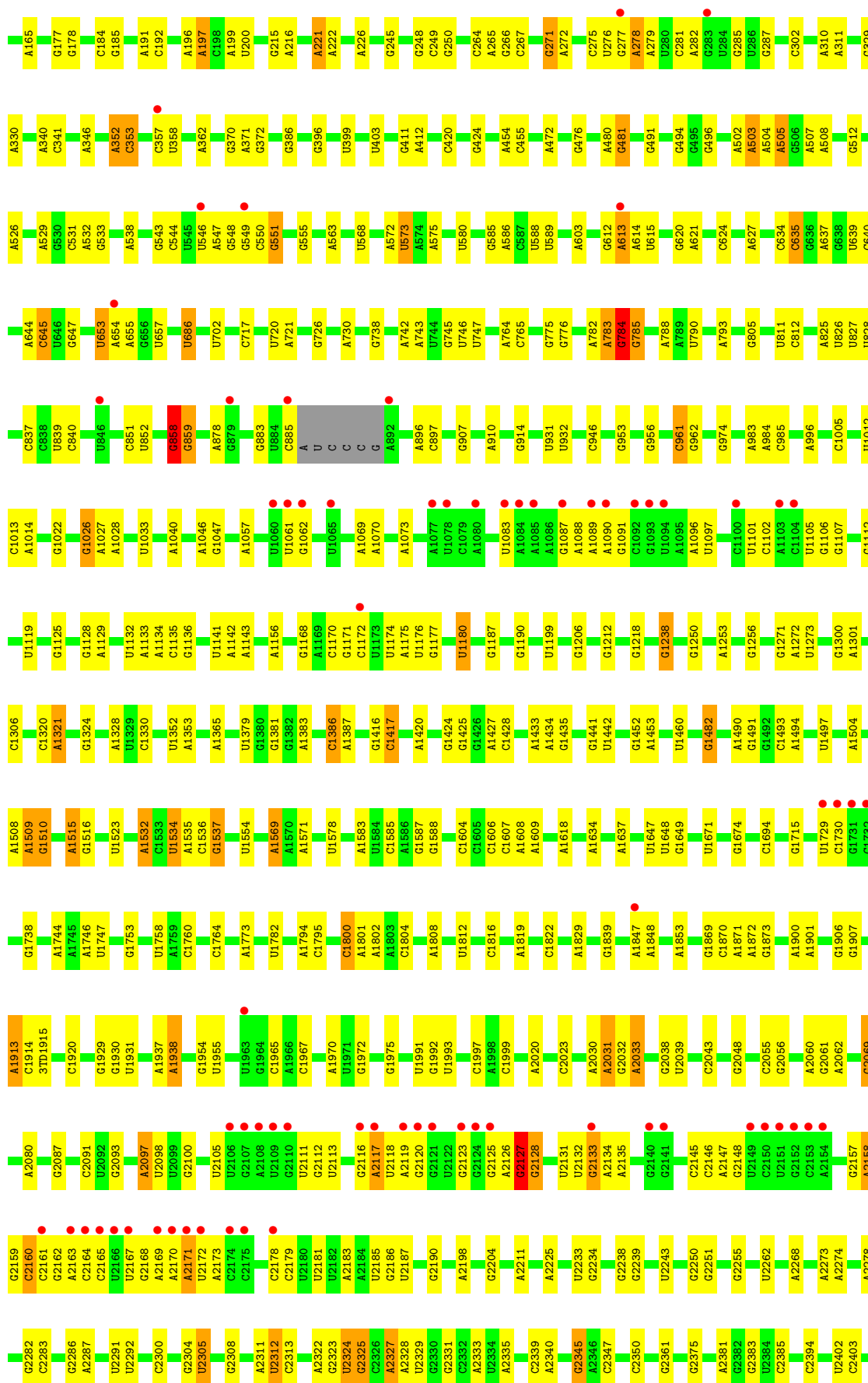


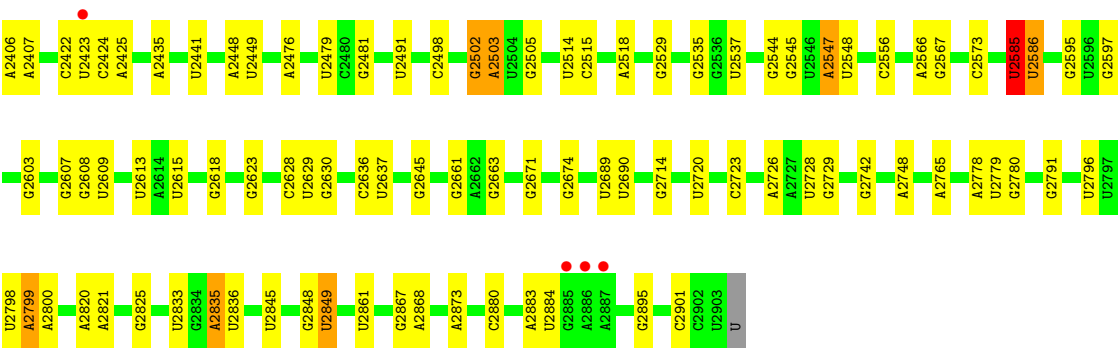
- Molecule 54: 50S ribosomal protein L10



- Molecule 55: 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	211.72Å 435.19Å 622.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.53 – 3.10 48.53 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.53-3.10) 99.7 (48.53-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 3.12Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, R_{free}	0.171 , 0.192 0.185 , 0.207	Depositor DCC
R_{free} test set	4087 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 106.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	295207	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: D2T, H2U, 3TD, TRS, PSU, T1C, 1PE, MA6, MEQ, 1MG, 6MZ, 2MA, ACY, MPD, ZN, 5MU, SPD, EDO, PEG, MG, 7MG, UR3, GUN, PGE, 4D4, OMC, OMU, OMG, PUT, 2MG, PG4, 5MC, 4OC

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	0.67	11/36597 (0.0%)	0.67	1/57088 (0.0%)
1	BA	0.68	7/36572 (0.0%)	0.67	2/57049 (0.0%)
2	AB	0.79	0/1784	1.36	5/2403 (0.2%)
2	BB	0.78	0/1784	1.37	5/2403 (0.2%)
3	AC	0.81	0/1652	1.29	2/2225 (0.1%)
3	BC	0.82	0/1652	1.31	6/2225 (0.3%)
4	AD	0.73	0/1665	1.38	7/2227 (0.3%)
4	BD	0.73	0/1665	1.38	7/2227 (0.3%)
5	AE	0.79	0/1157	1.40	8/1557 (0.5%)
5	BE	0.83	0/1118	1.41	6/1504 (0.4%)
6	AF	0.78	0/881	1.31	4/1189 (0.3%)
6	BF	0.80	0/835	1.41	10/1128 (0.9%)
7	AG	0.80	0/1196	1.38	4/1602 (0.2%)
7	BG	0.81	0/1196	1.38	3/1602 (0.2%)
8	AH	0.73	0/989	1.32	1/1326 (0.1%)
8	BH	0.74	0/989	1.32	1/1326 (0.1%)
9	AI	0.78	0/1034	1.32	2/1375 (0.1%)
9	BI	0.78	0/1034	1.31	2/1375 (0.1%)
10	AJ	0.76	0/806	1.26	2/1089 (0.2%)
10	BJ	0.87	0/797	1.31	4/1077 (0.4%)
11	AK	0.78	0/893	1.20	3/1205 (0.2%)
11	BK	0.76	0/893	1.24	3/1205 (0.2%)
12	AL	0.74	0/960	1.24	4/1286 (0.3%)
12	BL	0.76	0/960	1.24	2/1286 (0.2%)
13	AM	0.90	0/893	1.51	9/1193 (0.8%)
13	BM	0.91	0/893	1.50	10/1193 (0.8%)
14	AN	0.81	0/817	1.36	1/1088 (0.1%)
14	BN	0.78	0/817	1.35	1/1088 (0.1%)
15	AO	0.73	0/722	1.46	1/964 (0.1%)
15	BO	0.73	0/722	1.50	0/964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	AP	0.79	0/659	1.31	4/884 (0.5%)
16	BP	0.83	0/659	1.38	5/884 (0.6%)
17	AQ	0.81	0/658	1.22	2/881 (0.2%)
17	BQ	0.86	0/658	1.32	4/881 (0.5%)
18	AR	0.83	0/463	1.40	3/621 (0.5%)
18	BR	0.81	0/463	1.35	2/621 (0.3%)
19	AS	0.87	0/653	1.23	0/877
19	BS	0.86	0/653	1.23	0/877
20	AT	0.79	0/676	1.54	4/895 (0.4%)
20	BT	0.89	1/671 (0.1%)	1.63	5/888 (0.6%)
21	AU	0.71	0/472	1.35	4/627 (0.6%)
21	BU	0.69	0/472	1.37	2/627 (0.3%)
22	C1	0.87	0/450	1.29	0/599
22	D1	0.86	0/450	1.28	1/599 (0.2%)
23	C2	0.81	0/416	1.24	0/554
23	D2	0.80	0/421	1.24	1/561 (0.2%)
24	C3	0.71	0/380	1.46	0/498
24	D3	0.82	0/380	1.49	1/498 (0.2%)
25	C4	0.74	0/513	1.20	0/676
25	D4	0.80	0/513	1.23	0/676
26	C5	0.76	0/303	1.22	2/397 (0.5%)
26	D5	0.82	0/303	1.13	0/397
27	C0	0.84	0/453	1.38	1/605 (0.2%)
27	D0	0.87	0/467	1.33	2/623 (0.3%)
28	CB	0.64	0/2828	0.67	1/4410 (0.0%)
28	DB	0.67	0/2872	0.69	0/4478
29	CC	0.73	0/2121	1.25	9/2852 (0.3%)
29	DC	0.74	0/2121	1.22	6/2852 (0.2%)
30	CD	0.75	1/1586 (0.1%)	1.15	1/2134 (0.0%)
31	CA	0.69	33/69165 (0.0%)	0.68	5/107896 (0.0%)
32	DD	0.76	0/1576	1.14	3/2119 (0.1%)
33	CE	0.76	0/1571	1.36	10/2113 (0.5%)
33	DE	0.77	0/1570	1.32	6/2113 (0.3%)
34	CF	0.75	0/1434	1.36	8/1926 (0.4%)
34	DF	0.78	0/1434	1.36	12/1926 (0.6%)
35	CG	0.74	0/1343	1.27	6/1816 (0.3%)
35	DG	0.73	0/1343	1.23	2/1816 (0.1%)
36	CH	0.84	0/1121	1.35	2/1515 (0.1%)
36	DH	0.85	1/1121 (0.1%)	1.35	2/1515 (0.1%)
37	CJ	0.93	0/993	1.35	3/1341 (0.2%)
37	DJ	0.93	0/993	1.34	3/1341 (0.2%)
38	CK	0.69	0/1152	1.28	4/1551 (0.3%)
38	DK	0.80	0/1152	1.26	6/1551 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	CL	0.78	0/947	1.20	2/1268 (0.2%)
39	DL	0.80	1/955 (0.1%)	1.17	0/1279
40	CM	0.77	1/1062 (0.1%)	1.36	8/1413 (0.6%)
40	DM	0.73	0/1062	1.25	1/1413 (0.1%)
41	CN	0.74	0/1081	1.27	6/1443 (0.4%)
41	DN	0.76	0/1092	1.25	1/1457 (0.1%)
42	CO	0.74	0/973	1.29	1/1301 (0.1%)
42	DO	0.82	0/1006	1.35	3/1345 (0.2%)
43	CP	0.74	0/902	1.41	6/1209 (0.5%)
43	DP	0.78	0/910	1.38	4/1219 (0.3%)
44	CQ	0.69	0/929	1.15	0/1242
44	DQ	0.73	0/929	1.15	1/1242 (0.1%)
45	CR	0.75	0/960	1.39	3/1278 (0.2%)
45	DR	0.81	0/960	1.36	3/1278 (0.2%)
46	CS	0.72	0/829	1.22	5/1107 (0.5%)
46	DS	0.76	0/829	1.23	1/1107 (0.1%)
47	CT	0.71	0/864	1.34	2/1156 (0.2%)
47	DT	0.78	0/864	1.33	1/1156 (0.1%)
48	CU	0.76	0/745	1.27	3/994 (0.3%)
48	DU	0.76	0/744	1.30	5/994 (0.5%)
49	CV	0.78	0/787	1.30	4/1051 (0.4%)
49	DV	0.76	0/787	1.30	10/1051 (1.0%)
50	CW	0.71	0/766	1.24	0/1025
50	DW	0.76	0/766	1.26	1/1025 (0.1%)
51	CX	0.65	0/576	1.08	1/762 (0.1%)
51	DX	0.72	1/598 (0.2%)	1.09	0/790
52	CY	0.67	0/635	1.33	3/848 (0.4%)
52	DY	0.73	0/635	1.30	2/848 (0.2%)
53	CZ	0.71	0/502	1.51	0/667
53	DZ	0.73	0/502	1.51	0/667
54	DI	0.89	0/1037	1.47	7/1402 (0.5%)
55	DA	0.72	19/69364 (0.0%)	0.71	2/108207 (0.0%)
All	All	0.72	76/309273 (0.0%)	0.90	334/462224 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
41	CN	0	1
55	DA	0	25
All	All	0	26

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2095	A	O5'-C5'	-9.45	1.28	1.42
55	DA	12	U	C1'-N1	8.21	1.60	1.48
55	DA	2585	U	C1'-N1	8.10	1.59	1.47
55	DA	2097	A	O5'-C5'	-7.60	1.31	1.42
31	CA	2425	A	C3'-O3'	7.52	1.54	1.43
1	BA	5	U	C1'-N1	7.29	1.59	1.48
31	CA	451	U	C1'-N1	7.18	1.58	1.47
31	CA	12	U	C1'-N1	6.86	1.58	1.48
1	AA	5	U	C1'-N1	6.62	1.58	1.48
31	CA	769	U	C1'-N1	6.55	1.58	1.48
31	CA	546	U	C1'-N1	6.36	1.57	1.48
55	DA	1306	C	C1'-N1	6.24	1.57	1.48
1	BA	1008	U	O5'-C5'	-6.22	1.33	1.42
31	CA	2465	C	C1'-N1	6.16	1.57	1.48
31	CA	2354	C	C1'-N1	6.08	1.57	1.48
31	CA	995	C	O5'-C5'	-6.05	1.33	1.42
55	DA	140	C	C1'-N1	6.00	1.56	1.47
31	CA	1825	U	C1'-N1	5.96	1.57	1.48
55	DA	1170	C	C1'-N1	5.95	1.57	1.48
31	CA	692	C	C1'-N1	5.90	1.57	1.48
31	CA	2225	A	C3'-O3'	5.88	1.51	1.43
1	AA	1397	C	C1'-N1	5.84	1.56	1.47
55	DA	1534	U	C1'-N1	5.77	1.57	1.48
1	AA	528	C	C1'-N1	5.76	1.57	1.48
31	CA	1376	C	C1'-N1	5.73	1.57	1.48
55	DA	1920	C	C1'-N1	5.72	1.57	1.48
1	AA	932	C	C1'-N1	5.72	1.57	1.48
31	CA	961	C	C1'-N1	5.72	1.56	1.47
31	CA	946	C	C1'-N1	5.72	1.57	1.48
31	CA	1777	U	C1'-N1	5.67	1.56	1.48
1	BA	1493	A	C3'-O3'	5.67	1.50	1.42
31	CA	2232	C	C1'-N1	5.60	1.56	1.48
31	CA	1306	C	C1'-N1	5.58	1.56	1.48
55	DA	139	U	C1'-N1	5.57	1.55	1.47
1	AA	955	U	C1'-N1	5.57	1.56	1.48
55	DA	2586	U	C1'-N1	5.55	1.56	1.48
31	CA	1658	C	C1'-N1	5.52	1.56	1.48
55	DA	2127	G	C3'-O3'	5.49	1.50	1.42
31	CA	2586	U	C1'-N1	5.48	1.56	1.48
55	DA	784	G	C3'-O3'	5.47	1.50	1.42
1	AA	485	U	C1'-N1	5.46	1.55	1.47
1	BA	955	U	C1'-N1	5.45	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	956	U	C1'-N1	5.44	1.56	1.48
31	CA	817	C	C1'-N1	5.42	1.56	1.48
31	CA	1379	U	C3'-O3'	5.40	1.50	1.42
30	CD	193	VAL	CA-C	5.37	1.57	1.52
31	CA	1788	C	C1'-N1	5.36	1.56	1.48
31	CA	461	C	C1'-N1	5.35	1.56	1.48
40	CM	77	ILE	CG1-CD1	-5.29	1.31	1.51
1	BA	1298	U	C1'-N1	5.28	1.55	1.47
31	CA	29	U	C1'-N1	5.26	1.56	1.48
1	AA	1203	C	C1'-N1	5.25	1.56	1.48
1	AA	1298	U	C1'-N1	5.22	1.55	1.47
31	CA	140	C	C1'-N1	5.22	1.55	1.47
55	DA	2901	C	C1'-N1	5.19	1.56	1.48
31	CA	653	U	C1'-N1	5.17	1.56	1.48
1	AA	632	U	C1'-N1	5.17	1.56	1.48
1	AA	1498	UR3	O3'-P	5.16	1.61	1.56
31	CA	557	C	C1'-N1	5.15	1.56	1.48
55	DA	114	U	C1'-N1	5.15	1.56	1.48
55	DA	653	U	C1'-N1	5.14	1.56	1.48
55	DA	635	C	C1'-N1	5.14	1.56	1.48
55	DA	961	C	C1'-N1	5.10	1.55	1.47
31	CA	2715	C	C1'-N1	5.06	1.56	1.48
1	BA	956	U	C1'-N1	5.06	1.56	1.48
55	DA	2300	C	C1'-N1	5.04	1.56	1.48
31	CA	635	C	C1'-N1	5.03	1.55	1.48
39	DL	113	MET	SD-CE	5.03	1.92	1.79
55	DA	275	C	C1'-N1	5.02	1.55	1.48
31	CA	1656	C	C1'-N1	5.02	1.55	1.48
31	CA	2006	C	C1'-N1	5.01	1.55	1.48
31	CA	198	C	C1'-N1	5.01	1.55	1.48
36	DH	31	VAL	CA-C	5.01	1.57	1.52
1	BA	737	C	C1'-N1	5.01	1.55	1.48
20	BT	5	LYS	CA-C	5.00	1.59	1.52
51	DX	82	ILE	CG1-CD1	-5.00	1.32	1.51

All (334) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	BE	50	TYR	CA-C-O	-10.54	113.12	119.55
54	DI	132	TYR	CA-C-N	9.87	139.46	121.70
54	DI	132	TYR	C-N-CA	9.87	139.46	121.70
34	DF	10	ASP	CA-CB-CG	9.17	121.77	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DI	106	PHE	CA-CB-CG	8.37	122.17	113.80
46	CS	51	VAL	N-CA-C	-7.70	102.88	109.19
41	CN	106	ASP	CA-CB-CG	7.66	120.26	112.60
41	DN	106	ASP	CA-CB-CG	7.54	120.14	112.60
29	DC	260	ASN	CA-C-N	7.52	130.35	120.28
29	DC	260	ASN	C-N-CA	7.52	130.35	120.28
41	CN	69	PRO	CA-C-N	7.30	135.49	121.54
41	CN	69	PRO	C-N-CA	7.30	135.49	121.54
34	DF	107	ALA	CA-C-N	7.26	124.82	120.24
34	DF	107	ALA	C-N-CA	7.26	124.82	120.24
34	CF	107	ALA	CA-C-N	7.21	124.78	120.24
34	CF	107	ALA	C-N-CA	7.21	124.78	120.24
17	BQ	51	ASN	CA-CB-CG	7.18	119.78	112.60
20	BT	6	SER	N-CA-C	-7.08	104.67	113.38
27	D0	10	THR	N-CA-CB	-7.07	101.50	110.90
40	CM	68	SER	CA-C-N	7.00	134.92	121.54
40	CM	68	SER	C-N-CA	7.00	134.92	121.54
20	BT	43	ASP	CA-CB-CG	6.97	119.57	112.60
5	AE	55	GLU	CA-C-N	6.89	127.05	120.43
5	AE	55	GLU	C-N-CA	6.89	127.05	120.43
23	D2	5	ILE	N-CA-C	-6.86	105.84	112.29
40	CM	15	ALA	N-CA-C	6.75	118.64	111.28
34	CF	21	ASN	CA-CB-CG	6.71	119.31	112.60
43	DP	78	VAL	N-CA-CB	6.71	118.40	110.55
38	CK	80	HIS	CA-C-N	6.68	134.00	121.97
38	CK	80	HIS	C-N-CA	6.68	134.00	121.97
43	CP	78	VAL	N-CA-CB	6.68	118.36	110.55
4	AD	131	ASN	CA-CB-CG	6.63	119.23	112.60
13	AM	54	ASP	CA-CB-CG	6.61	119.20	112.60
40	CM	68	SER	N-CA-C	6.60	119.07	111.02
6	BF	79	ARG	CA-C-N	6.56	129.07	120.28
6	BF	79	ARG	C-N-CA	6.56	129.07	120.28
35	CG	175	LYS	CA-C-N	6.55	134.06	121.54
35	CG	175	LYS	C-N-CA	6.55	134.06	121.54
47	DT	65	ASP	CA-CB-CG	6.55	119.15	112.60
55	DA	271	G	C2'-C3'-O3'	6.54	119.31	109.50
2	BB	126	PHE	CA-CB-CG	6.52	120.32	113.80
36	CH	8	LYS	CA-C-N	6.51	133.69	121.97
36	CH	8	LYS	C-N-CA	6.51	133.69	121.97
34	CF	134	GLU	CB-CG-CD	6.51	123.67	112.60
6	AF	55	HIS	N-CA-C	-6.50	98.38	109.24
2	AB	126	PHE	CA-CB-CG	6.49	120.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	BJ	37	ARG	CA-C-N	6.48	132.04	121.87
10	BJ	37	ARG	C-N-CA	6.48	132.04	121.87
10	AJ	76	ILE	CA-C-N	6.46	128.83	120.56
10	AJ	76	ILE	C-N-CA	6.46	128.83	120.56
5	BE	55	GLU	CA-C-N	6.44	126.61	120.43
5	BE	55	GLU	C-N-CA	6.44	126.61	120.43
3	BC	61	ALA	CA-C-N	6.43	131.26	122.19
3	BC	61	ALA	C-N-CA	6.43	131.26	122.19
6	BF	55	HIS	N-CA-C	-6.42	98.52	109.24
13	AM	96	PRO	CA-C-N	6.38	128.72	120.56
13	AM	96	PRO	C-N-CA	6.38	128.72	120.56
18	AR	34	THR	CA-C-N	6.36	128.80	120.28
18	AR	34	THR	C-N-CA	6.36	128.80	120.28
3	BC	178	LEU	CA-C-N	6.34	129.41	120.28
3	BC	178	LEU	C-N-CA	6.34	129.41	120.28
40	DM	22	GLY	N-CA-C	6.31	119.36	112.29
13	BM	96	PRO	CA-C-N	6.26	128.58	120.56
13	BM	96	PRO	C-N-CA	6.26	128.58	120.56
34	CF	46	ASP	CA-CB-CG	6.23	118.83	112.60
46	DS	38	VAL	N-CA-CB	6.22	118.46	110.99
48	DU	74	ILE	CA-C-N	6.17	125.84	121.65
48	DU	74	ILE	C-N-CA	6.17	125.84	121.65
3	AC	178	LEU	CA-C-N	6.16	129.14	120.28
3	AC	178	LEU	C-N-CA	6.16	129.14	120.28
34	DF	46	ASP	CA-CB-CG	6.14	118.74	112.60
6	BF	92	THR	CA-C-N	6.11	131.06	122.08
6	BF	92	THR	C-N-CA	6.11	131.06	122.08
45	CR	91	ASP	CA-CB-CG	6.11	118.71	112.60
4	AD	99	ASP	CA-CB-CG	6.09	118.69	112.60
33	CE	82	GLY	CA-C-N	6.08	132.92	121.97
33	CE	82	GLY	C-N-CA	6.08	132.92	121.97
49	DV	53	ASN	CA-C-N	6.07	128.91	120.65
49	DV	53	ASN	C-N-CA	6.07	128.91	120.65
4	BD	99	ASP	CA-CB-CG	6.04	118.64	112.60
54	DI	7	ASP	CA-CB-CG	6.02	118.62	112.60
43	DP	19	GLN	CA-C-N	6.00	128.32	120.28
43	DP	19	GLN	C-N-CA	6.00	128.32	120.28
27	D0	40	ASP	CA-CB-CG	5.99	118.59	112.60
49	DV	74	ASN	CA-C-N	5.99	128.59	120.38
49	DV	74	ASN	C-N-CA	5.99	128.59	120.38
20	BT	6	SER	CA-C-N	5.97	129.39	120.31
20	BT	6	SER	C-N-CA	5.97	129.39	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AQ	48	ASP	CA-CB-CG	5.97	118.57	112.60
46	CS	50	GLY	CA-C-N	5.96	130.08	121.68
46	CS	50	GLY	C-N-CA	5.96	130.08	121.68
6	AF	79	ARG	CA-C-N	5.94	128.24	120.28
6	AF	79	ARG	C-N-CA	5.94	128.24	120.28
12	AL	38	TYR	N-CA-C	5.94	115.93	108.45
29	DC	70	ASN	CA-CB-CG	5.92	118.52	112.60
45	CR	12	ALA	CA-C-N	5.91	128.19	120.28
45	CR	12	ALA	C-N-CA	5.91	128.19	120.28
13	BM	11	ASP	CA-C-N	5.91	130.96	122.40
13	BM	11	ASP	C-N-CA	5.91	130.96	122.40
54	DI	20	LYS	CA-C-N	5.90	126.49	119.94
54	DI	20	LYS	C-N-CA	5.90	126.49	119.94
27	C0	40	ASP	CA-CB-CG	5.90	118.50	112.60
37	CJ	22	PRO	N-CA-C	5.87	117.87	110.70
38	DK	9	GLU	CB-CG-CD	5.86	122.55	112.60
37	DJ	22	PRO	N-CA-C	5.84	117.83	110.70
40	CM	67	THR	CA-C-N	5.84	128.90	120.79
40	CM	67	THR	C-N-CA	5.84	128.90	120.79
26	C5	19	ARG	CA-C-N	5.83	132.68	121.54
26	C5	19	ARG	C-N-CA	5.83	132.68	121.54
11	BK	71	ALA	N-CA-C	-5.80	104.56	111.69
12	AL	42	PRO	CA-C-N	5.77	131.22	120.95
12	AL	42	PRO	C-N-CA	5.77	131.22	120.95
7	BG	18	PHE	CA-CB-CG	5.77	119.57	113.80
43	CP	19	GLN	CA-C-N	5.76	128.00	120.28
43	CP	19	GLN	C-N-CA	5.76	128.00	120.28
13	BM	86	TYR	CA-C-N	5.72	127.94	120.28
13	BM	86	TYR	C-N-CA	5.72	127.94	120.28
39	CL	121	GLU	CA-C-N	5.71	131.99	121.70
39	CL	121	GLU	C-N-CA	5.71	131.99	121.70
45	DR	91	ASP	CA-CB-CG	5.70	118.30	112.60
12	BL	38	TYR	N-CA-C	5.70	115.63	108.45
13	AM	86	TYR	CA-C-N	5.68	127.89	120.28
13	AM	86	TYR	C-N-CA	5.68	127.89	120.28
16	BP	23	ASP	CA-CB-CG	5.67	118.27	112.60
29	CC	157	SER	CA-C-N	5.63	132.30	121.54
29	CC	157	SER	C-N-CA	5.63	132.30	121.54
29	CC	195	VAL	N-CA-CB	5.63	116.67	110.53
40	CM	30	THR	N-CA-CB	5.63	120.01	110.49
15	AO	88	ARG	N-CA-C	-5.62	100.13	109.46
29	CC	204	VAL	N-CA-CB	5.62	120.30	111.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	AP	23	ASP	CA-CB-CG	5.61	118.21	112.60
9	BI	99	ARG	CA-C-N	5.60	128.05	120.38
9	BI	99	ARG	C-N-CA	5.60	128.05	120.38
49	DV	29	LEU	CA-C-N	5.60	128.55	120.38
49	DV	29	LEU	C-N-CA	5.60	128.55	120.38
16	BP	19	VAL	N-CA-CB	5.59	117.22	110.95
16	AP	47	GLU	CA-C-N	5.59	132.21	121.54
16	AP	47	GLU	C-N-CA	5.59	132.21	121.54
52	CY	17	ASN	CA-CB-CG	5.59	118.19	112.60
31	CA	271	G	C2'-C3'-O3'	5.59	117.88	109.50
41	CN	69	PRO	CA-C-O	-5.59	110.43	120.60
33	CE	83	VAL	CA-C-N	5.58	128.03	120.44
33	CE	83	VAL	C-N-CA	5.58	128.03	120.44
8	BH	109	GLY	N-CA-C	5.57	117.70	112.08
2	BB	204	ASP	CA-CB-CG	5.56	118.16	112.60
49	CV	53	ASN	CA-C-N	5.56	127.04	120.09
49	CV	53	ASN	C-N-CA	5.56	127.04	120.09
36	DH	26	ALA	CA-C-N	5.55	127.66	120.44
36	DH	26	ALA	C-N-CA	5.55	127.66	120.44
4	AD	39	GLY	CA-C-N	5.55	127.65	120.44
4	AD	39	GLY	C-N-CA	5.55	127.65	120.44
29	CC	13	ARG	N-CA-C	-5.55	106.64	113.41
2	AB	204	ASP	CA-CB-CG	5.54	118.14	112.60
6	BF	98	GLU	CA-C-N	5.54	132.13	121.54
6	BF	98	GLU	C-N-CA	5.54	132.13	121.54
29	DC	45	ASN	CA-CB-CG	5.54	118.14	112.60
37	CJ	118	THR	CA-C-N	5.54	125.36	120.10
37	CJ	118	THR	C-N-CA	5.54	125.36	120.10
37	DJ	118	THR	CA-C-N	5.54	125.36	120.10
37	DJ	118	THR	C-N-CA	5.54	125.36	120.10
8	AH	109	GLY	N-CA-C	5.53	117.68	112.04
45	DR	7	GLY	CA-C-N	5.53	127.61	120.70
45	DR	7	GLY	C-N-CA	5.53	127.61	120.70
48	DU	92	ASN	CA-C-N	5.52	131.64	121.70
48	DU	92	ASN	C-N-CA	5.52	131.64	121.70
4	BD	131	ASN	CA-CB-CG	5.52	118.12	112.60
18	BR	34	THR	CA-C-N	5.50	127.66	120.28
18	BR	34	THR	C-N-CA	5.50	127.66	120.28
31	CA	2095	A	C5'-C4'-C3'	-5.50	107.75	116.00
32	DD	32	ASN	CA-CB-CG	5.50	118.09	112.60
11	BK	118	HIS	CA-C-N	5.49	132.02	121.54
11	BK	118	HIS	C-N-CA	5.49	132.02	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AF	80	PHE	CA-CB-CG	5.47	119.27	113.80
38	CK	89	PHE	CA-C-N	5.47	127.87	120.38
38	CK	89	PHE	C-N-CA	5.47	127.87	120.38
7	AG	151	PHE	CA-CB-CG	5.46	119.26	113.80
34	DF	146	VAL	N-CA-CB	5.46	116.89	110.82
1	AA	413	G	C1'-O4'-C4'	-5.46	104.24	109.70
11	AK	120	GLY	N-CA-C	5.46	115.18	110.21
29	CC	252	THR	N-CA-C	-5.45	103.49	110.53
4	BD	25	VAL	N-CA-C	-5.45	105.19	110.42
35	DG	80	THR	CA-C-N	5.43	127.50	120.44
35	DG	80	THR	C-N-CA	5.43	127.50	120.44
2	AB	124	GLY	CA-C-N	5.42	131.90	121.54
2	AB	124	GLY	C-N-CA	5.42	131.90	121.54
7	AG	62	PHE	CA-C-N	5.42	127.54	120.28
7	AG	62	PHE	C-N-CA	5.42	127.54	120.28
31	CA	974	G	N9-C1'-C2'	5.42	122.12	114.00
33	CE	171	ASP	CA-CB-CG	5.42	118.02	112.60
32	DD	108	ASP	CA-CB-CG	5.41	118.00	112.60
4	BD	39	GLY	CA-C-N	5.40	127.47	120.44
4	BD	39	GLY	C-N-CA	5.40	127.47	120.44
2	BB	124	GLY	CA-C-N	5.40	131.86	121.54
2	BB	124	GLY	C-N-CA	5.40	131.86	121.54
30	CD	108	ASP	CA-CB-CG	5.40	118.00	112.60
20	AT	23	SER	CA-C-N	5.39	127.50	120.28
20	AT	23	SER	C-N-CA	5.39	127.50	120.28
9	AI	99	ARG	CA-C-N	5.38	127.75	120.38
9	AI	99	ARG	C-N-CA	5.38	127.75	120.38
43	CP	17	LYS	CA-C-N	5.38	127.48	120.28
43	CP	17	LYS	C-N-CA	5.38	127.48	120.28
48	CU	74	ILE	CA-C-N	5.37	125.30	121.65
48	CU	74	ILE	C-N-CA	5.37	125.30	121.65
42	DO	76	VAL	N-CA-CB	5.37	118.64	110.58
11	AK	118	HIS	CA-C-N	5.37	131.79	121.54
11	AK	118	HIS	C-N-CA	5.37	131.79	121.54
33	CE	7	ASP	CA-CB-CG	5.36	117.96	112.60
6	BF	90	MET	CA-C-N	5.36	131.78	121.54
6	BF	90	MET	C-N-CA	5.36	131.78	121.54
14	BN	84	VAL	N-CA-C	-5.34	105.51	110.53
35	CG	69	ARG	CA-C-N	5.34	127.70	120.38
35	CG	69	ARG	C-N-CA	5.34	127.70	120.38
38	DK	71	ASP	CA-CB-CG	5.34	117.94	112.60
13	AM	14	HIS	CA-C-N	5.34	128.83	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	AM	14	HIS	C-N-CA	5.34	128.83	120.82
43	CP	93	ASP	CA-CB-CG	5.34	117.94	112.60
5	AE	62	LYS	CA-C-N	5.33	127.37	120.44
5	AE	62	LYS	C-N-CA	5.33	127.37	120.44
12	AL	64	THR	CB-CA-C	5.32	118.53	109.75
13	BM	14	HIS	CA-C-N	5.32	128.80	120.82
13	BM	14	HIS	C-N-CA	5.32	128.80	120.82
48	CU	79	ASP	CA-CB-CG	5.32	117.92	112.60
17	BQ	48	ASP	CA-CB-CG	5.32	117.92	112.60
4	AD	107	PHE	CA-C-N	5.31	125.26	121.65
4	AD	107	PHE	C-N-CA	5.31	125.26	121.65
7	BG	62	PHE	CA-C-N	5.31	127.40	120.28
7	BG	62	PHE	C-N-CA	5.31	127.40	120.28
33	DE	64	GLY	N-CA-C	5.31	122.17	115.42
17	BQ	57	ASP	CA-CB-CG	5.31	117.91	112.60
42	DO	99	LYS	CA-C-N	-5.30	117.46	123.13
42	DO	99	LYS	C-N-CA	-5.30	117.46	123.13
7	AG	18	PHE	CA-CB-CG	5.30	119.10	113.80
5	BE	51	GLY	CA-C-N	5.29	131.02	122.29
5	BE	51	GLY	C-N-CA	5.29	131.02	122.29
13	AM	12	HIS	CA-C-N	5.29	132.00	122.64
13	AM	12	HIS	C-N-CA	5.29	132.00	122.64
16	BP	42	ILE	N-CA-C	-5.29	107.20	111.91
54	DI	134	GLU	N-CA-C	-5.29	108.59	114.62
52	DY	17	ASN	CA-CB-CG	5.28	117.88	112.60
46	CS	53	PHE	CA-C-N	5.26	127.55	120.50
46	CS	53	PHE	C-N-CA	5.26	127.55	120.50
41	CN	111	GLU	CB-CG-CD	5.26	121.54	112.60
16	BP	42	ILE	CA-C-N	5.25	129.53	121.19
16	BP	42	ILE	C-N-CA	5.25	129.53	121.19
33	DE	198	GLU	CA-C-N	5.25	127.26	120.44
33	DE	198	GLU	C-N-CA	5.25	127.26	120.44
14	AN	84	VAL	N-CA-C	-5.24	105.60	110.53
29	CC	208	ALA	CA-C-N	5.24	125.89	120.03
29	CC	208	ALA	C-N-CA	5.24	125.89	120.03
33	DE	122	GLU	CB-CG-CD	5.23	121.50	112.60
49	DV	53	ASN	N-CA-C	-5.23	106.48	112.86
5	AE	50	TYR	CA-C-N	-5.22	118.10	121.65
5	AE	50	TYR	C-N-CA	-5.22	118.10	121.65
12	BL	64	THR	CB-CA-C	5.22	118.37	109.75
31	CA	2326	C	C4'-C3'-O3'	5.22	117.23	109.40
29	DC	264	ASP	CA-CB-CG	5.22	117.82	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	CX	44	LYS	N-CA-C	-5.21	105.60	111.28
5	AE	137	VAL	N-CA-CB	5.21	117.63	110.54
4	BD	107	PHE	CA-C-N	5.21	125.19	121.65
4	BD	107	PHE	C-N-CA	5.21	125.19	121.65
34	CF	146	VAL	N-CA-CB	5.21	116.60	110.82
5	BE	41	ASP	CA-CB-CG	5.21	117.81	112.60
21	AU	33	ARG	CA-C-N	5.21	127.26	120.28
21	AU	33	ARG	C-N-CA	5.21	127.26	120.28
1	BA	1362	A	C1'-O4'-C4'	-5.21	104.49	109.70
43	DP	93	ASP	CA-CB-CG	5.20	117.80	112.60
49	DV	51	ALA	CA-C-N	5.19	131.45	121.54
49	DV	51	ALA	C-N-CA	5.19	131.45	121.54
21	BU	45	ARG	CA-C-N	5.18	127.48	120.44
21	BU	45	ARG	C-N-CA	5.18	127.48	120.44
44	DQ	3	ASN	N-CA-C	-5.18	106.11	112.90
49	DV	28	VAL	N-CA-CB	5.18	118.29	111.25
55	DA	784	G	P-O3'-C3'	5.18	127.96	120.20
21	AU	45	ARG	CA-C-N	5.17	127.48	120.44
21	AU	45	ARG	C-N-CA	5.17	127.48	120.44
33	CE	198	GLU	CA-C-N	5.17	127.16	120.44
33	CE	198	GLU	C-N-CA	5.17	127.16	120.44
38	DK	33	ALA	CA-C-N	5.17	127.16	120.44
38	DK	33	ALA	C-N-CA	5.17	127.16	120.44
13	BM	6	GLY	CA-C-N	5.16	131.26	121.97
13	BM	6	GLY	C-N-CA	5.16	131.26	121.97
2	AB	93	ASN	CA-CB-CG	5.16	117.76	112.60
10	BJ	58	ASN	CA-C-N	5.16	127.61	120.29
10	BJ	58	ASN	C-N-CA	5.16	127.61	120.29
29	CC	239	ASN	CA-CB-CG	5.15	117.75	112.60
20	BT	84	ASN	CA-CB-CG	5.14	117.74	112.60
52	CY	70	GLU	CA-C-N	5.14	127.17	120.28
52	CY	70	GLU	C-N-CA	5.14	127.17	120.28
24	D3	44	VAL	N-CA-CB	5.13	116.85	111.00
1	BA	842	U	C2'-C3'-O3'	5.13	117.19	109.50
42	CO	76	VAL	N-CA-CB	5.12	118.27	110.58
6	BF	80	PHE	CA-CB-CG	5.12	118.92	113.80
33	CE	113	VAL	CA-C-N	5.12	127.39	120.38
33	CE	113	VAL	C-N-CA	5.12	127.39	120.38
34	DF	5	HIS	N-CA-C	-5.12	105.78	111.36
34	DF	167	ARG	CA-C-N	5.12	127.14	120.28
34	DF	167	ARG	C-N-CA	5.12	127.14	120.28
28	CB	15	A	O4'-C1'-N9	5.11	115.86	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AQ	57	ASP	CA-CB-CG	5.11	117.71	112.60
17	BQ	22	VAL	N-CA-CB	5.10	117.17	111.21
49	CV	29	LEU	CA-C-N	5.10	127.82	120.38
49	CV	29	LEU	C-N-CA	5.10	127.82	120.38
29	DC	252	THR	N-CA-C	-5.10	103.32	110.35
33	DE	113	VAL	CA-C-N	5.09	127.36	120.38
33	DE	113	VAL	C-N-CA	5.09	127.36	120.38
3	BC	26	THR	CA-C-N	5.09	127.37	120.65
3	BC	26	THR	C-N-CA	5.09	127.37	120.65
52	DY	60	ASP	CA-CB-CG	5.09	117.69	112.60
34	CF	147	ASP	CA-CB-CG	5.09	117.69	112.60
4	AD	25	VAL	N-CA-C	-5.08	105.54	110.42
34	DF	146	VAL	CA-C-N	5.08	127.05	120.44
34	DF	146	VAL	C-N-CA	5.08	127.05	120.44
20	AT	22	ALA	CA-C-N	5.08	127.36	120.65
20	AT	22	ALA	C-N-CA	5.08	127.36	120.65
2	BB	93	ASN	CA-CB-CG	5.08	117.68	112.60
22	D1	26	THR	CB-CA-C	5.07	117.90	109.38
34	CF	5	HIS	N-CA-C	-5.06	105.84	111.36
48	DU	79	ASP	CA-CB-CG	5.05	117.65	112.60
40	CM	91	ASP	CA-CB-CG	5.05	117.65	112.60
31	CA	271	G	P-O3'-C3'	5.04	127.76	120.20
5	AE	123	VAL	N-CA-C	5.04	115.62	108.42
34	DF	59	ALA	CA-C-N	5.03	126.90	120.56
34	DF	59	ALA	C-N-CA	5.03	126.90	120.56
16	AP	42	ILE	N-CA-C	-5.03	107.44	111.91
18	AR	25	ASP	CA-CB-CG	5.03	117.63	112.60
35	CG	80	THR	CA-C-N	5.02	126.97	120.44
35	CG	80	THR	C-N-CA	5.02	126.97	120.44
32	DD	127	PHE	CA-CB-CG	5.02	118.82	113.80
41	CN	13	HIS	CA-CB-CG	5.01	118.81	113.80
50	DW	8	VAL	N-CA-CB	5.01	117.12	110.26
38	DK	89	PHE	CA-C-N	5.00	127.24	120.38
38	DK	89	PHE	C-N-CA	5.00	127.24	120.38
47	CT	64	ALA	CA-C-N	5.00	131.09	121.54
47	CT	64	ALA	C-N-CA	5.00	131.09	121.54

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
41	CN	69	PRO	Mainchain

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Mol	Chain	Res	Type	Group
55	DA	1324	G	Sidechain
55	DA	1425	G	Sidechain
55	DA	15	G	Sidechain
55	DA	1753	G	Sidechain
55	DA	177	G	Sidechain
55	DA	1938	A	Sidechain
55	DA	1954	G	Sidechain
55	DA	2048	G	Sidechain
55	DA	221	A	Sidechain
55	DA	2250	G	Sidechain
55	DA	2323	G	Sidechain
55	DA	2375	G	Sidechain
55	DA	2481	G	Sidechain
55	DA	249	C	Sidechain
55	DA	250	G	Sidechain
55	DA	2595	G	Sidechain
55	DA	2597	G	Sidechain
55	DA	2645	G	Sidechain
55	DA	2835	A	Sidechain
55	DA	2848	G	Sidechain
55	DA	512	G	Sidechain
55	DA	555	G	Sidechain
55	DA	726	G	Sidechain
55	DA	858	G	Sidechain
55	DA	956	G	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32933	0	16593	79	0
1	BA	32911	0	16582	95	0
2	AB	1753	0	1780	8	0
2	BB	1753	0	1780	9	0
3	AC	1625	0	1696	12	0
3	BC	1625	0	1696	13	0
4	AD	1643	0	1707	11	0
4	BD	1643	0	1707	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AE	1144	0	1185	10	0
5	BE	1105	0	1148	19	0
6	AF	862	0	864	7	0
6	BF	817	0	808	7	0
7	AG	1182	0	1238	5	0
7	BG	1182	0	1238	3	0
8	AH	979	0	1031	11	0
8	BH	979	0	1031	9	0
9	AI	1022	0	1070	10	0
9	BI	1022	0	1070	11	0
10	AJ	796	0	836	10	0
10	BJ	787	0	828	8	0
11	AK	877	0	887	11	0
11	BK	877	0	887	14	0
12	AL	957	0	1017	6	0
12	BL	957	0	1017	8	0
13	AM	884	0	941	11	0
13	BM	884	0	941	16	0
14	AN	805	0	844	7	0
14	BN	805	0	844	6	0
15	AO	714	0	734	0	0
15	BO	714	0	734	1	0
16	AP	649	0	666	6	0
16	BP	649	0	666	6	0
17	AQ	649	0	691	4	0
17	BQ	649	0	691	11	0
18	AR	456	0	478	3	0
18	BR	456	0	478	3	0
19	AS	638	0	665	4	0
19	BS	638	0	665	6	0
20	AT	670	0	719	1	0
20	BT	665	0	714	7	0
21	AU	465	0	491	3	0
21	BU	465	0	491	3	0
22	C1	444	0	458	4	0
22	D1	444	0	458	10	0
23	C2	409	0	440	7	0
23	D2	414	0	442	5	0
24	C3	377	0	418	4	0
24	D3	377	0	418	2	0
25	C4	504	0	572	2	0
25	D4	504	0	572	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	C5	302	0	340	9	0
26	D5	302	0	340	3	0
27	C0	449	0	488	3	0
27	D0	463	0	504	0	0
28	CB	2529	0	1281	7	0
28	DB	2569	0	1301	2	0
29	CC	2082	0	2154	20	0
29	DC	2082	0	2154	11	0
30	CD	1565	0	1616	12	0
31	CA	62229	0	31319	203	0
32	DD	1576	0	1627	11	0
33	CE	1552	0	1619	15	0
33	DE	1551	0	1619	10	0
34	CF	1410	0	1444	19	0
34	DF	1410	0	1444	14	0
35	CG	1323	0	1371	7	0
35	DG	1323	0	1371	6	0
36	CH	1110	0	1148	10	0
36	DH	1110	0	1148	7	0
37	CJ	979	0	1028	7	0
37	DJ	979	0	1028	5	0
38	CK	1129	0	1162	6	0
38	DK	1129	0	1162	5	0
39	CL	938	0	1012	9	0
39	DL	946	0	1023	10	0
40	CM	1053	0	1129	16	0
40	DM	1053	0	1129	7	0
41	CN	1075	0	1154	8	0
41	DN	1092	0	1177	8	0
42	CO	960	0	1000	7	0
42	DO	993	0	1034	6	0
43	CP	892	0	923	6	0
43	DP	900	0	935	6	0
44	CQ	917	0	962	4	0
44	DQ	917	0	962	7	0
45	CR	947	0	1019	11	0
45	DR	947	0	1019	13	0
46	CS	816	0	839	8	0
46	DS	816	0	839	4	0
47	CT	857	0	922	12	0
47	DT	857	0	922	10	0
48	CU	739	0	807	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	DU	738	0	807	4	0
49	CV	779	0	831	6	0
49	DV	779	0	831	6	0
50	CW	753	0	780	7	0
50	DW	753	0	780	7	0
51	CX	569	0	581	4	0
51	DX	591	0	606	4	0
52	CY	625	0	652	4	0
52	DY	625	0	652	4	0
53	CZ	501	0	531	1	0
53	DZ	501	0	531	2	0
54	DI	1023	0	1052	20	0
55	DA	62423	0	31412	163	0
56	AA	72	0	0	0	0
56	BA	45	0	0	0	0
56	CA	156	0	0	0	0
56	CB	3	0	0	0	0
56	DA	184	0	0	0	0
56	DB	9	0	0	0	0
56	DD	1	0	0	0	0
56	DM	1	0	0	0	0
56	DR	1	0	0	0	0
57	AA	13	0	18	1	0
57	BA	13	0	18	1	0
57	DA	26	0	36	0	0
57	DQ	13	0	18	0	0
57	DR	13	0	18	4	0
57	DS	13	0	18	1	0
58	AA	16	0	28	0	0
58	DA	40	0	70	2	0
58	DE	16	0	28	0	0
58	DK	8	0	14	0	0
58	DN	8	0	14	1	0
58	DS	8	0	14	0	0
58	DT	16	0	28	0	0
59	AA	24	0	48	0	0
59	DA	72	0	144	3	0
60	AA	42	0	39	2	0
60	BA	42	0	38	0	0
61	AB	1	0	0	0	0
61	C5	1	0	0	0	0
61	D5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	AL	7	0	10	0	0
62	D1	7	0	10	1	0
62	D3	7	0	10	0	0
62	DA	35	0	50	0	0
62	DL	7	0	10	0	0
62	DP	7	0	10	0	0
62	DQ	7	0	10	0	0
63	D1	4	0	6	0	0
63	DA	28	0	42	1	0
63	DB	16	0	24	0	0
64	D1	10	0	14	2	0
64	D3	10	0	14	0	0
64	DA	50	0	70	5	0
64	DS	10	0	14	1	0
64	DU	10	0	14	1	0
65	DA	40	0	76	2	0
66	DA	32	0	44	3	0
67	DA	12	0	9	0	0
68	DA	11	0	5	0	0
69	DA	8	0	12	1	0
70	AA	500	0	0	0	0
70	AC	5	0	0	0	0
70	AD	2	0	0	0	0
70	AE	4	0	0	0	0
70	AF	1	0	0	0	0
70	AG	1	0	0	0	0
70	AH	1	0	0	0	0
70	AJ	2	0	0	0	0
70	AK	6	0	0	0	0
70	AL	10	0	0	0	0
70	AM	4	0	0	1	0
70	AN	7	0	0	1	0
70	AO	2	0	0	0	0
70	AP	2	0	0	0	0
70	AR	1	0	0	0	0
70	AT	3	0	0	0	0
70	AU	2	0	0	0	0
70	BA	288	0	0	1	0
70	BD	12	0	0	0	0
70	BE	1	0	0	0	0
70	BF	2	0	0	0	0
70	BK	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	BL	2	0	0	0	0
70	BN	2	0	0	0	0
70	BO	1	0	0	0	0
70	BP	3	0	0	0	0
70	BT	4	0	0	0	0
70	BU	1	0	0	0	0
70	C3	3	0	0	0	0
70	C4	1	0	0	0	0
70	CA	692	0	0	2	0
70	CB	13	0	0	0	0
70	CC	12	0	0	0	0
70	CD	6	0	0	0	0
70	CE	4	0	0	0	0
70	CL	1	0	0	0	0
70	CM	4	0	0	0	0
70	CO	1	0	0	0	0
70	CU	3	0	0	0	0
70	CV	1	0	0	0	0
70	CW	1	0	0	0	0
70	CY	1	0	0	0	0
70	D0	21	0	0	0	0
70	D1	45	0	0	0	0
70	D2	7	0	0	0	0
70	D3	23	0	0	0	0
70	D4	39	0	0	0	0
70	D5	12	0	0	0	0
70	DA	4829	0	0	13	0
70	DB	213	0	0	0	0
70	DC	104	0	0	0	0
70	DD	92	0	0	2	0
70	DE	60	0	0	2	0
70	DF	15	0	0	0	0
70	DG	6	0	0	0	0
70	DH	2	0	0	0	0
70	DK	64	0	0	2	0
70	DL	51	0	0	0	0
70	DM	64	0	0	0	0
70	DN	73	0	0	0	0
70	DO	46	0	0	0	0
70	DP	40	0	0	0	0
70	DQ	32	0	0	0	0
70	DR	63	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	DS	44	0	0	0	0
70	DT	69	0	0	1	0
70	DU	21	0	0	0	0
70	DV	20	0	0	0	0
70	DW	31	0	0	0	0
70	DX	26	0	0	0	0
70	DY	11	0	0	0	0
70	DZ	7	0	0	1	0
All	All	295207	0	194493	1142	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 2.

All (1142) 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)
46:CS:14:VAL:HG21	46:CS:98:ILE:HG13	1.26	1.10
31:CA:1936:A:H2	31:CA:1943:U:H3	1.01	0.98
2:BB:20:THR:HA	2:BB:39:HIS:CE1	1.98	0.97
1:BA:1052:G:H22	1:BA:1206:G:H1	0.98	0.94
55:DA:2796:U:H3	55:DA:2799:A:H61	1.20	0.88
46:CS:14:VAL:CG2	46:CS:98:ILE:HG13	2.05	0.87
14:AN:66:GLN:HB2	70:AN:207:HOH:O	1.74	0.87
31:CA:1005:C:O2'	38:CK:30:THR:HG21	1.73	0.87
46:CS:14:VAL:HG21	46:CS:98:ILE:CG1	2.05	0.86
1:BA:1052:G:N2	1:BA:1206:G:H1	1.75	0.85
31:CA:2796:U:H3	31:CA:2799:A:H61	1.23	0.85
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.60	0.84
40:CM:77:ILE:HD11	40:CM:108:ALA:HB1	1.60	0.84
31:CA:528:A:C2	31:CA:2043:C:H4'	2.13	0.83
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.61	0.82
1:BA:664:G:H22	1:BA:741:G:H1	1.28	0.81
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.64	0.80
11:BK:88:GLY:H	11:BK:114:THR:HG22	1.46	0.80
55:DA:135:U:H3	55:DA:144:A:H61	1.30	0.80
13:BM:6:GLY:HA3	13:BM:66:GLU:HG3	1.62	0.80
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.63	0.80
1:AA:73:C:HO2'	1:AA:74:A:H8	1.28	0.79
31:CA:135:U:H3	31:CA:144:A:H61	1.30	0.79
1:AA:1492:A:H5''	12:AL:44:LYS:HG2	1.65	0.78
1:AA:664:G:H22	1:AA:741:G:H1	1.29	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:CM:82:LEU:HD11	40:CM:116:VAL:HG23	1.64	0.78
1:AA:1305:G:H21	1:AA:1332:A:H2	1.30	0.78
13:BM:114:LYS:HB3	13:BM:115:PRO:HD3	1.65	0.78
12:BL:80:ILE:HD12	12:BL:97:THR:HG22	1.66	0.78
1:BA:1305:G:H21	1:BA:1332:A:H2	1.30	0.76
1:BA:841:C:H3'	1:BA:842:U:H5''	1.66	0.76
3:BC:123:GLN:HB3	3:BC:128:VAL:HG21	1.69	0.75
31:CA:740:C:H5'	31:CA:1784:A:H3'	1.68	0.74
35:CG:80:THR:HG23	35:CG:81:GLU:H	1.52	0.74
1:BA:9:G:H5'	5:BE:108:GLY:HA3	1.70	0.73
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.70	0.73
10:AJ:7:ARG:HB3	10:AJ:101:SER:HB2	1.71	0.73
31:CA:846:U:H1'	31:CA:847:U:H5	1.52	0.73
45:DR:20:GLN:HG3	57:DR:202:PG4:H42	1.70	0.73
4:AD:107:PHE:HB3	4:AD:145:ILE:HD11	1.70	0.72
45:DR:20:GLN:CG	57:DR:202:PG4:H42	2.20	0.72
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.71	0.72
4:BD:107:PHE:HB3	4:BD:145:ILE:HD11	1.70	0.72
30:CD:133:THR:HG22	31:CA:1993:U:H4'	1.70	0.72
35:CG:24:ILE:HD11	35:CG:43:VAL:HG11	1.72	0.72
55:DA:2127:G:H4'	55:DA:2128:G:OP1	1.90	0.71
31:CA:1936:A:H2	31:CA:1943:U:N3	1.83	0.71
8:BH:87:LYS:HB2	8:BH:125:ILE:HD11	1.73	0.71
31:CA:1779:U:H5	31:CA:1784:A:N7	1.89	0.70
6:BF:38:ARG:HH12	6:BF:99:ALA:HB3	1.55	0.70
1:BA:522:C:H5	12:BL:50:ARG:HH12	1.37	0.70
13:AM:33:ILE:HD11	13:AM:63:PHE:HE1	1.57	0.69
1:BA:841:C:H3'	1:BA:842:U:C5'	2.22	0.69
2:BB:20:THR:HA	2:BB:39:HIS:HE1	1.55	0.69
3:BC:40:ARG:HH11	3:BC:55:ILE:HG23	1.56	0.69
47:CT:73:LYS:HB2	47:CT:106:VAL:HB	1.75	0.69
55:DA:1105:U:H2'	55:DA:1106:G:H8	1.58	0.68
55:DA:2033:A:H5'	70:DA:3343:HOH:O	1.92	0.68
48:CU:28:ASN:HD21	48:CU:91:GLN:HB3	1.58	0.68
35:DG:24:ILE:HD11	35:DG:43:VAL:HG11	1.74	0.68
13:BM:83:LEU:HD21	19:BS:65:GLU:HB2	1.74	0.68
43:DP:39:VAL:HB	43:DP:49:VAL:HG23	1.74	0.68
31:CA:1105:U:H2'	31:CA:1106:G:H8	1.58	0.68
55:DA:568:U:H1'	55:DA:2030:6MZ:H9C1	1.76	0.67
36:DH:41:LYS:HA	36:DH:44:ILE:HG12	1.76	0.67
33:CE:149:ILE:HG12	33:CE:188:MET:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:CL:38:ILE:HD11	39:CL:112:PHE:HZ	1.59	0.67
24:C3:12:ARG:HD2	24:C3:44:VAL:HG11	1.75	0.67
39:DL:113:MET:HE1	39:DL:116:ILE:HD11	1.77	0.67
11:BK:89:PRO:HG3	21:BU:32:VAL:HG11	1.77	0.67
1:BA:451:A:H2'	70:BA:1701:HOH:O	1.95	0.66
31:CA:910:A:H62	41:CN:12:MET:HA	1.60	0.66
8:AH:87:LYS:HB2	8:AH:125:ILE:HD11	1.75	0.66
1:BA:619:U:H3	4:BD:131:ASN:HB3	1.60	0.66
55:DA:1913:A:H4'	55:DA:1913:A:OP1	1.96	0.66
36:CH:41:LYS:HA	36:CH:44:ILE:HG12	1.77	0.66
12:BL:65:SER:HB2	12:BL:82:ILE:HD11	1.77	0.66
31:CA:1105:U:H2'	31:CA:1106:G:C8	2.30	0.65
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.79	0.65
31:CA:1847:A:HO2'	31:CA:1848:A:H8	1.42	0.65
55:DA:1105:U:H2'	55:DA:1106:G:C8	2.30	0.65
47:DT:73:LYS:HB2	47:DT:106:VAL:HB	1.77	0.65
55:DA:1847:A:HO2'	55:DA:1848:A:H8	1.43	0.65
20:BT:9:LYS:O	20:BT:12:ILE:HG13	1.96	0.65
31:CA:1311:G:H21	31:CA:1603:A:H62	1.43	0.65
55:DA:1853:A:N1	55:DA:2087:G:H1'	2.12	0.65
47:CT:86:MET:HB2	47:CT:96:ILE:HD11	1.77	0.65
31:CA:2291:U:H2'	31:CA:2292:U:C6	2.31	0.65
36:CH:15:LEU:HD22	36:CH:15:LEU:H	1.62	0.64
48:CU:18:GLU:H	48:CU:18:GLU:CD	2.05	0.64
31:CA:699:A:H2'	31:CA:700:G:O4'	1.96	0.64
39:DL:38:ILE:HD11	39:DL:112:PHE:HZ	1.63	0.64
5:BE:72:ILE:HG12	5:BE:145:GLU:HG3	1.81	0.63
45:DR:31:VAL:HG13	55:DA:580:U:O3'	1.99	0.63
55:DA:1746:A:H2'	55:DA:1747:U:C6	2.34	0.63
5:AE:77:ASN:HB2	5:AE:82:GLN:NE2	2.14	0.63
55:DA:2628:C:H5'	59:DA:3195:PUT:H12	1.81	0.63
2:AB:20:THR:HG22	2:AB:39:HIS:CE1	2.34	0.63
26:C5:16:ILE:HD13	26:C5:25:VAL:HG22	1.81	0.63
11:BK:23:ILE:HG22	11:BK:32:VAL:HG13	1.81	0.63
17:BQ:8:LEU:HD23	17:BQ:25:ILE:HG21	1.80	0.63
22:D1:9:THR:CG2	55:DA:2020:A:H5'	2.28	0.62
11:AK:31:ILE:HG12	11:AK:46:THR:HG22	1.79	0.62
25:D4:8:ARG:HD3	55:DA:245:G:O6	1.99	0.62
11:AK:23:ILE:HG22	11:AK:32:VAL:HG13	1.80	0.62
33:DE:33:VAL:HG22	58:DA:3192:MPD:H12	1.81	0.62
22:C1:43:ILE:HG22	22:C1:49:TYR:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2291:U:H2'	55:DA:2292:U:C6	2.34	0.62
5:BE:77:ASN:HB2	5:BE:82:GLN:NE2	2.15	0.61
55:DA:2128:G:H1	55:DA:2160:C:H42	1.48	0.61
7:AG:22:LEU:HD12	7:AG:62:PHE:HE2	1.65	0.61
22:D1:43:ILE:HG22	22:D1:49:TYR:HB2	1.82	0.61
54:DI:69:PHE:HB3	54:DI:72:LEU:HD12	1.82	0.61
1:AA:1012:A:H61	1:AA:1017:U:H3	1.48	0.61
1:BA:1012:A:H61	1:BA:1017:U:H3	1.48	0.61
1:BA:1060:U:C5	3:BC:2:GLY:HA3	2.34	0.61
2:BB:23:TRP:HB3	2:BB:39:HIS:CE1	2.35	0.61
1:BA:73:C:HO2'	1:BA:74:A:H8	1.47	0.61
1:AA:81:A:H61	1:AA:86:G:H1	1.49	0.61
23:C2:22:THR:HG21	31:CA:2419:U:H5''	1.82	0.61
34:CF:36:LEU:HD21	34:CF:91:LEU:HD11	1.81	0.61
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.83	0.61
29:DC:29:PRO:HG2	29:DC:34:LEU:HD11	1.83	0.61
32:DD:140:HIS:HB3	70:DD:481:HOH:O	2.01	0.61
6:BF:38:ARG:NH1	6:BF:99:ALA:HB3	2.15	0.60
1:AA:209:U:H4'	1:AA:210:C:OP2	2.01	0.60
29:CC:210:ALA:HA	29:CC:213:TRP:CE2	2.37	0.60
1:AA:412:A:H3'	1:AA:413:G:H5'	1.84	0.60
1:AA:774:G:H21	57:AA:1670:PG4:H51	1.67	0.60
7:BG:113:ASP:HB2	7:BG:119:ARG:HG3	1.84	0.59
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.83	0.59
16:BP:4:ILE:HG12	16:BP:21:VAL:HG22	1.84	0.59
26:D5:16:ILE:HD13	26:D5:25:VAL:HG22	1.82	0.59
29:CC:29:PRO:HG2	29:CC:34:LEU:HD11	1.83	0.59
1:AA:1144:G:H21	1:AA:1146:A:H62	1.50	0.59
1:BA:1151:A:HO2'	1:BA:1152:A:H8	1.50	0.59
25:C4:60:ALA:O	40:CM:48:ARG:HD2	2.03	0.59
40:DM:53:GLY:HA3	55:DA:826:U:O2'	2.03	0.59
44:DQ:29:LYS:HB3	44:DQ:40:LEU:HD13	1.83	0.59
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.83	0.59
1:BA:209:U:H4'	1:BA:210:C:OP2	2.02	0.59
31:CA:450:G:H2'	31:CA:451:U:H5''	1.82	0.59
46:CS:78:ARG:HB2	46:CS:83:TYR:HD1	1.66	0.59
1:BA:1144:G:H21	1:BA:1146:A:H62	1.50	0.59
1:BA:1226:C:H2'	13:BM:102:THR:HB	1.85	0.59
33:DE:189:THR:HG22	33:DE:192:ALA:H	1.68	0.59
54:DI:57:ASN:HB3	54:DI:76:PHE:HB3	1.85	0.59
1:AA:1226:C:H2'	13:AM:102:THR:HB	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1394:U:H4'	31:CA:1603:A:H4'	1.85	0.59
45:DR:28:ARG:HD3	70:DR:306:HOH:O	2.02	0.59
46:DS:83:TYR:CE1	55:DA:1187:G:H5''	2.38	0.59
1:BA:1323:G:H2'	1:BA:1324:A:C8	2.38	0.58
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.39	0.58
19:AS:15:LEU:HD13	19:AS:33:THR:HG21	1.85	0.58
11:BK:88:GLY:N	11:BK:114:THR:HG22	2.16	0.58
29:CC:227:PRO:HA	29:CC:233:GLY:HA2	1.85	0.58
17:BQ:17:MET:HB3	17:BQ:20:SER:HB3	1.85	0.58
47:CT:59:GLU:HA	47:CT:64:ALA:HA	1.84	0.58
55:DA:1028:A:N6	55:DA:1125:G:H2'	2.18	0.58
34:CF:31:VAL:CG1	34:CF:97:TRP:CH2	2.86	0.58
45:CR:58:ARG:HH11	45:CR:62:ILE:HD11	1.69	0.58
31:CA:674:G:H1'	33:CE:69:ARG:HH11	1.68	0.58
50:CW:63:ILE:HD12	50:CW:72:VAL:HG21	1.86	0.58
29:DC:227:PRO:HA	29:DC:233:GLY:HA2	1.84	0.58
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	1.84	0.58
31:CA:1847:A:O2'	31:CA:1848:A:H8	1.86	0.58
54:DI:64:VAL:HG22	54:DI:69:PHE:HB2	1.85	0.57
51:CX:37:ILE:HG21	51:CX:80:ILE:HG21	1.85	0.57
51:DX:37:ILE:HG21	51:DX:80:ILE:HG21	1.87	0.57
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.87	0.57
55:DA:62:U:O4'	58:DA:3204:MPD:H31	2.04	0.57
47:CT:17:VAL:HG11	47:CT:103:ILE:HG12	1.86	0.57
25:D4:54:ASP:HB3	40:DM:57:LEU:HD22	1.87	0.57
45:CR:58:ARG:NH1	45:CR:62:ILE:HD11	2.19	0.57
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.87	0.57
28:CB:55:U:H1'	34:CF:26:MET:HG3	1.87	0.57
31:CA:1936:A:N6	31:CA:1963:U:H3	2.02	0.57
17:BQ:68:SER:OG	17:BQ:71:LYS:HB3	2.04	0.56
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.86	0.56
32:DD:99:GLU:HG2	32:DD:182:ALA:HB2	1.87	0.56
32:DD:150[A]:MEQ:HG2	70:DA:3371:HOH:O	2.05	0.56
36:CH:4:ILE:HD11	36:CH:44:ILE:HG22	1.87	0.56
17:BQ:14:SER:HB3	17:BQ:22:VAL:HG12	1.87	0.56
8:BH:96:MET:HE2	8:BH:130:ALA:HB1	1.86	0.56
19:BS:6:LYS:HD2	19:BS:7:LYS:H	1.69	0.56
30:CD:4:LEU:HD22	30:CD:101:PHE:CE2	2.40	0.56
5:AE:38:VAL:HG11	5:AE:114:VAL:HG22	1.87	0.56
3:BC:77:ILE:HA	3:BC:84:VAL:HG23	1.87	0.56
31:CA:457:A:N1	31:CA:470:A:H5''	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2019:A:H4'	45:CR:34:VAL:HG21	1.88	0.56
33:CE:189:THR:HG22	33:CE:192:ALA:H	1.69	0.56
39:DL:113:MET:CE	39:DL:116:ILE:HD11	2.35	0.56
47:CT:69:LEU:HG	47:CT:107:VAL:HG22	1.88	0.56
55:DA:1847:A:O2'	55:DA:1848:A:H8	1.88	0.56
1:AA:451:A:H61	1:AA:481:G:H5'	1.71	0.56
29:CC:17:VAL:HB	29:CC:204:VAL:HG13	1.88	0.56
32:DD:150[A]:MEQ:HE3	55:DA:2032:G:C8	2.41	0.56
44:DQ:53:ARG:NH2	55:DA:2720:U:OP1	2.39	0.56
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.52	0.56
13:AM:33:ILE:HD11	13:AM:63:PHE:CE1	2.40	0.55
5:BE:90:THR:HG22	5:BE:91:GLY:H	1.70	0.55
1:BA:769:G:H4'	1:BA:1513:A:H4'	1.87	0.55
37:CJ:19:ASN:H	37:CJ:20:PRO:HD2	1.72	0.55
49:CV:74:ASN:HD22	49:CV:77:THR:H	1.53	0.55
34:DF:61:SER:HB2	34:DF:91:LEU:HD21	1.88	0.55
10:AJ:35:GLN:HB2	10:AJ:77:VAL:HB	1.88	0.55
47:DT:72:THR:HG21	47:DT:108:SER:HB3	1.89	0.55
55:DA:793:A:OP1	65:DA:3224:SPD:H81	2.07	0.55
11:AK:34:ILE:HB	11:AK:74:VAL:HG11	1.87	0.55
39:CL:43:ILE:HD12	39:CL:56:ASP:HB2	1.88	0.55
49:DV:52:LEU:HB3	49:DV:54:GLN:HB2	1.89	0.55
55:DA:1482:G:H1'	55:DA:1509:A:H61	1.71	0.55
55:DA:2304:G:H22	55:DA:2312:U:H3	1.55	0.55
30:CD:99:GLU:HG2	30:CD:182:ALA:HB2	1.87	0.55
31:CA:2502:G:H5''	31:CA:2503:2MA:H5''	1.88	0.55
47:DT:17:VAL:HG11	47:DT:103:ILE:HG12	1.88	0.55
4:BD:197:GLU:HA	4:BD:200:ILE:HD12	1.87	0.55
31:CA:1779:U:C5	31:CA:1784:A:N7	2.72	0.55
47:DT:6:LYS:HB2	55:DA:494:G:H4'	1.89	0.55
47:CT:66:ILE:HA	47:CT:69:LEU:HD22	1.89	0.55
43:DP:31:THR:HG22	43:DP:34:HIS:H	1.72	0.55
50:DW:63:ILE:HD12	50:DW:72:VAL:HG21	1.87	0.55
31:CA:796:C:H2'	31:CA:797:G:C8	2.41	0.55
4:AD:197:GLU:HA	4:AD:200:ILE:HD12	1.88	0.54
26:C5:2:LYS:HE3	26:C5:4:ARG:HH11	1.70	0.54
31:CA:118:A:N3	31:CA:178:G:H1'	2.22	0.54
41:CN:41:LEU:HD21	41:CN:124:LEU:HD22	1.88	0.54
42:CO:95:THR:HG21	42:CO:113:ILE:HD11	1.89	0.54
52:CY:12:PRO:HB3	52:CY:30:LEU:HD23	1.90	0.54
16:BP:20:VAL:HG13	16:BP:32:PHE:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BT:28:MET:HE1	20:BT:67:ILE:HG12	1.89	0.54
31:CA:2304:G:H22	31:CA:2312:U:H3	1.55	0.54
37:DJ:19:ASN:H	37:DJ:20:PRO:HD2	1.72	0.54
22:D1:25:VAL:HG11	47:DT:38:TYR:HB2	1.90	0.54
23:D2:35:GLU:HG2	23:D2:50:LYS:HG2	1.89	0.54
43:CP:31:THR:HG22	43:CP:34:HIS:H	1.72	0.54
34:DF:131:GLY:HA3	55:DA:2305:U:H5''	1.90	0.54
31:CA:1482:G:H1'	31:CA:1509:A:H61	1.72	0.54
3:AC:40:ARG:HG2	3:AC:55:ILE:HG21	1.90	0.54
13:AM:12:HIS:HB3	70:AM:303:HOH:O	2.08	0.54
31:CA:833:A:H2'	31:CA:834:G:C8	2.42	0.54
39:DL:43:ILE:HD12	39:DL:56:ASP:HB2	1.88	0.54
49:DV:26:LYS:HE2	49:DV:37:GLU:HG3	1.89	0.54
12:BL:110:ARG:HB2	12:BL:119:VAL:HG21	1.89	0.54
31:CA:1936:A:H62	31:CA:1963:U:H3	1.54	0.54
31:CA:206:U:H2'	31:CA:207:A:H8	1.73	0.54
52:DY:56:MET:HE1	55:DA:2091:C:O2'	2.07	0.54
2:AB:129:LEU:HD13	2:AB:134:ALA:HB2	1.90	0.54
2:BB:129:LEU:HD13	2:BB:134:ALA:HB2	1.90	0.54
29:CC:174:LEU:CD2	29:CC:184:VAL:HB	2.38	0.54
5:AE:90:THR:HG22	5:AE:91:GLY:H	1.72	0.53
43:DP:51:ALA:HB3	43:DP:78:VAL:HG13	1.90	0.53
55:DA:1026:G:H2'	55:DA:1027:A:C8	2.43	0.53
1:AA:1054:C:O2'	60:AA:1680:T1C:H921	2.08	0.53
11:AK:67:ALA:HB2	11:AK:96:THR:HG23	1.90	0.53
11:AK:84:VAL:HG21	11:AK:97:ILE:HG23	1.90	0.53
26:C5:3:VAL:HG11	31:CA:2539:C:C5'	2.38	0.53
1:BA:451:A:H61	1:BA:481:G:H5'	1.73	0.53
47:CT:82:MET:HB2	47:CT:98:LYS:HB2	1.89	0.53
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.44	0.53
66:DA:3202:1PE:H231	70:DA:3315:HOH:O	2.08	0.53
23:C2:35:GLU:HG2	23:C2:50:LYS:HG2	1.91	0.53
31:CA:694:U:OP1	31:CA:1569:A:H1'	2.08	0.53
34:DF:88:LYS:HD3	55:DA:2313:C:H5''	1.91	0.53
1:AA:412:A:H3'	1:AA:413:G:C5'	2.39	0.53
43:CP:51:ALA:HB3	43:CP:78:VAL:HG13	1.90	0.53
1:AA:86:G:H21	1:AA:87:C:H41	1.57	0.53
1:BA:1218:C:H2'	1:BA:1219:A:C8	2.44	0.53
32:DD:186:LEU:HD21	44:DQ:4:ILE:HG21	1.90	0.53
26:C5:3:VAL:HG11	31:CA:2539:C:H5'	1.91	0.52
45:DR:20:GLN:HG2	57:DR:202:PG4:H42	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.39	0.52
7:AG:22:LEU:HD12	7:AG:62:PHE:CE2	2.43	0.52
31:CA:2498:OMC:HM22	31:CA:2499:C:H5'	1.91	0.52
36:DH:4:ILE:HD11	36:DH:44:ILE:HG22	1.91	0.52
44:DQ:52:ASN:O	55:DA:2845:U:H5''	2.09	0.52
52:DY:12:PRO:HB3	52:DY:30:LEU:HD23	1.91	0.52
55:DA:2623:G:OP1	64:DA:3203:PGE:H12	2.08	0.52
31:CA:674:G:H1'	33:CE:69:ARG:HD2	1.91	0.52
49:CV:13:VAL:HG21	49:CV:39:ILE:HG21	1.92	0.52
31:CA:320:A:H2'	33:CE:131:THR:HG21	1.92	0.52
39:CL:121:GLU:HG2	39:CL:122:VAL:HG23	1.91	0.52
40:CM:79:LEU:HD11	40:CM:112:LEU:HD12	1.91	0.52
22:D1:9:THR:HG22	55:DA:2020:A:H5'	1.91	0.52
29:CC:105:LEU:H	29:CC:105:LEU:HD12	1.75	0.52
36:CH:27:ARG:HH11	52:CY:60:ASP:HA	1.75	0.52
47:DT:82:MET:HB2	47:DT:98:LYS:HB2	1.90	0.52
9:AI:19:VAL:HG22	9:AI:65:ILE:HG22	1.92	0.52
11:BK:67:ALA:HB2	11:BK:96:THR:HG23	1.91	0.52
34:CF:61:SER:HB2	34:CF:91:LEU:HD21	1.89	0.52
1:AA:299:G:H2'	1:AA:300:A:C8	2.43	0.52
43:DP:31:THR:HG21	28:DB:28:C:OP1	2.08	0.52
48:DU:80:TRP:HB3	64:DU:101:PGE:H32	1.91	0.52
55:DA:551:G:H8	55:DA:551:G:H5''	1.75	0.52
13:BM:22:ILE:HB	13:BM:25:VAL:CG1	2.40	0.52
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.92	0.52
7:BG:69:VAL:HG23	7:BG:100:ALA:HB1	1.92	0.52
11:BK:84:VAL:HG21	11:BK:97:ILE:HG23	1.92	0.52
40:CM:77:ILE:CD1	40:CM:108:ALA:HB1	2.37	0.52
12:AL:33:VAL:HG22	12:AL:79:VAL:HG22	1.92	0.51
54:DI:44:ALA:HB1	54:DI:95:LEU:HD11	1.92	0.51
8:AH:2:SER:HB2	8:AH:4:GLN:HE21	1.75	0.51
1:BA:518:C:H2'	1:BA:530:G:C8	2.45	0.51
31:CA:639:U:H2'	31:CA:640:C:C6	2.45	0.51
40:CM:19:LEU:HD23	40:CM:31:GLY:O	2.10	0.51
1:AA:518:C:H2'	1:AA:530:G:C8	2.45	0.51
1:BA:299:G:H2'	1:BA:300:A:C8	2.44	0.51
8:BH:87:LYS:HB2	8:BH:125:ILE:CD1	2.38	0.51
1:AA:528:C:H5''	1:AA:528:C:H6	1.75	0.51
10:AJ:5:ARG:HE	10:AJ:77:VAL:HG22	1.75	0.51
31:CA:528:A:H8	31:CA:528:A:H3'	1.76	0.51
48:CU:54:GLU:HB3	48:CU:88:LYS:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:102:U:H2'	55:DA:102:U:O2	2.11	0.51
55:DA:639:U:H2'	55:DA:640:C:C6	2.46	0.51
1:BA:8:A:C6	4:BD:206:LYS:HB3	2.46	0.51
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.41	0.51
9:BI:19:VAL:HG22	9:BI:65:ILE:HG22	1.92	0.51
31:CA:1447:C:H2'	31:CA:1448:G:C8	2.46	0.51
42:CO:33:ILE:HD12	42:CO:114:GLU:HB3	1.92	0.51
34:DF:106:ILE:HD12	34:DF:139:PRO:HG2	1.93	0.51
16:AP:6:LEU:HB3	16:AP:17:TYR:HB3	1.92	0.51
1:BA:845:A:O5'	1:BA:845:A:H8	1.94	0.51
6:BF:45:ARG:O	6:BF:56:LYS:HA	2.11	0.51
17:BQ:8:LEU:HD13	17:BQ:73:TRP:CH2	2.46	0.51
29:CC:154:LEU:HD13	29:CC:176:LEU:HD21	1.92	0.51
31:CA:320:A:H4'	31:CA:322:A:N7	2.25	0.51
1:BA:374:A:OP1	1:BA:452:A:N1	2.44	0.51
55:DA:1509:A:HO2'	55:DA:1510:G:H8	1.57	0.51
2:AB:41:ILE:HD13	2:AB:202:GLY:HA2	1.93	0.51
1:BA:202:G:H1	1:BA:215:C:H42	1.58	0.51
2:BB:41:ILE:HD13	2:BB:202:GLY:HA2	1.93	0.51
14:BN:89:MET:HE1	14:BN:98:LYS:HD2	1.93	0.51
47:CT:72:THR:HG21	47:CT:108:SER:HB3	1.92	0.51
50:CW:51:GLN:HG2	50:CW:86:LEU:HD11	1.93	0.51
47:DT:74:ILE:HD12	47:DT:105:VAL:HG22	1.91	0.51
1:BA:269:C:H2'	1:BA:270:A:C8	2.46	0.51
48:DU:54:GLU:HB3	48:DU:88:LYS:HD2	1.92	0.51
16:BP:6:LEU:HB3	16:BP:17:TYR:HB3	1.93	0.50
6:AF:45:ARG:O	6:AF:56:LYS:HA	2.10	0.50
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.93	0.50
5:BE:72:ILE:HG13	5:BE:73:ASN:N	2.25	0.50
14:AN:89:MET:HE1	14:AN:98:LYS:HD2	1.92	0.50
10:BJ:5:ARG:HG2	10:BJ:79:PRO:HG3	1.93	0.50
30:CD:133:THR:CG2	31:CA:1993:U:H4'	2.41	0.50
49:CV:7:ARG:O	49:CV:25:VAL:HB	2.10	0.50
47:CT:74:ILE:HD12	47:CT:105:VAL:HG22	1.93	0.50
42:DO:33:ILE:HD12	42:DO:114:GLU:HB3	1.92	0.50
12:BL:33:VAL:HG22	12:BL:79:VAL:HG22	1.93	0.50
55:DA:1554:U:H1'	59:DA:3219:PUT:H32	1.94	0.50
1:AA:269:C:H2'	1:AA:270:A:C8	2.46	0.50
8:AH:87:LYS:HB2	8:AH:125:ILE:CD1	2.41	0.50
12:AL:110:ARG:HB2	12:AL:119:VAL:HG21	1.91	0.50
29:CC:158:ALA:HB3	31:CA:1820:U:O2'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:634:C:H2'	31:CA:635:C:C6	2.47	0.50
31:CA:974:G:H8	31:CA:990:A:H62	1.60	0.50
29:DC:154:LEU:HD13	29:DC:176:LEU:HD21	1.94	0.50
31:CA:784:G:H5'	31:CA:785:G:OP1	2.12	0.50
29:DC:16:VAL:HG22	29:DC:206:GLY:HA3	1.94	0.50
1:AA:845:A:O4'	1:AA:845:A:P	2.69	0.50
21:AU:51:SER:HA	21:AU:54:LYS:HE3	1.94	0.50
33:DE:189:THR:HG21	70:DE:441:HOH:O	2.11	0.50
1:AA:619:U:C2	4:AD:132:ILE:HD11	2.47	0.49
22:D1:4:GLN:HA	55:DA:2615:U:C2	2.47	0.49
23:D2:25:LYS:HE2	23:D2:30:LYS:O	2.12	0.49
31:CA:551:G:H5''	31:CA:551:G:H8	1.76	0.49
31:CA:2043:C:C6	31:CA:2043:C:H5''	2.47	0.49
31:CA:2189:U:H2'	31:CA:2190:G:H8	1.77	0.49
26:C5:6:SER:HB3	31:CA:2466:C:H5''	1.94	0.49
31:CA:2796:U:H3	31:CA:2799:A:N6	2.02	0.49
34:CF:106:ILE:HD12	34:CF:139:PRO:HG2	1.94	0.49
55:DA:118:A:N3	55:DA:178:G:H1'	2.26	0.49
55:DA:136:G:H1	55:DA:143:C:H42	1.60	0.49
5:AE:157:ARG:HD2	8:AH:43:GLU:O	2.13	0.49
8:BH:2:SER:HB2	8:BH:4:GLN:HE21	1.77	0.49
55:DA:12:U:O2	55:DA:12:U:H2'	2.12	0.49
55:DA:2273:A:H2'	55:DA:2274:A:C8	2.47	0.49
55:DA:2796:U:H3	55:DA:2799:A:N6	1.99	0.49
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	1.94	0.49
9:AI:116:VAL:HG21	10:AJ:62:ARG:HB2	1.94	0.49
18:AR:36:SER:HA	18:AR:72:ASP:HB3	1.94	0.49
24:C3:2:LYS:HE2	31:CA:687:C:H5''	1.94	0.49
39:CL:103:VAL:O	39:CL:122:VAL:HB	2.12	0.49
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.77	0.49
11:BK:43:GLY:HA3	11:BK:74:VAL:HG12	1.93	0.49
31:CA:2822:G:H2'	31:CA:2823:A:H5''	1.95	0.49
49:DV:13:VAL:HG21	49:DV:39:ILE:HG21	1.93	0.49
50:DW:63:ILE:HG22	50:DW:65:VAL:HG23	1.94	0.49
3:AC:47:LEU:HD22	3:AC:76:VAL:HG22	1.95	0.49
3:AC:151:VAL:HG12	3:AC:200:VAL:HG22	1.94	0.49
55:DA:1180:U:H5''	55:DA:1180:U:H6	1.78	0.49
13:BM:90:ARG:HH21	13:BM:95:LEU:HB3	1.78	0.49
31:CA:2394:C:H5''	40:CM:63:LYS:HE2	1.94	0.49
40:CM:28:GLY:O	40:CM:29:LYS:O	2.30	0.49
54:DI:132:TYR:H	54:DI:133:GLU:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AL:79:VAL:HG12	12:AL:102:LEU:HD23	1.94	0.49
32:DD:121:THR:HB	32:DD:127:PHE:CD2	2.48	0.49
48:CU:69:ARG:HB2	48:CU:74:ILE:HG22	1.95	0.49
37:DJ:103:ARG:HA	37:DJ:106:LEU:HD12	1.94	0.49
39:DL:30:ARG:HD2	55:DA:2674:G:H4'	1.94	0.49
40:DM:21:ARG:HA	55:DA:811:U:H2'	1.93	0.49
8:AH:96:MET:HE3	8:AH:130:ALA:HB1	1.94	0.49
13:AM:86:TYR:CZ	13:AM:90:ARG:HD2	2.47	0.49
3:BC:47:LEU:HD22	3:BC:76:VAL:HG22	1.95	0.49
5:BE:90:THR:HG22	5:BE:91:GLY:N	2.28	0.49
31:CA:2095:A:H8	31:CA:2095:A:H5''	1.78	0.49
35:CG:17:VAL:HG11	35:CG:50:LEU:HD21	1.95	0.49
37:CJ:103:ARG:HA	37:CJ:106:LEU:HD12	1.93	0.49
35:DG:19:ILE:HG12	35:DG:24:ILE:HG12	1.94	0.49
55:DA:1417:C:H5'	55:DA:1588:G:H1'	1.95	0.49
1:AA:1492:A:C5'	12:AL:44:LYS:HG2	2.39	0.49
1:BA:404:G:N7	4:BD:2:ALA:HB3	2.28	0.49
13:BM:86:TYR:CZ	13:BM:90:ARG:HD2	2.47	0.49
31:CA:2074:U:H2'	31:CA:2075:U:C6	2.48	0.49
31:CA:136:G:H1	31:CA:143:C:H42	1.61	0.48
33:CE:21:ARG:HD3	33:CE:106:LYS:HB3	1.95	0.48
34:CF:44:ILE:HG21	34:CF:79:ILE:HG22	1.95	0.48
70:DK:307:HOH:O	45:DR:93:LYS:HD2	2.13	0.48
54:DI:23:LEU:HD13	54:DI:89:PRO:HD3	1.94	0.48
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	1.95	0.48
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	1.95	0.48
19:BS:15:LEU:HD13	19:BS:33:THR:HG21	1.94	0.48
31:CA:1703:G:H2'	31:CA:1704:C:C6	2.48	0.48
31:CA:1794:A:H2'	31:CA:1795:C:C6	2.49	0.48
33:DE:21:ARG:HD2	70:DE:416:HOH:O	2.13	0.48
50:DW:51:GLN:HG2	50:DW:86:LEU:HD11	1.94	0.48
1:BA:209:U:H2'	1:BA:209:U:O2	2.13	0.48
5:BE:105:ILE:H	5:BE:123:VAL:H	1.61	0.48
31:CA:1274:A:N3	31:CA:1297:C:H1'	2.28	0.48
31:CA:2630:G:O4'	31:CA:2894:G:H1'	2.13	0.48
29:DC:199:GLU:O	29:DC:202:LEU:HB2	2.13	0.48
54:DI:31:ARG:HB2	54:DI:79:PRO:HG2	1.93	0.48
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	1.95	0.48
1:AA:413:G:H5''	1:AA:414:A:H5'	1.96	0.48
10:AJ:52:LEU:HB2	14:AN:81:ARG:HD2	1.96	0.48
5:BE:106:ILE:HD11	5:BE:124:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:45:G:H5''	31:CA:46:G:H5'	1.96	0.48
31:CA:668:A:H2'	31:CA:670:A:H62	1.78	0.48
31:CA:2327:A:H2'	31:CA:2328:A:C8	2.49	0.48
54:DI:26:VAL:HB	54:DI:83:ALA:HB3	1.95	0.48
55:DA:2187:U:H5''	70:DA:4577:HOH:O	2.12	0.48
55:DA:2728:U:O2'	55:DA:2729:G:H5''	2.13	0.48
50:CW:63:ILE:HG22	50:CW:65:VAL:HG23	1.95	0.48
52:CY:4:VAL:HG22	52:CY:11:ARG:HG3	1.95	0.48
55:DA:45:G:H5''	55:DA:46:G:H5'	1.95	0.48
1:AA:202:G:H21	1:AA:466:A:H61	1.60	0.48
1:AA:404:G:N7	4:AD:2:ALA:HB3	2.28	0.48
27:C0:9:GLN:HB3	27:C0:32:ILE:HA	1.95	0.48
6:BF:3:HIS:H	6:BF:92:THR:HG23	1.78	0.48
31:CA:586:A:H5'	33:CE:84:THR:HG21	1.96	0.48
31:CA:822:G:O6	31:CA:943:A:H2	1.96	0.48
31:CA:948:C:H1'	31:CA:984:A:C8	2.48	0.48
45:CR:87:SER:HB3	46:CS:52:PRO:HD3	1.94	0.48
19:BS:29:LYS:HB3	19:BS:30:PRO:HD2	1.96	0.48
31:CA:2636:C:H2'	31:CA:2637:U:C6	2.49	0.48
38:DK:9:GLU:HG2	70:DA:5165:HOH:O	2.13	0.48
1:AA:202:G:H1	1:AA:215:C:H42	1.62	0.48
24:D3:19:ARG:HG3	55:DA:126:A:O5'	2.14	0.48
31:CA:528:A:H3'	31:CA:528:A:C8	2.48	0.48
53:CZ:56:LEU:HA	53:CZ:59:GLU:HG2	1.96	0.48
55:DA:1975:G:H21	64:DA:3225:PGE:H22	1.79	0.48
32:DD:3:GLY:HA3	32:DD:204:LYS:HG2	1.95	0.48
39:CL:58:LEU:HD11	39:CL:86:LEU:HD13	1.96	0.48
41:DN:92:TRP:HE1	58:DN:201:MPD:HM1	1.78	0.48
22:C1:53:LYS:HE3	22:C1:56:ALA:HA	1.95	0.48
43:DP:35:ILE:HG21	43:DP:71:ALA:HA	1.96	0.48
51:DX:59:LEU:HD12	51:DX:80:ILE:HD12	1.96	0.48
55:DA:1536:C:H4'	55:DA:1537:G:H5''	1.95	0.48
17:AQ:15:ASP:HA	17:AQ:21:ILE:HG22	1.95	0.47
19:AS:29:LYS:HB3	19:AS:30:PRO:HD2	1.96	0.47
31:CA:1709:U:H2'	31:CA:1710:G:C8	2.49	0.47
34:CF:36:LEU:HD21	34:CF:91:LEU:CD1	2.45	0.47
40:DM:85:VAL:HB	40:DM:94:THR:HG22	1.96	0.47
8:AH:105:SER:HB2	8:AH:126:ILE:HD11	1.96	0.47
11:BK:24:HIS:HB3	11:BK:31:ILE:HG23	1.96	0.47
48:CU:28:ASN:ND2	48:CU:91:GLN:HB3	2.28	0.47
55:DA:2636:C:H2'	55:DA:2637:U:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:DA:3224:SPD:H82	70:DA:4835:HOH:O	2.14	0.47
1:BA:108:G:H5''	1:BA:108:G:N3	2.30	0.47
13:BM:22:ILE:HB	13:BM:25:VAL:HG12	1.97	0.47
17:BQ:51:ASN:N	17:BQ:51:ASN:HD22	2.13	0.47
31:CA:532:A:N3	31:CA:532:A:H2'	2.30	0.47
35:CG:19:ILE:HG12	35:CG:24:ILE:HG12	1.96	0.47
42:CO:103:ARG:HD3	42:CO:110:MET:SD	2.55	0.47
2:BB:97:LEU:H	2:BB:100:MET:HE3	1.80	0.47
3:BC:20:SER:HB3	14:BN:94:PRO:HG3	1.96	0.47
30:CD:3:GLY:HA3	30:CD:204:LYS:HG2	1.97	0.47
34:DF:44:ILE:HG21	34:DF:79:ILE:HG22	1.96	0.47
5:AE:90:THR:HG22	5:AE:91:GLY:N	2.29	0.47
23:C2:25:LYS:HE2	23:C2:30:LYS:O	2.14	0.47
31:CA:373:U:H2'	31:CA:374:A:H8	1.78	0.47
31:CA:782:A:H5'	31:CA:783:A:C2	2.50	0.47
51:CX:37:ILE:HG22	51:CX:38:VAL:HG23	1.94	0.47
35:DG:86:LYS:HG2	35:DG:132:VAL:HG22	1.96	0.47
41:DN:3:GLN:HG3	41:DN:92:TRP:CD1	2.49	0.47
55:DA:2547:A:H2'	55:DA:2548:U:C6	2.50	0.47
22:C1:8:PRO:HG2	31:CA:1264:A:H5'	1.96	0.47
9:BI:116:VAL:HG21	10:BJ:62:ARG:HB2	1.97	0.47
20:BT:4:ILE:HA	20:BT:8:LYS:HE2	1.96	0.47
23:D2:6:ARG:HG2	23:D2:24:THR:HB	1.96	0.47
29:CC:3:VAL:HG21	29:CC:202:LEU:HD23	1.97	0.47
41:CN:3:GLN:HG3	41:CN:92:TRP:CD1	2.49	0.47
42:CO:71:ARG:HG3	42:CO:71:ARG:O	2.15	0.47
43:CP:7:ARG:HA	43:CP:10:ARG:HE	1.80	0.47
1:AA:946:A:H2'	1:AA:947:G:C8	2.50	0.47
22:C1:25:VAL:HG13	22:C1:26:THR:H	1.78	0.47
4:BD:201:VAL:HG11	5:BE:103:THR:HB	1.96	0.47
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.79	0.47
29:CC:174:LEU:HD21	29:CC:184:VAL:HB	1.95	0.47
29:CC:199:GLU:O	29:CC:202:LEU:HB2	2.13	0.47
31:CA:1936:A:C2	31:CA:1943:U:N3	2.62	0.47
51:CX:59:LEU:HD12	51:CX:80:ILE:HD12	1.96	0.47
53:DZ:56:LEU:HA	53:DZ:59:GLU:HG2	1.96	0.47
55:DA:851:C:H2'	55:DA:852:U:C6	2.50	0.47
55:DA:2502:G:H5''	55:DA:2503:2MA:H5''	1.95	0.47
12:BL:79:VAL:HG12	12:BL:102:LEU:HD23	1.95	0.47
35:DG:17:VAL:HG11	35:DG:50:LEU:HD21	1.96	0.47
35:DG:164:TYR:HB2	35:DG:167:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:97:LEU:H	2:AB:100:MET:HE3	1.80	0.47
23:C2:6:ARG:HG2	23:C2:24:THR:HB	1.97	0.47
25:C4:8:ARG:HG3	31:CA:253:C:N4	2.30	0.47
1:BA:376:G:H5''	16:BP:5:ARG:HB2	1.97	0.47
22:D1:24:ALA:HB3	64:D1:102:PGE:H5	1.96	0.47
30:CD:121:THR:HB	30:CD:127:PHE:CD2	2.50	0.47
31:CA:12:U:H2'	31:CA:12:U:O2	2.15	0.47
31:CA:17:G:H4'	45:CR:25:TYR:HE2	1.80	0.47
31:CA:1956:U:O2	31:CA:1985:C:H4'	2.15	0.47
29:DC:160:THR:HG21	55:DA:1819:A:H5''	1.96	0.47
35:CG:164:TYR:HB2	35:CG:167:GLU:HB2	1.96	0.47
41:DN:33:LEU:HD13	41:DN:117:PHE:HB3	1.97	0.47
1:AA:411:A:P	4:AD:26:ARG:HH12	2.38	0.47
5:AE:57:PRO:O	5:AE:60:ILE:HG13	2.15	0.47
5:AE:107:ALA:HB2	5:AE:125:ALA:HB3	1.96	0.47
17:BQ:76:VAL:HG12	17:BQ:77:ARG:HG3	1.97	0.47
31:CA:1441:G:H2'	31:CA:1442:U:C6	2.50	0.47
35:CG:86:LYS:HG2	35:CG:132:VAL:HG22	1.97	0.47
33:DE:21:ARG:HD3	33:DE:106:LYS:HB3	1.96	0.47
39:DL:58:LEU:HD11	39:DL:86:LEU:HD13	1.96	0.47
39:DL:101:GLY:O	39:DL:120:PRO:HD2	2.15	0.47
8:AH:66:PHE:CD2	8:AH:67:GLN:HG2	2.51	0.46
24:C3:19:ARG:HG3	31:CA:126:A:O5'	2.15	0.46
1:BA:946:A:H2'	1:BA:947:G:C8	2.50	0.46
20:BT:44:LYS:HB3	20:BT:87:ALA:HB2	1.96	0.46
31:CA:321:U:H5''	33:CE:131:THR:HG23	1.98	0.46
31:CA:851:C:H2'	31:CA:852:U:C6	2.50	0.46
31:CA:2845:U:H5''	44:CQ:52:ASN:O	2.15	0.46
1:AA:604:G:H2'	1:AA:605:U:O4'	2.15	0.46
23:C2:37:LYS:HG2	23:C2:48:ILE:HG13	1.97	0.46
20:BT:24:ARG:O	20:BT:27:MET:HG3	2.15	0.46
30:CD:13:ARG:HH11	44:CQ:56:HIS:HA	1.79	0.46
47:DT:20:VAL:HG11	47:DT:44:ALA:HA	1.97	0.46
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.81	0.46
17:AQ:76:VAL:HG12	17:AQ:77:ARG:HG3	1.96	0.46
5:BE:105:ILE:HA	5:BE:123:VAL:HG23	1.98	0.46
31:CA:608:A:H2'	31:CA:609:A:C8	2.50	0.46
31:CA:998:C:OP2	45:CR:58:ARG:NH2	2.48	0.46
43:CP:35:ILE:HG21	43:CP:71:ALA:HA	1.98	0.46
41:DN:18[B]:ARG:HG3	28:DB:90:C:H5''	1.97	0.46
1:AA:108:G:N3	1:AA:108:G:H5''	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:129:LEU:H	2:AB:129:LEU:HG	1.53	0.46
3:AC:20:SER:HB3	14:AN:94:PRO:HG3	1.96	0.46
1:BA:1001:C:H2'	1:BA:1002:G:H8	1.81	0.46
31:CA:2842:G:H2'	31:CA:2843:G:O4'	2.15	0.46
29:DC:3:VAL:HG21	29:DC:202:LEU:HD23	1.97	0.46
55:DA:1014:A:H1'	70:DA:6962:HOH:O	2.14	0.46
55:DA:1999:C:H5''	55:DA:2723:C:O2'	2.15	0.46
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.80	0.46
8:BH:105:SER:HB2	8:BH:126:ILE:HD11	1.97	0.46
31:CA:1509:A:HO2'	31:CA:1510:G:H8	1.63	0.46
47:CT:20:VAL:HG11	47:CT:44:ALA:HA	1.98	0.46
40:DM:63:LYS:HE2	55:DA:2394:C:H5''	1.98	0.46
55:DA:858:G:H3'	55:DA:859:G:C8	2.51	0.46
8:AH:29:SER:HB3	8:AH:57:PRO:HB2	1.97	0.46
9:AI:98:LEU:HB3	9:AI:104:VAL:HG13	1.97	0.46
12:AL:3:THR:HB	12:AL:6:GLN:HG3	1.98	0.46
27:C0:14:ILE:HG12	31:CA:989:G:C8	2.50	0.46
1:BA:73:C:O2'	1:BA:74:A:H8	1.98	0.46
18:BR:36:SER:HA	18:BR:72:ASP:HB3	1.98	0.46
31:CA:1783:A:H5'	31:CA:2608:G:H4'	1.97	0.46
55:DA:287:G:H1	55:DA:353:C:H42	1.64	0.46
1:AA:79:G:H22	1:AA:90:C:H42	1.64	0.46
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.81	0.46
1:BA:374:A:H5''	1:BA:452:A:C2	2.51	0.46
1:BA:374:A:H5''	1:BA:452:A:N1	2.29	0.46
29:CC:228:VAL:HG21	70:CA:3406:HOH:O	2.16	0.46
31:CA:7:G:H4'	38:CK:15:TRP:CZ2	2.50	0.46
42:CO:2:ARG:HA	42:CO:5:LYS:HD2	1.98	0.46
45:CR:90:ILE:HG22	45:CR:95:LEU:HG	1.97	0.46
41:DN:16:ARG:HG3	41:DN:18[B]:ARG:HH11	1.81	0.46
1:BA:604:G:H2'	1:BA:605:U:O4'	2.16	0.46
5:BE:88:VAL:HG12	5:BE:93:ARG:HG2	1.97	0.46
10:BJ:52:LEU:HB2	14:BN:81:ARG:HD2	1.98	0.46
31:CA:2815:C:H2'	31:CA:2816:G:O4'	2.15	0.46
39:CL:101:GLY:O	39:CL:120:PRO:HD2	2.15	0.46
41:DN:20:LEU:HD22	50:DW:81:PRO:HG2	1.98	0.46
45:DR:4:VAL:HG22	55:DA:1199:U:H1'	1.98	0.46
1:AA:56:U:H2'	1:AA:57:G:C8	2.51	0.46
31:CA:443:A:H2'	33:CE:40:ARG:NH1	2.30	0.46
31:CA:532:A:N1	31:CA:2020:A:H1'	2.31	0.46
31:CA:1028:A:N6	31:CA:1125:G:H2'	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1587:G:H2'	31:CA:1588:G:H8	1.81	0.46
40:CM:85:VAL:HG11	40:CM:90:VAL:HG22	1.98	0.46
45:CR:76:TYR:CZ	45:CR:80:ILE:HG13	2.51	0.46
55:DA:2133:G:H21	55:DA:2158:A:N6	2.13	0.46
1:AA:967:5MC:O3'	9:AI:127:PHE:HE1	1.98	0.46
4:AD:177:LYS:HB3	4:AD:179:GLU:HG2	1.98	0.46
1:BA:1478:U:H2'	1:BA:1479:C:C6	2.51	0.46
31:CA:1405:U:H2'	31:CA:1406:U:C6	2.51	0.46
31:CA:1430:G:H2'	31:CA:1431:A:O4'	2.15	0.46
41:CN:33:LEU:HD13	41:CN:117:PHE:HB3	1.98	0.46
38:DK:7:LYS:HG2	55:DA:538:A:H4'	1.97	0.46
55:DA:1794:A:H2'	55:DA:1795:C:C6	2.50	0.46
5:AE:76:LEU:HD11	5:AE:120:VAL:HG22	1.99	0.45
1:BA:972:C:H4'	10:BJ:59:LYS:HG2	1.98	0.45
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	1.97	0.45
30:CD:186:LEU:HD21	44:CQ:4:ILE:HG21	1.98	0.45
33:CE:75:SER:O	33:CE:78:TRP:HB2	2.15	0.45
45:DR:6:ARG:HD3	55:DA:1250:G:C5'	2.46	0.45
55:DA:191:A:H2'	55:DA:192:C:C6	2.51	0.45
1:AA:1478:U:H2'	1:AA:1479:C:C6	2.51	0.45
4:BD:177:LYS:HB3	4:BD:179:GLU:HG2	1.97	0.45
5:BE:57:PRO:O	5:BE:60:ILE:HG13	2.16	0.45
9:BI:7:TYR:HE1	9:BI:18:ARG:HB2	1.79	0.45
31:CA:244:A:H5''	40:CM:67:THR:HG21	1.98	0.45
31:CA:2305:U:H5''	34:CF:131:GLY:HA3	1.97	0.45
1:AA:403:C:H5'	4:AD:132:ILE:HG23	1.97	0.45
26:C5:3:VAL:CG1	31:CA:2539:C:H5'	2.46	0.45
1:BA:774:G:H21	57:BA:1642:PG4:H62	1.81	0.45
31:CA:804:A:H2'	31:CA:806:C:C4	2.51	0.45
33:CE:149:ILE:HD12	33:CE:172:ALA:HA	1.98	0.45
40:DM:32:GLY:HA2	55:DA:1190:G:H5''	1.98	0.45
55:DA:1587:G:H2'	55:DA:1588:G:H8	1.82	0.45
1:AA:376:G:H5''	16:AP:5:ARG:HB2	1.98	0.45
1:AA:923:A:OP1	5:AE:26:LYS:HG2	2.16	0.45
31:CA:1380:G:H1'	31:CA:1569:A:N6	2.32	0.45
31:CA:2350:C:H2'	31:CA:2351:G:O4'	2.17	0.45
45:DR:76:TYR:CZ	45:DR:80:ILE:HG13	2.52	0.45
22:D1:22:LEU:HD23	62:D1:103:PEG:H31	1.99	0.45
31:CA:310:A:H5''	49:CV:15:THR:HG23	1.97	0.45
43:DP:27:VAL:HG21	43:DP:40:ILE:HD12	1.98	0.45
55:DA:2128:G:H1	55:DA:2160:C:N4	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:111:ILE:HD12	2:AB:152:LYS:HA	1.98	0.45
28:CB:57:A:C4'	34:CF:27:GLN:HG3	2.47	0.45
44:DQ:106:LYS:HA	44:DQ:109:ARG:HD3	1.99	0.45
55:DA:1424:G:H21	64:DA:3214:PGE:H32	1.82	0.45
14:BN:31:ILE:HG23	14:BN:42:TRP:HZ2	1.81	0.45
30:CD:62:LYS:HE2	31:CA:2810:A:H5''	1.99	0.45
31:CA:720:U:H2'	31:CA:721:A:C8	2.52	0.45
55:DA:742:A:H2'	55:DA:743:A:C8	2.52	0.45
2:AB:188:ASP:HB2	2:AB:204:ASP:OD2	2.16	0.45
1:BA:56:U:H2'	1:BA:57:G:C8	2.52	0.45
45:DR:16:LYS:HE2	63:DA:3209:EDO:H21	1.98	0.45
55:DA:2233:U:H2'	55:DA:2234:G:C8	2.52	0.45
21:AU:4:ILE:HG13	21:AU:19:PHE:HA	1.99	0.45
1:BA:1003:G:H21	1:BA:1005:A:H5'	1.82	0.45
9:BI:57:MET:HG3	9:BI:61:LEU:HG	1.99	0.45
24:D3:12:ARG:HB2	55:DA:686:U:O4	2.17	0.45
38:DK:46:PRO:HD2	70:DK:360:HOH:O	2.17	0.45
41:DN:77:PRO:HG2	41:DN:80:VAL:HG21	1.98	0.45
2:BB:188:ASP:HB2	2:BB:204:ASP:OD2	2.17	0.45
32:DD:150[B]:MEQ:HG3	55:DA:2032:G:N3	2.31	0.45
46:CS:49:ILE:HB	46:CS:51:VAL:O	2.17	0.45
54:DI:126:LEU:HA	54:DI:129:LEU:HD12	1.98	0.45
55:DA:31:C:O3'	55:DA:1238:G:H5''	2.17	0.45
1:AA:109:A:H2'	1:AA:326:G:N2	2.31	0.44
5:BE:157:ARG:HG3	8:BH:43:GLU:O	2.17	0.44
31:CA:191:A:H2'	31:CA:192:C:C6	2.52	0.44
42:DO:55:ALA:HA	42:DO:80:PHE:CE2	2.53	0.44
66:DA:3202:1PE:H162	70:DA:3315:HOH:O	2.16	0.44
11:AK:52:PHE:HE2	11:AK:65:VAL:HG21	1.82	0.44
1:BA:109:A:H2'	1:BA:326:G:N2	2.32	0.44
1:BA:1106:G:H5''	3:BC:172:ARG:HG3	1.99	0.44
2:BB:129:LEU:H	2:BB:129:LEU:HG	1.53	0.44
11:BK:52:PHE:HE2	11:BK:65:VAL:HG21	1.81	0.44
13:BM:77:ILE:HG22	13:BM:81:MET:HE2	1.99	0.44
28:CB:28:C:OP1	43:CP:31:THR:HG21	2.16	0.44
31:CA:247:G:H4'	31:CA:386:G:C5	2.52	0.44
31:CA:287:G:H1	31:CA:353:C:H42	1.65	0.44
41:CN:69:PRO:HA	41:CN:94:ALA:HB2	1.99	0.44
43:CP:27:VAL:HG21	43:CP:40:ILE:HD12	2.00	0.44
1:BA:322:C:H5	1:BA:328:C:C5	2.36	0.44
13:BM:16:VAL:HG13	13:BM:34:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
31:CA:2607:G:H2'	31:CA:2608:G:O4'	2.16	0.44
50:CW:38:LEU:HD21	50:CW:65:VAL:HG11	1.99	0.44
1:AA:715:A:H2'	1:AA:716:A:C8	2.53	0.44
1:AA:1329:A:H5''	13:AM:26:GLY:H	1.81	0.44
1:BA:328:C:H2'	1:BA:328:C:O2	2.17	0.44
1:BA:923:A:OP1	5:BE:26:LYS:HG2	2.18	0.44
1:BA:1329:A:H5''	13:BM:26:GLY:H	1.82	0.44
17:BQ:31:HIS:HE1	17:BQ:33:ILE:HD12	1.82	0.44
20:BT:69:LYS:H	20:BT:69:LYS:HG3	1.57	0.44
21:BU:4:ILE:HG13	21:BU:19:PHE:HA	1.99	0.44
31:CA:1638:C:H4'	31:CA:2710:C:O2	2.17	0.44
50:CW:63:ILE:CD1	50:CW:72:VAL:HG21	2.47	0.44
50:DW:63:ILE:CD1	50:DW:72:VAL:HG21	2.47	0.44
20:BT:58:VAL:HG13	20:BT:72:ALA:HB1	1.98	0.44
28:CB:14:U:H2'	28:CB:15:A:C2	2.52	0.44
31:CA:582:A:H2'	31:CA:583:G:C8	2.53	0.44
31:CA:588:U:H2'	31:CA:589:U:C6	2.53	0.44
33:CE:149:ILE:HD11	33:CE:188:MET:HE3	1.99	0.44
35:CG:76:VAL:O	35:CG:80:THR:HG22	2.18	0.44
44:DQ:31:TRP:CE2	44:DQ:40:LEU:HD21	2.52	0.44
55:DA:2324:U:H3'	55:DA:2325:G:H5''	2.00	0.44
8:AH:94:LYS:HB3	8:AH:117:ARG:HH22	1.82	0.44
9:AI:57:MET:HG3	9:AI:61:LEU:HG	1.99	0.44
13:AM:90:ARG:HD3	13:AM:97:VAL:HA	1.99	0.44
1:BA:439:U:H5''	4:BD:121:LYS:HD2	1.99	0.44
1:BA:1496:C:H2'	1:BA:1497:G:O4'	2.17	0.44
13:BM:90:ARG:HD3	13:BM:97:VAL:HA	1.99	0.44
21:BU:51:SER:HA	21:BU:54:LYS:HE3	2.00	0.44
29:CC:155:ALA:HB2	29:CC:162:VAL:HG23	1.98	0.44
31:CA:686:U:H2'	31:CA:788:A:N1	2.32	0.44
31:CA:1327:A:H2'	31:CA:1328:A:O4'	2.17	0.44
31:CA:1636:U:H2'	31:CA:1637:A:C8	2.52	0.44
45:CR:112:LYS:HD3	46:CS:48:LYS:HG3	2.00	0.44
55:DA:136:G:H1	55:DA:143:C:N4	2.16	0.44
55:DA:783:A:N3	55:DA:783:A:H2'	2.33	0.44
55:DA:2262:U:H4'	55:DA:2328:A:C2	2.53	0.44
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	2.00	0.44
17:AQ:31:HIS:HE1	17:AQ:33:ILE:HD12	1.83	0.44
27:C0:7:ILE:HD13	27:C0:27:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BG:111:ARG:HB3	7:BG:119:ARG:HG2	2.00	0.44
8:BH:29:SER:HB3	8:BH:57:PRO:HB2	2.00	0.44
26:C5:38:GLY:HA2	31:CA:1125:G:H5'	1.99	0.44
1:BA:967:5MC:O3'	9:BI:127:PHE:HE1	2.00	0.44
9:BI:98:LEU:HB3	9:BI:104:VAL:HG13	1.98	0.44
31:CA:587:C:O2'	40:CM:19:LEU:HD13	2.17	0.44
31:CA:1680:U:H2'	31:CA:1681:G:O4'	2.18	0.44
31:CA:2190:G:H2'	31:CA:2191:A:H8	1.83	0.44
29:DC:97:LYS:HA	29:DC:97:LYS:HD3	1.68	0.44
47:DT:73:LYS:HD3	66:DA:3185:1PE:H232	2.00	0.44
50:DW:38:LEU:HD21	50:DW:65:VAL:HG11	1.99	0.44
1:AA:328:C:H2'	1:AA:328:C:O2	2.17	0.44
1:AA:439:U:H5''	4:AD:121:LYS:HD2	1.99	0.44
1:AA:1003:G:H21	1:AA:1005:A:H5'	1.82	0.44
24:C3:9:VAL:HG23	31:CA:1309:G:H5''	2.00	0.44
29:CC:160:THR:HG21	31:CA:1819:A:H5''	2.00	0.44
31:CA:826:U:O2'	40:CM:53:GLY:HA3	2.17	0.44
31:CA:1363:C:H2'	31:CA:1364:G:C8	2.53	0.44
34:CF:31:VAL:HG11	34:CF:97:TRP:CH2	2.53	0.44
37:DJ:14:ALA:HB3	37:DJ:17:MET:HB2	2.00	0.44
54:DI:3:LEU:HD12	54:DI:56:ARG:NH2	2.33	0.44
55:DA:720:U:H2'	55:DA:721:A:C8	2.53	0.44
55:DA:1101:U:H2'	55:DA:1102:C:C6	2.53	0.44
55:DA:1328:A:H2'	55:DA:1330:C:C5	2.53	0.44
55:DA:1975:G:H21	64:DA:3225:PGE:C2	2.31	0.44
6:AF:38:ARG:HE	6:AF:63:ASN:ND2	2.16	0.43
13:AM:77:ILE:HG22	13:AM:81:MET:HE2	2.00	0.43
8:BH:102:ALA:HB3	8:BH:113:ASP:HB3	2.00	0.43
12:BL:64:THR:HG23	12:BL:93:VAL:HA	1.99	0.43
14:BN:31:ILE:HG23	14:BN:42:TRP:CZ2	2.53	0.43
22:D1:9:THR:HG21	55:DA:2020:A:H5'	2.00	0.43
26:D5:2:LYS:HE2	26:D5:4:ARG:HH11	1.83	0.43
31:CA:328:U:O3'	49:CV:66:GLN:HG3	2.18	0.43
31:CA:729:G:H2'	31:CA:1775:U:H1'	1.99	0.43
31:CA:1324:G:H1'	31:CA:1616:A:N6	2.33	0.43
29:DC:155:ALA:HB2	29:DC:162:VAL:HG23	2.00	0.43
36:CH:82:SER:HB2	36:CH:94:ILE:HD11	2.00	0.43
38:CK:117:ALA:HA	38:CK:120:ARG:HD2	2.00	0.43
44:CQ:106:LYS:HA	44:CQ:109:ARG:HD3	1.99	0.43
55:DA:588:U:H2'	55:DA:589:U:C6	2.53	0.43
55:DA:2607:G:H2'	55:DA:2608:G:O4'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:202:G:O2'	1:BA:468:A:H8	2.01	0.43
1:BA:438:U:H5'	4:BD:120:HIS:HB3	1.99	0.43
9:BI:120:LYS:HB2	9:BI:123:ARG:HB3	2.00	0.43
38:DK:117:ALA:HA	38:DK:120:ARG:HD2	2.00	0.43
55:DA:1637:A:H5'	55:DA:1760:C:O2'	2.18	0.43
1:AA:438:U:H5'	4:AD:120:HIS:HB3	2.00	0.43
10:AJ:49:PHE:CE1	14:AN:77:PHE:HZ	2.36	0.43
4:BD:85:ASN:HA	5:BE:102:GLY:CA	2.41	0.43
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	1.99	0.43
31:CA:357:C:H2'	31:CA:358:U:C6	2.53	0.43
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.54	0.43
34:CF:36:LEU:HB2	34:CF:57:LEU:HD21	2.00	0.43
51:DX:41[A]:ARG:HH12	55:DA:2262:U:H5''	1.84	0.43
55:DA:357:C:H2'	55:DA:358:U:C6	2.53	0.43
55:DA:1433:A:O2'	55:DA:1434:A:H5'	2.19	0.43
1:BA:79:G:H22	1:BA:90:C:H42	1.65	0.43
1:BA:1493:A:H1'	31:CA:1913:A:H61	1.82	0.43
3:BC:113:ALA:O	3:BC:200:VAL:HG11	2.18	0.43
26:D5:36:ARG:HD3	55:DA:2742:G:OP1	2.19	0.43
31:CA:373:U:H2'	31:CA:374:A:C8	2.53	0.43
31:CA:460:A:H2'	31:CA:461:C:O4'	2.18	0.43
45:DR:19:LYS:HB3	57:DR:202:PG4:H41	2.00	0.43
45:DR:90:ILE:HG22	45:DR:95:LEU:HG	2.00	0.43
54:DI:27:VAL:HG13	54:DI:80:THR:HG23	2.00	0.43
55:DA:138:U:H5'	55:DA:139:U:H5'	1.99	0.43
55:DA:278:A:N3	55:DA:278:A:H2'	2.33	0.43
55:DA:686:U:H2'	55:DA:788:A:N1	2.33	0.43
1:AA:649:A:H2'	1:AA:650:G:O4'	2.17	0.43
8:AH:102:ALA:HB3	8:AH:113:ASP:HB3	2.01	0.43
1:BA:1062:U:H2'	1:BA:1063:C:C6	2.54	0.43
17:BQ:28:PHE:HD2	17:BQ:37:PHE:HB3	1.84	0.43
30:CD:101:PHE:O	30:CD:104:VAL:HG22	2.19	0.43
30:CD:141:ARG:HB2	31:CA:1656:C:H5''	2.01	0.43
31:CA:278:A:N3	31:CA:278:A:H2'	2.33	0.43
32:DD:155:VAL:HG21	55:DA:2618:G:H21	1.84	0.43
36:DH:104:THR:HG22	36:DH:109:GLU:HA	1.99	0.43
55:DA:2800:A:C2	55:DA:2895:G:H1'	2.53	0.43
1:AA:1496:C:H2'	1:AA:1497:G:O4'	2.18	0.43
9:AI:99:ARG:HG2	9:AI:104:VAL:HG21	2.01	0.43
31:CA:20:C:H2'	31:CA:21:A:C8	2.53	0.43
31:CA:136:G:H1	31:CA:143:C:N4	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:DO:51:LEU:HD23	42:DO:51:LEU:HA	1.88	0.43
55:DA:57:C:H2'	55:DA:58:G:O4'	2.19	0.43
55:DA:340:A:H2'	55:DA:341:C:O4'	2.19	0.43
55:DA:2031:A:C6	55:DA:2498:OMC:H1'	2.53	0.43
55:DA:2251:OMG:H1'	55:DA:2251:OMG:HM23	1.73	0.43
55:DA:2479:U:OP1	55:DA:2537:U:H1'	2.19	0.43
1:AA:202:G:O2'	1:AA:468:A:H8	2.02	0.43
7:AG:111:ARG:HB3	7:AG:119:ARG:HG2	2.00	0.43
1:BA:649:A:H2'	1:BA:650:G:O4'	2.18	0.43
1:BA:840:C:H2'	1:BA:841:C:O4'	2.19	0.43
28:CB:57:A:O4'	34:CF:27:GLN:HG3	2.18	0.43
31:CA:1101:U:H2'	31:CA:1102:C:C6	2.53	0.43
36:DH:82:SER:HB2	36:DH:94:ILE:HD11	1.99	0.43
55:DA:784:G:H5'	55:DA:785:G:OP1	2.18	0.43
11:BK:84:VAL:HG11	11:BK:97:ILE:HG12	2.01	0.43
31:CA:2031:A:C6	31:CA:2498:OMC:H1'	2.54	0.43
33:DE:32:VAL:HG21	40:DM:6:LEU:HD13	2.00	0.43
49:DV:51:ALA:O	49:DV:52:LEU:HB2	2.18	0.43
54:DI:132:TYR:N	54:DI:133:GLU:HB2	2.33	0.43
55:DA:142:A:H2'	55:DA:143:C:C6	2.53	0.43
55:DA:184:C:H2'	55:DA:185:G:H8	1.84	0.43
55:DA:2849:U:H4'	55:DA:2868:A:C2	2.54	0.43
1:AA:957:U:O2	1:AA:959:A:H8	2.02	0.43
3:BC:22:TRP:HB3	3:BC:59:ARG:H	1.84	0.43
5:BE:104:GLY:HA3	5:BE:122:ASN:HA	2.01	0.43
8:BH:94:LYS:HB3	8:BH:117:ARG:HH22	1.84	0.43
22:D1:12:LYS:HD2	22:D1:12:LYS:HA	1.85	0.43
22:D1:50:ARG:NH2	55:DA:2884[A]:U:H4'	2.33	0.43
29:CC:88:SER:HB2	29:CC:158:ALA:HB2	2.01	0.43
29:DC:35:GLU:HG3	29:DC:64:ILE:HD11	2.00	0.43
33:CE:149:ILE:CD1	33:CE:188:MET:HE3	2.49	0.43
42:CO:55:ALA:HA	42:CO:80:PHE:CE2	2.53	0.43
46:CS:38:VAL:HG22	46:CS:57:GLY:HA3	2.01	0.43
33:DE:3:LEU:HD12	33:DE:14:VAL:HG11	2.00	0.43
55:DA:526:A:H2'	70:DA:3565:HOH:O	2.19	0.43
1:AA:1358:U:H3	1:AA:1363:A:H62	1.67	0.43
20:AT:24:ARG:HD3	20:AT:24:ARG:N	2.34	0.43
13:BM:11:ASP:HA	13:BM:45:ILE:HD13	1.99	0.43
31:CA:2025:C:H2'	31:CA:2026:U:C6	2.54	0.43
31:CA:2469:A:H4'	41:CN:55:ARG:HD3	2.00	0.43
31:CA:2514:U:H2'	31:CA:2515:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:DT:72:THR:CG2	47:DT:108:SER:HB3	2.48	0.43
48:DU:28:ASN:OD1	48:DU:91:GLN:HB3	2.19	0.43
52:DY:7:VAL:HG23	52:DY:51:VAL:HG12	2.01	0.43
53:DZ:47:ARG:HD3	70:DZ:102:HOH:O	2.19	0.43
1:BA:12:U:H4'	1:BA:526:C:H4'	1.99	0.42
3:BC:47:LEU:HB3	3:BC:50:ALA:HB3	2.01	0.42
32:DD:150[A]:MEQ:OE1	55:DA:2032:G:H1'	2.19	0.42
41:CN:69:PRO:O	41:CN:93:VAL:O	2.37	0.42
51:DX:21:LEU:HD11	51:DX:41[A]:ARG:HE	1.83	0.42
1:BA:957:U:O2	1:BA:959:A:H8	2.02	0.42
28:CB:14:U:H2'	28:CB:15:A:H2	1.84	0.42
31:CA:184:C:H2'	31:CA:185:G:H8	1.83	0.42
37:CJ:14:ALA:HB3	37:CJ:17:MET:HB2	2.00	0.42
1:AA:1346:A:H61	1:AA:1374:A:H3'	1.84	0.42
11:AK:84:VAL:HG11	11:AK:97:ILE:HG12	2.00	0.42
13:AM:80:LEU:HD22	13:AM:87:ARG:HB3	2.01	0.42
1:BA:429:U:H1'	1:BA:430:A:H5''	2.01	0.42
9:BI:19:VAL:HG11	9:BI:83:ILE:HA	2.01	0.42
31:CA:685:A:H1'	31:CA:688:U:O4	2.20	0.42
31:CA:1182:G:H2'	31:CA:1183:U:O4'	2.19	0.42
31:CA:2261:C:H5''	51:CX:19:LYS:HZ1	1.84	0.42
36:CH:3:VAL:HG12	36:CH:38:PRO:HA	2.01	0.42
39:CL:35:VAL:HG12	39:CL:106:GLU:HG2	1.99	0.42
41:CN:77:PRO:HG2	41:CN:80:VAL:HG21	2.02	0.42
48:DU:11:LEU:HD22	48:DU:32:LEU:HD13	2.01	0.42
6:AF:16:GLU:HB3	4:BD:189:SER:HA	2.01	0.42
1:BA:1068:G:N7	1:BA:1094:G:H2'	2.35	0.42
4:BD:48:LEU:HD21	4:BD:56:ARG:HG3	2.01	0.42
13:BM:54:ASP:HA	13:BM:57:ARG:HD2	2.01	0.42
29:CC:35:GLU:HG3	29:CC:64:ILE:HD11	2.01	0.42
31:CA:571:U:H4'	31:CA:573:U:H5	1.84	0.42
31:CA:1250:G:C5'	45:CR:6:ARG:HD3	2.49	0.42
31:CA:2339:C:H2'	31:CA:2340:A:C8	2.55	0.42
33:CE:3:LEU:HD12	33:CE:14:VAL:HG11	2.01	0.42
36:CH:104:THR:HG22	36:CH:109:GLU:HA	1.99	0.42
38:CK:58:ASN:HA	38:CK:126:ALA:O	2.19	0.42
40:CM:28:GLY:O	40:CM:29:LYS:C	2.61	0.42
37:DJ:11:LEU:HD22	37:DJ:24:VAL:HG23	2.01	0.42
54:DI:50:VAL:HG11	54:DI:92:ALA:HB2	2.00	0.42
10:AJ:19:ASP:HA	10:AJ:22:THR:HB	2.02	0.42
10:BJ:26:VAL:HG21	10:BJ:39:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:142:A:H2'	31:CA:143:C:C6	2.54	0.42
40:CM:95:LEU:HD22	40:CM:100:ILE:HG12	2.01	0.42
44:DQ:92:VAL:HG21	44:DQ:97:LEU:HD11	2.02	0.42
46:DS:79:ARG:NH2	55:DA:572:A:H5'	2.34	0.42
55:DA:634:C:H2'	55:DA:635:C:C6	2.55	0.42
55:DA:2327:A:H5''	70:DA:7160:HOH:O	2.19	0.42
55:DA:2328:A:H2'	55:DA:2329:U:C6	2.54	0.42
6:AF:102:MET:HE1	18:AR:24:LYS:HB3	2.02	0.42
23:D2:15:ALA:HB2	23:D2:47:VAL:HG21	2.02	0.42
31:CA:580:U:O3'	45:CR:31:VAL:HG13	2.20	0.42
31:CA:976:G:H2'	31:CA:977:G:H8	1.84	0.42
31:CA:1386:C:H2'	31:CA:1387:A:C8	2.55	0.42
34:CF:104:ILE:HG23	34:CF:176:PRO:HD3	2.01	0.42
1:AA:1289:A:H3'	1:AA:1290:G:H8	1.85	0.42
4:AD:48:LEU:HD21	4:AD:56:ARG:HG3	2.02	0.42
26:C5:4:ARG:HB2	31:CA:2466:C:OP1	2.19	0.42
1:BA:76:G:H1	1:BA:93:U:H3	1.68	0.42
1:BA:1508:A:H2'	1:BA:1509:C:O4'	2.20	0.42
30:CD:3:GLY:O	30:CD:4:LEU:HD13	2.20	0.42
31:CA:2060:A:N6	33:CE:69:ARG:NH2	2.67	0.42
31:CA:2328:A:H2'	31:CA:2329:U:C6	2.55	0.42
34:CF:130:MET:HE2	34:CF:154:ILE:HD12	2.01	0.42
49:CV:94:ARG:HB3	49:CV:103:ILE:HD12	2.02	0.42
41:DN:16:ARG:HG3	41:DN:18[B]:ARG:NH1	2.34	0.42
54:DI:12:VAL:O	54:DI:16:SER:HB2	2.19	0.42
55:DA:1381:G:H1'	55:DA:1571:A:N1	2.34	0.42
11:AK:31:ILE:HG12	11:AK:46:THR:CG2	2.47	0.42
1:BA:1346:A:H61	1:BA:1374:A:H3'	1.85	0.42
37:CJ:11:LEU:HD22	37:CJ:24:VAL:HG23	2.02	0.42
37:CJ:19:ASN:N	37:CJ:20:PRO:HD2	2.34	0.42
55:DA:476:G:H4'	55:DA:502:A:N1	2.35	0.42
55:DA:644:A:H2'	55:DA:645:C:O4'	2.20	0.42
1:AA:429:U:H1'	1:AA:430:A:H5''	2.01	0.42
1:AA:1250:A:O3'	9:AI:69:GLY:HA2	2.20	0.42
6:AF:47:LEU:HD13	6:AF:51:ILE:HG12	2.01	0.42
16:AP:61:VAL:HG21	16:AP:67:ILE:HD11	2.01	0.42
26:C5:8:LYS:HE3	31:CA:1031:G:H5''	2.02	0.42
1:BA:214:C:H2'	1:BA:215:C:H6	1.85	0.42
5:BE:81:LEU:HB3	5:BE:147:MET:SD	2.60	0.42
31:CA:1077:A:H4'	37:CJ:94:ASN:HB2	2.02	0.42
37:CJ:24:VAL:HG22	37:CJ:28:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DJ:19:ASN:N	37:DJ:20:PRO:HD2	2.34	0.42
50:DW:51:GLN:HB2	50:DW:57:TYR:OH	2.19	0.42
55:DA:624:C:O2'	55:DA:657:U:H5''	2.20	0.42
55:DA:2262:U:H4'	55:DA:2328:A:H2	1.85	0.42
55:DA:2514:U:H2'	55:DA:2515:C:C6	2.54	0.42
1:AA:1057:G:O3'	3:AC:197:GLY:HA3	2.20	0.42
1:AA:1238:A:H5'	1:AA:1336:C:H41	1.84	0.42
10:AJ:5:ARG:HG3	10:AJ:77:VAL:HA	2.02	0.42
1:BA:17:U:H2'	1:BA:18:C:C6	2.55	0.42
9:BI:6:TYR:HB2	9:BI:21:ILE:HB	2.02	0.42
31:CA:782:A:H4'	31:CA:783:A:O5'	2.19	0.42
31:CA:2626:C:H2'	31:CA:2627:G:O4'	2.19	0.42
33:DE:131:THR:HG23	33:DE:160:ALA:O	2.19	0.42
45:DR:6:ARG:NH1	55:DA:585:G:N7	2.67	0.42
55:DA:1353:A:O4'	55:DA:1569:A:H2	2.01	0.42
55:DA:2339:C:H2'	55:DA:2340:A:C8	2.55	0.42
55:DA:2585:U:O2'	55:DA:2586:U:H5'	2.20	0.42
1:AA:322:C:H5	1:AA:328:C:C5	2.37	0.41
1:AA:1108:G:H5''	3:AC:176:HIS:ND1	2.35	0.41
4:BD:130:VAL:HG11	4:BD:135:TYR:CG	2.54	0.41
5:BE:126:LYS:HG2	5:BE:128:TYR:CZ	2.55	0.41
13:BM:6:GLY:O	13:BM:7:ILE:HG13	2.20	0.41
29:CC:85:PRO:HG3	31:CA:1567:G:H3'	2.02	0.41
31:CA:538:A:H4'	38:CK:7:LYS:HG2	2.02	0.41
42:DO:28:LEU:HD23	42:DO:48:VAL:HG21	2.02	0.41
46:DS:21:ARG:HH21	57:DS:202:PG4:H71	1.85	0.41
49:DV:17:LYS:HE3	49:DV:40:ASN:HA	2.02	0.41
55:DA:503:A:H5'	55:DA:505:A:OP1	2.20	0.41
1:AA:77:A:H2'	1:AA:78:A:C8	2.55	0.41
3:AC:7:PRO:HD2	3:AC:184:TYR:CD1	2.55	0.41
11:AK:25:ALA:HA	11:AK:30:THR:HG22	2.02	0.41
1:BA:1308:U:H2'	1:BA:1309:G:H8	1.85	0.41
6:BF:99:ALA:O	6:BF:100:SER:HB3	2.19	0.41
31:CA:340:A:H2'	31:CA:341:C:O4'	2.20	0.41
31:CA:2313:C:H5''	34:CF:88:LYS:HD3	2.02	0.41
31:CA:2728:U:O2'	31:CA:2729:G:H5''	2.20	0.41
70:DD:411:HOH:O	55:DA:1671:U:H4'	2.20	0.41
39:CL:1:MET:HE3	39:CL:32:TYR:CZ	2.55	0.41
42:CO:28:LEU:HD23	42:CO:48:VAL:HG21	2.01	0.41
50:CW:77:VAL:HG23	50:CW:89:ILE:HG12	2.02	0.41
1:AA:1151:A:O2'	1:AA:1152:A:H8	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1338:G:H2'	1:AA:1339:A:C8	2.56	0.41
9:AI:19:VAL:HG11	9:AI:83:ILE:HA	2.02	0.41
1:BA:1277:C:HO2'	1:BA:1279:G:H8	1.67	0.41
10:BJ:19:ASP:HA	10:BJ:22:THR:HB	2.02	0.41
31:CA:78:U:H2'	31:CA:79:C:C6	2.56	0.41
31:CA:550:C:H2'	31:CA:551:G:H5''	2.03	0.41
48:CU:45:ALA:O	48:CU:49:LYS:HG2	2.19	0.41
50:CW:51:GLN:HB2	50:CW:57:TYR:OH	2.21	0.41
38:DK:58:ASN:HA	38:DK:126:ALA:O	2.21	0.41
54:DI:94:ARG:HG2	54:DI:127:ALA:HA	2.01	0.41
55:DA:825:A:H5''	59:DA:3223:PUT:H12	2.02	0.41
1:AA:1508:A:H2'	1:AA:1509:C:O4'	2.21	0.41
31:CA:1101:U:H2'	31:CA:1102:C:H6	1.86	0.41
31:CA:1326:U:H2'	31:CA:1327:A:H8	1.85	0.41
34:CF:40:VAL:HG23	34:CF:86:GLY:HA2	2.02	0.41
34:DF:34:ILE:HG12	34:DF:156:ILE:HG12	2.02	0.41
34:DF:36:LEU:HB2	34:DF:57:LEU:HD21	2.02	0.41
55:DA:825:A:H2'	55:DA:826:U:O4'	2.21	0.41
55:DA:1515:A:H2'	55:DA:1516:G:O4'	2.20	0.41
55:DA:2255:G:H21	69:DA:3220:TRS:H12	1.85	0.41
55:DA:2324:U:H3'	55:DA:2325:G:C5'	2.51	0.41
2:AB:187:VAL:HG13	2:AB:191:SER:HB2	2.03	0.41
14:AN:46:LEU:HA	14:AN:49:GLN:HE21	1.85	0.41
16:AP:57:ILE:O	16:AP:61:VAL:HG23	2.20	0.41
23:C2:15:ALA:HB2	23:C2:47:VAL:HG21	2.03	0.41
1:BA:1238:A:H5'	1:BA:1336:C:H41	1.85	0.41
13:BM:80:LEU:HD22	13:BM:87:ARG:HB3	2.02	0.41
31:CA:2579:C:H2'	31:CA:2580:PSU:O4'	2.20	0.41
5:AE:15:LEU:HA	5:AE:37:THR:HG22	2.03	0.41
8:AH:96:MET:CE	8:AH:130:ALA:HB1	2.49	0.41
1:BA:715:A:H2'	1:BA:716:A:C8	2.54	0.41
31:CA:477:A:H2'	31:CA:478:A:C8	2.55	0.41
31:CA:784:G:H3'	70:CA:3540:HOH:O	2.20	0.41
31:CA:1141:U:H4'	31:CA:1142:A:O4'	2.20	0.41
31:CA:1363:C:H2'	31:CA:1364:G:H8	1.85	0.41
36:CH:27:ARG:HA	36:CH:27:ARG:HD3	1.92	0.41
33:DE:45:ALA:HB3	55:DA:38:A:H5'	2.02	0.41
39:DL:1:MET:HE3	39:DL:32:TYR:CZ	2.55	0.41
52:DY:29:PHE:HB3	55:DA:396:G:H1'	2.02	0.41
54:DI:130:PRO:HG2	54:DI:134:GLU:HG2	2.02	0.41
55:DA:68:G:H2'	55:DA:69:C:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:572:A:H5''	55:DA:573:U:OP2	2.21	0.41
55:DA:1386:C:H2'	55:DA:1387:A:C8	2.55	0.41
55:DA:2117:A:H61	55:DA:2171:A:H61	1.69	0.41
1:BA:216:U:H4'	1:BA:464:U:H4'	2.02	0.41
1:BA:310:G:H5''	16:BP:31:ARG:HB2	2.02	0.41
1:BA:1250:A:O3'	9:BI:69:GLY:HA2	2.21	0.41
9:BI:99:ARG:HG2	9:BI:104:VAL:HG21	2.01	0.41
11:BK:45:ALA:HB3	11:BK:70:CYS:HB2	2.03	0.41
19:BS:30:PRO:HB2	19:BS:50:ALA:HB2	2.03	0.41
31:CA:1294:U:H5''	31:CA:1294:U:H6	1.85	0.41
31:CA:1311:G:N2	31:CA:1603:A:H62	2.14	0.41
31:CA:1638:C:H5''	31:CA:2710:C:O2'	2.21	0.41
31:CA:2641:G:H5''	38:CK:78:THR:HB	2.02	0.41
34:DF:132:VAL:HG22	34:DF:152:LEU:HG	2.03	0.41
35:DG:52:PHE:CD1	35:DG:52:PHE:N	2.89	0.41
36:DH:126:GLY:H	36:DH:146:VAL:HB	1.85	0.41
49:DV:94:ARG:HB3	49:DV:103:ILE:HD12	2.01	0.41
55:DA:1804:C:H6	55:DA:1804:C:O5'	2.03	0.41
1:AA:1052:G:H22	1:AA:1206:G:H1	1.69	0.41
1:BA:815:A:H4'	1:BA:817:C:C4	2.56	0.41
1:BA:1289:A:H3'	1:BA:1290:G:H8	1.85	0.41
1:BA:1391:U:H2'	1:BA:1392:G:C8	2.56	0.41
23:D2:11:LEU:HD21	23:D2:34:LEU:HD23	2.03	0.41
31:CA:184:C:H2'	31:CA:185:G:C8	2.55	0.41
29:DC:146:MET:HE1	55:DA:1800:C:H5''	2.02	0.41
36:CH:126:GLY:H	36:CH:146:VAL:HB	1.86	0.41
33:DE:49:ARG:O	33:DE:74:LYS:HD2	2.21	0.41
34:DF:130:MET:HE2	34:DF:154:ILE:HD12	2.02	0.41
1:AA:17:U:H2'	1:AA:18:C:C6	2.56	0.41
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.56	0.41
11:AK:34:ILE:HG12	11:AK:70:CYS:SG	2.61	0.41
1:BA:23:C:H5	1:BA:561:U:O4	2.04	0.41
1:BA:129:A:H1'	1:BA:130:A:C8	2.56	0.41
6:BF:91:ARG:HD2	18:BR:61:ARG:HH22	1.85	0.41
11:BK:31:ILE:HB	11:BK:46:THR:HG22	2.03	0.41
16:BP:61:VAL:HG21	16:BP:67:ILE:HD11	2.03	0.41
31:CA:685:A:H5''	31:CA:774:G:O6	2.21	0.41
31:CA:1808:A:N1	52:CY:28:ARG:HD2	2.35	0.41
31:CA:1957:C:H5'	31:CA:1984:G:O2'	2.21	0.41
31:CA:2114:A:N6	31:CA:2119:A:H62	2.18	0.41
31:CA:2304:G:H5'	34:CF:121:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DF:104:ILE:HG23	34:DF:176:PRO:HD3	2.02	0.41
36:DH:3:VAL:HG12	36:DH:38:PRO:HA	2.03	0.41
42:DO:8:ARG:HB3	42:DO:10:LEU:HG	2.03	0.41
42:DO:53:THR:HA	42:DO:56:LYS:HD2	2.03	0.41
55:DA:839:U:H2'	55:DA:840:C:C6	2.56	0.41
55:DA:1321:A:C2	64:DA:3217:PGE:H12	2.56	0.41
55:DA:1604:C:H5'	70:DA:3811:HOH:O	2.21	0.41
55:DA:2345:G:N3	55:DA:2381:A:H2'	2.36	0.41
1:AA:1141:C:O2'	1:AA:1142:G:H8	2.04	0.41
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.55	0.41
6:AF:70:VAL:HA	6:AF:73:GLU:HG2	2.04	0.41
1:BA:502:A:OP1	12:BL:115:SER:HB2	2.21	0.41
1:BA:1060:U:H4'	10:BJ:53:ILE:HG23	2.03	0.41
4:BD:10:LYS:HG2	4:BD:38:PRO:HB3	2.03	0.41
11:BK:25:ALA:HA	11:BK:30:THR:HG22	2.03	0.41
11:BK:72:ASP:C	11:BK:74:VAL:H	2.29	0.41
31:CA:574:A:C6	31:CA:2033:A:H5'	2.55	0.41
31:CA:666:A:H4'	40:CM:48:ARG:HD3	2.02	0.41
31:CA:1203:U:H1'	40:CM:4:ASN:HB3	2.03	0.41
31:CA:1494:A:H2'	31:CA:1495:A:C8	2.55	0.41
31:CA:2038:G:H2'	31:CA:2039:U:O4'	2.21	0.41
32:DD:152:PRO:HG3	32:DD:156:PHE:CZ	2.56	0.41
55:DA:78:U:H2'	55:DA:79:C:C6	2.56	0.41
55:DA:1802:A:N1	55:DA:1822:C:H1'	2.35	0.41
55:DA:2422:C:H1'	70:DA:3441:HOH:O	2.20	0.41
60:AA:1680:T1C:O1C	60:AA:1680:T1C:H422	2.21	0.40
1:BA:302:G:N3	1:BA:556:C:H4'	2.36	0.40
1:BA:1069:C:H4'	1:BA:1192:C:O2	2.20	0.40
29:CC:171:TYR:CD1	29:CC:185:GLU:HA	2.56	0.40
31:CA:494:G:H4'	47:CT:6:LYS:HB2	2.02	0.40
31:CA:2680:U:H2'	31:CA:2681:C:C6	2.56	0.40
34:CF:8:TYR:HA	34:CF:12:VAL:HB	2.03	0.40
36:CH:94:ILE:HB	36:CH:122:LEU:HB2	2.03	0.40
34:DF:121:SER:HB2	55:DA:2304:G:H5'	2.02	0.40
54:DI:70:GLU:HG2	54:DI:73:LYS:HE3	2.02	0.40
55:DA:281:C:H2'	55:DA:282:A:C8	2.56	0.40
55:DA:455:C:N3	55:DA:472:A:H2'	2.36	0.40
55:DA:837:C:H5	70:DA:6009:HOH:O	2.04	0.40
55:DA:2544:G:H2'	55:DA:2545:G:O4'	2.22	0.40
1:AA:129:A:H1'	1:AA:130:A:C8	2.57	0.40
1:AA:310:G:H5''	16:AP:31:ARG:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:340:U:H2'	1:AA:341:C:C6	2.57	0.40
1:AA:502:A:H2'	1:AA:503:C:O4'	2.22	0.40
9:AI:6:TYR:HB2	9:AI:21:ILE:HB	2.02	0.40
1:BA:1141:C:O2'	1:BA:1142:G:H8	2.04	0.40
4:BD:102:VAL:HG13	4:BD:107:PHE:HB2	2.03	0.40
15:BO:64:ARG:HH22	15:BO:88:ARG:NH2	2.19	0.40
31:CA:1469:A:H2'	31:CA:1470:A:C8	2.57	0.40
54:DI:28:ALA:HA	54:DI:109:LYS:H	1.86	0.40
54:DI:29:ASP:HB3	54:DI:106:PHE:HB2	2.03	0.40
54:DI:56:ARG:HA	55:DA:1107:G:OP1	2.22	0.40
55:DA:481:G:C4	55:DA:507:A:C2	3.09	0.40
1:AA:1322:C:P	19:AS:78:ARG:HH22	2.44	0.40
23:C2:11:LEU:HD21	23:C2:34:LEU:HD23	2.03	0.40
1:BA:579:A:H2'	1:BA:580:C:C6	2.56	0.40
1:BA:1057:G:O3'	3:BC:197:GLY:HA3	2.21	0.40
17:BQ:46:VAL:HG11	17:BQ:61:ILE:CG2	2.52	0.40
31:CA:352:A:H8	31:CA:352:A:H5''	1.87	0.40
31:CA:1914:C:H2'	31:CA:1915:3TD:H6	2.02	0.40
34:CF:34:ILE:HG12	34:CF:156:ILE:HG12	2.03	0.40
34:DF:40:VAL:HG23	34:DF:86:GLY:HA2	2.03	0.40
55:DA:612:G:H4'	55:DA:613:A:C2	2.56	0.40
1:AA:620:C:H2'	1:AA:621:A:O4'	2.21	0.40
10:AJ:65:TYR:HB2	14:AN:96:LEU:HD11	2.04	0.40
1:BA:224:U:H2'	1:BA:225:C:C6	2.57	0.40
1:BA:368:U:O4	36:DH:83:LYS:HB2	2.21	0.40
64:D1:102:PGE:H4	70:DT:319:HOH:O	2.21	0.40
29:CC:76:ALA:HB2	29:CC:96:TYR:CD1	2.56	0.40
29:CC:105:LEU:HD12	29:CC:105:LEU:N	2.36	0.40
31:CA:2353:G:H2'	31:CA:2354:C:O4'	2.20	0.40
34:DF:8:TYR:HA	34:DF:12:VAL:HB	2.03	0.40
34:DF:36:LEU:HD22	34:DF:154:ILE:HG12	2.02	0.40
39:DL:7:MET:HE1	39:DL:44:LYS:HG3	2.02	0.40
39:DL:113:MET:O	39:DL:116:ILE:HG13	2.22	0.40
55:DA:1441:G:H2'	55:DA:1442:U:C6	2.55	0.40
55:DA:1532:A:H8	55:DA:1532:A:H5''	1.85	0.40
3:AC:5:VAL:HG21	3:AC:10:ILE:HD13	2.04	0.40
4:AD:10:LYS:HG2	4:AD:38:PRO:HB3	2.03	0.40
1:BA:33:A:H2'	1:BA:34:C:C6	2.56	0.40
1:BA:202:G:H21	1:BA:466:A:H61	1.68	0.40
1:BA:591:U:H2'	1:BA:592:G:C8	2.57	0.40
1:BA:1338:G:H2'	1:BA:1339:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:BR:28:THR:HG22	18:BR:32:TYR:HE1	1.87	0.40
28:CB:111:U:H2'	28:CB:112:G:H8	1.87	0.40
31:CA:569:U:H5''	31:CA:821:A:C2	2.56	0.40
31:CA:1510:G:H2'	31:CA:1511:G:O4'	2.22	0.40
39:CL:113:MET:O	39:CL:116:ILE:HG13	2.21	0.40
47:CT:69:LEU:HG	47:CT:107:VAL:CG2	2.50	0.40
46:DS:24:LYS:HD2	64:DS:201:PGE:H22	2.03	0.40
55:DA:352:A:H8	55:DA:352:A:H5''	1.86	0.40
55:DA:2038:G:H2'	55:DA:2039:U:O4'	2.22	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%)	6	28
2	BB	222/224 (99%)	207 (93%)	11 (5%)	4 (2%)	6	28
3	AC	204/206 (99%)	194 (95%)	9 (4%)	1 (0%)	24	57
3	BC	204/206 (99%)	195 (96%)	7 (3%)	2 (1%)	12	41
4	AD	203/205 (99%)	197 (97%)	6 (3%)	0	100	100
4	BD	203/205 (99%)	197 (97%)	6 (3%)	0	100	100
5	AE	153/155 (99%)	144 (94%)	7 (5%)	2 (1%)	9	35
5	BE	148/155 (96%)	131 (88%)	14 (10%)	3 (2%)	6	25
6	AF	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
6	BF	98/106 (92%)	91 (93%)	5 (5%)	2 (2%)	6	25
7	AG	149/151 (99%)	135 (91%)	13 (9%)	1 (1%)	18	49
7	BG	149/151 (99%)	137 (92%)	12 (8%)	0	100	100
8	AH	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	BH	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	7	30
9	AI	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
9	BI	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
10	AJ	97/99 (98%)	89 (92%)	7 (7%)	1 (1%)	12	41
10	BJ	96/99 (97%)	77 (80%)	13 (14%)	6 (6%)	1	6
11	AK	115/117 (98%)	105 (91%)	9 (8%)	1 (1%)	14	44
11	BK	115/117 (98%)	104 (90%)	10 (9%)	1 (1%)	14	44
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
12	BL	120/123 (98%)	111 (92%)	8 (7%)	1 (1%)	16	47
13	AM	112/114 (98%)	102 (91%)	7 (6%)	3 (3%)	4	20
13	BM	112/114 (98%)	101 (90%)	6 (5%)	5 (4%)	2	12
14	AN	98/100 (98%)	87 (89%)	9 (9%)	2 (2%)	6	25
14	BN	98/100 (98%)	87 (89%)	10 (10%)	1 (1%)	12	41
15	AO	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
15	BO	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	10	37
16	AP	80/82 (98%)	73 (91%)	5 (6%)	2 (2%)	4	21
16	BP	80/82 (98%)	68 (85%)	10 (12%)	2 (2%)	4	21
17	AQ	78/80 (98%)	71 (91%)	6 (8%)	1 (1%)	9	35
17	BQ	78/80 (98%)	67 (86%)	7 (9%)	4 (5%)	1	10
18	AR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
19	BS	77/79 (98%)	66 (86%)	10 (13%)	1 (1%)	9	35
20	AT	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
20	BT	83/86 (96%)	79 (95%)	3 (4%)	1 (1%)	10	37
21	AU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
21	BU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
22	C1	54/56 (96%)	47 (87%)	4 (7%)	3 (6%)	1	8
22	D1	54/56 (96%)	54 (100%)	0	0	100	100
23	C2	48/51 (94%)	43 (90%)	3 (6%)	2 (4%)	2	13
23	D2	49/51 (96%)	47 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	C3	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	5	23
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	C4	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
25	D4	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
26	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	20
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	51 (91%)	3 (5%)	2 (4%)	2	16
27	D0	57/58 (98%)	53 (93%)	4 (7%)	0	100	100
29	CC	269/272 (99%)	249 (93%)	15 (6%)	5 (2%)	6	27
29	DC	269/272 (99%)	251 (93%)	16 (6%)	2 (1%)	18	49
30	CD	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
32	DD	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
33	CE	199/201 (99%)	189 (95%)	7 (4%)	3 (2%)	8	32
33	DE	199/201 (99%)	191 (96%)	7 (4%)	1 (0%)	24	57
34	CF	175/178 (98%)	166 (95%)	9 (5%)	0	100	100
34	DF	175/178 (98%)	166 (95%)	9 (5%)	0	100	100
35	CG	174/176 (99%)	162 (93%)	7 (4%)	5 (3%)	3	19
35	DG	174/176 (99%)	165 (95%)	7 (4%)	2 (1%)	11	39
36	CH	147/149 (99%)	130 (88%)	11 (8%)	6 (4%)	2	13
36	DH	147/149 (99%)	133 (90%)	11 (8%)	3 (2%)	6	25
37	CJ	132/135 (98%)	125 (95%)	3 (2%)	4 (3%)	3	19
37	DJ	132/135 (98%)	125 (95%)	3 (2%)	4 (3%)	3	19
38	CK	140/142 (99%)	135 (96%)	2 (1%)	3 (2%)	5	25
38	DK	140/142 (99%)	136 (97%)	2 (1%)	2 (1%)	9	34
39	CL	120/123 (98%)	114 (95%)	4 (3%)	2 (2%)	7	30
39	DL	121/123 (98%)	116 (96%)	4 (3%)	1 (1%)	16	47
40	CM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	5	25
40	DM	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	18	49
41	CN	133/136 (98%)	125 (94%)	7 (5%)	1 (1%)	16	47
41	DN	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
42	CO	118/125 (94%)	110 (93%)	6 (5%)	2 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	DO	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
43	CP	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
43	DP	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
44	CQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	14	44
44	DQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	14	44
45	CR	115/117 (98%)	110 (96%)	4 (4%)	1 (1%)	14	44
45	DR	115/117 (98%)	110 (96%)	4 (4%)	1 (1%)	14	44
46	CS	101/103 (98%)	91 (90%)	7 (7%)	3 (3%)	3	19
46	DS	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	12	41
47	CT	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
47	DT	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
48	CU	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
48	DU	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
49	CV	100/103 (97%)	90 (90%)	6 (6%)	4 (4%)	2	13
49	DV	100/103 (97%)	96 (96%)	2 (2%)	2 (2%)	6	25
50	CW	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
50	DW	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
51	CX	73/83 (88%)	72 (99%)	1 (1%)	0	100	100
51	DX	75/83 (90%)	74 (99%)	1 (1%)	0	100	100
52	CY	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
52	DY	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
53	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	30
53	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
54	DI	133/135 (98%)	112 (84%)	15 (11%)	6 (4%)	2	12
All	All	11407/11651 (98%)	10682 (94%)	590 (5%)	135 (1%)	10	37

All (135) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
23	C2	5	ILE
2	BB	126	PHE
3	BC	156	ARG
6	BF	98	GLU
10	BJ	38	GLY
10	BJ	91	ASP
13	BM	7	ILE
17	BQ	82	ALA
20	BT	5	LYS
29	CC	158	ALA
33	CE	83	VAL
35	CG	119	ALA
35	CG	175	LYS
35	CG	176	LYS
36	CH	10	ALA
37	CJ	19	ASN
38	CK	81	ILE
39	CL	35	VAL
40	CM	29	LYS
41	CN	70	ASP
49	CV	7	ARG
36	DH	11	ASN
37	DJ	19	ASN
49	DV	52	LEU
54	DI	91	ALA
5	AE	109	GLY
7	AG	56	LYS
10	AJ	57	VAL
13	AM	105	ASN
14	AN	38	ASP
27	C0	14	ILE
3	BC	61	ALA
10	BJ	57	VAL
13	BM	5	ALA
13	BM	105	ASN
13	BM	114	LYS
14	BN	38	ASP
16	BP	80	LYS
17	BQ	70	THR
19	BS	6	LYS
29	CC	233	GLY
29	DC	233	GLY

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Mol	Chain	Res	Type
33	CE	6	LYS
33	CE	82	GLY
35	CG	46	ALA
37	CJ	25	GLY
39	CL	108	ARG
40	CM	69	ARG
49	CV	16	GLY
49	CV	17	LYS
33	DE	6	LYS
35	DG	46	ALA
37	DJ	25	GLY
44	DQ	105	GLY
2	AB	95	ARG
2	AB	125	THR
11	AK	89	PRO
22	C1	26	THR
22	C1	27	SER
24	C3	45	SER
2	BB	95	ARG
2	BB	125	THR
5	BE	103	THR
10	BJ	95	GLY
11	BK	89	PRO
12	BL	44	LYS
15	BO	88	ARG
29	CC	197	ASN
29	CC	253	LYS
29	DC	253	LYS
36	CH	11	ASN
36	CH	122	LEU
38	CK	95	ARG
40	CM	36	LYS
42	CO	118	ARG
42	CO	119	SER
49	CV	89	ASP
36	DH	122	LEU
38	DK	95	ARG
40	DM	36	LYS
49	DV	89	ASP
54	DI	130	PRO
2	AB	127	ASP
8	AH	66	PHE

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Mol	Chain	Res	Type
16	AP	24	SER
23	C2	51	GLU
26	C5	21	GLY
27	C0	4	THR
2	BB	127	ASP
5	BE	24	THR
5	BE	157	ARG
8	BH	66	PHE
8	BH	67	GLN
10	BJ	36	VAL
13	BM	4	ILE
16	BP	24	SER
36	CH	9	VAL
38	CK	25	LEU
46	CS	43	ASN
46	CS	48	LYS
38	DK	25	LEU
46	DS	44	GLY
54	DI	70	GLU
54	DI	88	HIS
5	AE	162	GLU
13	AM	7	ILE
16	AP	45	GLU
17	BQ	17	MET
17	BQ	18	GLU
29	CC	108	LYS
35	CG	45	HIS
37	CJ	23	PRO
35	DG	45	HIS
37	DJ	23	PRO
39	DL	108	ARG
54	DI	108	VAL
14	AN	81	ARG
6	BF	92	THR
10	BJ	93	ALA
36	CH	8	LYS
37	CJ	32	GLY
44	CQ	105	GLY
46	CS	53	PHE
53	CZ	62	GLY
37	DJ	32	GLY
45	DR	7	GLY

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Mol	Chain	Res	Type
54	DI	109	LYS
36	DH	118	PRO
36	CH	118	PRO
45	CR	7	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/186 (100%)	170 (91%)	16 (9%)	10	34
2	BB	186/186 (100%)	171 (92%)	15 (8%)	11	36
3	AC	170/170 (100%)	156 (92%)	14 (8%)	10	36
3	BC	170/170 (100%)	156 (92%)	14 (8%)	10	36
4	AD	172/172 (100%)	165 (96%)	7 (4%)	27	59
4	BD	172/172 (100%)	165 (96%)	7 (4%)	27	59
5	AE	118/118 (100%)	101 (86%)	17 (14%)	3	14
5	BE	113/118 (96%)	90 (80%)	23 (20%)	1	5
6	AF	92/92 (100%)	84 (91%)	8 (9%)	9	34
6	BF	87/92 (95%)	75 (86%)	12 (14%)	3	15
7	AG	124/124 (100%)	111 (90%)	13 (10%)	6	26
7	BG	124/124 (100%)	108 (87%)	16 (13%)	4	18
8	AH	104/104 (100%)	89 (86%)	15 (14%)	3	14
8	BH	104/104 (100%)	90 (86%)	14 (14%)	4	16
9	AI	105/105 (100%)	99 (94%)	6 (6%)	18	49
9	BI	105/105 (100%)	99 (94%)	6 (6%)	18	49
10	AJ	87/87 (100%)	79 (91%)	8 (9%)	8	31
10	BJ	86/87 (99%)	74 (86%)	12 (14%)	3	15
11	AK	90/90 (100%)	90 (100%)	0	100	100
11	BK	90/90 (100%)	85 (94%)	5 (6%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	102/102 (100%)	94 (92%)	8 (8%)	11	38
12	BL	102/102 (100%)	91 (89%)	11 (11%)	6	25
13	AM	92/92 (100%)	84 (91%)	8 (9%)	9	34
13	BM	92/92 (100%)	87 (95%)	5 (5%)	20	50
14	AN	83/83 (100%)	81 (98%)	2 (2%)	43	69
14	BN	83/83 (100%)	81 (98%)	2 (2%)	43	69
15	AO	76/76 (100%)	72 (95%)	4 (5%)	20	51
15	BO	76/76 (100%)	73 (96%)	3 (4%)	28	60
16	AP	65/65 (100%)	63 (97%)	2 (3%)	35	64
16	BP	65/65 (100%)	57 (88%)	8 (12%)	4	20
17	AQ	74/74 (100%)	65 (88%)	9 (12%)	5	20
17	BQ	74/74 (100%)	66 (89%)	8 (11%)	6	25
18	AR	48/48 (100%)	45 (94%)	3 (6%)	16	45
18	BR	48/48 (100%)	47 (98%)	1 (2%)	47	71
19	AS	70/70 (100%)	61 (87%)	9 (13%)	4	18
19	BS	70/70 (100%)	63 (90%)	7 (10%)	7	29
20	AT	65/65 (100%)	60 (92%)	5 (8%)	12	38
20	BT	65/65 (100%)	53 (82%)	12 (18%)	1	8
21	AU	48/48 (100%)	44 (92%)	4 (8%)	10	35
21	BU	48/48 (100%)	44 (92%)	4 (8%)	10	35
22	C1	47/47 (100%)	46 (98%)	1 (2%)	47	71
22	D1	47/47 (100%)	46 (98%)	1 (2%)	47	71
23	C2	45/46 (98%)	41 (91%)	4 (9%)	9	33
23	D2	45/46 (98%)	39 (87%)	6 (13%)	4	17
24	C3	38/38 (100%)	36 (95%)	2 (5%)	20	51
24	D3	38/38 (100%)	37 (97%)	1 (3%)	40	68
25	C4	51/51 (100%)	49 (96%)	2 (4%)	28	60
25	D4	51/51 (100%)	50 (98%)	1 (2%)	48	72
26	C5	34/34 (100%)	33 (97%)	1 (3%)	37	66
26	D5	34/34 (100%)	34 (100%)	0	100	100
27	C0	48/48 (100%)	39 (81%)	9 (19%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	D0	49/48 (102%)	46 (94%)	3 (6%)	17	46
29	CC	216/217 (100%)	200 (93%)	16 (7%)	13	40
29	DC	216/217 (100%)	206 (95%)	10 (5%)	24	55
30	CD	164/164 (100%)	156 (95%)	8 (5%)	22	53
32	DD	163/163 (100%)	157 (96%)	6 (4%)	30	61
33	CE	165/165 (100%)	151 (92%)	14 (8%)	10	35
33	DE	165/165 (100%)	160 (97%)	5 (3%)	36	65
34	CF	148/149 (99%)	129 (87%)	19 (13%)	4	18
34	DF	148/149 (99%)	132 (89%)	16 (11%)	6	25
35	CG	137/137 (100%)	131 (96%)	6 (4%)	25	56
35	DG	137/137 (100%)	131 (96%)	6 (4%)	25	56
36	CH	114/114 (100%)	99 (87%)	15 (13%)	4	17
36	DH	114/114 (100%)	98 (86%)	16 (14%)	3	15
37	CJ	104/105 (99%)	97 (93%)	7 (7%)	15	43
37	DJ	104/105 (99%)	97 (93%)	7 (7%)	15	43
38	CK	116/116 (100%)	112 (97%)	4 (3%)	32	63
38	DK	116/116 (100%)	113 (97%)	3 (3%)	40	68
39	CL	103/104 (99%)	98 (95%)	5 (5%)	22	53
39	DL	104/104 (100%)	101 (97%)	3 (3%)	37	66
40	CM	103/103 (100%)	96 (93%)	7 (7%)	14	42
40	DM	103/103 (100%)	98 (95%)	5 (5%)	22	53
41	CN	108/108 (100%)	101 (94%)	7 (6%)	15	44
41	DN	109/108 (101%)	105 (96%)	4 (4%)	30	61
42	CO	100/102 (98%)	92 (92%)	8 (8%)	11	37
42	DO	102/102 (100%)	98 (96%)	4 (4%)	28	60
43	CP	86/87 (99%)	77 (90%)	9 (10%)	6	26
43	DP	87/87 (100%)	81 (93%)	6 (7%)	14	41
44	CQ	99/99 (100%)	91 (92%)	8 (8%)	11	36
44	DQ	99/99 (100%)	93 (94%)	6 (6%)	17	46
45	CR	89/89 (100%)	84 (94%)	5 (6%)	19	49
45	DR	89/89 (100%)	86 (97%)	3 (3%)	32	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	CS	84/84 (100%)	78 (93%)	6 (7%)	13	41
46	DS	84/84 (100%)	82 (98%)	2 (2%)	43	69
47	CT	93/93 (100%)	87 (94%)	6 (6%)	15	44
47	DT	93/93 (100%)	90 (97%)	3 (3%)	34	64
48	CU	80/80 (100%)	71 (89%)	9 (11%)	5	23
48	DU	80/80 (100%)	76 (95%)	4 (5%)	22	53
49	CV	83/84 (99%)	77 (93%)	6 (7%)	13	40
49	DV	83/84 (99%)	79 (95%)	4 (5%)	23	54
50	CW	78/78 (100%)	72 (92%)	6 (8%)	12	38
50	DW	78/78 (100%)	74 (95%)	4 (5%)	21	52
51	CX	56/62 (90%)	53 (95%)	3 (5%)	20	50
51	DX	58/62 (94%)	55 (95%)	3 (5%)	21	51
52	CY	67/67 (100%)	62 (92%)	5 (8%)	12	39
52	DY	67/67 (100%)	64 (96%)	3 (4%)	24	56
53	CZ	54/54 (100%)	48 (89%)	6 (11%)	6	24
53	DZ	54/54 (100%)	50 (93%)	4 (7%)	13	40
54	DI	103/103 (100%)	95 (92%)	8 (8%)	11	38
All	All	9461/9494 (100%)	8767 (93%)	694 (7%)	13	40

All (694) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	44	GLU
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	183	VAL
2	AB	205	ASP

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Mol	Chain	Res	Type
2	AB	207	ILE
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	75	ILE
3	AC	107	ARG
3	AC	121	THR
3	AC	128	VAL
3	AC	175	LEU
3	AC	178	LEU
3	AC	185	ASN
3	AC	186	THR
3	AC	207	ILE
4	AD	17	THR
4	AD	22	LYS
4	AD	26	ARG
4	AD	28	ILE
4	AD	132	ILE
4	AD	143	VAL
4	AD	151	LYS
5	AE	11	LEU
5	AE	14	LYS
5	AE	32	SER
5	AE	46	VAL
5	AE	71	MET
5	AE	76	LEU
5	AE	78	ASN
5	AE	81	LEU
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	149	SER
5	AE	159	LYS
6	AF	36	ILE
6	AF	39	LEU

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Mol	Chain	Res	Type
6	AF	68	GLN
6	AF	69	GLU
6	AF	71	ILE
6	AF	74	LEU
6	AF	89	VAL
6	AF	93	LYS
7	AG	22	LEU
7	AG	23	LEU
7	AG	30	LEU
7	AG	36	LYS
7	AG	58	GLU
7	AG	59	LEU
7	AG	63	GLU
7	AG	70	ARG
7	AG	76	LYS
7	AG	120	LEU
7	AG	131	LYS
7	AG	133	THR
7	AG	142	HIS
8	AH	3	MET
8	AH	31	LYS
8	AH	47	GLU
8	AH	51	VAL
8	AH	52	GLU
8	AH	54	ASP
8	AH	60	GLU
8	AH	63	LEU
8	AH	76	GLN
8	AH	83	LEU
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	36	GLU
9	AI	61	LEU
9	AI	63	LEU
9	AI	66	THR
9	AI	87	LEU
10	AJ	6	ILE
10	AJ	22	THR

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Mol	Chain	Res	Type
10	AJ	62	ARG
10	AJ	63	ASP
10	AJ	69	THR
10	AJ	88	MET
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	88	LYS
12	AL	90	LEU
12	AL	110	ARG
12	AL	121	ARG
13	AM	7	ILE
13	AM	13	LYS
13	AM	22	ILE
13	AM	27	LYS
13	AM	48	LEU
13	AM	58	ASP
13	AM	63	PHE
13	AM	64	VAL
14	AN	31	ILE
14	AN	80	SER
15	AO	24	SER
15	AO	40	GLN
15	AO	70	LEU
15	AO	89	ARG
16	AP	18	GLN
16	AP	48	GLU
17	AQ	5	ILE
17	AQ	16	LYS
17	AQ	21	ILE
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	34	THR
18	AR	47	THR
18	AR	66	SER

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Mol	Chain	Res	Type
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
19	AS	63	THR
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	16	LEU
21	AU	18	ARG
21	AU	56	HIS
22	C1	10	ARG
23	C2	8	LYS
23	C2	9	ILE
23	C2	46	HIS
23	C2	47	VAL
24	C3	1	MET
24	C3	44	VAL
25	C4	13	ARG
25	C4	52	LYS
26	C5	26	ILE
27	C0	3	LYS
27	C0	4	THR
27	C0	5	ILE
27	C0	10	THR
27	C0	25	LEU
27	C0	36	VAL
27	C0	39	GLU
27	C0	45	ARG
27	C0	59	GLU
2	BB	44	GLU
2	BB	73	LYS
2	BB	93	ASN
2	BB	105	LYS
2	BB	108	ARG

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Mol	Chain	Res	Type
2	BB	125	THR
2	BB	129	LEU
2	BB	130	THR
2	BB	135	LEU
2	BB	147	SER
2	BB	161	LEU
2	BB	183	VAL
2	BB	205	ASP
2	BB	207	ILE
2	BB	212	LEU
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	121	THR
3	BC	152	GLU
3	BC	175	LEU
3	BC	185	ASN
3	BC	186	THR
3	BC	207	ILE
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	206	LYS
5	BE	11	LEU
5	BE	14	LYS
5	BE	24	THR
5	BE	32	SER
5	BE	46	VAL
5	BE	71	MET
5	BE	76	LEU
5	BE	81	LEU
5	BE	82	GLN
5	BE	88	VAL
5	BE	94	VAL

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Mol	Chain	Res	Type
5	BE	101	GLU
5	BE	103	THR
5	BE	105	ILE
5	BE	106	ILE
5	BE	114	VAL
5	BE	115	LEU
5	BE	123	VAL
5	BE	126	LYS
5	BE	137	VAL
5	BE	149	SER
5	BE	151	GLU
5	BE	159	LYS
6	BF	7	VAL
6	BF	14	GLN
6	BF	16	GLU
6	BF	36	ILE
6	BF	39	LEU
6	BF	53	LYS
6	BF	68	GLN
6	BF	69	GLU
6	BF	71	ILE
6	BF	74	LEU
6	BF	89	VAL
6	BF	93	LYS
7	BG	5	ARG
7	BG	10	ARG
7	BG	23	LEU
7	BG	30	LEU
7	BG	36	LYS
7	BG	48	GLU
7	BG	50	LEU
7	BG	58	GLU
7	BG	59	LEU
7	BG	63	GLU
7	BG	70	ARG
7	BG	76	LYS
7	BG	120	LEU
7	BG	131	LYS
7	BG	133	THR
7	BG	142	HIS
8	BH	3	MET
8	BH	47	GLU

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Mol	Chain	Res	Type
8	BH	51	VAL
8	BH	52	GLU
8	BH	60	GLU
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	36	GLU
9	BI	61	LEU
9	BI	63	LEU
9	BI	66	THR
9	BI	87	LEU
10	BJ	5	ARG
10	BJ	6	ILE
10	BJ	22	THR
10	BJ	59	LYS
10	BJ	62	ARG
10	BJ	63	ASP
10	BJ	69	THR
10	BJ	77	VAL
10	BJ	78	GLU
10	BJ	88	MET
10	BJ	89	ARG
10	BJ	90	LEU
11	BK	18	ASP
11	BK	22	HIS
11	BK	31	ILE
11	BK	38	GLN
11	BK	72	ASP
12	BL	24	LEU
12	BL	43	LYS
12	BL	44	LYS
12	BL	55	VAL
12	BL	58	THR
12	BL	74	LEU
12	BL	82	ILE

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Mol	Chain	Res	Type
12	BL	88	LYS
12	BL	90	LEU
12	BL	110	ARG
12	BL	121	ARG
13	BM	11	ASP
13	BM	16	VAL
13	BM	22	ILE
13	BM	27	LYS
13	BM	48	LEU
14	BN	26	GLU
14	BN	80	SER
15	BO	40	GLN
15	BO	64	ARG
15	BO	70	LEU
16	BP	2	VAL
16	BP	18	GLN
16	BP	19	VAL
16	BP	20	VAL
16	BP	36	VAL
16	BP	46	LYS
16	BP	48	GLU
16	BP	76	LYS
17	BQ	17	MET
17	BQ	21	ILE
17	BQ	26	GLU
17	BQ	33	ILE
17	BQ	38	ILE
17	BQ	40	ARG
17	BQ	51	ASN
17	BQ	75	LEU
18	BR	47	THR
19	BS	6	LYS
19	BS	7	LYS
19	BS	11	ILE
19	BS	13	LEU
19	BS	33	THR
19	BS	37	ARG
19	BS	63	THR
20	BT	5	LYS
20	BT	12	ILE
20	BT	24	ARG
20	BT	43	ASP

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Mol	Chain	Res	Type
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	16	LEU
21	BU	18	ARG
21	BU	56	HIS
22	D1	26	THR
23	D2	5	ILE
23	D2	8	LYS
23	D2	9	ILE
23	D2	46	HIS
23	D2	47	VAL
23	D2	48	ILE
24	D3	1	MET
25	D4	52	LYS
27	D0	10	THR
27	D0	36	VAL
27	D0	39	GLU
29	CC	97	LYS
29	CC	110	LEU
29	CC	117	GLN
29	CC	120	VAL
29	CC	154	LEU
29	CC	156	ARG
29	CC	157	SER
29	CC	168	ASP
29	CC	174	LEU
29	CC	184	VAL
29	CC	195	VAL
29	CC	202	LEU
29	CC	204	VAL
29	CC	221	ARG
29	CC	236	GLU
29	CC	267	ILE
30	CD	2	ILE
30	CD	4	LEU

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Mol	Chain	Res	Type
30	CD	18	ASP
30	CD	52	THR
30	CD	95	SER
30	CD	97	SER
30	CD	129	THR
30	CD	138	LEU
29	DC	70	ASN
29	DC	97	LYS
29	DC	110	LEU
29	DC	117	GLN
29	DC	120	VAL
29	DC	154	LEU
29	DC	184	VAL
29	DC	202	LEU
29	DC	236	GLU
29	DC	267	ILE
32	DD	2	ILE
32	DD	18	ASP
32	DD	52	THR
32	DD	95	SER
32	DD	97	SER
32	DD	138	LEU
33	CE	7	ASP
33	CE	12	LEU
33	CE	25	GLU
33	CE	40	ARG
33	CE	44	ARG
33	CE	72	SER
33	CE	83	VAL
33	CE	93	SER
33	CE	122	GLU
33	CE	127	GLU
33	CE	149	ILE
33	CE	152	GLU
33	CE	163	ASN
33	CE	189	THR
34	CF	18	THR
34	CF	31	VAL
34	CF	35	THR
34	CF	36	LEU
34	CF	49	LEU
34	CF	57	LEU

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Mol	Chain	Res	Type
34	CF	72	LYS
34	CF	80	ARG
34	CF	94	GLU
34	CF	117	LEU
34	CF	123	ASP
34	CF	134	GLU
34	CF	136	ILE
34	CF	141	ILE
34	CF	149	VAL
34	CF	150	ARG
34	CF	152	LEU
34	CF	167	ARG
34	CF	174	ASP
35	CG	11	VAL
35	CG	18	LYS
35	CG	42	GLU
35	CG	72	LEU
35	CG	155	GLU
35	CG	168	VAL
36	CH	1	MET
36	CH	7	ASP
36	CH	15	LEU
36	CH	21	VAL
36	CH	51	ARG
36	CH	53	GLU
36	CH	55	GLU
36	CH	58	LEU
36	CH	62	LEU
36	CH	75	LEU
36	CH	76	GLU
36	CH	89	LYS
36	CH	112	LYS
36	CH	127	GLU
36	CH	145	ASN
37	CJ	11	LEU
37	CJ	13	VAL
37	CJ	28	LEU
37	CJ	53	LEU
37	CJ	55	ILE
37	CJ	101	ILE
37	CJ	113	LYS
38	CK	5	THR

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Mol	Chain	Res	Type
38	CK	81	ILE
38	CK	124	VAL
38	CK	142	ILE
39	CL	35	VAL
39	CL	58	LEU
39	CL	70	ARG
39	CL	76	VAL
39	CL	113	MET
40	CM	59	ARG
40	CM	92	LEU
40	CM	94	THR
40	CM	100	ILE
40	CM	103	ILE
40	CM	115	GLU
40	CM	120	VAL
41	CN	6	ARG
41	CN	14	LYS
41	CN	59	ARG
41	CN	75	GLU
41	CN	78	LEU
41	CN	100	LYS
41	CN	115	GLU
42	CO	2	ARG
42	CO	6	SER
42	CO	14	SER
42	CO	53	THR
42	CO	69	ARG
42	CO	71	ARG
42	CO	76	VAL
42	CO	95	THR
43	CP	18	LEU
43	CP	20	GLU
43	CP	31	THR
43	CP	38	GLN
43	CP	47	VAL
43	CP	48	LEU
43	CP	49	VAL
43	CP	78	VAL
43	CP	111	ARG
44	CQ	2	SER
44	CQ	26	VAL
44	CQ	39	ARG

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Mol	Chain	Res	Type
44	CQ	63	LYS
44	CQ	96	LYS
44	CQ	102	GLU
44	CQ	109	ARG
44	CQ	114	LEU
45	CR	5	LYS
45	CR	9	ILE
45	CR	51	ARG
45	CR	52	GLN
45	CR	117	LEU
46	CS	12	HIS
46	CS	45	GLU
46	CS	46	GLU
46	CS	48	LYS
46	CS	51	VAL
46	CS	102	SER
47	CT	29	VAL
47	CT	69	LEU
47	CT	76	VAL
47	CT	86	MET
47	CT	97	LEU
47	CT	109	ASP
48	CU	2	ILE
48	CU	10	VAL
48	CU	18	GLU
48	CU	24	MET
48	CU	30	ILE
48	CU	36	LYS
48	CU	49	LYS
48	CU	69	ARG
48	CU	93	LEU
49	CV	28	VAL
49	CV	29	LEU
49	CV	61	LYS
49	CV	72	ILE
49	CV	81	ASP
49	CV	98	SER
50	CW	1	MET
50	CW	7	GLU
50	CW	10	LYS
50	CW	18	ARG
50	CW	61	LEU

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Mol	Chain	Res	Type
50	CW	66	ASP
51	CX	39	ARG
51	CX	40	GLN
51	CX	82	ILE
52	CY	25	THR
52	CY	35	SER
52	CY	44	LYS
52	CY	48	THR
52	CY	71	LEU
53	CZ	7	ARG
53	CZ	12	GLU
53	CZ	18	LEU
53	CZ	19	LEU
53	CZ	38	GLN
53	CZ	58	ASN
33	DE	12	LEU
33	DE	80	SER
33	DE	127	GLU
33	DE	163	ASN
33	DE	189	THR
34	DF	10	ASP
34	DF	35	THR
34	DF	49	LEU
34	DF	57	LEU
34	DF	72	LYS
34	DF	94	GLU
34	DF	115	ARG
34	DF	117	LEU
34	DF	134	GLU
34	DF	136	ILE
34	DF	141	ILE
34	DF	149	VAL
34	DF	150	ARG
34	DF	152	LEU
34	DF	167	ARG
34	DF	174	ASP
35	DG	11	VAL
35	DG	18	LYS
35	DG	42	GLU
35	DG	72	LEU
35	DG	155	GLU
35	DG	168	VAL

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Mol	Chain	Res	Type
36	DH	1	MET
36	DH	7	ASP
36	DH	15	LEU
36	DH	21	VAL
36	DH	53	GLU
36	DH	54	LEU
36	DH	58	LEU
36	DH	60	GLU
36	DH	62	LEU
36	DH	75	LEU
36	DH	76	GLU
36	DH	89	LYS
36	DH	112	LYS
36	DH	117	LEU
36	DH	127	GLU
36	DH	145	ASN
37	DJ	11	LEU
37	DJ	13	VAL
37	DJ	28	LEU
37	DJ	53	LEU
37	DJ	55	ILE
37	DJ	101	ILE
37	DJ	113	LYS
38	DK	84	ILE
38	DK	124	VAL
38	DK	142	ILE
39	DL	58	LEU
39	DL	70	ARG
39	DL	110	GLU
40	DM	59	ARG
40	DM	92	LEU
40	DM	94	THR
40	DM	115	GLU
40	DM	120	VAL
41	DN	75	GLU
41	DN	100	LYS
41	DN	115	GLU
41	DN	126	ILE
42	DO	6	SER
42	DO	14	SER
42	DO	69	ARG
42	DO	76	VAL

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Mol	Chain	Res	Type
43	DP	20	GLU
43	DP	31	THR
43	DP	49	VAL
43	DP	56	LYS
43	DP	78	VAL
43	DP	111	ARG
44	DQ	26	VAL
44	DQ	40	LEU
44	DQ	63	LYS
44	DQ	96	LYS
44	DQ	102	GLU
44	DQ	109	ARG
45	DR	5	LYS
45	DR	9	ILE
45	DR	51	ARG
46	DS	38	VAL
46	DS	102	SER
47	DT	76	VAL
47	DT	86	MET
47	DT	109	ASP
48	DU	1	MET
48	DU	3	ARG
48	DU	10	VAL
48	DU	25	GLU
49	DV	28	VAL
49	DV	29	LEU
49	DV	52	LEU
49	DV	61	LYS
50	DW	7	GLU
50	DW	53	LYS
50	DW	61	LEU
50	DW	66	ASP
51	DX	11	ARG
51	DX	39	ARG
51	DX	82	ILE
52	DY	25	THR
52	DY	35	SER
52	DY	44	LYS
53	DZ	7	ARG
53	DZ	12	GLU
53	DZ	19	LEU
53	DZ	38	GLN

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Mol	Chain	Res	Type
54	DI	16	SER
54	DI	53	ARG
54	DI	57	ASN
54	DI	60	LEU
54	DI	64	VAL
54	DI	85	VAL
54	DI	117	LEU
54	DI	123	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	42	ASN
2	AB	93	ASN
2	AB	120	GLN
3	AC	41	GLN
3	AC	123	GLN
4	AD	136	GLN
4	AD	152	GLN
5	AE	70	ASN
5	AE	77	ASN
5	AE	89	HIS
5	AE	122	ASN
6	AF	17	GLN
6	AF	63	ASN
7	AG	86	GLN
7	AG	130	ASN
7	AG	142	HIS
7	AG	148	ASN
8	AH	4	GLN
8	AH	38	ASN
8	AH	67	GLN
9	AI	4	ASN
9	AI	50	GLN
9	AI	110	GLN
9	AI	126	GLN
10	AJ	35	GLN
10	AJ	56	HIS
12	AL	77	HIS
13	AM	12	HIS
14	AN	4	GLN
14	AN	35	ASN

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Mol	Chain	Res	Type
15	AO	28	GLN
15	AO	40	GLN
15	AO	50	HIS
16	AP	9	HIS
16	AP	40	ASN
16	AP	59	HIS
20	AT	48	GLN
22	C1	6	ASN
24	C3	13	ASN
27	C0	9	GLN
2	BB	39	HIS
2	BB	42	ASN
2	BB	93	ASN
2	BB	120	GLN
3	BC	25	ASN
4	BD	136	GLN
4	BD	152	GLN
5	BE	77	ASN
5	BE	89	HIS
5	BE	122	ASN
6	BF	3	HIS
6	BF	17	GLN
6	BF	46	GLN
7	BG	130	ASN
7	BG	148	ASN
8	BH	4	GLN
8	BH	38	ASN
8	BH	67	GLN
9	BI	4	ASN
9	BI	110	GLN
9	BI	126	GLN
10	BJ	56	HIS
11	BK	40	ASN
14	BN	4	GLN
15	BO	28	GLN
15	BO	40	GLN
15	BO	50	HIS
16	BP	9	HIS
16	BP	40	ASN
16	BP	63	GLN
17	BQ	51	ASN
20	BT	3	ASN

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Mol	Chain	Res	Type
20	BT	48	GLN
20	BT	52	ASN
20	BT	84	ASN
27	D0	20	HIS
29	CC	142	HIS
29	CC	260	ASN
30	CD	150	GLN
30	CD	173	GLN
29	DC	142	HIS
29	DC	153	GLN
32	DD	42	ASN
32	DD	173	GLN
33	CE	94	GLN
33	CE	136	GLN
34	CF	23	ASN
34	CF	52	ASN
35	CG	38	ASN
35	CG	73	ASN
35	CG	104	ASN
35	CG	128	GLN
35	CG	139	GLN
36	CH	2	GLN
36	CH	20	ASN
36	CH	43	ASN
36	CH	145	ASN
37	CJ	105	GLN
38	CK	47	HIS
39	CL	5	GLN
43	CP	29	HIS
43	CP	100	HIS
43	CP	116	GLN
44	CQ	41	GLN
45	CR	44	GLN
46	CS	12	HIS
47	CT	9	HIS
48	CU	28	ASN
48	CU	70	HIS
49	CV	74	ASN
50	CW	24	ASN
52	CY	36	HIS
53	CZ	45	GLN
33	DE	94	GLN

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Mol	Chain	Res	Type
34	DF	27	GLN
35	DG	104	ASN
35	DG	116	GLN
35	DG	128	GLN
36	DH	2	GLN
36	DH	20	ASN
36	DH	43	ASN
36	DH	73	ASN
36	DH	145	ASN
38	DK	47	HIS
39	DL	5	GLN
39	DL	93	GLN
42	DO	107	ASN
45	DR	44	GLN
45	DR	81	ASN
46	DS	87	GLN
47	DT	60	HIS
48	DU	70	HIS
52	DY	36	HIS
53	DZ	39	GLN
53	DZ	45	GLN
54	DI	88	HIS
54	DI	122	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1533/1534 (99%)	265 (17%)	31 (2%)
1	BA	1532/1534 (99%)	266 (17%)	36 (2%)
28	CB	117/120 (97%)	12 (10%)	0
28	DB	119/120 (99%)	10 (8%)	0
31	CA	2896/2904 (99%)	477 (16%)	78 (2%)
55	DA	2884/2904 (99%)	418 (14%)	62 (2%)
All	All	9081/9116 (99%)	1448 (15%)	207 (2%)

All (1448) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G

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Mol	Chain	Res	Type
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
1	AA	108	G
1	AA	116	A
1	AA	120	A
1	AA	127	G
1	AA	130	A
1	AA	131	A
1	AA	137	U
1	AA	141	G
1	AA	142	G
1	AA	143	A
1	AA	144	G
1	AA	149	A
1	AA	159	G
1	AA	163	C
1	AA	168	G

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Mol	Chain	Res	Type
1	AA	177	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	281	G
1	AA	289	G
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	348	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
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

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Mol	Chain	Res	Type
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	481	G
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	511	C
1	AA	527	7MG
1	AA	528	C
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	615	G
1	AA	632	U
1	AA	633	G
1	AA	650	G
1	AA	653	U
1	AA	661	G
1	AA	665	A
1	AA	682	G
1	AA	695	A
1	AA	702	A
1	AA	703	G
1	AA	721	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

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Mol	Chain	Res	Type
1	AA	799	G
1	AA	809	G
1	AA	814	A
1	AA	815	A
1	AA	817	C
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	934	C
1	AA	935	A
1	AA	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	987	G
1	AA	992	U
1	AA	993	G
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

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Mol	Chain	Res	Type
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	1066	C
1	AA	1070	U
1	AA	1086	U
1	AA	1087	G
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
1	AA	1160	G
1	AA	1168	U
1	AA	1182	G
1	AA	1184	G
1	AA	1196	A
1	AA	1197	A
1	AA	1200	C
1	AA	1202	U
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C

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Mol	Chain	Res	Type
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	1282	C
1	AA	1286	U
1	AA	1287	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1312	G
1	AA	1317	C
1	AA	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	1419	G
1	AA	1429	A
1	AA	1441	A
1	AA	1446	A
1	AA	1447	A
1	AA	1448	C
1	AA	1451	U
1	AA	1452	C
1	AA	1453	G
1	AA	1475	G
1	AA	1492	A
1	AA	1497	G

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Mol	Chain	Res	Type
1	AA	1499	A
1	AA	1503	A
1	AA	1505	G
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1533	C
1	AA	1534	A
1	BA	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	86	G
1	BA	87	C
1	BA	88	U
1	BA	89	U
1	BA	90	C
1	BA	94	G
1	BA	95	C
1	BA	108	G
1	BA	116	A

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Mol	Chain	Res	Type
1	BA	120	A
1	BA	127	G
1	BA	130	A
1	BA	131	A
1	BA	137	U
1	BA	141	G
1	BA	142	G
1	BA	143	A
1	BA	144	G
1	BA	149	A
1	BA	159	G
1	BA	163	C
1	BA	168	G
1	BA	177	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	281	G
1	BA	289	G
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	348	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	411	A
1	BA	412	A
1	BA	413	G
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	7MG
1	BA	531	U
1	BA	532	A
1	BA	533	A
1	BA	547	A
1	BA	559	A
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	596	A
1	BA	615	G
1	BA	632	U
1	BA	633	G
1	BA	650	G
1	BA	653	U
1	BA	661	G

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Mol	Chain	Res	Type
1	BA	665	A
1	BA	682	G
1	BA	695	A
1	BA	702	A
1	BA	703	G
1	BA	721	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	799	G
1	BA	814	A
1	BA	815	A
1	BA	817	C
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
1	BA	987	G
1	BA	992	U

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Mol	Chain	Res	Type
1	BA	993	G
1	BA	1004	A
1	BA	1008	U
1	BA	1009	U
1	BA	1015	G
1	BA	1019	A
1	BA	1024	G
1	BA	1026	G
1	BA	1027	C
1	BA	1029	U
1	BA	1030	U
1	BA	1031	C
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	1070	U
1	BA	1086	U
1	BA	1087	G
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	1182	G
1	BA	1196	A
1	BA	1197	A
1	BA	1200	C
1	BA	1202	U
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	1261	A
1	BA	1280	A
1	BA	1281	C
1	BA	1282	C
1	BA	1286	U
1	BA	1287	A
1	BA	1300	G
1	BA	1302	C
1	BA	1305	G
1	BA	1312	G
1	BA	1317	C
1	BA	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

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Mol	Chain	Res	Type
1	BA	1397	C
1	BA	1398	A
1	BA	1419	G
1	BA	1429	A
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	1493	A
1	BA	1497	G
1	BA	1499	A
1	BA	1503	A
1	BA	1505	G
1	BA	1506	U
1	BA	1507	A
1	BA	1517	G
1	BA	1529	G
1	BA	1530	G
1	BA	1533	C
1	BA	1534	A
28	CB	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	33	C
31	CA	34	U
31	CA	42	A
31	CA	46	G

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Mol	Chain	Res	Type
31	CA	49	A
31	CA	58	G
31	CA	63	A
31	CA	71	A
31	CA	74	A
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	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	196	A
31	CA	197	A
31	CA	198	C
31	CA	199	A
31	CA	200	U
31	CA	215	G
31	CA	216	A
31	CA	221	A
31	CA	222	A
31	CA	245	G
31	CA	248	G
31	CA	264	C
31	CA	265	A
31	CA	266	G
31	CA	267	C
31	CA	272	A
31	CA	276	U
31	CA	277	G
31	CA	278	A

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Mol	Chain	Res	Type
31	CA	279	A
31	CA	285	G
31	CA	310	A
31	CA	311	A
31	CA	329	G
31	CA	330	A
31	CA	343	C
31	CA	346	A
31	CA	352	A
31	CA	353	C
31	CA	362	A
31	CA	371	A
31	CA	372	G
31	CA	385	C
31	CA	386	G
31	CA	399	U
31	CA	403	U
31	CA	404	A
31	CA	405	U
31	CA	411	G
31	CA	412	A
31	CA	420	C
31	CA	424	G
31	CA	451	U
31	CA	480	A
31	CA	481	G
31	CA	491	G
31	CA	496	G
31	CA	503	A
31	CA	504	A
31	CA	505	A
31	CA	508	A
31	CA	528	A
31	CA	529	A
31	CA	531	C
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

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Mol	Chain	Res	Type
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
31	CA	615	U
31	CA	620	G
31	CA	621	A
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	730	A
31	CA	740	C
31	CA	747	5MU
31	CA	764	A
31	CA	765	C
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

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Mol	Chain	Res	Type
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	907	G
31	CA	910	A
31	CA	914	G
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	973	A
31	CA	974	G
31	CA	983	A
31	CA	984	A
31	CA	985	C
31	CA	995	C
31	CA	996	A
31	CA	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	1045	C
31	CA	1046	A
31	CA	1047	G
31	CA	1057	A
31	CA	1061	U
31	CA	1062	G
31	CA	1069	A

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Mol	Chain	Res	Type
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	1091	G
31	CA	1096	A
31	CA	1097	U
31	CA	1111	A
31	CA	1112	G
31	CA	1119	U
31	CA	1128	G
31	CA	1129	A
31	CA	1132	U
31	CA	1133	A
31	CA	1134	A
31	CA	1135	C
31	CA	1136	G
31	CA	1142	A
31	CA	1156	A
31	CA	1168	G
31	CA	1169	A
31	CA	1172	C
31	CA	1175	A
31	CA	1176	U
31	CA	1177	G
31	CA	1179	G
31	CA	1180	U
31	CA	1186	G
31	CA	1206	G
31	CA	1210	G
31	CA	1212	G
31	CA	1218	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

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Mol	Chain	Res	Type
31	CA	1273	U
31	CA	1288	G
31	CA	1289	C
31	CA	1300	G
31	CA	1301	A
31	CA	1313	U
31	CA	1320	C
31	CA	1321	A
31	CA	1328	A
31	CA	1329	U
31	CA	1330	C
31	CA	1352	U
31	CA	1365	A
31	CA	1376	C
31	CA	1379	U
31	CA	1380	G
31	CA	1383	A
31	CA	1386	C
31	CA	1395	A
31	CA	1416	G
31	CA	1417	C
31	CA	1419	A
31	CA	1420	A
31	CA	1428	C
31	CA	1437	C
31	CA	1438	U
31	CA	1452	G
31	CA	1453	A
31	CA	1460	U
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

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Mol	Chain	Res	Type
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	1606	C
31	CA	1607	C
31	CA	1608	A
31	CA	1616	A
31	CA	1634	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	1694	C
31	CA	1715	G
31	CA	1729	U
31	CA	1730	C
31	CA	1738	G
31	CA	1744	A
31	CA	1750	G
31	CA	1758	U
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	1829	A
31	CA	1869	G
31	CA	1870	C
31	CA	1871	A
31	CA	1872	A

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Mol	Chain	Res	Type
31	CA	1873	G
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	1991	U
31	CA	1993	U
31	CA	1997	C
31	CA	2022	U
31	CA	2023	C
31	CA	2031	A
31	CA	2033	A
31	CA	2035	G
31	CA	2036	C
31	CA	2043	C
31	CA	2046	G
31	CA	2049	G
31	CA	2055	C
31	CA	2056	G
31	CA	2060	A
31	CA	2061	G
31	CA	2062	A
31	CA	2069	7MG
31	CA	2072	C
31	CA	2080	A
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

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Mol	Chain	Res	Type
31	CA	2113	U
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
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	2178	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	2282	G

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Mol	Chain	Res	Type
31	CA	2283	C
31	CA	2287	A
31	CA	2305	U
31	CA	2311	A
31	CA	2322	A
31	CA	2324	U
31	CA	2325	G
31	CA	2326	C
31	CA	2327	A
31	CA	2331	G
31	CA	2333	A
31	CA	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
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	2436	G
31	CA	2441	U
31	CA	2448	A
31	CA	2465	C
31	CA	2469	A
31	CA	2476	A
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

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Mol	Chain	Res	Type
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	2582	G
31	CA	2585	U
31	CA	2586	U
31	CA	2603	G
31	CA	2609	U
31	CA	2613	U
31	CA	2621	G
31	CA	2629	U
31	CA	2630	G
31	CA	2646	C
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	2726	A
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	2820	A
31	CA	2821	A
31	CA	2825	G
31	CA	2833	U
31	CA	2835	A
31	CA	2836	U
31	CA	2849	U
31	CA	2850	A

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Mol	Chain	Res	Type
31	CA	2861	U
31	CA	2867	G
31	CA	2880	C
31	CA	2883	A
31	CA	2884	U
31	CA	2886	A
31	CA	2893	A
31	CA	2894	G
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
28	DB	88	C
28	DB	89	U
28	DB	90	C
28	DB	109	A
55	DA	10	A
55	DA	12	U
55	DA	34	U
55	DA	42	A
55	DA	46	G
55	DA	58	G
55	DA	63	A
55	DA	71	A
55	DA	74	A
55	DA	75	G
55	DA	80	G
55	DA	84	A
55	DA	101	A
55	DA	102	U
55	DA	118	A
55	DA	119	A
55	DA	120	U
55	DA	138	U
55	DA	139	U
55	DA	140	C
55	DA	141	G
55	DA	142	A
55	DA	143	C

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Mol	Chain	Res	Type
55	DA	165	A
55	DA	196	A
55	DA	197	A
55	DA	199	A
55	DA	200	U
55	DA	215	G
55	DA	216	A
55	DA	221	A
55	DA	222	A
55	DA	226	A
55	DA	248	G
55	DA	264	C
55	DA	265	A
55	DA	266	G
55	DA	267	C
55	DA	272	A
55	DA	276	U
55	DA	277	G
55	DA	278	A
55	DA	279	A
55	DA	285	G
55	DA	302	C
55	DA	310	A
55	DA	311	A
55	DA	329	G
55	DA	330	A
55	DA	346	A
55	DA	352	A
55	DA	353	C
55	DA	362	A
55	DA	370	G
55	DA	371	A
55	DA	372	G
55	DA	386	G
55	DA	399	U
55	DA	403	U
55	DA	411	G
55	DA	412	A
55	DA	420	C
55	DA	424	G
55	DA	454	A
55	DA	480	A

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Mol	Chain	Res	Type
55	DA	481	G
55	DA	491	G
55	DA	496	G
55	DA	503	A
55	DA	504	A
55	DA	505	A
55	DA	508	A
55	DA	529	A
55	DA	531	C
55	DA	532	A
55	DA	533	G
55	DA	543	G
55	DA	544	C
55	DA	546	U
55	DA	547	A
55	DA	548	G
55	DA	549	G
55	DA	550	C
55	DA	551	G
55	DA	563	A
55	DA	573	U
55	DA	575	A
55	DA	586	A
55	DA	603	A
55	DA	613	A
55	DA	614	A
55	DA	615	U
55	DA	620	G
55	DA	621	A
55	DA	627	A
55	DA	637	A
55	DA	645	C
55	DA	647	G
55	DA	653	U
55	DA	654	A
55	DA	655	A
55	DA	686	U
55	DA	702	U
55	DA	717	C
55	DA	730	A
55	DA	738	G
55	DA	747	5MU

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Mol	Chain	Res	Type
55	DA	764	A
55	DA	765	C
55	DA	775	G
55	DA	776	G
55	DA	782	A
55	DA	783	A
55	DA	784	G
55	DA	785	G
55	DA	790	U
55	DA	805	G
55	DA	812	C
55	DA	827	U
55	DA	828	U
55	DA	858	G
55	DA	859	G
55	DA	878	A
55	DA	883	G
55	DA	885	C
55	DA	896	A
55	DA	897	C
55	DA	907	G
55	DA	910	A
55	DA	914	G
55	DA	931	U
55	DA	932	U
55	DA	946	C
55	DA	953	G
55	DA	961	C
55	DA	962	G
55	DA	974	G
55	DA	983	A
55	DA	984	A
55	DA	985	C
55	DA	996	A
55	DA	1005	C
55	DA	1012	U
55	DA	1013	C
55	DA	1022	G
55	DA	1026	G
55	DA	1033	U
55	DA	1040	A
55	DA	1047	G

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Mol	Chain	Res	Type
55	DA	1057	A
55	DA	1061	U
55	DA	1062	G
55	DA	1069	A
55	DA	1070	A
55	DA	1073	A
55	DA	1083	U
55	DA	1088	A
55	DA	1089	A
55	DA	1090	A
55	DA	1091	G
55	DA	1096	A
55	DA	1097	U
55	DA	1112	G
55	DA	1119	U
55	DA	1128	G
55	DA	1129	A
55	DA	1132	U
55	DA	1133	A
55	DA	1134	A
55	DA	1135	C
55	DA	1136	G
55	DA	1142	A
55	DA	1143	A
55	DA	1156	A
55	DA	1168	G
55	DA	1171	G
55	DA	1172	C
55	DA	1174	U
55	DA	1175	A
55	DA	1176	U
55	DA	1177	G
55	DA	1180	U
55	DA	1206	G
55	DA	1212	G
55	DA	1218	G
55	DA	1238	G
55	DA	1253	A
55	DA	1256	G
55	DA	1271	G
55	DA	1272	A
55	DA	1273	U

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Mol	Chain	Res	Type
55	DA	1300	G
55	DA	1301	A
55	DA	1321	A
55	DA	1352	U
55	DA	1365	A
55	DA	1379	U
55	DA	1383	A
55	DA	1386	C
55	DA	1416	G
55	DA	1417	C
55	DA	1420	A
55	DA	1427	A
55	DA	1428	C
55	DA	1435	G
55	DA	1452	G
55	DA	1453	A
55	DA	1460	U
55	DA	1482	G
55	DA	1490	A
55	DA	1491	G
55	DA	1493	C
55	DA	1494	A
55	DA	1497	U
55	DA	1504	A
55	DA	1508	A
55	DA	1509	A
55	DA	1510	G
55	DA	1515	A
55	DA	1523	U
55	DA	1532	A
55	DA	1534	U
55	DA	1535	A
55	DA	1537	G
55	DA	1569	A
55	DA	1578	U
55	DA	1583	A
55	DA	1585	C
55	DA	1606	C
55	DA	1607	C
55	DA	1608	A
55	DA	1634	A
55	DA	1647	U

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Mol	Chain	Res	Type
55	DA	1648	U
55	DA	1649	G
55	DA	1674	G
55	DA	1694	C
55	DA	1715	G
55	DA	1729	U
55	DA	1730	C
55	DA	1738	G
55	DA	1744	A
55	DA	1758	U
55	DA	1764	C
55	DA	1773	A
55	DA	1782	U
55	DA	1800	C
55	DA	1801	A
55	DA	1808	A
55	DA	1812	U
55	DA	1816	C
55	DA	1829	A
55	DA	1839	G
55	DA	1869	G
55	DA	1870	C
55	DA	1871	A
55	DA	1872	A
55	DA	1873	G
55	DA	1900	A
55	DA	1901	A
55	DA	1906	G
55	DA	1907	G
55	DA	1913	A
55	DA	1914	C
55	DA	1929	G
55	DA	1930	G
55	DA	1931	U
55	DA	1937	A
55	DA	1938	A
55	DA	1955	U
55	DA	1965	C
55	DA	1967	C
55	DA	1970	A
55	DA	1972	G
55	DA	1991	U

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Mol	Chain	Res	Type
55	DA	1992	G
55	DA	1993	U
55	DA	1997	C
55	DA	2023	C
55	DA	2031	A
55	DA	2033	A
55	DA	2043	C
55	DA	2055	C
55	DA	2056	G
55	DA	2060	A
55	DA	2061	G
55	DA	2062	A
55	DA	2069	7MG
55	DA	2080	A
55	DA	2093	G
55	DA	2097	A
55	DA	2098	U
55	DA	2100	G
55	DA	2105	U
55	DA	2111	U
55	DA	2112	G
55	DA	2113	U
55	DA	2116	G
55	DA	2117	A
55	DA	2118	U
55	DA	2119	A
55	DA	2120	G
55	DA	2123	G
55	DA	2125	G
55	DA	2126	A
55	DA	2128	G
55	DA	2131	U
55	DA	2132	U
55	DA	2133	G
55	DA	2134	A
55	DA	2135	A
55	DA	2145	C
55	DA	2146	C
55	DA	2147	A
55	DA	2148	G
55	DA	2158	A
55	DA	2159	G

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Mol	Chain	Res	Type
55	DA	2160	C
55	DA	2161	C
55	DA	2162	G
55	DA	2163	A
55	DA	2164	C
55	DA	2165	C
55	DA	2167	U
55	DA	2168	G
55	DA	2169	A
55	DA	2170	A
55	DA	2171	A
55	DA	2172	U
55	DA	2173	A
55	DA	2178	C
55	DA	2179	C
55	DA	2181	U
55	DA	2183	A
55	DA	2185	U
55	DA	2186	G
55	DA	2190	G
55	DA	2198	A
55	DA	2204	G
55	DA	2211	A
55	DA	2225	A
55	DA	2238	G
55	DA	2239	G
55	DA	2243	U
55	DA	2268	A
55	DA	2278	A
55	DA	2283	C
55	DA	2286	G
55	DA	2287	A
55	DA	2305	U
55	DA	2308	G
55	DA	2311	A
55	DA	2312	U
55	DA	2322	A
55	DA	2324	U
55	DA	2325	G
55	DA	2327	A
55	DA	2331	G
55	DA	2333	A

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Mol	Chain	Res	Type
55	DA	2335	A
55	DA	2345	G
55	DA	2347	C
55	DA	2350	C
55	DA	2361	G
55	DA	2383	G
55	DA	2385	C
55	DA	2402	U
55	DA	2403	C
55	DA	2406	A
55	DA	2407	A
55	DA	2424	C
55	DA	2425	A
55	DA	2435	A
55	DA	2441	U
55	DA	2448	A
55	DA	2476	A
55	DA	2491	U
55	DA	2502	G
55	DA	2505	G
55	DA	2518	A
55	DA	2529	G
55	DA	2535	G
55	DA	2547	A
55	DA	2556	C
55	DA	2566	A
55	DA	2567	G
55	DA	2573	C
55	DA	2585	U
55	DA	2603	G
55	DA	2609	U
55	DA	2613	U
55	DA	2629	U
55	DA	2630	G
55	DA	2661	G
55	DA	2663	G
55	DA	2671	G
55	DA	2689	U
55	DA	2690	U
55	DA	2714	G
55	DA	2726	A
55	DA	2748	A

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Mol	Chain	Res	Type
55	DA	2765	A
55	DA	2778	A
55	DA	2779	U
55	DA	2780	G
55	DA	2791	G
55	DA	2798	U
55	DA	2799	A
55	DA	2820	A
55	DA	2821	A
55	DA	2825	G
55	DA	2833	U
55	DA	2835	A
55	DA	2836	U
55	DA	2861	U
55	DA	2867	G
55	DA	2880	C
55	DA	2883	A

All (207) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	7	A
1	AA	70	U
1	AA	88	U
1	AA	89	U
1	AA	209	U
1	AA	413	G
1	AA	422	C
1	AA	429	U
1	AA	438	U
1	AA	559	A
1	AA	576	C
1	AA	653	U
1	AA	702	A
1	AA	733	G
1	AA	793	U
1	AA	841	C
1	AA	884	U
1	AA	992	U
1	AA	1086	U
1	AA	1137	C

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Mol	Chain	Res	Type
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1196	A
1	AA	1225	A
1	AA	1281	C
1	AA	1299	A
1	AA	1397	C
1	AA	1447	A
1	AA	1452	C
1	BA	5	U
1	BA	7	A
1	BA	70	U
1	BA	86	G
1	BA	89	U
1	BA	209	U
1	BA	246	A
1	BA	422	C
1	BA	429	U
1	BA	438	U
1	BA	559	A
1	BA	560	A
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
1	BA	1140	C
1	BA	1141	C
1	BA	1196	A
1	BA	1225	A
1	BA	1281	C
1	BA	1299	A
1	BA	1362	A

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Mol	Chain	Res	Type
1	BA	1363	A
1	BA	1397	C
1	BA	1447	A
1	BA	1452	C
31	CA	33	C
31	CA	62	U
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	451	U
31	CA	455	C
31	CA	503	A
31	CA	506	G
31	CA	527	C
31	CA	555	G
31	CA	620	G
31	CA	686	U
31	CA	764	A
31	CA	784	G
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
31	CA	1070	A
31	CA	1088	A
31	CA	1089	A
31	CA	1128	G
31	CA	1133	A
31	CA	1286	A

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Mol	Chain	Res	Type
31	CA	1288	G
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	1730	C
31	CA	1786	A
31	CA	1870	C
31	CA	1871	A
31	CA	1900	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	2225	A
31	CA	2282	G
31	CA	2326	C
31	CA	2423	U
31	CA	2425	A
31	CA	2645	G
31	CA	2680	U
31	CA	2681	C
31	CA	2778	A
31	CA	2779	U
31	CA	2849	U
31	CA	2873	A
31	CA	2893	A
55	DA	62	U
55	DA	138	U

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Mol	Chain	Res	Type
55	DA	141	G
55	DA	196	A
55	DA	199	A
55	DA	271	G
55	DA	278	A
55	DA	310	A
55	DA	370	G
55	DA	371	A
55	DA	403	U
55	DA	503	A
55	DA	620	G
55	DA	764	A
55	DA	784	G
55	DA	961	C
55	DA	984	A
55	DA	1046	A
55	DA	1061	U
55	DA	1069	A
55	DA	1070	A
55	DA	1087	G
55	DA	1089	A
55	DA	1128	G
55	DA	1133	A
55	DA	1141	U
55	DA	1142	A
55	DA	1171	G
55	DA	1175	A
55	DA	1300	G
55	DA	1320	C
55	DA	1490	A
55	DA	1497	U
55	DA	1509	A
55	DA	1535	A
55	DA	1607	C
55	DA	1609	A
55	DA	1647	U
55	DA	1730	C
55	DA	1800	C
55	DA	1870	C
55	DA	1871	A
55	DA	1900	A
55	DA	2097	A

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Mol	Chain	Res	Type
55	DA	2119	A
55	DA	2127	G
55	DA	2146	C
55	DA	2157	G
55	DA	2158	A
55	DA	2164	C
55	DA	2282	G
55	DA	2286	G
55	DA	2311	A
55	DA	2324	U
55	DA	2406	A
55	DA	2423	U
55	DA	2585	U
55	DA	2779	U
55	DA	2798	U
55	DA	2820	A
55	DA	2849	U
55	DA	2873	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	5MU	DA	1939	55	19,22,23	0.48	0	27,32,35	0.43	0
55	2MG	DA	2445	55	23,26,27	0.51	0	33,38,41	0.39	0
31	1MG	CA	745	31	23,26,27	0.87	1 (4%)	33,39,42	0.69	2 (6%)
1	4OC	AA	1402	1	20,23,24	0.34	0	25,32,35	0.44	0
31	5MU	CA	747	31	19,22,23	0.39	0	27,32,35	0.30	0
55	PSU	DA	955	55	18,21,22	0.67	0	21,30,33	0.53	0
31	2MG	CA	1835	31	23,26,27	0.37	0	33,38,41	0.37	0
55	H2U	DA	2449	55	18,21,22	0.47	0	19,30,33	0.67	1 (5%)
41	4D4	CN	81	41	9,11,12	2.30	2 (22%)	7,13,15	2.55	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	BA	1516	1	23,26,27	0.36	0	33,38,41	0.58	0
55	PSU	DA	2457	55	18,21,22	0.54	0	21,30,33	0.46	0
12	D2T	BL	89	12	8,9,10	1.24	1 (12%)	6,11,13	1.33	1 (16%)
55	6MZ	DA	2030	55	22,25,26	0.63	0	29,36,39	0.50	0
55	PSU	DA	2604	55	18,21,22	0.79	0	21,30,33	0.52	0
31	6MZ	CA	1618	31	22,25,26	0.46	0	29,36,39	0.55	0
31	5MU	CA	1939	31	19,22,23	0.43	0	27,32,35	0.36	0
1	2MG	AA	1516	1	23,26,27	0.27	0	33,38,41	0.58	0
31	6MZ	CA	2030	31	22,25,26	0.35	0	29,36,39	0.46	0
12	D2T	AL	89	12	8,9,10	1.37	2 (25%)	6,11,13	1.15	0
1	5MC	BA	967	1	19,22,23	0.30	0	26,32,35	0.40	0
32	MEQ	DD	150[A]	32	8,9,10	0.39	0	5,10,12	0.53	0
1	2MG	BA	966	1	23,26,27	0.32	0	33,38,41	0.41	0
1	UR3	AA	1498	1	19,22,23	0.48	0	26,32,35	0.33	0
1	5MC	AA	967	1	19,22,23	0.32	0	26,32,35	0.42	0
1	PSU	AA	516	56,1	18,21,22	0.33	0	21,30,33	0.48	0
31	PSU	CA	1917	31	18,21,22	0.31	0	21,30,33	0.40	0
1	4OC	BA	1402	1	20,23,24	0.34	0	25,32,35	0.45	0
1	MA6	BA	1519	1	23,26,27	0.53	0	33,38,41	1.13	5 (15%)
32	MEQ	DD	150[B]	32	8,9,10	0.98	1 (12%)	5,10,12	0.73	0
55	PSU	DA	1917	55	18,21,22	0.35	0	21,30,33	0.41	0
1	MA6	AA	1519	1	23,26,27	0.54	0	33,38,41	1.10	4 (12%)
31	PSU	CA	955	31	18,21,22	0.31	0	21,30,33	0.50	0
55	OMU	DA	2552	55	19,22,23	0.47	0	25,31,34	0.31	0
31	PSU	CA	2504	31	18,21,22	0.36	0	21,30,33	0.43	0
55	PSU	DA	746	56,55	18,21,22	0.94	1 (5%)	21,30,33	0.32	0
1	5MC	BA	1407	1	19,22,23	0.41	0	26,32,35	0.51	0
55	PSU	DA	2605	55	18,21,22	0.45	0	21,30,33	0.53	0
55	5MC	DA	1962	55	19,22,23	0.54	0	26,32,35	0.44	0
1	2MG	AA	966	1	23,26,27	0.43	0	33,38,41	0.53	0
1	PSU	BA	516	1	18,21,22	0.37	0	21,30,33	0.46	0
31	PSU	CA	1911	31	18,21,22	0.27	0	21,30,33	0.40	0
31	5MC	CA	1962	31	19,22,23	0.28	0	26,32,35	0.37	0
31	2MG	CA	2445	31	23,26,27	0.42	0	33,38,41	0.44	0
31	2MA	CA	2503	31	22,25,26	0.72	0	32,37,40	1.98	6 (18%)
31	OMU	CA	2552	31	19,22,23	0.30	0	25,31,34	0.28	0
55	PSU	DA	1911	55	18,21,22	0.28	0	21,30,33	0.39	0
55	OMG	DA	2251	55	23,26,27	0.39	0	32,38,41	0.35	0
31	OMG	CA	2251	31	23,26,27	0.36	0	32,38,41	0.42	0
31	PSU	CA	746	56,31	18,21,22	0.54	1 (5%)	21,30,33	0.43	0
31	PSU	CA	2457	31	18,21,22	0.66	0	21,30,33	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	6MZ	DA	1618	55	22,25,26	0.44	0	29,36,39	1.40	1 (3%)
1	5MC	AA	1407	1	19,22,23	0.40	0	26,32,35	0.53	0
55	OMC	DA	2498	56,55	19,22,23	0.34	0	25,31,34	0.52	0
1	MA6	BA	1518	1	23,26,27	0.40	0	33,38,41	1.23	4 (12%)
1	2MG	BA	1207	1	23,26,27	0.29	0	33,38,41	0.42	0
1	UR3	BA	1498	1	19,22,23	0.85	0	26,32,35	0.72	1 (3%)
1	MA6	AA	1518	1	23,26,27	0.45	0	33,38,41	1.20	4 (12%)
41	4D4	DN	81[A]	-	9,11,12	1.77	2 (22%)	7,13,15	2.46	2 (28%)
55	7MG	DA	2069	55	23,26,27	4.17	3 (13%)	27,39,42	2.19	6 (22%)
55	5MU	DA	747	55	19,22,23	0.41	0	27,32,35	0.32	0
55	PSU	DA	2580	55	18,21,22	0.74	0	21,30,33	0.63	0
1	7MG	BA	527	1	23,26,27	4.15	2 (8%)	27,39,42	2.58	6 (22%)
55	1MG	DA	745	55	23,26,27	0.85	1 (4%)	33,39,42	0.58	1 (3%)
55	2MG	DA	1835	55	23,26,27	0.30	0	33,38,41	0.33	0
31	PSU	CA	2605	31	18,21,22	0.45	0	21,30,33	0.58	0
55	PSU	DA	2504	55	18,21,22	0.46	0	21,30,33	0.41	0
31	OMC	CA	2498	56,31	19,22,23	0.46	0	25,31,34	0.52	0
55	2MA	DA	2503	56,55	22,25,26	0.76	0	32,37,40	1.79	6 (18%)
41	4D4	DN	81[B]	-	9,11,12	1.85	2 (22%)	7,13,15	2.69	2 (28%)
1	2MG	AA	1207	1	23,26,27	0.23	0	33,38,41	0.36	0
55	3TD	DA	1915	55	19,22,23	0.51	0	23,32,35	0.90	1 (4%)
31	PSU	CA	2580	31	18,21,22	0.50	0	21,30,33	0.60	0
31	7MG	CA	2069	31	23,26,27	4.11	3 (13%)	27,39,42	2.35	6 (22%)
1	7MG	AA	527	1	23,26,27	4.19	2 (8%)	27,39,42	2.57	6 (22%)
31	3TD	CA	1915	31	19,22,23	0.51	0	23,32,35	0.85	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
55	5MU	DA	1939	55	-	0/7/25/26	0/2/2/2
55	2MG	DA	2445	55	-	2/9/27/28	0/3/3/3
31	1MG	CA	745	31	-	0/7/25/26	0/3/3/3
1	4OC	AA	1402	1	-	1/9/29/30	0/2/2/2
31	5MU	CA	747	31	-	0/7/25/26	0/2/2/2
55	PSU	DA	955	55	-	0/7/25/26	0/2/2/2
31	2MG	CA	1835	31	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	H2U	DA	2449	55	-	0/7/38/39	0/2/2/2
41	4D4	CN	81	41	-	1/11/12/14	-
1	2MG	BA	1516	1	-	0/9/27/28	0/3/3/3
55	PSU	DA	2457	55	-	0/7/25/26	0/2/2/2
12	D2T	BL	89	12	-	4/7/12/14	-
55	6MZ	DA	2030	55	-	2/9/27/28	0/3/3/3
55	PSU	DA	2604	55	-	0/7/25/26	0/2/2/2
31	6MZ	CA	1618	31	-	1/9/27/28	0/3/3/3
31	5MU	CA	1939	31	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3
31	6MZ	CA	2030	31	-	2/9/27/28	0/3/3/3
12	D2T	AL	89	12	-	1/7/12/14	-
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
32	MEQ	DD	150[A]	32	-	4/8/9/11	-
1	2MG	BA	966	1	-	0/9/27/28	0/3/3/3
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	56,1	-	0/7/25/26	0/2/2/2
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
1	4OC	BA	1402	1	-	1/9/29/30	0/2/2/2
1	MA6	BA	1519	1	-	2/11/29/30	0/3/3/3
32	MEQ	DD	150[B]	32	-	4/8/9/11	-
55	PSU	DA	1917	55	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	2/11/29/30	0/3/3/3
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
55	OMU	DA	2552	55	-	1/9/27/28	0/2/2/2
31	PSU	CA	2504	31	-	1/7/25/26	0/2/2/2
55	PSU	DA	746	56,55	-	2/7/25/26	0/2/2/2
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
55	PSU	DA	2605	55	-	0/7/25/26	0/2/2/2
55	5MC	DA	1962	55	-	2/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/9/27/28	0/3/3/3
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
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
31	2MG	CA	2445	31	-	0/9/27/28	0/3/3/3
31	2MA	CA	2503	31	-	1/7/25/26	0/3/3/3
31	OMU	CA	2552	31	-	1/9/27/28	0/2/2/2
55	PSU	DA	1911	55	-	0/7/25/26	0/2/2/2
55	OMG	DA	2251	55	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	OMG	CA	2251	31	-	0/9/27/28	0/3/3/3
31	PSU	CA	746	56,31	-	2/7/25/26	0/2/2/2
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
55	6MZ	DA	1618	55	-	0/9/27/28	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
55	OMC	DA	2498	56,55	-	0/9/27/28	0/2/2/2
1	MA6	BA	1518	1	-	0/11/29/30	0/3/3/3
1	2MG	BA	1207	1	-	0/9/27/28	0/3/3/3
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/11/29/30	0/3/3/3
41	4D4	DN	81[A]	-	-	1/11/12/14	-
55	7MG	DA	2069	55	-	1/7/37/38	0/3/3/3
55	5MU	DA	747	55	-	1/7/25/26	0/2/2/2
55	PSU	DA	2580	55	-	0/7/25/26	0/2/2/2
1	7MG	BA	527	1	-	2/7/37/38	0/3/3/3
55	1MG	DA	745	55	-	0/7/25/26	0/3/3/3
55	2MG	DA	1835	55	-	2/9/27/28	0/3/3/3
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
55	PSU	DA	2504	55	-	1/7/25/26	0/2/2/2
31	OMC	CA	2498	56,31	-	0/9/27/28	0/2/2/2
55	2MA	DA	2503	56,55	-	1/7/25/26	0/3/3/3
41	4D4	DN	81[B]	-	-	3/11/12/14	-
1	2MG	AA	1207	1	-	0/9/27/28	0/3/3/3
55	3TD	DA	1915	55	-	0/7/25/26	0/2/2/2
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
31	7MG	CA	2069	31	-	0/7/37/38	0/3/3/3
1	7MG	AA	527	1	-	2/7/37/38	0/3/3/3
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	527	7MG	C8-N9	-19.65	1.33	1.45
55	DA	2069	7MG	C8-N9	-19.53	1.33	1.45
1	BA	527	7MG	C8-N9	-19.48	1.33	1.45
31	CA	2069	7MG	C8-N9	-19.17	1.33	1.45
41	CN	81	4D4	CZ-NE	6.24	1.45	1.33
41	DN	81[B]	4D4	CZ-NE	4.83	1.42	1.33
41	DN	81[A]	4D4	CZ-NE	4.50	1.42	1.33
31	CA	745	1MG	C2-N1	3.77	1.44	1.37
55	DA	745	1MG	C2-N1	3.33	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	746	PSU	O4'-C1'	-3.14	1.39	1.43
12	AL	89	D2T	CB-SB	2.76	1.85	1.82
12	BL	89	D2T	CB-CG	2.74	1.56	1.52
32	DD	150[B]	MEQ	CB-CA	2.62	1.57	1.53
41	CN	81	4D4	CZ-NH1	2.62	1.43	1.34
31	CA	2069	7MG	C1'-N9	-2.50	1.42	1.46
55	DA	2069	7MG	C5-N7	2.49	1.38	1.35
41	DN	81[A]	4D4	CZ-NH1	2.48	1.43	1.34
41	DN	81[B]	4D4	CZ-NH1	2.46	1.43	1.34
1	AA	527	7MG	C5-N7	2.44	1.38	1.35
12	AL	89	D2T	CB-CG	2.07	1.55	1.52
31	CA	2069	7MG	C5-N7	2.06	1.38	1.35
31	CA	746	PSU	O4'-C1'	-2.04	1.41	1.43
1	BA	527	7MG	C5-N7	2.02	1.38	1.35
55	DA	2069	7MG	C8-N7	-2.01	1.32	1.42

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2503	2MA	N6-C6-N1	8.41	128.38	117.03
55	DA	2503	2MA	N6-C6-N1	7.51	127.16	117.03
55	DA	1618	6MZ	C9-N6-C6	-7.33	116.06	122.85
1	BA	527	7MG	C6-C5-N7	-6.55	121.78	131.93
1	AA	527	7MG	O4'-C1'-N9	6.49	118.14	109.30
31	CA	2069	7MG	C6-C5-C4	-6.46	111.04	122.40
1	BA	527	7MG	O4'-C1'-N9	6.34	117.94	109.30
55	DA	2069	7MG	O4'-C1'-N9	5.94	117.39	109.30
31	CA	2069	7MG	C6-C5-N7	-5.94	122.73	131.93
41	DN	81[B]	4D4	NE-CZ-NH2	5.93	130.85	120.67
1	AA	527	7MG	C6-C5-C4	-5.89	112.04	122.40
1	AA	527	7MG	C6-C5-N7	-5.78	122.98	131.93
41	CN	81	4D4	NE-CZ-NH2	5.72	130.49	120.67
1	BA	527	7MG	C6-C5-C4	-5.67	112.42	122.40
1	BA	527	7MG	C5-C4-N3	-5.61	117.60	128.13
1	AA	527	7MG	C5-C4-N3	-5.49	117.83	128.13
41	DN	81[A]	4D4	NE-CZ-NH2	5.34	129.84	120.67
55	DA	2069	7MG	C6-C5-N7	-5.20	123.88	131.93
1	AA	527	7MG	N9-C8-N7	4.63	109.92	103.37
55	DA	2069	7MG	N9-C8-N7	4.62	109.91	103.37
31	CA	2503	2MA	C2-N1-C6	4.60	125.18	118.10
31	CA	2069	7MG	O4'-C1'-N9	4.57	115.52	109.30
31	CA	2069	7MG	N9-C8-N7	4.56	109.82	103.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	527	7MG	N9-C8-N7	4.52	109.78	103.37
55	DA	2069	7MG	C6-C5-C4	-4.50	114.48	122.40
31	CA	2069	7MG	C5-C4-N3	-4.50	119.68	128.13
55	DA	2503	2MA	C2-N1-C6	4.12	124.44	118.10
1	BA	1518	MA6	C4-C5-C6	-3.93	111.85	115.91
55	DA	2069	7MG	C5-C4-N3	-3.76	121.07	128.13
1	AA	1518	MA6	C4-C5-C6	-3.69	112.09	115.91
55	DA	1915	3TD	C1'-C5-C4	3.67	123.17	117.61
1	BA	1519	MA6	C4-C5-C6	-3.64	112.15	115.91
1	BA	1518	MA6	N1-C6-N6	-3.62	112.45	116.86
41	DN	81[B]	4D4	NH1-CZ-NE	-3.59	111.11	119.27
1	AA	1518	MA6	N1-C6-N6	-3.57	112.51	116.86
31	CA	1915	3TD	C1'-C5-C4	3.45	122.85	117.61
1	AA	1519	MA6	C4-C5-C6	-3.43	112.36	115.91
31	CA	2503	2MA	C5-C6-N1	-3.37	113.66	118.90
41	DN	81[A]	4D4	NH1-CZ-NE	-3.31	111.75	119.27
1	BA	527	7MG	C4-C5-N7	-2.91	101.94	105.38
1	AA	527	7MG	C4-C5-N7	-2.86	102.00	105.38
41	CN	81	4D4	NH1-CZ-NE	-2.84	112.82	119.27
55	DA	2069	7MG	C4-C5-N7	-2.76	102.11	105.38
1	BA	1518	MA6	C5-C6-N1	2.70	124.14	118.55
1	AA	1518	MA6	C5-C6-N1	2.65	124.05	118.55
1	BA	1519	MA6	C5-C6-N1	2.57	123.89	118.55
55	DA	2503	2MA	C5-C6-N1	-2.55	114.93	118.90
1	BA	1518	MA6	C6-C5-N7	2.54	137.49	133.43
1	BA	1498	UR3	C4-N3-C2	-2.54	122.54	124.58
55	DA	2503	2MA	N3-C2-N1	-2.52	121.32	125.77
1	AA	1519	MA6	C5-C6-N1	2.49	123.72	118.55
55	DA	2449	H2U	O4'-C1'-N1	2.45	112.64	109.30
1	AA	1519	MA6	N1-C6-N6	-2.44	113.89	116.86
1	AA	1518	MA6	C6-C5-N7	2.43	137.31	133.43
1	BA	1519	MA6	N1-C6-N6	-2.40	113.93	116.86
55	DA	2503	2MA	CM2-C2-N3	2.36	120.66	117.13
31	CA	2503	2MA	N3-C2-N1	-2.33	121.65	125.77
1	BA	1519	MA6	C6-C5-N7	2.33	137.15	133.43
31	CA	2069	7MG	C4-C5-N7	-2.31	102.64	105.38
31	CA	2503	2MA	CM2-C2-N3	2.23	120.47	117.13
31	CA	745	1MG	N2-C2-N1	-2.23	116.99	118.79
1	AA	1519	MA6	C6-C5-N7	2.22	136.98	133.43
12	BL	89	D2T	OD1-CG-CB	2.20	127.06	122.44
55	DA	2503	2MA	C5-C6-N6	-2.17	117.91	123.29
31	CA	745	1MG	C6-C5-C4	-2.17	117.51	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2503	2MA	C5-C6-N6	-2.15	117.96	123.29
1	BA	1519	MA6	C5-C6-N6	-2.12	121.98	125.33
55	DA	745	1MG	C6-C5-C4	-2.02	117.68	119.97

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	7MG	O4'-C4'-C5'-O5'
1	BA	527	7MG	O4'-C4'-C5'-O5'
1	BA	527	7MG	C3'-C4'-C5'-O5'
32	DD	150[A]	MEQ	N-CA-CB-CG
32	DD	150[A]	MEQ	C-CA-CB-CG
32	DD	150[B]	MEQ	N-CA-CB-CG
32	DD	150[B]	MEQ	C-CA-CB-CG
32	DD	150[B]	MEQ	O-C-CA-CB
55	DA	2251	OMG	C1'-C2'-O2'-CM2
41	DN	81[B]	4D4	CA-CB-CG-CD
1	AA	527	7MG	C3'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
1	BA	1519	MA6	O4'-C4'-C5'-O5'
31	CA	2030	6MZ	O4'-C4'-C5'-O5'
31	CA	2030	6MZ	C3'-C4'-C5'-O5'
55	DA	2030	6MZ	O4'-C4'-C5'-O5'
55	DA	2030	6MZ	C3'-C4'-C5'-O5'
41	DN	81[B]	4D4	OB-CB-CG-CD
55	DA	2445	2MG	C3'-C4'-C5'-O5'
1	AA	1519	MA6	C3'-C4'-C5'-O5'
1	BA	1519	MA6	C3'-C4'-C5'-O5'
32	DD	150[B]	MEQ	CA-CB-CG-CD
32	DD	150[A]	MEQ	OE1-CD-CG-CB
12	AL	89	D2T	CG-CB-SB-CB1
12	BL	89	D2T	CG-CB-SB-CB1
55	DA	2445	2MG	O4'-C4'-C5'-O5'
32	DD	150[A]	MEQ	NE2-CD-CG-CB
55	DA	2069	7MG	C4'-C5'-O5'-P
41	DN	81[B]	4D4	N-CA-CB-CG
55	DA	747	5MU	C3'-C4'-C5'-O5'
41	DN	81[A]	4D4	CG-CD-NE-CZ
55	DA	1962	5MC	C2'-C1'-N1-C6
55	DA	1962	5MC	O4'-C1'-N1-C6
12	BL	89	D2T	SB-CB-CG-OD2

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Mol	Chain	Res	Type	Atoms
31	CA	746	PSU	O4'-C1'-C5-C6
55	DA	746	PSU	O4'-C1'-C5-C6
12	BL	89	D2T	CA-CB-CG-OD1
12	BL	89	D2T	CA-CB-CG-OD2
31	CA	746	PSU	C2'-C1'-C5-C6
55	DA	746	PSU	C2'-C1'-C5-C6
55	DA	1835	2MG	C3'-C4'-C5'-O5'
31	CA	2552	OMU	C3'-C2'-O2'-CM2
55	DA	2552	OMU	C3'-C2'-O2'-CM2
41	CN	81	4D4	O-C-CA-CB
1	AA	1402	4OC	O4'-C4'-C5'-O5'
1	BA	1402	4OC	O4'-C4'-C5'-O5'
31	CA	2504	PSU	O4'-C4'-C5'-O5'
55	DA	1835	2MG	O4'-C4'-C5'-O5'
55	DA	2504	PSU	O4'-C4'-C5'-O5'
31	CA	2503	2MA	C4'-C5'-O5'-P
55	DA	2503	2MA	C4'-C5'-O5'-P
31	CA	1618	6MZ	C4'-C5'-O5'-P
31	CA	1835	2MG	O4'-C4'-C5'-O5'

There are no ring outliers.

17 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	DA	2030	6MZ	1	0
31	CA	2030	6MZ	1	0
1	BA	967	5MC	1	0
32	DD	150[A]	MEQ	3	0
1	AA	967	5MC	1	0
1	BA	1519	MA6	1	0
32	DD	150[B]	MEQ	1	0
1	AA	1519	MA6	1	0
31	CA	2503	2MA	1	0
55	DA	2251	OMG	1	0
55	DA	2498	OMC	1	0
1	BA	1518	MA6	1	0
1	AA	1518	MA6	1	0
31	CA	2498	OMC	2	0
55	DA	2503	2MA	1	0
31	CA	2580	PSU	1	0
31	CA	1915	3TD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 557 ligands modelled in this entry, 475 are monoatomic - leaving 82 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	PUT	AA	1674	-	5,5,5	0.14	0	4,4,4	0.10	0
58	MPD	DT	201	-	7,7,7	0.46	0	9,10,10	0.35	0
59	PUT	DA	3223	-	5,5,5	0.16	0	4,4,4	0.12	0
59	PUT	DA	3189	-	5,5,5	0.29	0	4,4,4	0.20	0
59	PUT	DA	3195	-	5,5,5	0.31	0	4,4,4	0.36	0
64	PGE	DA	3214	-	9,9,9	0.19	0	8,8,8	0.27	0
63	EDO	DA	3197	-	3,3,3	0.60	0	2,2,2	0.24	0
59	PUT	AA	1675	-	5,5,5	0.20	0	4,4,4	0.13	0
59	PUT	DA	3184	-	5,5,5	0.15	0	4,4,4	0.11	0
57	PG4	DR	202	-	12,12,12	0.26	0	11,11,11	0.36	0
63	EDO	DB	201	-	3,3,3	0.61	0	2,2,2	0.19	0
67	ACY	DA	3201	-	3,3,3	0.76	0	3,3,3	1.05	0
64	PGE	DA	3217	-	9,9,9	0.16	0	8,8,8	0.13	0
64	PGE	DS	201	-	9,9,9	0.25	0	8,8,8	0.20	0
59	PUT	AA	1673	-	5,5,5	0.10	0	4,4,4	0.07	0
58	MPD	DN	201	-	7,7,7	0.79	0	9,10,10	0.54	0
63	EDO	DA	3208	-	3,3,3	0.60	0	2,2,2	0.22	0
63	EDO	DA	3215	-	3,3,3	0.62	0	2,2,2	0.23	0
59	PUT	DA	3188	-	5,5,5	0.20	0	4,4,4	0.13	0
65	SPD	DA	3224	-	9,9,9	0.19	0	8,8,8	0.40	0
59	PUT	DA	3222	-	5,5,5	0.44	0	4,4,4	0.58	0
59	PUT	DA	3213	-	5,5,5	0.16	0	4,4,4	0.17	0
63	EDO	DA	3002	-	3,3,3	0.62	0	2,2,2	0.24	0
64	PGE	D3	101	-	9,9,9	0.23	0	8,8,8	0.22	0
63	EDO	DA	3194	-	3,3,3	0.72	0	2,2,2	0.15	0
62	PEG	D3	102	-	6,6,6	0.21	0	5,5,5	0.19	0
58	MPD	DA	3204	-	7,7,7	0.69	0	9,10,10	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	PG4	DQ	202	-	12,12,12	0.20	0	11,11,11	0.14	0
58	MPD	DA	3190	-	7,7,7	0.32	0	9,10,10	0.52	0
59	PUT	DA	3221	-	5,5,5	0.16	0	4,4,4	0.11	0
58	MPD	AA	1671	-	7,7,7	0.58	0	9,10,10	0.55	0
58	MPD	DA	3210	-	7,7,7	0.56	0	9,10,10	0.30	0
59	PUT	AA	1672	-	5,5,5	0.19	0	4,4,4	0.21	0
58	MPD	DE	301	-	7,7,7	0.72	0	9,10,10	0.60	0
60	T1C	BA	1643	56	45,45,45	1.05	3 (6%)	56,72,72	1.64	7 (12%)
62	PEG	DA	3218	-	6,6,6	0.17	0	5,5,5	0.08	0
58	MPD	DK	201	-	7,7,7	0.58	0	9,10,10	0.28	0
62	PEG	DQ	201	-	6,6,6	0.13	0	5,5,5	0.09	0
63	EDO	D1	101	-	3,3,3	0.56	0	2,2,2	0.15	0
60	T1C	AA	1680	56	45,45,45	1.06	3 (6%)	56,72,72	1.56	4 (7%)
59	PUT	DA	3219	-	5,5,5	0.16	0	4,4,4	0.20	0
64	PGE	DA	3203	-	9,9,9	0.21	0	8,8,8	0.20	0
67	ACY	DA	3191	-	3,3,3	0.59	0	3,3,3	0.95	0
67	ACY	DA	3196	-	3,3,3	2.27	1 (33%)	3,3,3	2.32	2 (66%)
69	TRS	DA	3220	-	7,7,7	0.31	0	9,9,9	0.34	0
63	EDO	DA	3209	-	3,3,3	0.54	0	2,2,2	0.32	0
57	PG4	BA	1642	-	12,12,12	0.15	0	11,11,11	0.19	0
62	PEG	DA	3227	-	6,6,6	0.22	0	5,5,5	0.14	0
65	SPD	DA	3183	-	9,9,9	0.10	0	8,8,8	0.10	0
63	EDO	DA	3198	-	3,3,3	0.59	0	2,2,2	0.24	0
64	PGE	DA	3225	-	9,9,9	0.12	0	8,8,8	0.17	0
59	PUT	DA	3001	-	5,5,5	0.24	0	4,4,4	0.13	0
63	EDO	DB	211	-	3,3,3	0.64	0	2,2,2	0.14	0
62	PEG	DA	3226	-	6,6,6	0.24	0	5,5,5	0.12	0
62	PEG	DP	201	-	6,6,6	0.16	0	5,5,5	0.08	0
59	PUT	DA	3205	-	5,5,5	0.11	0	4,4,4	0.10	0
62	PEG	DA	3199	-	6,6,6	0.24	0	5,5,5	0.15	0
58	MPD	DT	202	-	7,7,7	0.62	0	9,10,10	0.38	0
63	EDO	DB	213	-	3,3,3	0.66	0	2,2,2	0.08	0
57	PG4	DA	3216	-	12,12,12	0.10	0	11,11,11	0.17	0
57	PG4	DA	3193	-	12,12,12	0.29	0	11,11,11	0.25	0
65	SPD	DA	3187	-	9,9,9	0.21	0	8,8,8	0.19	0
58	MPD	DS	203	-	7,7,7	0.31	0	9,10,10	0.52	0
62	PEG	DA	3200	-	6,6,6	0.35	0	5,5,5	0.21	0
66	1PE	DA	3185	-	15,15,15	0.19	0	14,14,14	0.21	0
57	PG4	DS	202	-	12,12,12	0.46	0	11,11,11	0.29	0
64	PGE	DA	3186	-	9,9,9	0.24	0	8,8,8	0.29	0
57	PG4	AA	1670	-	12,12,12	0.31	0	11,11,11	0.28	0
64	PGE	D1	102	-	9,9,9	0.20	0	8,8,8	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	MPD	DE	302	-	7,7,7	0.79	0	9,10,10	0.61	0
58	MPD	AA	1676	-	7,7,7	0.53	0	9,10,10	0.59	0
58	MPD	DA	3207	-	7,7,7	0.68	0	9,10,10	0.53	0
68	GUN	DA	3211	-	12,12,12	0.37	0	15,17,17	0.31	0
66	1PE	DA	3202	-	15,15,15	0.32	0	14,14,14	0.34	0
59	PUT	DA	3212	-	5,5,5	0.17	0	4,4,4	0.04	0
62	PEG	DL	201	-	6,6,6	0.07	0	5,5,5	0.10	0
58	MPD	DA	3192	-	7,7,7	0.45	0	9,10,10	0.58	0
63	EDO	DB	212	-	3,3,3	0.52	0	2,2,2	0.34	0
62	PEG	D1	103	-	6,6,6	0.31	0	5,5,5	0.15	0
65	SPD	DA	3206	-	9,9,9	0.20	0	8,8,8	0.17	0
64	PGE	DU	101	-	9,9,9	0.23	0	8,8,8	0.12	0
62	PEG	AL	201	-	6,6,6	0.23	0	5,5,5	0.12	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PUT	AA	1674	-	-	0/3/3/3	-
58	MPD	DT	201	-	-	3/5/5/5	-
59	PUT	DA	3223	-	-	1/3/3/3	-
59	PUT	DA	3189	-	-	0/3/3/3	-
59	PUT	DA	3195	-	-	1/3/3/3	-
64	PGE	DA	3214	-	-	2/7/7/7	-
63	EDO	DA	3197	-	-	0/1/1/1	-
59	PUT	AA	1675	-	-	1/3/3/3	-
59	PUT	DA	3184	-	-	0/3/3/3	-
57	PG4	DR	202	-	-	5/10/10/10	-
63	EDO	DB	201	-	-	1/1/1/1	-
64	PGE	DA	3217	-	-	4/7/7/7	-
64	PGE	DS	201	-	-	3/7/7/7	-
59	PUT	AA	1673	-	-	0/3/3/3	-
58	MPD	DN	201	-	-	2/5/5/5	-
63	EDO	DA	3208	-	-	0/1/1/1	-
63	EDO	DA	3215	-	-	1/1/1/1	-
59	PUT	DA	3188	-	-	0/3/3/3	-
65	SPD	DA	3224	-	-	3/7/7/7	-
59	PUT	DA	3222	-	-	0/3/3/3	-
59	PUT	DA	3213	-	-	0/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	EDO	DA	3002	-	-	0/1/1/1	-
64	PGE	D3	101	-	-	2/7/7/7	-
63	EDO	DA	3194	-	-	0/1/1/1	-
62	PEG	D3	102	-	-	1/4/4/4	-
58	MPD	DA	3204	-	-	4/5/5/5	-
57	PG4	DQ	202	-	-	1/10/10/10	-
58	MPD	DA	3190	-	-	2/5/5/5	-
59	PUT	DA	3221	-	-	0/3/3/3	-
58	MPD	AA	1671	-	-	0/5/5/5	-
58	MPD	DA	3210	-	-	0/5/5/5	-
59	PUT	AA	1672	-	-	0/3/3/3	-
58	MPD	DE	301	-	-	2/5/5/5	-
60	T1C	BA	1643	56	-	11/22/80/80	0/4/4/4
62	PEG	DA	3218	-	-	1/4/4/4	-
58	MPD	DK	201	-	-	2/5/5/5	-
62	PEG	DQ	201	-	-	1/4/4/4	-
63	EDO	D1	101	-	-	0/1/1/1	-
60	T1C	AA	1680	56	-	6/22/80/80	0/4/4/4
59	PUT	DA	3219	-	-	0/3/3/3	-
64	PGE	DA	3203	-	-	5/7/7/7	-
69	TRS	DA	3220	-	-	0/9/9/9	-
63	EDO	DA	3209	-	-	0/1/1/1	-
57	PG4	BA	1642	-	-	0/10/10/10	-
62	PEG	DA	3227	-	-	0/4/4/4	-
65	SPD	DA	3183	-	-	1/7/7/7	-
63	EDO	DA	3198	-	-	1/1/1/1	-
64	PGE	DA	3225	-	-	4/7/7/7	-
59	PUT	DA	3001	-	-	0/3/3/3	-
63	EDO	DB	211	-	-	0/1/1/1	-
62	PEG	DA	3226	-	-	2/4/4/4	-
62	PEG	DP	201	-	-	2/4/4/4	-
59	PUT	DA	3205	-	-	0/3/3/3	-
62	PEG	DA	3199	-	-	2/4/4/4	-
58	MPD	DT	202	-	-	2/5/5/5	-
63	EDO	DB	213	-	-	0/1/1/1	-
57	PG4	DA	3216	-	-	3/10/10/10	-
57	PG4	DA	3193	-	-	5/10/10/10	-
65	SPD	DA	3187	-	-	2/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	MPD	DS	203	-	-	1/5/5/5	-
62	PEG	DA	3200	-	-	2/4/4/4	-
66	1PE	DA	3185	-	-	5/13/13/13	-
57	PG4	DS	202	-	-	5/10/10/10	-
64	PGE	DA	3186	-	-	3/7/7/7	-
57	PG4	AA	1670	-	-	4/10/10/10	-
64	PGE	D1	102	-	-	3/7/7/7	-
58	MPD	DE	302	-	-	2/5/5/5	-
58	MPD	AA	1676	-	-	4/5/5/5	-
58	MPD	DA	3207	-	-	2/5/5/5	-
68	GUN	DA	3211	-	-	-	0/2/2/2
66	1PE	DA	3202	-	-	4/13/13/13	-
59	PUT	DA	3212	-	-	0/3/3/3	-
62	PEG	DL	201	-	-	2/4/4/4	-
58	MPD	DA	3192	-	-	1/5/5/5	-
63	EDO	DB	212	-	-	1/1/1/1	-
62	PEG	D1	103	-	-	0/4/4/4	-
65	SPD	DA	3206	-	-	3/7/7/7	-
64	PGE	DU	101	-	-	3/7/7/7	-
62	PEG	AL	201	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	DA	3196	ACY	O-C	3.74	1.38	1.22
60	BA	1643	T1C	C4-C3	3.30	1.58	1.51
60	AA	1680	T1C	C4-C3	2.99	1.57	1.51
60	AA	1680	T1C	C7-C61	2.96	1.43	1.40
60	BA	1643	T1C	C7-C61	2.91	1.43	1.40
60	BA	1643	T1C	C7-N7	2.61	1.49	1.42
60	AA	1680	T1C	C7-N7	2.54	1.49	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	1643	T1C	C92-N92-C93	7.92	125.80	115.77
60	AA	1680	T1C	C92-N92-C93	7.68	125.49	115.77
60	AA	1680	T1C	C8-C9-C10	-5.29	115.41	120.53
60	BA	1643	T1C	C8-C9-C10	-4.69	115.98	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	1643	T1C	C61-C6-C51	-3.60	108.36	113.12
67	DA	3196	ACY	OXT-C-CH3	3.06	127.87	115.05
67	DA	3196	ACY	O-C-CH3	-2.56	112.04	122.53
60	AA	1680	T1C	C1A-C10-C9	2.27	122.91	118.98
60	BA	1643	T1C	C1A-C10-C9	2.19	122.78	118.98
60	AA	1680	T1C	O3-C3-C2	2.16	126.56	122.93
60	BA	1643	T1C	C11-C1B-C12	2.16	120.51	118.80
60	BA	1643	T1C	O3-C3-C2	2.09	126.43	122.93
60	BA	1643	T1C	C5-C41-C4	-2.05	110.77	113.73

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AA	1676	MPD	C2-C3-C4-C5
58	DA	3192	MPD	C2-C3-C4-O4
60	AA	1680	T1C	C95-C93-N92-C92
60	AA	1680	T1C	C96-C93-N92-C92
60	AA	1680	T1C	C91-C92-N92-C93
60	BA	1643	T1C	C1-C2-C21-O21
60	BA	1643	T1C	C1-C2-C21-N21
66	DA	3202	1PE	OH5-C14-C24-OH4
57	DR	202	PG4	O2-C3-C4-O3
60	AA	1680	T1C	C94-C93-N92-C92
66	DA	3202	1PE	OH4-C13-C23-OH3
64	DU	101	PGE	O3-C5-C6-O4
64	DA	3203	PGE	O2-C3-C4-O3
60	BA	1643	T1C	C92-C91-N9-C9
57	DS	202	PG4	O1-C1-C2-O2
64	DU	101	PGE	O1-C1-C2-O2
57	DQ	202	PG4	O1-C1-C2-O2
65	DA	3183	SPD	C2-C3-C4-C5
57	DS	202	PG4	O4-C7-C8-O5
64	DA	3186	PGE	O3-C5-C6-O4
66	DA	3202	1PE	OH2-C12-C22-OH3
60	BA	1643	T1C	O91-C91-N9-C9
65	DA	3224	SPD	C4-C5-N6-C7
57	DA	3193	PG4	O3-C5-C6-O4
60	BA	1643	T1C	O91-C91-C92-N92
64	DA	3225	PGE	O3-C5-C6-O4
65	DA	3187	SPD	C2-C3-C4-C5
65	DA	3206	SPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
57	DA	3216	PG4	C3-C4-O3-C5
62	DA	3200	PEG	C1-C2-O2-C3
62	DA	3199	PEG	C4-C3-O2-C2
66	DA	3185	1PE	C12-C22-OH3-C23
64	DA	3186	PGE	C3-C4-O3-C5
62	DA	3218	PEG	C1-C2-O2-C3
57	DA	3193	PG4	C4-C3-O2-C2
64	DA	3217	PGE	C3-C4-O3-C5
57	DR	202	PG4	C4-C3-O2-C2
64	D3	101	PGE	C4-C3-O2-C2
64	DA	3214	PGE	C4-C3-O2-C2
59	DA	3223	PUT	C1-C2-C3-C4
57	DR	202	PG4	C6-C5-O3-C4
66	DA	3185	1PE	C16-C26-OH6-C15
57	AA	1670	PG4	C4-C3-O2-C2
66	DA	3185	1PE	C13-C23-OH3-C22
62	D3	102	PEG	C1-C2-O2-C3
64	DU	101	PGE	C6-C5-O3-C4
64	DA	3225	PGE	C1-C2-O2-C3
62	AL	201	PEG	C4-C3-O2-C2
64	DA	3225	PGE	O2-C3-C4-O3
60	BA	1643	T1C	N9-C91-C92-N92
64	DA	3203	PGE	C3-C4-O3-C5
64	DS	201	PGE	C4-C3-O2-C2
64	DA	3186	PGE	O1-C1-C2-O2
64	DA	3225	PGE	O1-C1-C2-O2
60	AA	1680	T1C	O91-C91-C92-N92
58	DK	201	MPD	O2-C2-C3-C4
58	DN	201	MPD	O2-C2-C3-C4
57	DA	3216	PG4	C8-C7-O4-C6
58	DE	302	MPD	C2-C3-C4-O4
58	DN	201	MPD	C2-C3-C4-O4
62	DP	201	PEG	C4-C3-O2-C2
64	D1	102	PGE	C4-C3-O2-C2
66	DA	3202	1PE	C12-C22-OH3-C23
57	DS	202	PG4	C4-C3-O2-C2
64	D3	101	PGE	C3-C4-O3-C5
58	DT	201	MPD	C1-C2-C3-C4
58	DA	3207	MPD	C1-C2-C3-C4
64	DA	3203	PGE	C4-C3-O2-C2
65	DA	3187	SPD	N6-C7-C8-C9
60	BA	1643	T1C	C91-C92-N92-C93

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Mol	Chain	Res	Type	Atoms
57	DA	3193	PG4	C6-C5-O3-C4
62	DA	3200	PEG	C4-C3-O2-C2
58	DE	301	MPD	C2-C3-C4-C5
58	DT	202	MPD	C2-C3-C4-C5
58	DA	3190	MPD	C2-C3-C4-C5
58	DA	3204	MPD	C2-C3-C4-C5
60	AA	1680	T1C	N9-C91-C92-N92
62	DA	3226	PEG	C4-C3-O2-C2
65	DA	3206	SPD	C8-C7-N6-C5
62	DQ	201	PEG	C1-C2-O2-C3
64	D1	102	PGE	C3-C4-O3-C5
59	AA	1675	PUT	C1-C2-C3-C4
59	DA	3195	PUT	C1-C2-C3-C4
65	DA	3224	SPD	C8-C7-N6-C5
65	DA	3224	SPD	C7-C8-C9-N10
57	DA	3193	PG4	C3-C4-O3-C5
64	DA	3203	PGE	C1-C2-O2-C3
63	DB	201	EDO	O1-C1-C2-O2
63	DA	3198	EDO	O1-C1-C2-O2
57	DR	202	PG4	O3-C5-C6-O4
64	DA	3217	PGE	C6-C5-O3-C4
62	AL	201	PEG	C1-C2-O2-C3
62	DL	201	PEG	C1-C2-O2-C3
63	DA	3215	EDO	O1-C1-C2-O2
57	AA	1670	PG4	C5-C6-O4-C7
62	DA	3226	PEG	O1-C1-C2-O2
57	AA	1670	PG4	C1-C2-O2-C3
66	DA	3185	1PE	C24-C14-OH5-C25
64	DA	3217	PGE	C1-C2-O2-C3
57	DS	202	PG4	C5-C6-O4-C7
63	DB	212	EDO	O1-C1-C2-O2
64	D1	102	PGE	O2-C3-C4-O3
64	DA	3217	PGE	C4-C3-O2-C2
65	DA	3206	SPD	C4-C5-N6-C7
62	DA	3199	PEG	C1-C2-O2-C3
66	DA	3185	1PE	C23-C13-OH4-C24
57	DS	202	PG4	C1-C2-O2-C3
62	DP	201	PEG	C1-C2-O2-C3
57	DA	3216	PG4	C1-C2-O2-C3
64	DA	3203	PGE	O3-C5-C6-O4
60	BA	1643	T1C	C61-C7-N7-C71
58	DE	302	MPD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
58	DT	201	MPD	O2-C2-C3-C4
58	DT	202	MPD	O2-C2-C3-C4
58	DA	3204	MPD	O2-C2-C3-C4
64	DS	201	PGE	C6-C5-O3-C4
58	AA	1676	MPD	C2-C3-C4-O4
58	DE	301	MPD	C2-C3-C4-O4
58	DK	201	MPD	C2-C3-C4-O4
58	DA	3190	MPD	C2-C3-C4-O4
58	DA	3204	MPD	C2-C3-C4-O4
62	DL	201	PEG	C4-C3-O2-C2
57	DA	3193	PG4	O1-C1-C2-O2
64	DA	3214	PGE	O3-C5-C6-O4
58	AA	1676	MPD	C1-C2-C3-C4
58	AA	1676	MPD	CM-C2-C3-C4
58	DS	203	MPD	C1-C2-C3-C4
58	DT	201	MPD	CM-C2-C3-C4
58	DA	3204	MPD	CM-C2-C3-C4
58	DA	3207	MPD	CM-C2-C3-C4
60	BA	1643	T1C	C3-C2-C21-N21
60	BA	1643	T1C	C61-C7-N7-C72
57	DR	202	PG4	C8-C7-O4-C6
60	BA	1643	T1C	C3-C2-C21-O21
57	AA	1670	PG4	O1-C1-C2-O2
64	DS	201	PGE	O2-C3-C4-O3

There are no ring outliers.

24 monomers are involved in 32 short contacts:

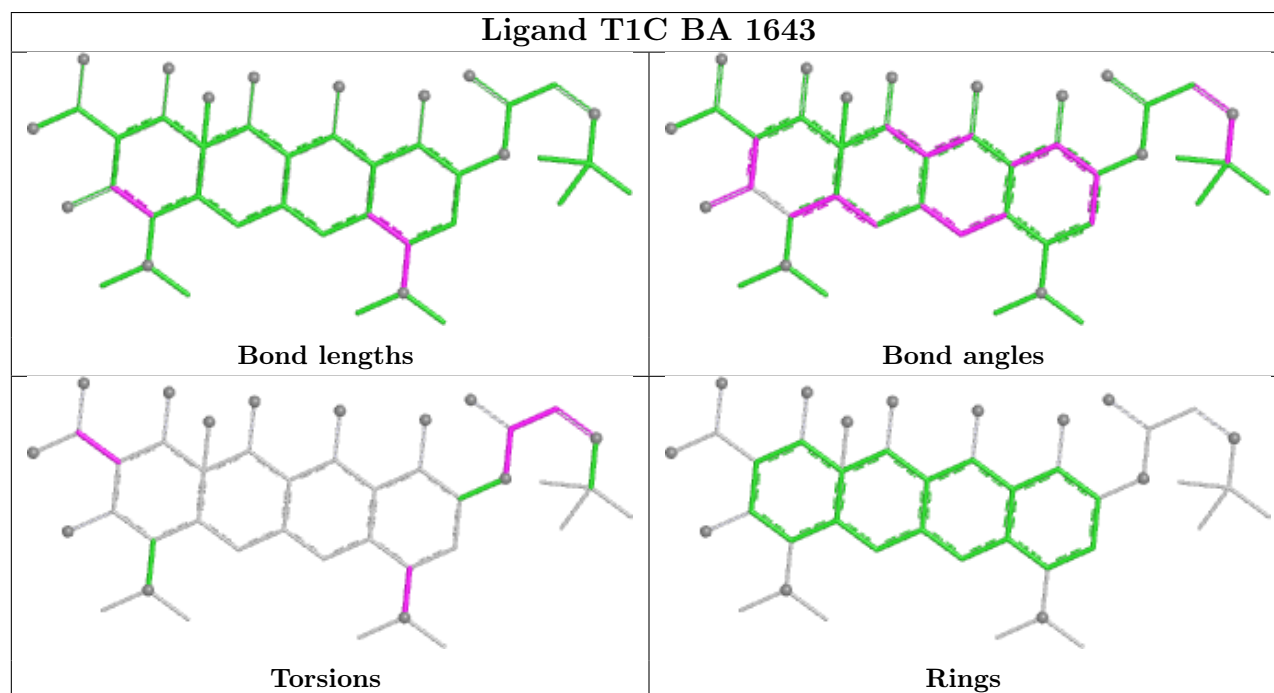
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	DA	3223	PUT	1	0
59	DA	3195	PUT	1	0
64	DA	3214	PGE	1	0
57	DR	202	PG4	4	0
64	DA	3217	PGE	1	0
64	DS	201	PGE	1	0
58	DN	201	MPD	1	0
65	DA	3224	SPD	2	0
58	DA	3204	MPD	1	0
60	AA	1680	T1C	2	0
59	DA	3219	PUT	1	0
64	DA	3203	PGE	1	0
69	DA	3220	TRS	1	0

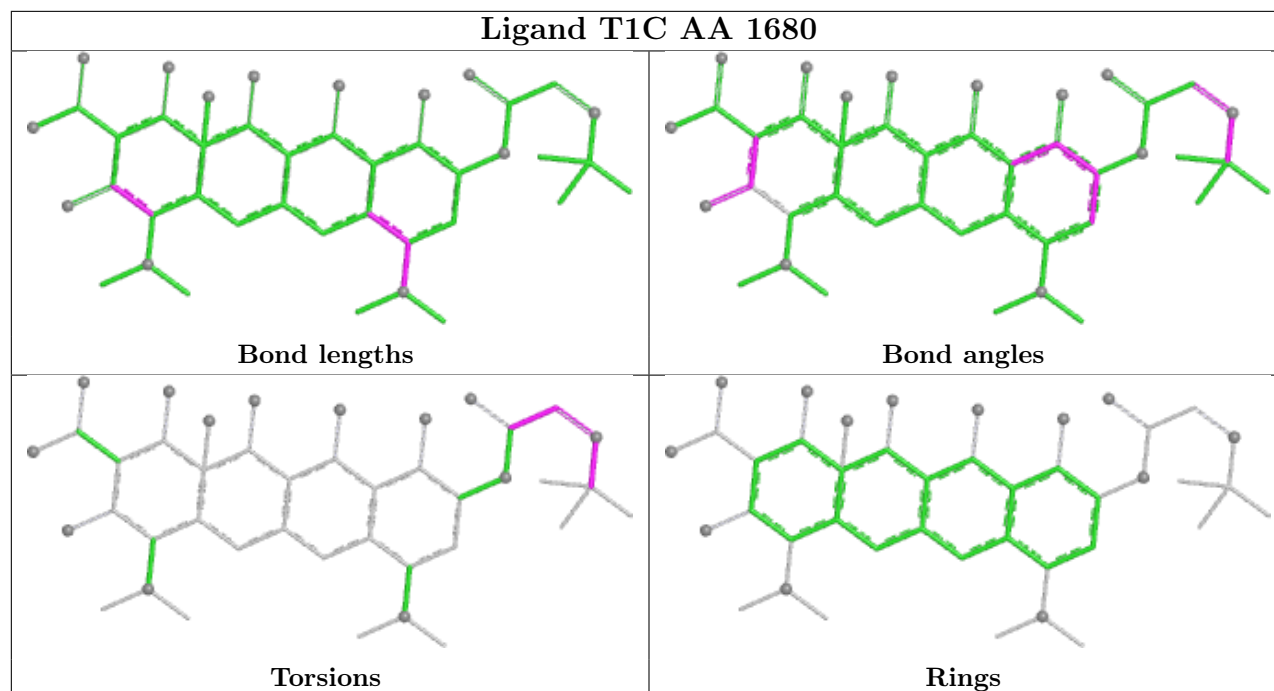
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	DA	3209	EDO	1	0
57	BA	1642	PG4	1	0
64	DA	3225	PGE	2	0
66	DA	3185	1PE	1	0
57	DS	202	PG4	1	0
57	AA	1670	PG4	1	0
64	D1	102	PGE	2	0
66	DA	3202	1PE	2	0
58	DA	3192	MPD	1	0
62	D1	103	PEG	1	0
64	DU	101	PGE	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	AA	1523/1534 (99%)	0.12	84 (5%)	30	16	43, 96, 240, 296	0
1	BA	1522/1534 (99%)	0.37	96 (6%)	26	14	59, 109, 268, 280	0
2	AB	224/224 (100%)	0.50	8 (3%)	46	26	72, 125, 197, 249	0
2	BB	224/224 (100%)	0.71	15 (6%)	24	13	101, 143, 205, 240	0
3	AC	206/206 (100%)	0.29	6 (2%)	53	32	78, 108, 137, 154	0
3	BC	206/206 (100%)	0.60	16 (7%)	19	10	103, 151, 181, 204	0
4	AD	205/205 (100%)	0.15	1 (0%)	87	73	71, 104, 137, 164	0
4	BD	205/205 (100%)	-0.07	0	100	100	51, 77, 108, 132	0
5	AE	155/155 (100%)	0.01	0	100	100	59, 84, 116, 155	0
5	BE	150/155 (96%)	0.41	5 (3%)	49	29	68, 94, 135, 207	0
6	AF	106/106 (100%)	0.29	1 (0%)	81	63	78, 107, 128, 148	0
6	BF	100/106 (94%)	0.34	3 (3%)	52	31	88, 124, 147, 160	0
7	AG	151/151 (100%)	0.96	19 (12%)	8	4	108, 141, 166, 178	0
7	BG	151/151 (100%)	1.34	35 (23%)	2	1	145, 205, 222, 231	0
8	AH	129/129 (100%)	0.19	4 (3%)	51	30	67, 89, 116, 132	0
8	BH	129/129 (100%)	0.34	6 (4%)	36	19	90, 113, 141, 157	0
9	AI	127/127 (100%)	1.05	20 (15%)	5	2	86, 142, 167, 175	0
9	BI	127/127 (100%)	1.47	27 (21%)	2	1	141, 172, 209, 221	0
10	AJ	99/99 (100%)	1.19	21 (21%)	2	1	91, 129, 150, 161	0
10	BJ	98/99 (98%)	1.53	30 (30%)	1	1	144, 175, 196, 202	0
11	AK	117/117 (100%)	0.48	4 (3%)	48	28	59, 117, 141, 150	0
11	BK	117/117 (100%)	0.64	9 (7%)	19	10	69, 115, 149, 175	0
12	AL	122/123 (99%)	-0.02	2 (1%)	70	49	50, 70, 99, 133	0
12	BL	122/123 (99%)	0.54	10 (8%)	17	10	71, 86, 117, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	1.14	23 (20%) 3 1	116, 139, 175, 182	0
13	BM	114/114 (100%)	1.17	14 (12%) 8 5	202, 239, 248, 254	0
14	AN	100/100 (100%)	1.46	27 (27%) 1 1	84, 124, 192, 203	0
14	BN	100/100 (100%)	1.38	17 (17%) 4 2	134, 185, 229, 236	0
15	AO	88/88 (100%)	0.22	2 (2%) 61 39	68, 92, 115, 136	0
15	BO	88/88 (100%)	0.32	1 (1%) 78 59	79, 113, 132, 152	0
16	AP	82/82 (100%)	0.42	5 (6%) 27 15	62, 86, 128, 142	0
16	BP	82/82 (100%)	0.95	11 (13%) 7 4	77, 94, 149, 159	0
17	AQ	80/80 (100%)	0.16	2 (2%) 58 37	64, 88, 118, 134	0
17	BQ	80/80 (100%)	0.72	4 (5%) 34 18	83, 120, 149, 157	0
18	AR	55/55 (100%)	0.46	2 (3%) 46 26	74, 101, 142, 166	0
18	BR	55/55 (100%)	0.55	4 (7%) 21 11	75, 97, 134, 166	0
19	AS	79/79 (100%)	1.43	18 (22%) 2 1	123, 139, 159, 165	0
19	BS	79/79 (100%)	1.17	15 (18%) 3 1	217, 233, 247, 254	0
20	AT	86/86 (100%)	0.44	2 (2%) 61 39	68, 86, 116, 133	0
20	BT	85/86 (98%)	1.24	17 (20%) 3 1	90, 119, 151, 161	0
21	AU	56/56 (100%)	0.63	4 (7%) 22 12	81, 118, 163, 176	0
21	BU	56/56 (100%)	0.64	5 (8%) 15 8	75, 110, 147, 155	0
22	C1	56/56 (100%)	1.74	17 (30%) 1 1	93, 147, 170, 185	0
22	D1	56/56 (100%)	-0.46	0 100 100	21, 47, 72, 112	0
23	C2	50/51 (98%)	1.63	17 (34%) 1 0	145, 160, 172, 198	0
23	D2	51/51 (100%)	0.10	1 (1%) 65 44	56, 69, 100, 116	0
24	C3	46/46 (100%)	2.37	26 (56%) 0 0	102, 130, 139, 152	0
24	D3	46/46 (100%)	-0.36	1 (2%) 62 41	30, 40, 58, 116	0
25	C4	64/64 (100%)	3.00	49 (76%) 0 0	108, 134, 150, 160	0
25	D4	64/64 (100%)	-0.28	0 100 100	32, 41, 57, 75	0
26	C5	38/38 (100%)	1.87	12 (31%) 1 1	115, 134, 145, 151	0
26	D5	38/38 (100%)	-0.35	0 100 100	43, 55, 72, 99	0
27	C0	58/58 (100%)	1.77	17 (29%) 1 1	109, 132, 151, 162	0
27	D0	58/58 (100%)	-0.33	2 (3%) 48 28	27, 37, 61, 83	2 (3%)
28	CB	118/120 (98%)	0.72	11 (9%) 14 8	110, 181, 234, 243	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	120/120 (100%)	-0.58	0 100 100	34, 63, 99, 131	0
29	CC	271/272 (99%)	0.75	39 (14%) 6 3	73, 100, 126, 136	0
29	DC	271/272 (99%)	-0.34	5 (1%) 67 47	26, 57, 84, 99	0
30	CD	209/209 (100%)	0.99	23 (11%) 10 5	79, 116, 143, 158	0
31	CA	2876/2904 (99%)	0.79	256 (8%) 15 8	64, 133, 248, 291	0
32	DD	208/209 (99%)	-0.55	1 (0%) 87 73	20, 41, 71, 100	0
33	CE	201/201 (100%)	1.19	35 (17%) 4 2	90, 160, 190, 200	0
33	DE	201/201 (100%)	-0.37	1 (0%) 87 73	25, 62, 104, 136	0
34	CF	177/178 (99%)	0.70	6 (3%) 48 28	201, 219, 227, 235	0
34	DF	177/178 (99%)	0.15	1 (0%) 85 70	54, 89, 132, 150	0
35	CG	176/176 (100%)	0.63	4 (2%) 61 39	140, 167, 194, 206	0
35	DG	176/176 (100%)	-0.05	5 (2%) 55 34	44, 75, 103, 136	0
36	CH	149/149 (100%)	0.46	3 (2%) 65 44	89, 149, 175, 187	0
36	DH	149/149 (100%)	0.62	5 (3%) 48 28	71, 150, 190, 207	0
37	CJ	134/135 (99%)	1.36	30 (22%) 2 1	241, 258, 269, 276	0
37	DJ	134/135 (99%)	1.43	32 (23%) 2 1	210, 234, 245, 252	0
38	CK	142/142 (100%)	0.85	11 (7%) 19 10	84, 109, 134, 142	0
38	DK	142/142 (100%)	-0.61	0 100 100	23, 37, 67, 88	0
39	CL	122/123 (99%)	0.64	8 (6%) 24 13	76, 99, 141, 159	0
39	DL	123/123 (100%)	-0.57	0 100 100	28, 44, 71, 110	0
40	CM	144/144 (100%)	1.33	33 (22%) 2 1	94, 152, 193, 222	0
40	DM	144/144 (100%)	-0.21	2 (1%) 73 53	18, 56, 88, 121	0
41	CN	135/136 (99%)	0.72	12 (8%) 15 8	76, 111, 139, 174	0
41	DN	135/136 (99%)	-0.49	0 100 100	18, 43, 73, 95	1 (0%)
42	CO	120/125 (96%)	1.34	34 (28%) 1 1	93, 124, 143, 189	0
42	DO	125/125 (100%)	-0.52	0 100 100	27, 40, 76, 125	0
43	CP	116/117 (99%)	0.84	12 (10%) 12 6	142, 164, 181, 187	0
43	DP	117/117 (100%)	-0.21	0 100 100	42, 61, 90, 99	0
44	CQ	114/114 (100%)	0.76	12 (10%) 11 6	96, 113, 138, 154	0
44	DQ	114/114 (100%)	-0.30	1 (0%) 81 63	28, 52, 86, 125	0
45	CR	117/117 (100%)	1.16	24 (20%) 2 1	82, 109, 134, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	DR	117/117 (100%)	-0.66	0 100 100	19, 34, 52, 82	0
46	CS	103/103 (100%)	1.03	19 (18%) 3 1	101, 124, 166, 174	0
46	DS	103/103 (100%)	-0.55	2 (1%) 66 45	22, 45, 74, 101	0
47	CT	110/110 (100%)	1.50	25 (22%) 2 1	99, 126, 157, 172	0
47	DT	110/110 (100%)	-0.34	0 100 100	26, 37, 67, 120	0
48	CU	93/93 (100%)	1.60	28 (30%) 1 1	124, 154, 178, 190	0
48	DU	93/93 (100%)	0.19	4 (4%) 40 22	41, 63, 120, 139	0
49	CV	102/103 (99%)	1.71	37 (36%) 1 0	132, 164, 197, 206	0
49	DV	102/103 (99%)	-0.04	4 (3%) 43 24	49, 67, 116, 143	0
50	CW	94/94 (100%)	0.49	6 (6%) 25 14	122, 144, 158, 167	0
50	DW	94/94 (100%)	-0.34	0 100 100	38, 58, 88, 96	0
51	CX	75/83 (90%)	1.05	10 (13%) 7 4	95, 126, 138, 176	0
51	DX	76/83 (91%)	-0.30	1 (1%) 75 56	20, 43, 72, 108	1 (1%)
52	CY	77/77 (100%)	1.14	11 (14%) 6 3	87, 116, 146, 163	0
52	DY	77/77 (100%)	-0.19	1 (1%) 75 56	34, 58, 96, 112	0
53	CZ	62/62 (100%)	1.20	9 (14%) 6 3	139, 171, 185, 191	0
53	DZ	62/62 (100%)	0.44	2 (3%) 50 30	51, 81, 123, 140	0
54	DI	135/135 (100%)	1.29	28 (20%) 2 1	82, 161, 211, 226	1 (0%)
55	DA	2873/2904 (98%)	-0.67	79 (2%) 56 35	18, 47, 217, 299	11 (0%)
All	All	20634/20767 (99%)	0.36	1609 (7%) 19 10	18, 106, 237, 299	16 (0%)

All (1609) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	CA	2172	U	11.1
7	AG	5	ARG	10.5
1	AA	121	U	9.9
25	C4	36	LYS	9.1
31	CA	331	C	8.7
55	DA	2120	G	8.5
25	C4	37	ALA	8.5
25	C4	40	ARG	8.4
40	CM	81	ASP	7.9
9	BI	16	ALA	7.8
10	BJ	41	PRO	7.3

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Mol	Chain	Res	Type	RSRZ
18	BR	20	GLU	7.2
55	DA	1731	G	7.1
9	BI	68	LYS	7.1
10	BJ	74	VAL	7.0
48	CU	43	ILE	6.9
31	CA	2174	C	6.7
31	CA	931	U	6.6
17	BQ	70	THR	6.5
49	CV	31	SER	6.4
55	DA	2886[A]	A	6.4
48	CU	36	LYS	6.3
18	BR	51	TYR	6.2
44	DQ	2	SER	6.2
25	C4	39	LYS	6.2
1	AA	984	C	6.1
10	BJ	8	ILE	6.1
20	BT	4	ILE	6.1
54	DI	40	GLU	6.1
21	BU	57	ALA	6.0
7	AG	4	ARG	6.0
31	CA	2402	U	5.9
7	BG	62	PHE	5.8
31	CA	1068	G	5.7
37	CJ	23	PRO	5.7
1	BA	1305	G	5.6
20	BT	5	LYS	5.6
31	CA	328	U	5.5
49	CV	5	ILE	5.5
55	DA	2172	U	5.5
22	C1	2	ALA	5.5
1	AA	1281	C	5.5
47	CT	97	LEU	5.5
8	BH	2	SER	5.5
22	C1	27	SER	5.4
37	CJ	13	VAL	5.4
1	BA	1243	C	5.4
23	C2	24	THR	5.4
54	DI	2	ALA	5.4
38	CK	81	ILE	5.3
31	CA	2383	G	5.3
37	DJ	54	PRO	5.3
9	BI	124	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
27	C0	24	LEU	5.2
25	C4	41	LYS	5.2
24	C3	35	ARG	5.2
7	BG	4	ARG	5.1
1	AA	985	C	5.1
37	DJ	135	SER	5.1
14	AN	4	GLN	5.0
40	DM	104	GLN	5.0
29	CC	242	LYS	5.0
1	AA	962	C	5.0
25	C4	12	LYS	5.0
30	CD	126	ASN	5.0
8	AH	2	SER	5.0
2	AB	30	PHE	5.0
1	AA	963	G	4.9
25	C4	28	ASN	4.9
10	AJ	75	ASP	4.9
31	CA	327	G	4.9
21	AU	57	ALA	4.9
1	BA	4	U	4.9
54	DI	83	ALA	4.9
1	BA	632	U	4.9
1	AA	983	A	4.8
30	CD	200	ASP	4.8
1	AA	1127	G	4.8
25	C4	38	THR	4.8
40	CM	100	ILE	4.8
1	BA	1242	G	4.8
31	CA	329	G	4.8
31	CA	1984	G	4.8
31	CA	2666	C	4.7
37	CJ	11	LEU	4.7
7	AG	109	ARG	4.7
9	BI	128	SER	4.7
49	DV	56	GLY	4.7
26	C5	18	LYS	4.7
43	CP	30	ARG	4.7
5	BE	91	GLY	4.7
49	CV	80	ALA	4.7
51	CX	17	GLU	4.7
20	BT	67	ILE	4.6
54	DI	93	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	AA	1126	U	4.6
54	DI	38	MET	4.6
1	BA	983	A	4.6
31	CA	829	A	4.6
1	BA	121	U	4.6
31	CA	386	G	4.6
31	CA	1067	A	4.6
31	CA	1238	G	4.6
25	C4	15	LYS	4.6
27	C0	48	ILE	4.6
30	CD	8	LYS	4.5
1	AA	951	G	4.5
31	CA	1215	G	4.5
9	AI	129	LYS	4.5
25	C4	3	LYS	4.5
1	BA	250	A	4.5
1	BA	1201	A	4.5
10	BJ	75	ASP	4.5
45	CR	2	ALA	4.5
1	AA	959	A	4.5
46	CS	78	ARG	4.5
47	CT	85	ILE	4.4
1	AA	1364	U	4.4
19	BS	49	ILE	4.4
37	CJ	56	PRO	4.4
31	CA	12	U	4.4
31	CA	330	A	4.4
47	CT	94	ASP	4.4
7	BG	5	ARG	4.4
9	BI	14	SER	4.4
49	CV	3	ALA	4.4
23	C2	36	LEU	4.4
31	CA	2173	A	4.4
2	BB	34	ALA	4.3
14	AN	8	ALA	4.3
55	DA	1087	G	4.3
31	CA	332	A	4.3
37	DJ	13	VAL	4.3
22	C1	5	GLN	4.3
55	DA	2141	G	4.3
13	BM	96	PRO	4.3
47	CT	43	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
14	AN	11	VAL	4.3
29	CC	241	GLY	4.3
42	CO	23	ASN	4.3
31	CA	326	G	4.3
26	C5	23	ILE	4.3
31	CA	2363	G	4.2
14	BN	47	LYS	4.2
45	CR	28	ARG	4.2
37	DJ	12	GLN	4.2
14	AN	71	HIS	4.2
31	CA	1214	A	4.2
24	C3	24	THR	4.2
13	AM	105	ASN	4.1
23	C2	22	THR	4.1
39	CL	122	VAL	4.1
13	AM	19	LEU	4.1
54	DI	126	LEU	4.1
1	AA	1019	A	4.1
42	CO	25	ALA	4.1
9	BI	125	PRO	4.1
6	BF	100	SER	4.1
51	CX	55	ARG	4.1
3	AC	74	GLY	4.1
2	AB	27	MET	4.1
43	CP	103	VAL	4.1
27	C0	56	LYS	4.1
38	CK	111	LYS	4.0
31	CA	335	C	4.0
25	C4	65	ALA	4.0
1	AA	1148	U	4.0
55	DA	2152	G	4.0
24	C3	28	ARG	4.0
55	DA	654	A	4.0
24	D3	46	LYS	4.0
1	AA	1125	U	4.0
13	AM	33	ILE	4.0
37	CJ	76	ALA	4.0
55	DA	879	G	4.0
10	AJ	74	VAL	4.0
42	CO	105	GLY	4.0
49	CV	30	SER	4.0
37	DJ	79	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
7	BG	45	SER	3.9
14	AN	5	SER	3.9
25	C4	14	PHE	3.9
25	C4	23	LYS	3.9
45	CR	22	LYS	3.9
33	CE	143	LEU	3.9
19	AS	58	VAL	3.9
29	CC	233	GLY	3.9
1	AA	1030	U	3.9
51	CX	54	GLY	3.9
33	CE	104	ALA	3.9
1	BA	1241	G	3.9
33	CE	178	VAL	3.9
37	CJ	24	VAL	3.9
27	C0	10	THR	3.9
33	CE	32	VAL	3.8
18	AR	51	TYR	3.8
52	CY	48	THR	3.8
1	BA	1236	A	3.8
30	CD	198	GLY	3.8
55	DA	2153	C	3.8
1	BA	82	G	3.8
44	CQ	95	ALA	3.8
1	AA	961	U	3.8
1	BA	1364	U	3.8
37	DJ	80	LEU	3.8
10	AJ	43	PRO	3.8
9	BI	119	ARG	3.8
14	AN	21	PHE	3.8
37	DJ	138	LEU	3.8
55	DA	2110	G	3.8
40	CM	80	SER	3.8
45	CR	9	ILE	3.8
47	CT	84	ARG	3.8
36	DH	12	LEU	3.8
31	CA	1325	U	3.8
31	CA	1167	C	3.7
51	CX	44	LYS	3.7
1	AA	1240	U	3.7
20	BT	6	SER	3.7
49	CV	35	ILE	3.7
13	BM	99	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
34	CF	32	GLU	3.7
19	AS	60	VAL	3.7
43	CP	7	ARG	3.7
10	AJ	6	ILE	3.7
31	CA	1460	U	3.7
25	C4	43	HIS	3.7
30	CD	192	ALA	3.7
31	CA	1084	A	3.7
37	DJ	24	VAL	3.7
45	CR	4	VAL	3.7
54	DI	131	THR	3.7
48	DU	70	HIS	3.7
37	DJ	76	ALA	3.6
47	CT	44	ALA	3.6
1	BA	1235	U	3.6
36	CH	27	ARG	3.6
24	C3	31	LEU	3.6
25	C4	5	LYS	3.6
25	C4	52	LYS	3.6
39	CL	94	PRO	3.6
9	BI	17	ALA	3.6
13	BM	106	ALA	3.6
45	CR	59	GLN	3.6
1	AA	1305	G	3.6
31	CA	53	A	3.6
9	BI	116	VAL	3.6
37	DJ	78	VAL	3.6
21	AU	36	GLU	3.6
55	DA	2174	C	3.6
2	AB	132	LYS	3.6
48	CU	73	ARG	3.6
32	DD	54	ALA	3.6
55	DA	277	G	3.6
27	C0	29	LEU	3.6
27	D0	3[A]	LYS	3.6
54	DI	24	SER	3.6
31	CA	1986	C	3.6
37	CJ	12	GLN	3.6
12	BL	4	VAL	3.6
33	CE	164	LEU	3.6
33	CE	73	ILE	3.6
35	CG	103	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
24	C3	43	THR	3.6
1	AA	994	A	3.5
24	C3	33	ARG	3.5
31	CA	1106	G	3.5
31	CA	1213	A	3.5
1	AA	1128	C	3.5
3	BC	71	ALA	3.5
26	C5	2	LYS	3.5
46	CS	73	LYS	3.5
29	CC	202	LEU	3.5
12	BL	70	GLU	3.5
31	CA	150	U	3.5
11	BK	14	LYS	3.5
19	AS	9	PRO	3.5
24	C3	32	ALA	3.5
24	C3	36	ALA	3.5
55	DA	1084	A	3.5
7	AG	23	LEU	3.5
47	CT	82	MET	3.5
29	DC	272	SER	3.5
29	CC	3	VAL	3.5
30	CD	9	VAL	3.5
48	CU	33	LYS	3.5
20	BT	63	ALA	3.5
19	AS	71	LEU	3.5
52	CY	49	LEU	3.5
20	BT	68	HIS	3.5
30	CD	10	GLY	3.5
47	CT	45	VAL	3.5
47	CT	86	MET	3.5
27	C0	32	ILE	3.5
1	AA	974	A	3.5
39	CL	35	VAL	3.5
24	C3	14	ARG	3.5
48	CU	10	VAL	3.4
54	DI	26	VAL	3.4
9	BI	9	THR	3.4
31	CA	765	C	3.4
1	AA	1049	U	3.4
55	DA	2125	G	3.4
24	C3	1	MET	3.4
43	CP	29	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
45	CR	52	GLN	3.4
31	CA	2107	G	3.4
47	CT	81	SER	3.4
37	CJ	79	LEU	3.4
45	CR	35	ALA	3.4
10	AJ	8	ILE	3.4
44	CQ	22	PRO	3.4
55	DA	2885[A]	G	3.4
23	C2	23	THR	3.4
31	CA	1085	A	3.3
37	DJ	53	LEU	3.3
28	CB	74	U	3.3
26	C5	21	GLY	3.3
14	AN	67	THR	3.3
9	BI	127	PHE	3.3
43	CP	97	PHE	3.3
55	DA	613	A	3.3
48	CU	83	ALA	3.3
1	BA	1126	U	3.3
1	BA	962	C	3.3
1	BA	1302	C	3.3
9	BI	122	ARG	3.3
9	AI	20	PHE	3.3
49	CV	13	VAL	3.3
1	BA	212	G	3.3
14	BN	82	ILE	3.3
1	AA	1236	A	3.3
1	AA	1243	C	3.3
14	BN	96	LEU	3.3
45	CR	8	VAL	3.3
30	CD	65	ALA	3.3
33	CE	77	ILE	3.3
9	AI	117	GLY	3.3
13	AM	30	SER	3.3
25	C4	64	TYR	3.3
30	CD	128	ARG	3.3
45	CR	3	ARG	3.3
24	C3	4	THR	3.3
55	DA	2107	G	3.3
23	C2	38	LYS	3.3
29	CC	245	VAL	3.3
31	CA	2126	A	3.3

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Mol	Chain	Res	Type	RSRZ
7	BG	106	GLU	3.3
31	CA	183	C	3.3
51	DX	17	GLU	3.3
25	C4	44	LEU	3.2
14	AN	7	LYS	3.2
30	CD	131	ASP	3.2
49	CV	33	LYS	3.2
7	AG	32	VAL	3.2
19	AS	39	THR	3.2
7	BG	39	ALA	3.2
10	AJ	25	ILE	3.2
1	BA	1148	U	3.2
1	BA	1386	G	3.2
31	CA	1396	U	3.2
31	CA	1963	U	3.2
55	DA	1060	U	3.2
31	CA	2800	A	3.2
7	BG	93	PRO	3.2
29	CC	39	LYS	3.2
55	DA	2150	C	3.2
54	DI	96	PHE	3.2
7	BG	43	VAL	3.2
29	CC	220	VAL	3.2
37	DJ	55	ILE	3.2
49	CV	39	ILE	3.2
12	BL	2	ALA	3.2
14	AN	9	ARG	3.2
1	AA	977	A	3.2
1	AA	1092	A	3.2
28	CB	98	G	3.2
31	CA	75	G	3.2
31	CA	1236	G	3.2
31	CA	2128	G	3.2
31	CA	2860	A	3.2
52	CY	20	HIS	3.2
1	AA	1317	C	3.2
31	CA	2260	C	3.2
38	CK	42	ALA	3.2
2	BB	131	LYS	3.2
2	BB	132	LYS	3.2
20	BT	69	LYS	3.2
16	AP	39	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	BA	1025	U	3.2
14	BN	4	GLN	3.2
55	DA	1103	A	3.2
14	BN	12	LYS	3.2
29	CC	213	TRP	3.2
31	CA	2150	C	3.2
11	BK	84	VAL	3.2
30	CD	26	VAL	3.2
7	BG	109	ARG	3.2
9	AI	72	ILE	3.2
48	DU	1	MET	3.2
7	BG	38	THR	3.2
9	BI	121	ALA	3.2
53	DZ	63	ALA	3.2
54	DI	111	ALA	3.2
47	CT	83	LYS	3.1
55	DA	102	U	3.1
31	CA	877	A	3.1
23	C2	47	VAL	3.1
49	CV	83	VAL	3.1
13	AM	112	PRO	3.1
23	C2	10	LYS	3.1
10	AJ	42	LEU	3.1
10	AJ	73	LEU	3.1
10	BJ	73	LEU	3.1
37	CJ	80	LEU	3.1
53	CZ	49	ASP	3.1
26	C5	22	VAL	3.1
40	CM	59	ARG	3.1
24	C3	22	MET	3.1
20	BT	64	LYS	3.1
14	BN	60	GLN	3.1
24	C3	23	ALA	3.1
3	BC	26	THR	3.1
10	AJ	54	SER	3.1
1	AA	933	G	3.1
1	AA	971	G	3.1
1	BA	108	G	3.1
31	CA	2110	G	3.1
9	BI	20	PHE	3.1
29	CC	228	VAL	3.1
42	CO	46	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	AA	1017	U	3.1
1	BA	252	U	3.1
13	BM	27	LYS	3.1
14	AN	12	LYS	3.1
31	CA	1105	U	3.1
46	CS	81	LYS	3.1
1	BA	1362	A	3.1
3	AC	78	GLY	3.1
14	AN	50	THR	3.1
31	CA	513	A	3.1
19	AS	73	GLU	3.1
19	BS	12	ASP	3.1
29	DC	240	PHE	3.1
19	BS	76	PRO	3.1
30	CD	23	PRO	3.1
37	CJ	74	PRO	3.1
1	AA	1244	G	3.1
1	BA	933	G	3.1
1	BA	1355	G	3.1
31	CA	776	G	3.1
41	CN	73	ILE	3.1
49	CV	103	ILE	3.1
52	CY	64	ILE	3.1
55	DA	141	G	3.1
11	BK	21	ALA	3.1
27	C0	27	LEU	3.1
45	CR	13	ARG	3.1
22	C1	3	VAL	3.1
14	BN	97	LYS	3.1
19	BS	17	LYS	3.1
25	C4	47	LYS	3.1
44	CQ	68	GLU	3.1
46	DS	26	ASP	3.1
22	C1	8	PRO	3.1
1	AA	1031	C	3.0
1	AA	1277	C	3.0
31	CA	2248	C	3.0
10	BJ	52	LEU	3.0
24	C3	10	LEU	3.0
1	BA	211	G	3.0
31	CA	411	G	3.0
10	AJ	36	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
22	C1	25	VAL	3.0
53	CZ	24	GLU	3.0
3	BC	196	ILE	3.0
16	AP	41	PRO	3.0
25	C4	2	PRO	3.0
26	C5	1	MET	3.0
37	CJ	55	ILE	3.0
47	CT	96	ILE	3.0
13	AM	11	ASP	3.0
24	C3	42	LEU	3.0
42	CO	28	LEU	3.0
48	CU	61	LEU	3.0
26	C5	38	GLY	3.0
31	CA	2175	C	3.0
31	CA	2667	C	3.0
49	CV	32	GLY	3.0
22	C1	12	LYS	3.0
47	CT	71	VAL	3.0
48	CU	47	VAL	3.0
50	CW	14	LYS	3.0
37	DJ	38	PHE	3.0
11	BK	110	ILE	3.0
39	CL	28	SER	3.0
55	DA	2167	U	3.0
25	C4	16	LYS	3.0
39	CL	68	GLY	3.0
26	C5	3	VAL	3.0
3	AC	103	ILE	3.0
11	AK	97	ILE	3.0
43	CP	48	LEU	3.0
47	CT	46	LEU	3.0
9	BI	64	TYR	3.0
23	C2	21	TYR	3.0
1	BA	1240	U	3.0
54	DI	36	ASP	3.0
55	DA	2151	U	3.0
1	AA	973	G	3.0
2	AB	210	VAL	3.0
47	CT	47	VAL	3.0
7	AG	7	ILE	3.0
7	AG	106	GLU	3.0
31	CA	311	A	3.0

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Mol	Chain	Res	Type	RSRZ
40	CM	8	PRO	3.0
45	CR	11	ARG	3.0
3	BC	30	ALA	3.0
37	DJ	133	ALA	3.0
14	AN	97	LYS	3.0
31	CA	225	C	3.0
31	CA	876	C	3.0
55	DA	1730	C	3.0
10	BJ	50	THR	3.0
11	AK	110	ILE	3.0
25	C4	6	THR	3.0
13	BM	89	LEU	2.9
1	BA	633	G	2.9
31	CA	930	G	2.9
31	CA	2525	G	2.9
37	DJ	96	ASP	2.9
1	AA	948	C	2.9
1	BA	207	C	2.9
31	CA	2364	C	2.9
7	BG	50	LEU	2.9
19	AS	33	THR	2.9
37	DJ	28	LEU	2.9
25	C4	25	LYS	2.9
47	CT	48	LYS	2.9
48	CU	35	ALA	2.9
31	CA	481	G	2.9
31	CA	619	G	2.9
31	CA	1324	G	2.9
40	CM	35	HIS	2.9
23	D2	54	ILE	2.9
37	CJ	122	ILE	2.9
1	AA	1016	A	2.9
10	AJ	7	ARG	2.9
55	DA	1090	A	2.9
19	BS	33	THR	2.9
37	DJ	94	ASN	2.9
40	CM	14	LYS	2.9
49	CV	26	LYS	2.9
1	BA	208	U	2.9
55	DA	1729	U	2.9
16	AP	1	MET	2.9
19	AS	3	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
8	BH	90	ASP	2.9
46	CS	76	LYS	2.9
1	AA	1020	G	2.9
36	DH	11	ASN	2.9
53	CZ	32	ALA	2.9
55	DA	549	G	2.9
31	CA	477	A	2.9
55	DA	2119	A	2.9
55	DA	2170	A	2.9
1	AA	1140	C	2.9
16	BP	17	TYR	2.9
31	CA	179	C	2.9
21	BU	19	PHE	2.9
25	C4	45	ARG	2.9
14	BN	93	ILE	2.9
37	DJ	35	ILE	2.9
38	CK	47	HIS	2.9
46	CS	82	HIS	2.9
7	BG	36	LYS	2.9
9	BI	120	LYS	2.9
11	BK	64	GLN	2.9
2	BB	192	ASP	2.9
9	BI	66	THR	2.9
14	AN	15	ALA	2.9
25	C4	27	ALA	2.9
37	DJ	118	THR	2.9
31	CA	675	A	2.9
48	CU	82	LYS	2.9
54	DI	3	LEU	2.9
1	BA	470	C	2.8
31	CA	815	C	2.8
31	CA	1880	U	2.8
43	CP	93	ASP	2.8
37	CJ	140	VAL	2.8
49	CV	69	ASN	2.8
25	C4	19	LYS	2.8
2	BB	129	LEU	2.8
19	AS	49	ILE	2.8
19	BS	71	LEU	2.8
1	AA	1306	A	2.8
1	BA	949	A	2.8
28	CB	29	A	2.8

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Mol	Chain	Res	Type	RSRZ
16	BP	27	ALA	2.8
27	C0	18	PRO	2.8
31	CA	1168	G	2.8
31	CA	1216	G	2.8
55	DA	1061	U	2.8
55	DA	2140	G	2.8
7	AG	38	THR	2.8
7	BG	49	THR	2.8
10	BJ	44	THR	2.8
31	CA	105	C	2.8
37	CJ	78	VAL	2.8
20	BT	3	ASN	2.8
37	DJ	11	LEU	2.8
44	CQ	4	ILE	2.8
51	CX	13	GLY	2.8
42	CO	3	HIS	2.8
40	CM	83	ALA	2.8
25	C4	63	PRO	2.8
14	AN	45	VAL	2.8
41	CN	93	VAL	2.8
40	CM	10	GLU	2.8
1	AA	199	A	2.8
1	BA	1049	U	2.8
8	BH	32	LEU	2.8
20	BT	86	LEU	2.8
40	CM	61	LEU	2.8
10	BJ	58	ASN	2.8
55	DA	846[A]	U	2.8
33	CE	81	GLY	2.8
1	BA	1343	G	2.8
31	CA	180	G	2.8
31	CA	1381	G	2.8
31	CA	1430	G	2.8
55	DA	1092	C	2.8
55	DA	2175	C	2.8
25	C4	61	CYS	2.8
27	C0	9	GLN	2.8
45	CR	56	GLN	2.8
48	CU	72	GLN	2.8
25	C4	13	ARG	2.8
37	CJ	54	PRO	2.8
49	CV	17	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
49	CV	70	VAL	2.8
8	BH	91	GLU	2.8
14	BN	16	LEU	2.8
17	BQ	63	GLU	2.8
41	CN	41	LEU	2.8
10	BJ	91	ASP	2.8
29	CC	30	PHE	2.8
37	CJ	129	ILE	2.8
31	CA	2891	U	2.8
55	DA	1078	U	2.8
19	AS	55	ARG	2.8
20	BT	72	ALA	2.8
24	C3	25	LYS	2.8
26	C5	32	LYS	2.8
29	DC	251	GLN	2.8
40	CM	15	ALA	2.8
31	CA	1193	G	2.8
55	DA	2124	G	2.8
48	CU	93	LEU	2.8
29	CC	240	PHE	2.7
38	CK	40	HIS	2.7
40	CM	78	ARG	2.7
14	AN	22	ALA	2.7
22	C1	21	ALA	2.7
33	CE	182	ALA	2.7
35	CG	175	LYS	2.7
49	CV	44	LYS	2.7
1	AA	950	U	2.7
1	AA	958	A	2.7
11	AK	129	VAL	2.7
29	CC	251	GLN	2.7
31	CA	508	A	2.7
31	CA	1572	A	2.7
13	BM	10	PRO	2.7
14	BN	70	PRO	2.7
20	BT	83	ILE	2.7
2	AB	9	MET	2.7
55	DA	2165	C	2.7
1	AA	1018	G	2.7
22	C1	20	ASP	2.7
55	DA	283	G	2.7
9	BI	11	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
50	CW	22	ALA	2.7
13	AM	16	VAL	2.7
49	CV	59	VAL	2.7
53	CZ	45	GLN	2.7
29	CC	205	LEU	2.7
54	DI	41	LEU	2.7
25	C4	32	ILE	2.7
27	C0	44	ILE	2.7
31	CA	615	U	2.7
37	DJ	117	MET	2.7
1	BA	1067	A	2.7
3	BC	158	GLY	2.7
45	CR	33	ARG	2.7
44	CQ	111	LYS	2.7
45	CR	5	LYS	2.7
1	AA	1149	C	2.7
1	BA	222	C	2.7
20	BT	36	TYR	2.7
2	AB	42	ASN	2.7
23	C2	42	VAL	2.7
48	CU	34	VAL	2.7
30	CD	201	LEU	2.7
37	DJ	106	LEU	2.7
54	DI	95	LEU	2.7
1	AA	1015	G	2.7
31	CA	805	G	2.7
22	C1	15	MET	2.7
54	DI	90	GLY	2.7
42	CO	15	SER	2.7
1	BA	1307	U	2.7
31	CA	1066	U	2.7
31	CA	412	A	2.7
31	CA	2171	A	2.7
2	BB	134	ALA	2.7
7	BG	134	ALA	2.7
12	AL	124	ALA	2.7
14	AN	54	ASP	2.7
46	DS	103	ALA	2.7
33	CE	134	LEU	2.7
19	AS	56	GLN	2.7
31	CA	1607	C	2.7
23	C2	51	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
23	C2	53	LYS	2.7
33	CE	42	GLY	2.7
31	CA	68	G	2.7
31	CA	117	G	2.7
31	CA	1235	G	2.7
31	CA	2127	G	2.7
31	CA	2410	G	2.7
20	AT	6	SER	2.7
30	CD	57	ALA	2.7
54	DI	92	ALA	2.7
1	AA	4	U	2.7
1	BA	1354	U	2.7
2	BB	187	VAL	2.7
55	DA	2109	U	2.7
7	BG	15	ASP	2.7
10	BJ	76	ILE	2.6
31	CA	2020	A	2.6
31	CA	2346	A	2.6
37	DJ	129	ILE	2.6
41	CN	22	GLN	2.6
42	CO	9	GLN	2.6
45	CR	90	ILE	2.6
52	CY	56	MET	2.6
41	CN	40	ARG	2.6
7	AG	8	GLY	2.6
13	AM	99	GLY	2.6
25	C4	9	GLY	2.6
1	BA	1217	C	2.6
1	BA	1369	C	2.6
31	CA	343	C	2.6
42	CO	36	THR	2.6
20	AT	2	ALA	2.6
25	C4	7	VAL	2.6
33	CE	36	ALA	2.6
33	CE	200	LEU	2.6
42	CO	104	ALA	2.6
54	DI	25	ALA	2.6
54	DI	55	VAL	2.6
1	BA	1024	G	2.6
12	BL	86	ARG	2.6
28	CB	7	G	2.6
31	CA	1627	G	2.6

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Mol	Chain	Res	Type	RSRZ
31	CA	2627	G	2.6
40	CM	77	ILE	2.6
44	CQ	110	ILE	2.6
50	CW	89	ILE	2.6
1	AA	632	U	2.6
9	BI	100	LYS	2.6
10	AJ	58	ASN	2.6
31	CA	2245	U	2.6
49	CV	24	LYS	2.6
1	BA	630	A	2.6
55	DA	2887[A]	A	2.6
25	C4	55	LEU	2.6
33	CE	153	LEU	2.6
37	CJ	106	LEU	2.6
47	CT	29	VAL	2.6
49	CV	29	LEU	2.6
1	AA	217	C	2.6
1	AA	470	C	2.6
1	BA	1218	C	2.6
31	CA	32	C	2.6
2	BB	126	PHE	2.6
13	AM	24	GLY	2.6
31	CA	288	U	2.6
1	BA	1304	G	2.6
1	BA	1370	G	2.6
31	CA	1107	G	2.6
31	CA	2125	G	2.6
10	BJ	69	THR	2.6
12	BL	3	THR	2.6
19	BS	13	LEU	2.6
25	C4	57	LEU	2.6
49	CV	67	VAL	2.6
33	CE	67	ARG	2.6
3	AC	207	ILE	2.6
41	CN	118	LYS	2.6
36	DH	25	TYR	2.6
52	CY	35	SER	2.6
50	CW	27	PRO	2.6
1	BA	948	C	2.6
14	BN	54	ASP	2.6
10	AJ	38	GLY	2.6
9	AI	35	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
9	BI	67	VAL	2.6
22	C1	33	THR	2.6
49	CV	64	ALA	2.6
16	BP	46	LYS	2.6
31	CA	767	U	2.6
31	CA	2629	U	2.6
10	BJ	100	ILE	2.6
8	BH	3	MET	2.6
1	AA	1331	G	2.6
13	AM	86	TYR	2.6
31	CA	107	G	2.6
31	CA	333	G	2.6
31	CA	1210	G	2.6
39	CL	32	TYR	2.6
42	CO	1	MET	2.6
25	C4	24	HIS	2.6
12	BL	91	PRO	2.6
1	AA	1441	A	2.6
31	CA	504	A	2.6
25	C4	54	ASP	2.6
51	CX	56	ASP	2.6
13	AM	95	LEU	2.6
40	CM	19	LEU	2.6
3	AC	82	GLU	2.6
31	CA	1518	C	2.6
31	CA	2628	C	2.6
37	DJ	9	VAL	2.6
42	CO	47	VAL	2.6
55	DA	1104	C	2.6
7	BG	35	LYS	2.6
22	C1	17	ARG	2.6
39	CL	33	ALA	2.6
1	AA	1183	U	2.5
1	AA	1286	U	2.5
31	CA	2871	U	2.5
3	BC	159	GLY	2.5
9	AI	40	GLY	2.5
46	CS	86	GLN	2.5
54	DI	72	LEU	2.5
5	BE	157	ARG	2.5
13	AM	44	LYS	2.5
19	BS	37	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
29	CC	238	ARG	2.5
31	CA	312	G	2.5
42	CO	29	VAL	2.5
44	CQ	92	VAL	2.5
46	CS	80	ARG	2.5
1	BA	1250	A	2.5
13	BM	18	ALA	2.5
22	C1	24	ALA	2.5
31	CA	1194	A	2.5
55	DA	1085	A	2.5
14	AN	42	TRP	2.5
1	BA	631	C	2.5
7	AG	26	PHE	2.5
31	CA	76	C	2.5
31	CA	2347	C	2.5
2	BB	147	SER	2.5
29	CC	209	GLY	2.5
31	CA	2585	U	2.5
35	CG	148	LEU	2.5
9	AI	13	LYS	2.5
9	BI	114	LYS	2.5
7	BG	87	VAL	2.5
10	AJ	60	ASP	2.5
20	BT	59	ASP	2.5
25	C4	60	ALA	2.5
26	C5	20	ASP	2.5
46	CS	49	ILE	2.5
13	AM	102	THR	2.5
1	AA	1014	A	2.5
1	AA	1289	A	2.5
31	CA	182	A	2.5
31	CA	46	G	2.5
31	CA	2693	G	2.5
31	CA	2877	G	2.5
55	DA	2133	G	2.5
29	CC	247	PRO	2.5
46	CS	12	HIS	2.5
25	C4	29	LEU	2.5
1	BA	985	C	2.5
10	BJ	7	ARG	2.5
31	CA	1178	C	2.5
40	CM	49	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
40	CM	53	GLY	2.5
46	CS	7	SER	2.5
13	AM	32	ALA	2.5
31	CA	355	U	2.5
3	BC	162	ILE	2.5
3	BC	207	ILE	2.5
33	CE	119	ILE	2.5
38	CK	119	PHE	2.5
42	CO	21	PHE	2.5
54	DI	106	PHE	2.5
9	AI	41	ARG	2.5
21	AU	16	LEU	2.5
23	C2	37	LYS	2.5
24	C3	3	ARG	2.5
27	C0	25	LEU	2.5
37	CJ	28	LEU	2.5
40	CM	84	LYS	2.5
41	CN	8	LYS	2.5
48	CU	66	LYS	2.5
31	CA	514	A	2.5
31	CA	1205	A	2.5
31	CA	2108	A	2.5
46	CS	50	GLY	2.5
55	DA	892	A	2.5
55	DA	1847	A	2.5
9	AI	111	VAL	2.5
29	CC	19	VAL	2.5
34	CF	31	VAL	2.5
48	CU	55	VAL	2.5
50	CW	87	GLN	2.5
1	AA	1260	G	2.5
1	BA	1353	G	2.5
14	AN	56	SER	2.5
19	BS	35	SER	2.5
29	CC	38	SER	2.5
29	CC	210	ALA	2.5
31	CA	317	G	2.5
31	CA	325	G	2.5
31	CA	1863	G	2.5
43	CP	95	SER	2.5
43	CP	107	ALA	2.5
55	DA	1093	G	2.5

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Mol	Chain	Res	Type	RSRZ
7	BG	12	ILE	2.5
7	BG	42	ILE	2.5
8	AH	91	GLU	2.5
10	BJ	40	ILE	2.5
17	BQ	21	ILE	2.5
25	C4	4	ILE	2.5
31	CA	1985	C	2.5
53	DZ	49	ASP	2.5
31	CA	2149	U	2.5
40	CM	30	THR	2.5
5	BE	23	LYS	2.5
13	AM	109	ARG	2.5
21	AU	55	ARG	2.5
27	C0	6	LYS	2.5
42	CO	10	LEU	2.5
34	CF	131	GLY	2.5
7	BG	65	ALA	2.4
13	AM	15	ALA	2.4
27	D0	2[A]	ALA	2.4
33	CE	39	ALA	2.4
45	CR	38	ALA	2.4
49	CV	75	ALA	2.4
1	AA	1201	A	2.4
1	BA	609	A	2.4
31	CA	480	A	2.4
21	BU	12	PHE	2.4
52	CY	46	PHE	2.4
24	C3	19	ARG	2.4
46	CS	84	ARG	2.4
1	AA	1290	G	2.4
1	BA	1356	G	2.4
5	BE	103	THR	2.4
31	CA	308	G	2.4
31	CA	1166	G	2.4
31	CA	1639	C	2.4
31	CA	1731	G	2.4
49	CV	77	THR	2.4
28	CB	28	C	2.4
55	DA	1062	G	2.4
26	C5	31	PRO	2.4
31	CA	224	U	2.4
2	BB	163	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
41	CN	23	GLY	2.4
49	CV	36	VAL	2.4
11	BK	99	ALA	2.4
11	BK	94	GLU	2.4
20	BT	33	LYS	2.4
24	C3	46	LYS	2.4
30	CD	62	LYS	2.4
33	CE	47	LYS	2.4
6	BF	39	LEU	2.4
19	BS	31	LEU	2.4
1	BA	1289	A	2.4
18	BR	71	THR	2.4
28	CB	99	A	2.4
31	CA	1393	A	2.4
55	DA	1077	A	2.4
47	CT	20	VAL	2.4
1	AA	1141	C	2.4
30	CD	132	ALA	2.4
1	BA	201	G	2.4
1	BA	1321	U	2.4
7	BG	7	ILE	2.4
31	CA	510	C	2.4
31	CA	1708	C	2.4
31	CA	375	G	2.4
48	CU	74	ILE	2.4
8	AH	3	MET	2.4
12	BL	14	ARG	2.4
24	C3	41	ARG	2.4
42	CO	40	LYS	2.4
48	CU	81	LYS	2.4
14	AN	55	SER	2.4
13	BM	19	LEU	2.4
19	AS	5	LEU	2.4
42	CO	79	LEU	2.4
7	AG	2	PRO	2.4
9	BI	111	VAL	2.4
10	BJ	84	VAL	2.4
19	AS	51	VAL	2.4
33	CE	33	VAL	2.4
40	CM	16	GLY	2.4
1	BA	532	A	2.4
8	BH	36	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
16	BP	42	ILE	2.4
18	BR	21	ILE	2.4
48	CU	30	ILE	2.4
48	CU	41	ALA	2.4
31	CA	1237	A	2.4
31	CA	2820	A	2.4
55	DA	1080	A	2.4
55	DA	2108	A	2.4
55	DA	2171	A	2.4
7	AG	25	LYS	2.4
42	CO	20	MET	2.4
29	CC	271	ARG	2.4
1	BA	1086	U	2.4
7	BG	23	LEU	2.4
10	BJ	42	LEU	2.4
28	CB	97	C	2.4
31	CA	334	C	2.4
31	CA	336	C	2.4
31	CA	1319	C	2.4
31	CA	1709	U	2.4
55	DA	1065	U	2.4
55	DA	1172	C	2.4
33	CE	72	SER	2.4
1	BA	976	G	2.4
31	CA	350	G	2.4
31	CA	830	G	2.4
31	CA	2895	G	2.4
55	DA	2121	G	2.4
2	BB	210	VAL	2.4
11	AK	84	VAL	2.4
49	CV	25	VAL	2.4
12	BL	5	ASN	2.4
52	DY	20	HIS	2.4
19	AS	50	ALA	2.4
33	CE	50	ALA	2.4
42	CO	113	ILE	2.4
49	DV	2	ALA	2.4
19	BS	66	MET	2.4
30	CD	77	ARG	2.4
41	CN	136	MET	2.4
9	BI	126	GLN	2.4
42	CO	18	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
14	AN	48	LEU	2.4
1	AA	1492	A	2.4
45	CR	29	SER	2.4
53	CZ	40	SER	2.4
1	AA	218	U	2.4
13	AM	96	PRO	2.4
31	CA	2151	U	2.4
55	DA	2149	U	2.4
1	AA	1119	C	2.3
1	AA	1120	C	2.3
1	AA	1282	C	2.3
1	AA	1302	C	2.3
31	CA	31	C	2.3
31	CA	456	C	2.3
31	CA	1064	C	2.3
3	BC	155	GLY	2.3
16	BP	10	GLY	2.3
24	C3	27	GLY	2.3
29	CC	41	GLY	2.3
3	AC	162	ILE	2.3
10	BJ	59	LYS	2.3
25	C4	35	LYS	2.3
48	CU	12	ARG	2.3
53	CZ	61	ALA	2.3
2	BB	82	ASP	2.3
7	AG	33	ASP	2.3
1	AA	540	G	2.3
31	CA	376	G	2.3
31	CA	2668	G	2.3
35	DG	116	GLN	2.3
37	DJ	57	VAL	2.3
41	CN	36	VAL	2.3
42	CO	116	VAL	2.3
46	CS	96	VAL	2.3
23	C2	41	PRO	2.3
7	AG	110	LYS	2.3
29	CC	9	THR	2.3
29	CC	27	GLY	2.3
29	CC	47	GLY	2.3
31	CA	482	A	2.3
31	CA	878	A	2.3
37	DJ	131	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
45	CR	23	GLY	2.3
47	CT	42	LYS	2.3
55	DA	2154	A	2.3
9	BI	108	ALA	2.3
29	CC	243	HIS	2.3
33	CE	135	ALA	2.3
37	DJ	18	ALA	2.3
1	AA	1086	U	2.3
31	CA	293	U	2.3
31	CA	1865	U	2.3
1	BA	984	C	2.3
10	BJ	10	LEU	2.3
10	BJ	102	LEU	2.3
31	CA	2045	C	2.3
31	CA	2362	C	2.3
37	CJ	138	LEU	2.3
15	BO	62	GLN	2.3
20	BT	13	GLN	2.3
11	BK	68	GLU	2.3
29	CC	236	GLU	2.3
1	BA	202	G	2.3
31	CA	108	G	2.3
31	CA	549	G	2.3
31	CA	1099	G	2.3
31	CA	1983	G	2.3
31	CA	2382	G	2.3
31	CA	2455	G	2.3
21	BU	54	LYS	2.3
25	C4	46	PRO	2.3
48	DU	73	ARG	2.3
54	DI	130	PRO	2.3
30	CD	151	THR	2.3
49	CV	15	THR	2.3
7	BG	22	LEU	2.3
29	CC	239	ASN	2.3
45	CR	18	LEU	2.3
1	BA	1280	A	2.3
31	CA	457	A	2.3
31	CA	764	A	2.3
31	CA	2070	A	2.3
37	DJ	67	PHE	2.3
55	DA	2163	A	2.3

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Mol	Chain	Res	Type	RSRZ
12	BL	109	ASP	2.3
22	C1	46	ASP	2.3
14	AN	66	GLN	2.3
31	CA	65	U	2.3
55	DA	1094	U	2.3
44	CQ	34	GLU	2.3
31	CA	816	C	2.3
44	CQ	94	LYS	2.3
2	AB	139	ARG	2.3
9	AI	119	ARG	2.3
25	C4	8	ARG	2.3
10	AJ	40	ILE	2.3
10	AJ	53	ILE	2.3
10	BJ	6	ILE	2.3
49	DV	55	PRO	2.3
27	C0	50	ALA	2.3
33	CE	172	ALA	2.3
42	CO	19	ALA	2.3
2	BB	136	MET	2.3
19	AS	35	SER	2.3
7	BG	59	LEU	2.3
13	BM	95	LEU	2.3
1	AA	1139	G	2.3
1	BA	844	G	2.3
30	CD	156	PHE	2.3
31	CA	512	G	2.3
31	CA	2067	G	2.3
35	DG	114	ASP	2.3
42	CO	5	LYS	2.3
49	CV	61	LYS	2.3
1	BA	196	A	2.3
1	BA	325	A	2.3
1	BA	1219	A	2.3
29	CC	212	ARG	2.3
30	CD	122	VAL	2.3
31	CA	181	A	2.3
31	CA	2406	A	2.3
1	BA	1125	U	2.3
55	DA	1963	U	2.3
55	DA	2166	U	2.3
16	BP	57	ILE	2.3
44	CQ	84	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
7	BG	46	ALA	2.3
29	CC	234	GLY	2.3
33	CE	34	ALA	2.3
37	CJ	114	ALA	2.3
1	BA	1322	C	2.3
55	DA	885	C	2.3
55	DA	2164	C	2.3
33	CE	101	TYR	2.3
34	CF	100	PHE	2.3
40	CM	107	PHE	2.3
10	BJ	64	GLN	2.3
14	AN	3	LYS	2.3
29	CC	18	LYS	2.3
38	CK	39	LYS	2.3
49	CV	66	GLN	2.3
3	BC	118	ASP	2.3
52	CY	47	VAL	2.3
1	AA	1142	G	2.2
31	CA	54	G	2.2
31	CA	1093	G	2.2
31	CA	2027	G	2.2
31	CA	2032	G	2.2
40	CM	37	GLY	2.2
54	DI	112	ALA	2.2
1	BA	1252	A	2.2
22	C1	39	LEU	2.2
31	CA	349	U	2.2
31	CA	501	A	2.2
31	CA	1065	U	2.2
31	CA	2861	U	2.2
42	CO	51	LEU	2.2
2	BB	130	THR	2.2
22	C1	19	HIS	2.2
19	BS	4	SER	2.2
27	C0	21	LYS	2.2
47	CT	16	LYS	2.2
47	CT	101	SER	2.2
1	AA	87	C	2.2
1	AA	1096	C	2.2
28	CB	8	C	2.2
31	CA	69	C	2.2
31	CA	1208	C	2.2

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Mol	Chain	Res	Type	RSRZ
33	CE	79	ARG	2.2
55	DA	2161	C	2.2
49	CV	40	ASN	2.2
40	CM	106	GLU	2.2
34	CF	156	ILE	2.2
10	BJ	34	ALA	2.2
29	CC	8	PRO	2.2
26	C5	10	LEU	2.2
34	DF	117	LEU	2.2
37	CJ	14	ALA	2.2
51	CX	52	GLY	2.2
7	BG	76	LYS	2.2
31	CA	377	G	2.2
31	CA	1087	G	2.2
35	DG	44	LYS	2.2
10	BJ	48	ARG	2.2
1	AA	1332	A	2.2
1	BA	1363	A	2.2
31	CA	608	A	2.2
37	CJ	21	SER	2.2
37	CJ	128	SER	2.2
55	DA	1089	A	2.2
3	BC	198	VAL	2.2
7	BG	94	VAL	2.2
11	BK	86	VAL	2.2
36	CH	108	VAL	2.2
38	CK	48	VAL	2.2
23	C2	5	ILE	2.2
43	CP	35	ILE	2.2
1	BA	1281	C	2.2
31	CA	1092	C	2.2
31	CA	1320	C	2.2
31	CA	1574	C	2.2
42	CO	24	MET	2.2
12	BL	15	LYS	2.2
27	C0	16	ARG	2.2
42	CO	4	ARG	2.2
42	CO	22	ARG	2.2
29	CC	223	THR	2.2
29	DC	243	HIS	2.2
33	CE	131	THR	2.2
7	BG	64	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
17	BQ	29	VAL	2.2
24	C3	45	SER	2.2
37	DJ	128	SER	2.2
1	AA	1205	U	2.2
1	BA	471	U	2.2
9	AI	110	GLN	2.2
31	CA	790	U	2.2
14	AN	30	ILE	2.2
1	AA	1353	G	2.2
31	CA	289	G	2.2
10	AJ	52	LEU	2.2
10	BJ	90	LEU	2.2
19	BS	15	LEU	2.2
31	CA	472	A	2.2
31	CA	515	A	2.2
9	BI	69	GLY	2.2
37	DJ	14	ALA	2.2
46	CS	88	GLY	2.2
20	BT	8	LYS	2.2
33	DE	7	ASP	2.2
3	BC	37	PHE	2.2
13	AM	101	ARG	2.2
24	C3	18	PHE	2.2
31	CA	455	C	2.2
31	CA	623	C	2.2
31	CA	1732	C	2.2
33	CE	78	TRP	2.2
55	DA	1732	C	2.2
7	AG	6	VAL	2.2
13	AM	25	VAL	2.2
13	AM	43	VAL	2.2
29	CC	216	VAL	2.2
48	CU	62	VAL	2.2
48	CU	63	VAL	2.2
9	AI	21	ILE	2.2
14	BN	80	SER	2.2
38	CK	103	ILE	2.2
45	CR	37	GLN	2.2
45	CR	44	GLN	2.2
54	DI	82	ILE	2.2
23	C2	34	LEU	2.2
42	CO	111	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
42	CO	114	GLU	2.2
9	BI	60	LYS	2.2
35	CG	172	LYS	2.2
47	CT	10	ALA	2.2
1	BA	472	U	2.2
1	BA	1017	U	2.2
10	BJ	39	PRO	2.2
37	DJ	137	GLY	2.2
40	CM	11	GLY	2.2
6	BF	91	ARG	2.2
37	DJ	39	CYS	2.2
47	CT	11	ARG	2.2
9	AI	39	PHE	2.2
1	BA	574	A	2.2
1	BA	1493	A	2.2
31	CA	354	A	2.2
31	CA	1103	A	2.2
31	CA	1616	A	2.2
31	CA	2435	A	2.2
1	AA	203	G	2.2
1	AA	1387	G	2.2
1	BA	1387	G	2.2
31	CA	291	G	2.2
31	CA	409	G	2.2
31	CA	1770	G	2.2
31	CA	2677	G	2.2
5	BE	140	THR	2.1
13	AM	104	THR	2.1
19	BS	58	VAL	2.1
37	CJ	58	VAL	2.1
52	CY	13	VAL	2.1
1	BA	1209	C	2.1
13	BM	22	ILE	2.1
13	BM	45	ILE	2.1
23	C2	48	ILE	2.1
49	CV	12	ILE	2.1
49	CV	72	ILE	2.1
55	DA	143	C	2.1
7	BG	47	LEU	2.1
13	BM	48	LEU	2.1
47	CT	19	LEU	2.1
14	AN	32	SER	2.1

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Mol	Chain	Res	Type	RSRZ
16	AP	24	SER	2.1
22	C1	7	LYS	2.1
42	CO	27	SER	2.1
10	BJ	9	ARG	2.1
35	DG	173	GLU	2.1
40	CM	51	GLU	2.1
42	CO	43	GLU	2.1
25	C4	53	GLY	2.1
46	CS	52	PRO	2.1
51	CX	41	ARG	2.1
1	BA	843	U	2.1
1	BA	989	U	2.1
31	CA	1340	U	2.1
31	CA	1390	U	2.1
55	DA	1083	U	2.1
25	C4	58	VAL	2.1
37	CJ	139	VAL	2.1
46	CS	20	VAL	2.1
33	CE	173	THR	2.1
48	CU	60	THR	2.1
1	AA	1280	A	2.1
1	BA	974	A	2.1
1	BA	1204	A	2.1
9	AI	90	TYR	2.1
10	AJ	76	ILE	2.1
31	CA	443	A	2.1
31	CA	1321	A	2.1
31	CA	2602	A	2.1
55	DA	2117	A	2.1
29	CC	36	LYS	2.1
36	DH	41	LYS	2.1
40	CM	92	LEU	2.1
44	CQ	106	LYS	2.1
31	CA	30	G	2.1
31	CA	408	G	2.1
31	CA	1444	G	2.1
34	CF	130	MET	2.1
48	DU	69	ARG	2.1
55	DA	2116	G	2.1
55	DA	2123	G	2.1
9	AI	17	ALA	2.1
16	BP	82	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
7	BG	41	SER	2.1
10	BJ	38	GLY	2.1
33	CE	70	SER	2.1
40	DM	102	GLY	2.1
49	CV	20	GLY	2.1
1	BA	634	C	2.1
1	BA	932	C	2.1
1	BA	1147	C	2.1
31	CA	106	C	2.1
31	CA	854	C	2.1
49	DV	48	PRO	2.1
25	C4	22	PHE	2.1
7	BG	135	VAL	2.1
10	BJ	77	VAL	2.1
16	BP	23	ASP	2.1
24	C3	30	VAL	2.1
27	C0	51	VAL	2.1
42	CO	48	VAL	2.1
1	BA	1351	U	2.1
10	AJ	10	LEU	2.1
13	AM	73	ILE	2.1
13	BM	103	LYS	2.1
31	CA	135	U	2.1
31	CA	234	U	2.1
31	CA	1234	U	2.1
31	CA	1647	U	2.1
37	CJ	53	LEU	2.1
38	CK	44	TYR	2.1
51	CX	75	LYS	2.1
55	DA	2423	U	2.1
15	AO	17	ARG	2.1
40	CM	18	ARG	2.1
19	AS	75	ALA	2.1
1	BA	1274	A	2.1
31	CA	348	A	2.1
31	CA	415	A	2.1
31	CA	2665	A	2.1
52	CY	55	GLY	2.1
53	CZ	17	GLU	2.1
7	AG	62	PHE	2.1
10	AJ	101	SER	2.1
9	BI	31	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	AA	94	G	2.1
19	BS	19	VAL	2.1
28	CB	23	G	2.1
31	CA	39	G	2.1
31	CA	442	G	2.1
31	CA	620	G	2.1
31	CA	1026	G	2.1
31	CA	1239	G	2.1
31	CA	1346	G	2.1
33	CE	83	VAL	2.1
1	BA	1237	C	2.1
12	AL	15	LYS	2.1
14	BN	7	LYS	2.1
3	BC	33	LEU	2.1
7	BG	124	LEU	2.1
9	AI	28	ILE	2.1
23	C2	19	HIS	2.1
29	CC	232	HIS	2.1
29	CC	255	LYS	2.1
41	CN	133	LYS	2.1
43	CP	4	LYS	2.1
48	CU	68	LYS	2.1
49	CV	43	LYS	2.1
33	CE	159	LEU	2.1
40	CM	3	LEU	2.1
9	AI	130	ARG	2.1
27	C0	11	ARG	2.1
33	CE	69	ARG	2.1
42	CO	2	ARG	2.1
45	CR	6	ARG	2.1
45	CR	30	ARG	2.1
40	CM	58	TYR	2.1
36	DH	74	ALA	2.1
7	AG	34	GLY	2.1
38	CK	66	GLY	2.1
40	CM	52	GLY	2.1
4	AD	88	GLU	2.1
7	AG	93	PRO	2.1
30	CD	127	PHE	2.1
48	CU	42	GLU	2.1
3	BC	53	SER	2.1
13	BM	21	SER	2.1

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Mol	Chain	Res	Type	RSRZ
33	CE	80	SER	2.1
1	BA	223	A	2.1
7	BG	137	LYS	2.1
29	DC	239	ASN	2.1
31	CA	73	A	2.1
31	CA	320	A	2.1
31	CA	654	A	2.1
31	CA	1598	A	2.1
35	DG	30	ASN	2.1
40	CM	36	LYS	2.1
42	CO	11	ASN	2.1
55	DA	2169	A	2.1
14	AN	16	LEU	2.1
14	BN	51	LEU	2.1
19	AS	37	ARG	2.1
30	CD	80	TRP	2.1
43	CP	106	LEU	2.1
49	CV	58	ILE	2.1
53	CZ	57	LEU	2.1
54	DI	123	ILE	2.1
16	AP	23	ASP	2.1
25	C4	49	MET	2.1
1	BA	1244	G	2.1
1	BA	1371	G	2.1
16	BP	22	ALA	2.1
24	C3	40	ALA	2.1
28	CB	47	C	2.1
31	CA	33	C	2.1
31	CA	128	C	2.1
31	CA	237	C	2.1
31	CA	318	C	2.1
31	CA	385	C	2.1
31	CA	1350	C	2.1
31	CA	1730	C	2.1
31	CA	2078	C	2.1
49	CV	2	ALA	2.1
55	DA	1100	C	2.1
31	CA	26	G	2.1
31	CA	2190	G	2.1
31	CA	2802	G	2.1
8	AH	76	GLN	2.1
29	CC	249	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
21	BU	44	GLU	2.1
41	CN	98	PRO	2.1
49	CV	37	GLU	2.1
1	AA	965	U	2.0
7	AG	35	LYS	2.0
31	CA	810	U	2.0
31	CA	2249	U	2.0
37	CJ	9	VAL	2.0
51	CX	16	SER	2.0
10	AJ	100	ILE	2.0
14	AN	46	LEU	2.0
33	CE	175	ILE	2.0
44	CQ	66	ASN	2.0
1	AA	949	A	2.0
1	AA	1130	A	2.0
3	BC	168	TYR	2.0
7	BG	128	ALA	2.0
14	BN	29	ALA	2.0
25	C4	10	ALA	2.0
31	CA	1596	A	2.0
37	CJ	73	THR	2.0
3	BC	197	GLY	2.0
17	AQ	9	GLN	2.0
14	AN	52	PRO	2.0
14	BN	52	PRO	2.0
36	CH	29	PHE	2.0
37	CJ	22	PRO	2.0
7	BG	11	LYS	2.0
31	CA	1606	C	2.0
39	CL	67	LYS	2.0
46	CS	71	LYS	2.0
48	CU	19	LYS	2.0
54	DI	85	VAL	2.0
55	DA	357	C	2.0
55	DA	2178	C	2.0
1	BA	954	G	2.0
6	AF	61	LEU	2.0
18	AR	43	ARG	2.0
24	C3	34	ARG	2.0
25	C4	42	ARG	2.0
31	CA	301	G	2.0
31	CA	2862	G	2.0

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Mol	Chain	Res	Type	RSRZ
47	CT	36	LEU	2.0
53	CZ	6	LEU	2.0
25	C4	51	SER	2.0
40	CM	101	ILE	2.0
54	DI	30	SER	2.0
1	AA	1235	U	2.0
1	BA	1286	U	2.0
28	CB	48	U	2.0
55	DA	546	U	2.0
55	DA	2106	U	2.0
29	CC	225	MET	2.0
48	CU	70	HIS	2.0
2	AB	46	THR	2.0
2	BB	166	ALA	2.0
10	BJ	61	ALA	2.0
16	BP	11	ALA	2.0
13	AM	23	TYR	2.0
15	AO	69	TYR	2.0
17	AQ	70	THR	2.0
37	CJ	83	ALA	2.0
54	DI	135	ALA	2.0
46	CS	83	TYR	2.0
9	AI	125	PRO	2.0
16	BP	12	LYS	2.0
19	AS	7	LYS	2.0
30	CD	7	LYS	2.0
40	CM	13	LYS	2.0
40	CM	56	PRO	2.0
46	CS	48	LYS	2.0
50	CW	84	PRO	2.0
1	AA	1150	A	2.0
1	BA	1145	A	2.0
1	BA	1251	A	2.0
9	AI	48	VAL	2.0
9	AI	55	VAL	2.0
31	CA	616	A	2.0
31	CA	2872	A	2.0
48	CU	67	VAL	2.0
52	CY	28	ARG	2.0
14	BN	74	LEU	2.0
1	BA	972	C	2.0
31	CA	129	C	2.0

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Mol	Chain	Res	Type	RSRZ
31	CA	444	C	2.0
31	CA	1104	C	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	2MG	BA	966	24/25	0.62	0.14	161,163,169,169	0
1	2MG	BA	1207	24/25	0.64	0.13	169,172,175,177	0
1	5MC	BA	967	21/22	0.72	0.14	156,162,165,165	0
31	PSU	CA	1917	20/21	0.79	0.12	106,115,121,121	0
1	2MG	AA	1207	24/25	0.82	0.12	124,129,130,132	0
31	3TD	CA	1915	21/22	0.85	0.08	132,137,140,141	0
31	PSU	CA	2457	20/21	0.87	0.14	83,88,93,96	0
31	PSU	CA	2504	20/21	0.87	0.15	87,89,95,96	0
1	PSU	BA	516	20/21	0.88	0.10	93,98,101,102	0
31	2MA	CA	2503	23/24	0.88	0.15	90,95,99,100	0
31	PSU	CA	1911	20/21	0.88	0.07	112,123,126,126	0
1	2MG	AA	966	24/25	0.89	0.13	84,94,103,105	0
31	PSU	CA	955	20/21	0.89	0.12	92,93,95,95	0
31	6MZ	CA	1618	23/24	0.90	0.14	112,116,119,120	0
55	PSU	DA	1917	20/21	0.90	0.09	79,84,93,93	0
1	PSU	AA	516	20/21	0.91	0.09	81,85,86,87	0
31	PSU	CA	2580	20/21	0.91	0.09	86,88,93,94	0
55	3TD	DA	1915	21/22	0.91	0.09	105,109,117,117	0
31	6MZ	CA	2030	23/24	0.91	0.12	82,91,100,102	0
12	D2T	AL	89	10/11	0.92	0.12	61,65,85,86	0
1	5MC	BA	1407	21/22	0.92	0.11	81,92,94,95	0
55	PSU	DA	1911	20/21	0.92	0.08	82,85,87,88	0
12	D2T	BL	89	10/11	0.92	0.13	77,82,93,93	0
31	PSU	CA	746	20/21	0.92	0.08	98,101,104,104	0
31	2MG	CA	2445	24/25	0.93	0.15	74,83,85,89	0
31	1MG	CA	745	24/25	0.93	0.10	92,96,97,98	0
1	5MC	AA	967	21/22	0.93	0.12	90,100,103,105	0
31	7MG	CA	2069	24/25	0.93	0.15	84,89,94,94	0
41	4D4	CN	81	12/13	0.93	0.12	85,88,108,110	0
31	OMC	CA	2498	21/22	0.94	0.13	82,84,89,92	0
1	UR3	BA	1498	21/22	0.94	0.09	81,84,87,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	5MC	CA	1962	21/22	0.94	0.12	67,69,73,76	0
31	5MU	CA	747	21/22	0.94	0.10	95,101,103,106	0
1	7MG	AA	527	24/25	0.95	0.08	60,65,72,74	0
31	OMU	CA	2552	21/22	0.95	0.14	80,82,86,88	0
31	OMG	CA	2251	24/25	0.95	0.10	69,79,82,84	0
1	2MG	BA	1516	24/25	0.95	0.08	67,75,78,81	0
31	5MU	CA	1939	21/22	0.95	0.09	70,73,82,85	0
31	2MG	CA	1835	24/25	0.95	0.09	61,72,77,78	0
1	7MG	BA	527	24/25	0.95	0.08	76,81,88,89	0
31	PSU	CA	2605	20/21	0.96	0.07	73,75,78,80	0
1	MA6	BA	1518	24/25	0.96	0.08	67,73,76,77	0
1	MA6	BA	1519	24/25	0.96	0.09	74,77,81,83	0
1	MA6	AA	1518	24/25	0.96	0.08	51,55,58,61	0
1	UR3	AA	1498	21/22	0.96	0.09	58,63,67,70	0
41	4D4	DN	81[A]	12/13	0.96	0.10	32,40,49,51	9
41	4D4	DN	81[B]	12/13	0.96	0.10	12,25,36,36	9
1	5MC	AA	1407	21/22	0.97	0.07	55,57,60,62	0
55	PSU	DA	2604	20/21	0.97	0.07	41,46,56,56	0
1	4OC	BA	1402	22/23	0.97	0.07	79,83,83,84	0
1	4OC	AA	1402	22/23	0.97	0.07	53,61,66,66	0
1	2MG	AA	1516	24/25	0.97	0.07	58,62,63,63	0
32	MEQ	DD	150[B]	10/11	0.98	0.08	23,32,41,41	10
55	5MU	DA	1939	21/22	0.98	0.07	35,37,41,47	0
55	5MC	DA	1962	21/22	0.98	0.08	36,44,48,49	0
55	7MG	DA	2069	24/25	0.98	0.08	32,37,41,43	0
55	2MG	DA	2445	24/25	0.98	0.07	26,29,35,37	0
55	2MA	DA	2503	23/24	0.98	0.06	21,35,41,42	0
55	PSU	DA	2504	20/21	0.98	0.09	37,40,44,44	0
55	OMU	DA	2552	21/22	0.98	0.07	31,34,39,46	0
55	5MU	DA	747	21/22	0.98	0.06	28,33,36,41	0
55	PSU	DA	2605	20/21	0.98	0.06	31,41,43,43	0
55	2MG	DA	1835	24/25	0.98	0.06	41,47,52,52	0
1	MA6	AA	1519	24/25	0.98	0.07	53,56,61,64	0
32	MEQ	DD	150[A]	10/11	0.98	0.08	7,15,29,31	10
55	OMC	DA	2498	21/22	0.99	0.05	21,26,29,30	0
55	PSU	DA	746	20/21	0.99	0.04	21,28,31,35	0
55	1MG	DA	745	24/25	0.99	0.05	25,29,37,41	0
55	6MZ	DA	2030	23/24	0.99	0.05	22,25,29,34	0
55	PSU	DA	2580	20/21	0.99	0.06	20,25,32,34	0
55	PSU	DA	955	20/21	0.99	0.06	25,27,30,30	0
55	OMG	DA	2251	24/25	0.99	0.05	27,32,37,42	0
55	6MZ	DA	1618	23/24	0.99	0.05	26,33,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	H2U	DA	2449	20/21	0.99	0.06	25,29,31,32	0
55	PSU	DA	2457	20/21	0.99	0.04	27,31,37,37	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3168	1/1	0.26	0.31	141,141,141,141	0
56	MG	CA	3154	1/1	0.32	0.36	147,147,147,147	0
56	MG	BA	1624	1/1	0.34	0.14	262,262,262,262	0
56	MG	AA	1628	1/1	0.38	0.18	159,159,159,159	0
56	MG	BA	1639	1/1	0.40	0.32	94,94,94,94	0
56	MG	AA	1677	1/1	0.41	0.18	194,194,194,194	0
56	MG	CA	3122	1/1	0.43	0.58	126,126,126,126	0
56	MG	CA	3038	1/1	0.46	0.11	263,263,263,263	0
56	MG	BA	1641	1/1	0.48	0.23	120,120,120,120	0
56	MG	CA	3132	1/1	0.49	0.27	105,105,105,105	0
56	MG	BA	1640	1/1	0.50	0.54	124,124,124,124	0
56	MG	CA	3060	1/1	0.52	0.15	234,234,234,234	0
56	MG	CA	3075	1/1	0.53	0.26	230,230,230,230	0
56	MG	CA	3077	1/1	0.54	0.15	249,249,249,249	0
56	MG	BA	1603	1/1	0.57	0.13	263,263,263,263	0
56	MG	CA	3124	1/1	0.58	0.20	118,118,118,118	0
56	MG	BA	1625	1/1	0.65	0.18	256,256,256,256	0
56	MG	CA	3005	1/1	0.66	0.21	237,237,237,237	0
56	MG	CA	3061	1/1	0.67	0.12	247,247,247,247	0
56	MG	CA	3028	1/1	0.67	0.17	278,278,278,278	0
56	MG	CA	3115	1/1	0.68	0.20	84,84,84,84	0
56	MG	CA	3155	1/1	0.69	0.16	156,156,156,156	0
56	MG	CA	3021	1/1	0.69	0.51	264,264,264,264	0
56	MG	CA	3139	1/1	0.70	0.28	87,87,87,87	0
58	MPD	DE	301	8/8	0.70	0.25	139,140,142,142	0
63	EDO	DB	212	4/4	0.71	0.31	115,115,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3067	1/1	0.72	0.14	277,277,277,277	0
56	MG	AA	1678	1/1	0.72	0.22	78,78,78,78	0
56	MG	CA	3156	1/1	0.72	0.17	232,232,232,232	0
56	MG	DA	3146	1/1	0.73	0.28	122,122,122,122	0
56	MG	CA	3009	1/1	0.73	0.25	243,243,243,243	0
56	MG	BA	1606	1/1	0.74	0.21	227,227,227,227	0
56	MG	CA	3002	1/1	0.75	0.16	265,265,265,265	0
56	MG	DA	3143	1/1	0.75	0.31	114,114,114,114	0
56	MG	AA	1622	1/1	0.75	0.36	100,100,100,100	0
56	MG	DA	3129	1/1	0.76	0.38	102,102,102,102	0
62	PEG	DP	201	7/7	0.76	0.16	126,127,131,132	0
56	MG	CA	3145	1/1	0.76	0.20	73,73,73,73	0
67	ACY	DA	3196	4/4	0.76	0.25	84,85,87,87	0
59	PUT	AA	1672	6/6	0.77	0.41	99,100,102,103	0
56	MG	CA	3034	1/1	0.77	0.25	246,246,246,246	0
56	MG	CA	3129	1/1	0.78	0.24	104,104,104,104	0
56	MG	CA	3147	1/1	0.78	0.52	58,58,58,58	1
56	MG	CA	3148	1/1	0.78	0.53	51,51,51,51	1
56	MG	CA	3112	1/1	0.79	0.10	75,75,75,75	0
56	MG	BA	1623	1/1	0.79	0.26	248,248,248,248	0
56	MG	CA	3146	1/1	0.79	0.19	144,144,144,144	0
56	MG	BA	1612	1/1	0.79	0.36	182,182,182,182	0
56	MG	DA	3180	1/1	0.79	0.28	106,106,106,106	0
56	MG	CA	3130	1/1	0.80	0.31	89,89,89,89	0
56	MG	BA	1646	1/1	0.80	0.15	108,108,108,108	0
56	MG	CA	3135	1/1	0.80	0.36	101,101,101,101	0
56	MG	AA	1660	1/1	0.80	0.17	284,284,284,284	0
56	MG	CA	3014	1/1	0.80	0.14	216,216,216,216	0
56	MG	CA	3003	1/1	0.80	0.33	278,278,278,278	0
56	MG	CA	3104	1/1	0.80	0.16	258,258,258,258	0
56	MG	CA	3142	1/1	0.81	0.10	78,78,78,78	0
56	MG	AA	1614	1/1	0.81	0.21	85,85,85,85	0
56	MG	CA	3068	1/1	0.81	0.17	216,216,216,216	0
56	MG	CA	3123	1/1	0.81	0.11	113,113,113,113	0
56	MG	AA	1654	1/1	0.81	0.34	262,262,262,262	0
56	MG	CA	3126	1/1	0.81	0.24	86,86,86,86	0
56	MG	CA	3032	1/1	0.82	0.12	241,241,241,241	0
56	MG	CA	3106	1/1	0.82	0.12	83,83,83,83	0
56	MG	CA	3108	1/1	0.82	0.19	83,83,83,83	0
56	MG	AA	1661	1/1	0.82	0.16	173,173,173,173	0
56	MG	CA	3152	1/1	0.82	0.10	151,151,151,151	0
56	MG	CA	3007	1/1	0.82	0.10	214,214,214,214	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MPD	DK	201	8/8	0.83	0.17	120,121,123,124	0
56	MG	CA	3125	1/1	0.83	0.19	89,89,89,89	0
59	PUT	AA	1675	6/6	0.83	0.24	106,109,109,109	0
56	MG	DA	3061	1/1	0.83	0.13	233,233,233,233	0
56	MG	AA	1608	1/1	0.83	0.39	96,96,96,96	0
56	MG	CA	3090	1/1	0.83	0.13	185,185,185,185	0
60	T1C	BA	1643	42/42	0.84	0.18	170,174,179,179	0
56	MG	CA	3072	1/1	0.84	0.12	249,249,249,249	0
63	EDO	DB	211	4/4	0.84	0.36	88,90,92,92	0
56	MG	CA	3140	1/1	0.84	0.10	84,84,84,84	0
64	PGE	D1	102	10/10	0.84	0.28	122,127,128,128	0
56	MG	CA	3047	1/1	0.84	0.32	229,229,229,229	0
59	PUT	DA	3222	6/6	0.85	0.20	48,52,57,58	0
56	MG	AA	1603	1/1	0.85	0.12	83,83,83,83	0
62	PEG	D3	102	7/7	0.85	0.28	114,119,124,125	0
56	MG	BA	1629	1/1	0.85	0.18	168,168,168,168	0
56	MG	CA	3107	1/1	0.85	0.26	83,83,83,83	0
56	MG	CA	3026	1/1	0.85	0.20	173,173,173,173	0
56	MG	CA	3080	1/1	0.85	0.18	151,151,151,151	0
56	MG	BA	1636	1/1	0.85	0.23	72,72,72,72	0
56	MG	DA	3178	1/1	0.86	0.38	88,88,88,88	0
56	MG	CA	3056	1/1	0.86	0.39	71,71,71,71	0
56	MG	AA	1609	1/1	0.86	0.31	89,89,89,89	0
58	MPD	DE	302	8/8	0.86	0.26	93,97,102,102	0
56	MG	AA	1611	1/1	0.86	0.22	108,108,108,108	0
58	MPD	DA	3190	8/8	0.86	0.19	95,97,99,102	0
56	MG	CA	3151	1/1	0.86	0.18	71,71,71,71	0
56	MG	AA	1624	1/1	0.86	0.19	95,95,95,95	0
56	MG	CA	3036	1/1	0.86	0.15	193,193,193,193	0
56	MG	CA	3037	1/1	0.86	0.25	189,189,189,189	0
56	MG	CA	3111	1/1	0.86	0.12	83,83,83,83	0
56	MG	CA	3022	1/1	0.86	0.21	195,195,195,195	0
56	MG	CA	3076	1/1	0.86	0.13	182,182,182,182	0
56	MG	CA	3116	1/1	0.86	0.25	95,95,95,95	0
56	MG	CA	3117	1/1	0.86	0.30	67,67,67,67	0
56	MG	BA	1647	1/1	0.86	0.38	91,91,91,91	0
67	ACY	DA	3201	4/4	0.86	0.25	78,79,79,79	0
69	TRS	DA	3220	8/8	0.86	0.17	125,128,134,134	0
56	MG	CA	3099	1/1	0.87	0.13	160,160,160,160	0
59	PUT	AA	1673	6/6	0.87	0.11	100,102,103,104	0
59	PUT	AA	1674	6/6	0.87	0.33	133,134,135,135	0
56	MG	CA	3136	1/1	0.87	0.37	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3149	1/1	0.87	0.13	67,67,67,67	0
56	MG	CA	3137	1/1	0.87	0.17	106,106,106,106	0
56	MG	DA	3176	1/1	0.87	0.28	98,98,98,98	0
56	MG	AA	1618	1/1	0.87	0.32	92,92,92,92	0
56	MG	AA	1664	1/1	0.87	0.15	212,212,212,212	0
57	PG4	AA	1670	13/13	0.87	0.12	78,87,97,97	0
63	EDO	DA	3002	4/4	0.87	0.43	93,94,95,95	0
56	MG	AA	1605	1/1	0.87	0.51	89,89,89,89	0
56	MG	CA	3055	1/1	0.87	0.07	169,169,169,169	0
56	MG	BA	1607	1/1	0.87	0.17	207,207,207,207	0
56	MG	DA	3125	1/1	0.87	0.31	59,59,59,59	0
56	MG	CA	3084	1/1	0.88	0.20	174,174,174,174	0
56	MG	BA	1604	1/1	0.88	0.09	153,153,153,153	0
56	MG	CA	3110	1/1	0.88	0.09	93,93,93,93	0
56	MG	CA	3094	1/1	0.88	0.13	105,105,105,105	0
57	PG4	DA	3193	13/13	0.88	0.24	85,95,100,101	0
56	MG	DA	3126	1/1	0.88	0.31	61,61,61,61	0
62	PEG	DQ	201	7/7	0.88	0.18	124,127,128,129	0
62	PEG	DA	3199	7/7	0.88	0.21	80,89,93,95	0
56	MG	AA	1615	1/1	0.88	0.33	83,83,83,83	0
56	MG	BA	1644	1/1	0.88	0.18	133,133,133,133	0
58	MPD	DN	201	8/8	0.88	0.18	106,111,116,117	0
56	MG	CA	3127	1/1	0.88	0.24	73,73,73,73	0
58	MPD	DA	3204	8/8	0.88	0.25	112,114,117,117	0
56	MG	DA	3152	1/1	0.88	0.54	66,66,66,66	0
56	MG	BA	1614	1/1	0.88	0.15	171,171,171,171	0
56	MG	CA	3039	1/1	0.89	0.13	175,175,175,175	0
56	MG	DA	3132	1/1	0.89	0.12	70,70,70,70	0
60	T1C	AA	1680	42/42	0.89	0.15	96,107,123,124	0
57	PG4	DQ	202	13/13	0.89	0.11	60,63,76,76	0
61	ZN	C5	101	1/1	0.89	0.10	149,149,149,149	0
62	PEG	AL	201	7/7	0.89	0.13	83,85,94,95	0
56	MG	DA	3136	1/1	0.89	0.27	77,77,77,77	0
56	MG	CA	3073	1/1	0.89	0.17	222,222,222,222	0
56	MG	AA	1616	1/1	0.89	0.54	85,85,85,85	0
56	MG	CA	3092	1/1	0.89	0.07	152,152,152,152	0
56	MG	DA	3164	1/1	0.89	0.32	71,71,71,71	0
58	MPD	DT	201	8/8	0.89	0.27	102,108,109,109	0
56	MG	DA	3167	1/1	0.89	0.29	102,102,102,102	0
56	MG	CA	3138	1/1	0.89	0.20	66,66,66,66	0
64	PGE	DS	201	10/10	0.89	0.12	77,89,91,92	0
56	MG	DA	3170	1/1	0.89	0.25	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CB	201	1/1	0.89	0.08	168,168,168,168	0
68	GUN	DA	3211	11/11	0.89	0.18	98,100,101,102	0
56	MG	CA	3001	1/1	0.89	0.17	296,296,296,296	0
57	PG4	DA	3216	13/13	0.90	0.16	99,104,109,110	0
56	MG	AA	1627	1/1	0.90	0.34	91,91,91,91	0
56	MG	CA	3141	1/1	0.90	0.38	80,80,80,80	0
56	MG	DA	3163	1/1	0.90	0.36	91,91,91,91	0
56	MG	BA	1638	1/1	0.90	0.40	78,78,78,78	0
56	MG	CA	3131	1/1	0.90	0.26	78,78,78,78	0
56	MG	AA	1612	1/1	0.90	0.32	77,77,77,77	0
56	MG	CA	3006	1/1	0.90	0.10	155,155,155,155	0
56	MG	BA	1645	1/1	0.90	0.21	102,102,102,102	0
56	MG	CA	3083	1/1	0.90	0.17	204,204,204,204	0
64	PGE	D3	101	10/10	0.90	0.18	97,99,102,103	0
56	MG	CA	3113	1/1	0.90	0.32	71,71,71,71	0
64	PGE	DA	3203	10/10	0.90	0.19	83,85,88,90	0
56	MG	DA	3141	1/1	0.90	0.33	86,86,86,86	0
57	PG4	BA	1642	13/13	0.90	0.11	88,89,99,100	0
56	MG	CA	3105	1/1	0.90	0.21	262,262,262,262	0
56	MG	DA	3145	1/1	0.90	0.18	79,79,79,79	0
56	MG	CA	3029	1/1	0.91	0.15	143,143,143,143	0
59	PUT	DA	3223	6/6	0.91	0.22	61,62,65,67	0
56	MG	CA	3010	1/1	0.91	0.10	234,234,234,234	0
57	PG4	DS	202	13/13	0.91	0.12	43,51,72,73	0
56	MG	CA	3114	1/1	0.91	0.14	66,66,66,66	0
56	MG	DA	3110	1/1	0.91	0.27	295,295,295,295	0
56	MG	DA	3120	1/1	0.91	0.20	70,70,70,70	0
62	PEG	DL	201	7/7	0.91	0.15	82,85,87,87	0
56	MG	DA	3124	1/1	0.91	0.24	65,65,65,65	0
56	MG	AA	1647	1/1	0.91	0.11	179,179,179,179	0
56	MG	AA	1642	1/1	0.91	0.13	158,158,158,158	0
62	PEG	DA	3226	7/7	0.91	0.23	89,91,98,98	0
56	MG	CA	3150	1/1	0.91	0.19	75,75,75,75	0
56	MG	DA	3172	1/1	0.91	0.49	103,103,103,103	0
58	MPD	DA	3192	8/8	0.91	0.27	95,100,104,105	0
63	EDO	DA	3198	4/4	0.91	0.24	78,81,83,83	0
56	MG	CA	3064	1/1	0.91	0.17	249,249,249,249	0
56	MG	DA	3177	1/1	0.91	0.41	77,77,77,77	0
56	MG	CA	3054	1/1	0.91	0.12	156,156,156,156	0
56	MG	DA	3137	1/1	0.91	0.50	37,37,37,37	1
65	SPD	DA	3183	10/10	0.91	0.15	79,83,87,87	0
56	MG	CA	3078	1/1	0.91	0.09	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	PUT	DA	3189	6/6	0.91	0.16	45,54,56,56	0
59	PUT	DA	3212	6/6	0.91	0.24	81,84,85,85	0
59	PUT	DA	3221	6/6	0.91	0.25	138,140,141,141	0
59	PUT	DA	3213	6/6	0.92	0.27	105,107,110,110	0
59	PUT	DA	3219	6/6	0.92	0.18	70,75,78,79	0
56	MG	CA	3109	1/1	0.92	0.13	62,62,62,62	0
56	MG	AA	1679	1/1	0.92	0.20	77,77,77,77	0
56	MG	DA	3142	1/1	0.92	0.16	62,62,62,62	0
56	MG	AA	1656	1/1	0.92	0.10	196,196,196,196	0
57	PG4	DR	202	13/13	0.92	0.24	109,117,120,121	0
56	MG	AA	1602	1/1	0.92	0.24	78,78,78,78	0
56	MG	BA	1627	1/1	0.92	0.14	124,124,124,124	0
62	PEG	D1	103	7/7	0.92	0.26	85,90,91,91	0
56	MG	AA	1623	1/1	0.92	0.14	69,69,69,69	0
56	MG	DA	3158	1/1	0.92	0.18	191,191,191,191	0
56	MG	DA	3160	1/1	0.92	0.36	74,74,74,74	0
56	MG	DA	3162	1/1	0.92	0.11	85,85,85,85	0
56	MG	DA	3122	1/1	0.92	0.32	100,100,100,100	0
62	PEG	DA	3200	7/7	0.92	0.30	83,85,95,96	0
62	PEG	DA	3218	7/7	0.92	0.33	123,129,133,134	0
56	MG	DA	3123	1/1	0.92	0.30	62,62,62,62	0
58	MPD	DT	202	8/8	0.92	0.25	128,128,130,130	0
56	MG	CA	3008	1/1	0.92	0.17	136,136,136,136	0
56	MG	CA	3057	1/1	0.92	0.09	133,133,133,133	0
56	MG	AA	1621	1/1	0.92	0.46	77,77,77,77	0
58	MPD	DA	3207	8/8	0.92	0.21	77,78,80,80	0
56	MG	DA	3171	1/1	0.92	0.10	73,73,73,73	0
56	MG	CA	3118	1/1	0.92	0.26	59,59,59,59	0
56	MG	DA	3131	1/1	0.92	0.21	62,62,62,62	0
56	MG	AA	1625	1/1	0.92	0.17	86,86,86,86	0
56	MG	AA	1626	1/1	0.92	0.11	99,99,99,99	0
59	PUT	DA	3195	6/6	0.92	0.28	87,91,91,92	0
59	PUT	DA	3205	6/6	0.92	0.35	108,109,111,111	0
56	MG	DA	3179	1/1	0.92	0.22	104,104,104,104	0
62	PEG	DA	3227	7/7	0.93	0.20	97,99,103,104	0
56	MG	CA	3119	1/1	0.93	0.25	89,89,89,89	0
56	MG	CA	3012	1/1	0.93	0.08	95,95,95,95	0
56	MG	DB	208	1/1	0.93	0.10	76,76,76,76	0
56	MG	DA	3173	1/1	0.93	0.20	98,98,98,98	0
63	EDO	DA	3209	4/4	0.93	0.26	135,136,137,138	0
56	MG	DA	3147	1/1	0.93	0.34	65,65,65,65	0
56	MG	DB	209	1/1	0.93	0.12	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3065	1/1	0.93	0.09	109,109,109,109	0
64	PGE	DU	101	10/10	0.93	0.15	89,97,104,105	0
56	MG	CA	3101	1/1	0.93	0.08	151,151,151,151	0
56	MG	DA	3133	1/1	0.93	0.13	91,91,91,91	0
65	SPD	DA	3224	10/10	0.93	0.15	50,54,66,68	0
66	1PE	DA	3185	16/16	0.93	0.12	50,55,84,87	0
56	MG	DA	3119	1/1	0.93	0.26	57,57,57,57	0
56	MG	BA	1637	1/1	0.93	0.12	85,85,85,85	0
56	MG	AA	1606	1/1	0.93	0.31	91,91,91,91	0
56	MG	CB	203	1/1	0.93	0.06	145,145,145,145	0
56	MG	DA	3155	1/1	0.94	0.15	58,58,58,58	0
56	MG	CA	3134	1/1	0.94	0.16	108,108,108,108	0
56	MG	DA	3130	1/1	0.94	0.29	54,54,54,54	0
56	MG	AA	1601	1/1	0.94	0.35	67,67,67,67	0
63	EDO	DB	201	4/4	0.94	0.23	94,97,98,99	0
56	MG	AA	1636	1/1	0.94	0.09	97,97,97,97	0
56	MG	CA	3071	1/1	0.94	0.06	166,166,166,166	0
63	EDO	DB	213	4/4	0.94	0.20	82,82,84,84	0
56	MG	DA	3118	1/1	0.94	0.14	68,68,68,68	0
58	MPD	AA	1671	8/8	0.94	0.24	88,88,90,92	0
58	MPD	AA	1676	8/8	0.94	0.22	95,99,100,101	0
56	MG	AA	1659	1/1	0.94	0.08	115,115,115,115	0
56	MG	DA	3169	1/1	0.94	0.20	69,69,69,69	0
56	MG	AA	1619	1/1	0.94	0.22	92,92,92,92	0
56	MG	AA	1617	1/1	0.94	0.33	96,96,96,96	0
56	MG	CA	3153	1/1	0.94	0.10	64,64,64,64	0
64	PGE	DA	3214	10/10	0.94	0.13	72,73,77,78	0
64	PGE	DA	3225	10/10	0.94	0.16	73,83,94,96	0
56	MG	CA	3093	1/1	0.94	0.07	88,88,88,88	0
65	SPD	DA	3206	10/10	0.94	0.25	87,102,109,110	0
56	MG	BA	1633	1/1	0.94	0.15	229,229,229,229	0
56	MG	BA	1616	1/1	0.94	0.10	122,122,122,122	0
66	1PE	DA	3202	16/16	0.94	0.15	61,64,72,73	0
56	MG	DA	3150	1/1	0.94	0.18	51,51,51,51	0
56	MG	DA	3151	1/1	0.94	0.28	82,82,82,82	0
56	MG	DA	3128	1/1	0.94	0.26	72,72,72,72	0
56	MG	DA	3182	1/1	0.94	0.20	61,61,61,61	0
56	MG	CA	3066	1/1	0.95	0.10	89,89,89,89	0
56	MG	CA	3019	1/1	0.95	0.08	58,58,58,58	0
56	MG	CA	3133	1/1	0.95	0.17	72,72,72,72	0
56	MG	BA	1619	1/1	0.95	0.09	96,96,96,96	0
63	EDO	D1	101	4/4	0.95	0.07	59,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3070	1/1	0.95	0.07	91,91,91,91	0
56	MG	DA	3138	1/1	0.95	0.13	59,59,59,59	0
56	MG	DR	201	1/1	0.95	0.11	42,42,42,42	0
59	PUT	DA	3188	6/6	0.95	0.15	50,53,55,56	0
56	MG	DB	206	1/1	0.95	0.32	80,80,80,80	0
56	MG	DB	207	1/1	0.95	0.13	92,92,92,92	0
56	MG	BA	1635	1/1	0.95	0.07	102,102,102,102	0
63	EDO	DA	3215	4/4	0.95	0.12	65,66,68,70	0
56	MG	CA	3051	1/1	0.95	0.07	80,80,80,80	0
56	MG	CA	3023	1/1	0.95	0.09	158,158,158,158	0
56	MG	CA	3120	1/1	0.95	0.14	102,102,102,102	0
56	MG	CA	3121	1/1	0.95	0.10	64,64,64,64	0
56	MG	CA	3074	1/1	0.95	0.07	131,131,131,131	0
56	MG	AA	1655	1/1	0.95	0.07	163,163,163,163	0
56	MG	DA	3157	1/1	0.95	0.23	73,73,73,73	0
56	MG	CA	3143	1/1	0.95	0.08	70,70,70,70	0
56	MG	BA	1609	1/1	0.95	0.07	166,166,166,166	0
56	MG	AA	1665	1/1	0.95	0.13	161,161,161,161	0
56	MG	CB	202	1/1	0.95	0.12	116,116,116,116	0
56	MG	AA	1604	1/1	0.95	0.42	70,70,70,70	0
56	MG	DA	3165	1/1	0.95	0.26	62,62,62,62	0
56	MG	CA	3128	1/1	0.95	0.13	75,75,75,75	0
56	MG	AA	1657	1/1	0.95	0.14	136,136,136,136	0
56	MG	BA	1630	1/1	0.95	0.12	153,153,153,153	0
56	MG	CA	3016	1/1	0.96	0.14	107,107,107,107	0
56	MG	DA	3181	1/1	0.96	0.33	83,83,83,83	0
59	PUT	DA	3184	6/6	0.96	0.16	78,80,81,82	0
56	MG	AA	1644	1/1	0.96	0.17	106,106,106,106	0
56	MG	DA	3156	1/1	0.96	0.27	62,62,62,62	0
56	MG	CA	3062	1/1	0.96	0.06	175,175,175,175	0
56	MG	CA	3063	1/1	0.96	0.15	125,125,125,125	0
63	EDO	DA	3194	4/4	0.96	0.13	76,77,78,78	0
63	EDO	DA	3197	4/4	0.96	0.12	65,67,68,69	0
56	MG	CA	3031	1/1	0.96	0.05	64,64,64,64	0
63	EDO	DA	3208	4/4	0.96	0.18	89,90,90,91	0
56	MG	DA	3161	1/1	0.96	0.17	61,61,61,61	0
56	MG	DA	3011	1/1	0.96	0.07	115,115,115,115	0
56	MG	DA	3036	1/1	0.96	0.10	24,24,24,24	0
56	MG	CA	3048	1/1	0.96	0.06	76,76,76,76	0
56	MG	DA	3097	1/1	0.96	0.12	128,128,128,128	0
56	MG	DA	3166	1/1	0.96	0.22	81,81,81,81	0
64	PGE	DA	3186	10/10	0.96	0.09	39,48,55,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	1618	1/1	0.96	0.07	129,129,129,129	0
56	MG	DA	3140	1/1	0.96	0.10	54,54,54,54	0
64	PGE	DA	3217	10/10	0.96	0.13	85,88,91,92	0
56	MG	AA	1669	1/1	0.96	0.08	134,134,134,134	0
56	MG	CA	3082	1/1	0.96	0.14	114,114,114,114	0
56	MG	CA	3035	1/1	0.96	0.18	91,91,91,91	0
56	MG	DA	3144	1/1	0.96	0.09	72,72,72,72	0
56	MG	DA	3121	1/1	0.96	0.45	68,68,68,68	0
56	MG	CA	3069	1/1	0.96	0.08	88,88,88,88	0
67	ACY	DA	3191	4/4	0.96	0.10	68,70,70,71	0
56	MG	CA	3088	1/1	0.96	0.09	62,62,62,62	0
58	MPD	DA	3210	8/8	0.96	0.15	87,89,90,91	0
56	MG	AA	1663	1/1	0.96	0.04	90,90,90,90	0
56	MG	AA	1607	1/1	0.96	0.20	65,65,65,65	0
56	MG	CA	3018	1/1	0.97	0.05	85,85,85,85	0
56	MG	DA	3116	1/1	0.97	0.24	72,72,72,72	0
56	MG	CA	3058	1/1	0.97	0.12	98,98,98,98	0
56	MG	CA	3004	1/1	0.97	0.08	159,159,159,159	0
56	MG	AA	1630	1/1	0.97	0.10	134,134,134,134	0
56	MG	BA	1622	1/1	0.97	0.05	85,85,85,85	0
61	ZN	AB	301	1/1	0.97	0.09	171,171,171,171	0
56	MG	BA	1610	1/1	0.97	0.05	93,93,93,93	0
56	MG	CA	3102	1/1	0.97	0.06	113,113,113,113	0
56	MG	CA	3046	1/1	0.97	0.10	111,111,111,111	0
56	MG	DA	3174	1/1	0.97	0.11	74,74,74,74	0
56	MG	AA	1658	1/1	0.97	0.12	98,98,98,98	0
56	MG	CA	3079	1/1	0.97	0.06	115,115,115,115	0
56	MG	DA	3127	1/1	0.97	0.43	53,53,53,53	0
56	MG	DA	3153	1/1	0.97	0.23	52,52,52,52	0
56	MG	DA	3154	1/1	0.97	0.20	59,59,59,59	0
56	MG	BA	1605	1/1	0.97	0.07	107,107,107,107	0
56	MG	AA	1633	1/1	0.97	0.06	123,123,123,123	0
56	MG	BA	1617	1/1	0.97	0.05	131,131,131,131	0
56	MG	DB	210	1/1	0.97	0.13	97,97,97,97	0
56	MG	AA	1610	1/1	0.97	0.21	90,90,90,90	0
56	MG	CA	3086	1/1	0.97	0.05	68,68,68,68	0
56	MG	DA	3135	1/1	0.97	0.14	72,72,72,72	0
56	MG	BA	1632	1/1	0.97	0.09	75,75,75,75	0
56	MG	CA	3089	1/1	0.97	0.11	68,68,68,68	0
56	MG	BA	1631	1/1	0.98	0.03	55,55,55,55	0
56	MG	DA	3117	1/1	0.98	0.03	56,56,56,56	0
56	MG	BA	1613	1/1	0.98	0.08	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1613	1/1	0.98	0.35	65,65,65,65	0
56	MG	CA	3042	1/1	0.98	0.04	88,88,88,88	0
56	MG	BA	1601	1/1	0.98	0.06	106,106,106,106	0
58	MPD	DS	203	8/8	0.98	0.11	48,52,58,59	0
56	MG	BA	1602	1/1	0.98	0.04	68,68,68,68	0
56	MG	CA	3097	1/1	0.98	0.05	90,90,90,90	0
56	MG	CA	3098	1/1	0.98	0.04	77,77,77,77	0
56	MG	AA	1651	1/1	0.98	0.05	76,76,76,76	0
56	MG	CA	3100	1/1	0.98	0.12	92,92,92,92	0
56	MG	AA	1638	1/1	0.98	0.05	114,114,114,114	0
56	MG	CA	3053	1/1	0.98	0.09	65,65,65,65	0
56	MG	CA	3024	1/1	0.98	0.08	102,102,102,102	0
56	MG	AA	1639	1/1	0.98	0.05	118,118,118,118	0
56	MG	AA	1641	1/1	0.98	0.05	67,67,67,67	0
56	MG	AA	1667	1/1	0.98	0.07	47,47,47,47	0
59	PUT	DA	3001	6/6	0.98	0.09	46,50,58,60	0
56	MG	BA	1608	1/1	0.98	0.06	102,102,102,102	0
56	MG	DA	3134	1/1	0.98	0.04	96,96,96,96	0
56	MG	CA	3059	1/1	0.98	0.04	86,86,86,86	0
56	MG	AA	1629	1/1	0.98	0.07	93,93,93,93	0
56	MG	CA	3081	1/1	0.98	0.04	104,104,104,104	0
56	MG	DA	3005	1/1	0.98	0.05	94,94,94,94	0
56	MG	DA	3139	1/1	0.98	0.11	67,67,67,67	0
56	MG	DA	3007	1/1	0.98	0.05	82,82,82,82	0
56	MG	CA	3033	1/1	0.98	0.14	110,110,110,110	0
56	MG	AA	1634	1/1	0.98	0.07	130,130,130,130	0
65	SPD	DA	3187	10/10	0.98	0.10	34,42,45,48	0
56	MG	DA	3042	1/1	0.98	0.09	40,40,40,40	0
56	MG	DA	3043	1/1	0.98	0.08	80,80,80,80	0
56	MG	DA	3053	1/1	0.98	0.07	89,89,89,89	0
56	MG	AA	1645	1/1	0.98	0.06	66,66,66,66	0
56	MG	DA	3079	1/1	0.98	0.07	119,119,119,119	0
56	MG	DA	3148	1/1	0.98	0.06	61,61,61,61	0
56	MG	DA	3149	1/1	0.98	0.07	62,62,62,62	0
56	MG	CA	3085	1/1	0.98	0.04	74,74,74,74	0
56	MG	CA	3013	1/1	0.98	0.04	86,86,86,86	0
56	MG	AA	1640	1/1	0.99	0.05	73,73,73,73	0
56	MG	CA	3025	1/1	0.99	0.04	82,82,82,82	0
56	MG	DA	3003	1/1	0.99	0.05	85,85,85,85	0
56	MG	DA	3004	1/1	0.99	0.09	77,77,77,77	0
56	MG	AA	1648	1/1	0.99	0.05	70,70,70,70	0
56	MG	DA	3006	1/1	0.99	0.03	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3091	1/1	0.99	0.06	68,68,68,68	0
56	MG	BA	1634	1/1	0.99	0.08	99,99,99,99	0
56	MG	DA	3014	1/1	0.99	0.03	45,45,45,45	0
56	MG	DA	3025	1/1	0.99	0.06	108,108,108,108	0
56	MG	DA	3027	1/1	0.99	0.05	94,94,94,94	0
56	MG	DA	3029	1/1	0.99	0.04	46,46,46,46	0
56	MG	AA	1649	1/1	0.99	0.04	68,68,68,68	0
56	MG	CA	3030	1/1	0.99	0.05	78,78,78,78	0
56	MG	CA	3095	1/1	0.99	0.07	63,63,63,63	0
56	MG	DA	3048	1/1	0.99	0.04	57,57,57,57	0
56	MG	DA	3051	1/1	0.99	0.03	73,73,73,73	0
56	MG	CA	3096	1/1	0.99	0.02	61,61,61,61	0
56	MG	DA	3159	1/1	0.99	0.07	72,72,72,72	0
56	MG	AA	1662	1/1	0.99	0.05	79,79,79,79	0
56	MG	DA	3063	1/1	0.99	0.12	72,72,72,72	0
56	MG	DA	3064	1/1	0.99	0.03	25,25,25,25	0
56	MG	DA	3069	1/1	0.99	0.08	79,79,79,79	0
56	MG	DA	3071	1/1	0.99	0.07	68,68,68,68	0
56	MG	DA	3073	1/1	0.99	0.04	45,45,45,45	0
56	MG	DA	3077	1/1	0.99	0.04	63,63,63,63	0
56	MG	DA	3078	1/1	0.99	0.04	96,96,96,96	0
56	MG	AA	1650	1/1	0.99	0.04	114,114,114,114	0
56	MG	DA	3080	1/1	0.99	0.03	44,44,44,44	0
56	MG	DA	3081	1/1	0.99	0.04	65,65,65,65	0
56	MG	DA	3084	1/1	0.99	0.07	54,54,54,54	0
56	MG	DA	3092	1/1	0.99	0.09	35,35,35,35	0
56	MG	DA	3093	1/1	0.99	0.05	20,20,20,20	0
56	MG	DA	3094	1/1	0.99	0.09	80,80,80,80	0
56	MG	DA	3175	1/1	0.99	0.06	63,63,63,63	0
56	MG	BA	1620	1/1	0.99	0.03	94,94,94,94	0
56	MG	BA	1621	1/1	0.99	0.12	33,33,33,33	0
56	MG	AA	1635	1/1	0.99	0.04	104,104,104,104	0
56	MG	CA	3011	1/1	0.99	0.03	59,59,59,59	0
56	MG	CA	3103	1/1	0.99	0.06	82,82,82,82	0
56	MG	AA	1632	1/1	0.99	0.04	94,94,94,94	0
56	MG	AA	1666	1/1	0.99	0.04	57,57,57,57	0
56	MG	DA	3230	1/1	0.99	0.05	55,55,55,55	0
56	MG	DA	3231	1/1	0.99	0.12	39,39,39,39	0
56	MG	AA	1643	1/1	0.99	0.03	65,65,65,65	0
56	MG	CA	3040	1/1	0.99	0.05	76,76,76,76	0
56	MG	CA	3144	1/1	0.99	0.03	49,49,49,49	0
56	MG	CA	3041	1/1	0.99	0.05	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3015	1/1	0.99	0.13	51,51,51,51	0
56	MG	CA	3043	1/1	0.99	0.05	81,81,81,81	0
56	MG	CA	3044	1/1	0.99	0.06	57,57,57,57	0
56	MG	CA	3045	1/1	0.99	0.06	84,84,84,84	0
56	MG	BA	1626	1/1	0.99	0.03	102,102,102,102	0
56	MG	AA	1668	1/1	0.99	0.09	75,75,75,75	0
56	MG	BA	1628	1/1	0.99	0.05	89,89,89,89	0
56	MG	CA	3049	1/1	0.99	0.03	48,48,48,48	0
56	MG	CA	3050	1/1	0.99	0.04	54,54,54,54	0
56	MG	CA	3020	1/1	0.99	0.06	86,86,86,86	0
56	MG	CA	3052	1/1	0.99	0.06	68,68,68,68	0
56	MG	AA	1620	1/1	0.99	0.25	78,78,78,78	0
56	MG	DB	202	1/1	0.99	0.06	62,62,62,62	0
56	MG	AA	1631	1/1	0.99	0.05	53,53,53,53	0
56	MG	AA	1646	1/1	0.99	0.05	66,66,66,66	0
56	MG	CA	3087	1/1	0.99	0.05	77,77,77,77	0
56	MG	DA	3085	1/1	1.00	0.01	31,31,31,31	0
56	MG	DA	3086	1/1	1.00	0.01	34,34,34,34	0
56	MG	DA	3087	1/1	1.00	0.02	54,54,54,54	0
56	MG	DA	3088	1/1	1.00	0.03	24,24,24,24	0
56	MG	DA	3089	1/1	1.00	0.02	26,26,26,26	0
56	MG	DA	3090	1/1	1.00	0.04	24,24,24,24	0
56	MG	DA	3228	1/1	1.00	0.04	41,41,41,41	0
56	MG	DA	3229	1/1	1.00	0.02	54,54,54,54	0
56	MG	DA	3091	1/1	1.00	0.02	30,30,30,30	0
56	MG	DA	3019	1/1	1.00	0.03	65,65,65,65	0
56	MG	DA	3020	1/1	1.00	0.04	31,31,31,31	0
56	MG	DA	3021	1/1	1.00	0.05	34,34,34,34	0
56	MG	DA	3095	1/1	1.00	0.05	36,36,36,36	0
56	MG	DA	3096	1/1	1.00	0.03	33,33,33,33	0
56	MG	DA	3022	1/1	1.00	0.05	36,36,36,36	0
56	MG	DA	3098	1/1	1.00	0.03	23,23,23,23	0
56	MG	DA	3099	1/1	1.00	0.01	31,31,31,31	0
56	MG	DA	3100	1/1	1.00	0.03	61,61,61,61	0
56	MG	DA	3101	1/1	1.00	0.02	42,42,42,42	0
56	MG	DA	3102	1/1	1.00	0.05	34,34,34,34	0
56	MG	DA	3103	1/1	1.00	0.05	30,30,30,30	0
56	MG	DA	3104	1/1	1.00	0.03	29,29,29,29	0
56	MG	DA	3105	1/1	1.00	0.10	37,37,37,37	0
56	MG	DA	3106	1/1	1.00	0.02	36,36,36,36	0
56	MG	DA	3107	1/1	1.00	0.02	39,39,39,39	0
56	MG	DA	3108	1/1	1.00	0.02	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3109	1/1	1.00	0.03	26,26,26,26	0
56	MG	DA	3023	1/1	1.00	0.04	29,29,29,29	0
56	MG	DA	3111	1/1	1.00	0.02	25,25,25,25	0
56	MG	DA	3112	1/1	1.00	0.04	83,83,83,83	0
56	MG	DA	3113	1/1	1.00	0.05	37,37,37,37	0
56	MG	DA	3114	1/1	1.00	0.01	31,31,31,31	0
56	MG	DA	3115	1/1	1.00	0.01	32,32,32,32	0
56	MG	DA	3024	1/1	1.00	0.01	39,39,39,39	0
56	MG	AA	1653	1/1	1.00	0.03	50,50,50,50	0
56	MG	DA	3026	1/1	1.00	0.03	51,51,51,51	0
56	MG	CA	3027	1/1	1.00	0.07	73,73,73,73	0
56	MG	DA	3028	1/1	1.00	0.08	27,27,27,27	0
56	MG	AA	1637	1/1	1.00	0.03	51,51,51,51	0
56	MG	DA	3030	1/1	1.00	0.02	22,22,22,22	0
56	MG	DA	3031	1/1	1.00	0.07	29,29,29,29	0
56	MG	DA	3032	1/1	1.00	0.02	27,27,27,27	0
56	MG	DA	3033	1/1	1.00	0.01	13,13,13,13	0
56	MG	DA	3034	1/1	1.00	0.06	35,35,35,35	0
56	MG	DA	3035	1/1	1.00	0.04	34,34,34,34	0
56	MG	AA	1652	1/1	1.00	0.14	25,25,25,25	0
56	MG	DA	3037	1/1	1.00	0.03	30,30,30,30	0
56	MG	DA	3038	1/1	1.00	0.07	35,35,35,35	0
56	MG	DA	3039	1/1	1.00	0.07	55,55,55,55	0
56	MG	DA	3040	1/1	1.00	0.14	24,24,24,24	0
56	MG	DA	3041	1/1	1.00	0.03	52,52,52,52	0
61	ZN	D5	101	1/1	1.00	0.02	66,66,66,66	0
56	MG	CA	3017	1/1	1.00	0.08	88,88,88,88	0
56	MG	DD	301	1/1	1.00	0.03	35,35,35,35	0
56	MG	DA	3044	1/1	1.00	0.03	53,53,53,53	0
56	MG	DA	3045	1/1	1.00	0.03	24,24,24,24	0
56	MG	DA	3046	1/1	1.00	0.02	47,47,47,47	0
56	MG	DA	3047	1/1	1.00	0.05	36,36,36,36	0
56	MG	DM	201	1/1	1.00	0.04	56,56,56,56	0
56	MG	DA	3049	1/1	1.00	0.02	20,20,20,20	0
56	MG	DA	3050	1/1	1.00	0.02	24,24,24,24	0
56	MG	BA	1615	1/1	1.00	0.03	72,72,72,72	0
56	MG	DA	3052	1/1	1.00	0.03	41,41,41,41	0
56	MG	BA	1611	1/1	1.00	0.04	53,53,53,53	0
56	MG	DA	3054	1/1	1.00	0.04	30,30,30,30	0
56	MG	DA	3055	1/1	1.00	0.02	34,34,34,34	0
56	MG	DA	3056	1/1	1.00	0.04	23,23,23,23	0
56	MG	DA	3057	1/1	1.00	0.01	27,27,27,27	0

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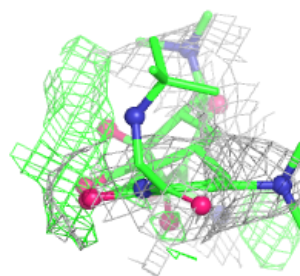
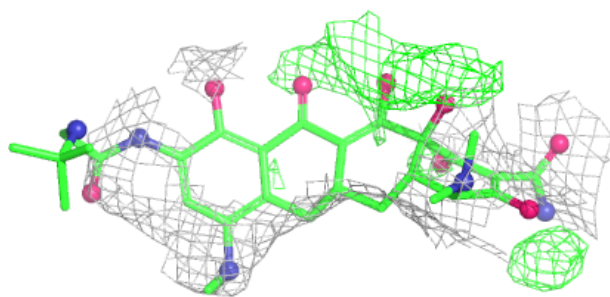
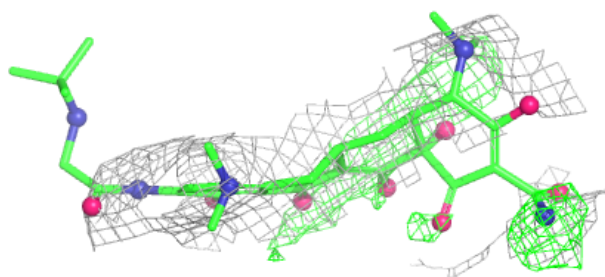
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3058	1/1	1.00	0.03	27,27,27,27	0
56	MG	DA	3059	1/1	1.00	0.03	33,33,33,33	0
56	MG	DA	3060	1/1	1.00	0.04	41,41,41,41	0
56	MG	DB	203	1/1	1.00	0.04	41,41,41,41	0
56	MG	DA	3062	1/1	1.00	0.04	73,73,73,73	0
56	MG	DA	3008	1/1	1.00	0.03	27,27,27,27	0
56	MG	DA	3009	1/1	1.00	0.04	27,27,27,27	0
56	MG	DA	3065	1/1	1.00	0.06	45,45,45,45	0
56	MG	DA	3066	1/1	1.00	0.03	49,49,49,49	0
56	MG	DA	3067	1/1	1.00	0.06	46,46,46,46	0
56	MG	DA	3068	1/1	1.00	0.09	59,59,59,59	0
56	MG	DA	3010	1/1	1.00	0.02	26,26,26,26	0
56	MG	DA	3070	1/1	1.00	0.05	55,55,55,55	0
56	MG	DB	204	1/1	1.00	0.06	37,37,37,37	0
56	MG	DA	3072	1/1	1.00	0.01	38,38,38,38	0
56	MG	DA	3012	1/1	1.00	0.03	25,25,25,25	0
56	MG	DA	3074	1/1	1.00	0.02	33,33,33,33	0
56	MG	DA	3075	1/1	1.00	0.03	40,40,40,40	0
56	MG	DA	3076	1/1	1.00	0.03	31,31,31,31	0
56	MG	DA	3013	1/1	1.00	0.02	20,20,20,20	0
56	MG	DB	205	1/1	1.00	0.04	63,63,63,63	0
56	MG	DA	3015	1/1	1.00	0.03	72,72,72,72	0
56	MG	DA	3016	1/1	1.00	0.01	26,26,26,26	0
56	MG	DA	3017	1/1	1.00	0.04	44,44,44,44	0
56	MG	DA	3082	1/1	1.00	0.06	56,56,56,56	0
56	MG	DA	3083	1/1	1.00	0.06	30,30,30,30	0
56	MG	DA	3018	1/1	1.00	0.11	8,8,8,8	0

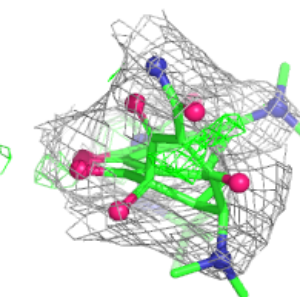
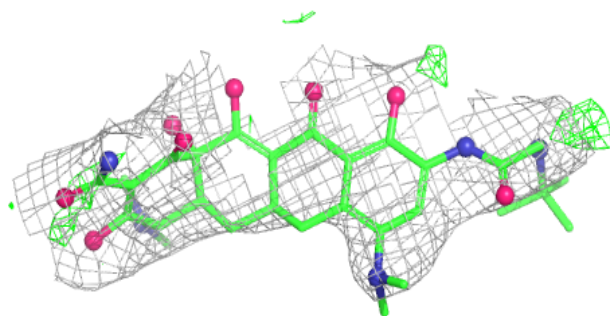
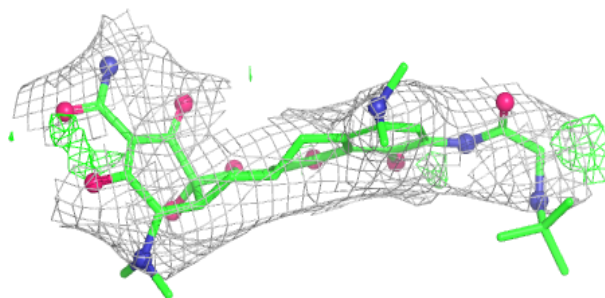
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around T1C 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 T1C 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.