



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 01:40 PM EDT

PDB ID : 5IT8 / pdb_00005it8
Title : High-resolution structure of the Escherichia coli ribosome
Authors : Cocozaki, A.; Ferguson, A.
Deposited on : 2016-03-16
Resolution : 3.12 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

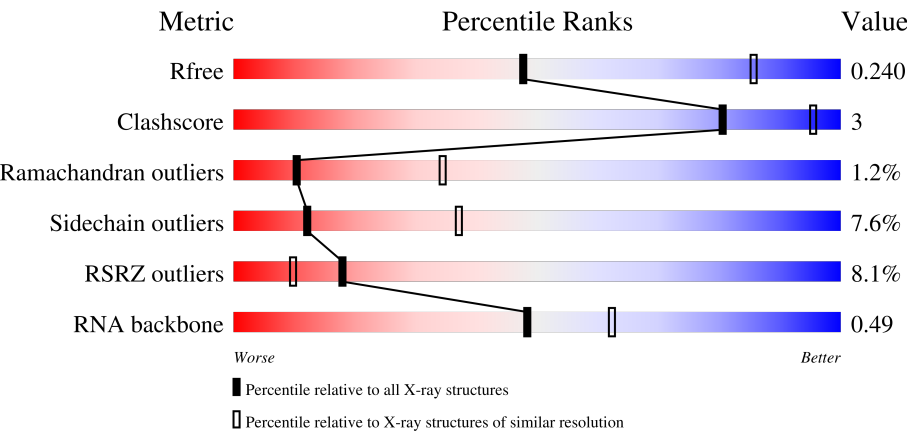
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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.



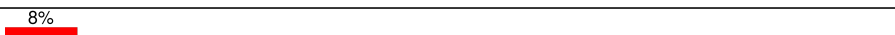
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)
RNA backbone	3983	1017 (3.34-2.90)

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	74%23%.
1	BA	1534	5%74%23%.
2	AB	224	3%82%16%.
2	BB	224	4%81%17%.

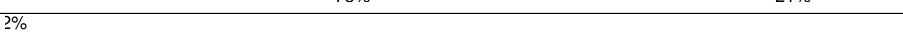
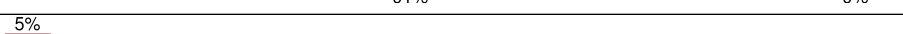
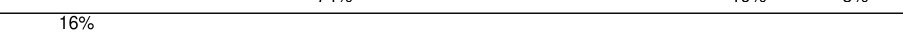
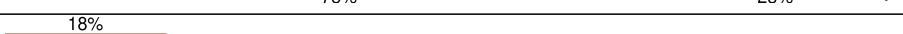
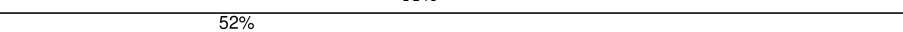
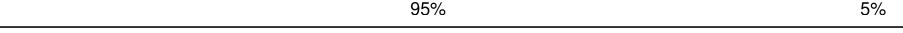
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Mol	Chain	Length	Quality of chain
3	AC	206	
3	BC	206	
4	AD	205	
4	BD	205	
5	AE	155	
5	BE	155	
6	AF	106	
6	BF	106	
7	AG	151	
7	BG	151	
8	AH	129	
8	BH	129	
9	AI	127	
9	BI	127	
10	AJ	99	
10	BJ	99	
11	AK	117	
11	BK	117	
12	AL	123	
12	BL	123	
13	AM	114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

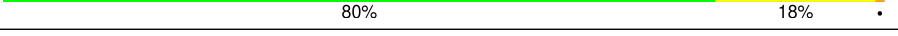
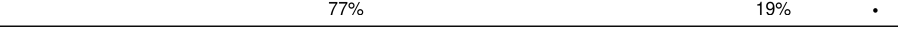
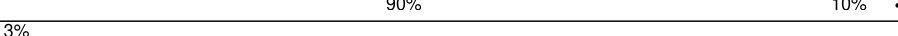
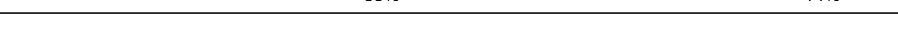
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Mol	Chain	Length	Quality of chain
15	BO	88	
16	AP	82	
16	BP	82	
17	AQ	80	
17	BQ	80	
18	AR	55	
18	BR	55	
19	AS	79	
19	BS	79	
20	AT	86	
20	BT	86	
21	AU	56	
21	BU	56	
22	C1	56	
22	D1	56	
23	C2	51	
23	D2	51	
24	C3	46	
24	D3	46	
25	C4	64	
25	D4	64	
26	C5	38	
26	D5	38	
27	C0	58	
27	D0	58	

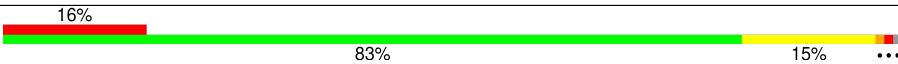
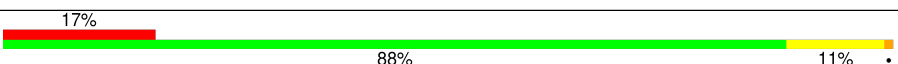
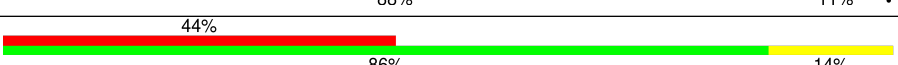
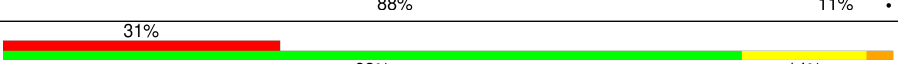
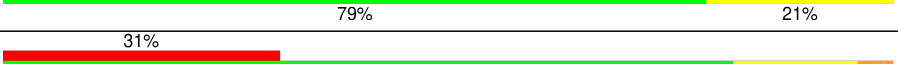
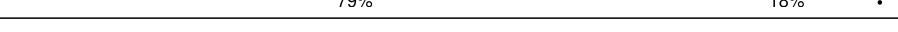
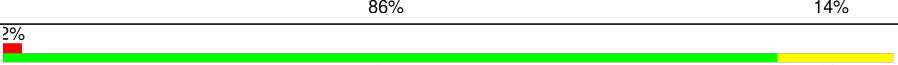
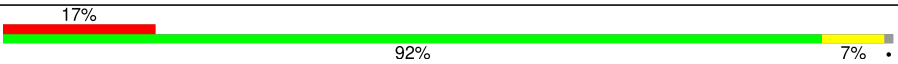
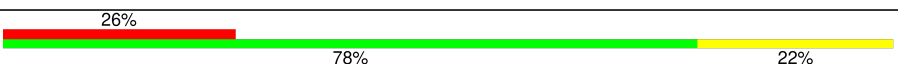
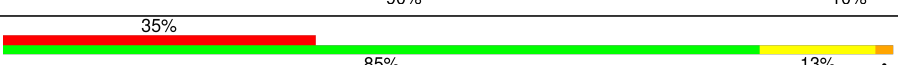
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Mol	Chain	Length	Quality of chain
28	CB	120	
28	DB	120	
29	CC	271	
29	DC	271	
30	CD	209	
31	CA	2904	
32	DD	209	
33	DA	2903	
34	CE	201	
34	DE	201	
35	CF	177	
35	DF	177	
36	CG	176	
36	DG	176	
37	CH	149	
37	DH	149	
38	CJ	134	
38	DJ	134	
39	CK	142	
39	DK	142	
40	CL	123	
40	DL	123	
41	CM	144	
41	DM	144	
42	CN	136	

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Mol	Chain	Length	Quality of chain
42	DN	136	
43	CO	125	
43	DO	125	
44	CP	117	
44	DP	117	
45	CQ	114	
45	DQ	114	
46	CR	117	
46	DR	117	
47	CS	103	
47	DS	103	
48	CT	110	
48	DT	110	
49	CU	93	
49	DU	93	
50	CV	102	
50	DV	102	
51	CW	94	
51	DW	94	
52	CX	76	
52	DX	76	
53	CY	77	
53	DY	77	
54	CZ	62	
54	DZ	62	

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Mol	Chain	Length	Quality of chain
55	DI	135	

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	AA	1606	-	-	-	X
56	MG	CA	3110	-	-	-	X
56	MG	CA	3115	-	-	-	X
66	ACY	DA	3194	-	X	-	-

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295125 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
			32930	14694	6041	10661	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32908	14684	6036	10655	1533			

- 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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
29	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

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

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

- 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 RNA chain called 23S rRNA.

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

- Molecule 34 is a protein called 50S ribosomal protein L4.

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

- Molecule 35 is a protein called 50S ribosomal protein L5.

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

- Molecule 36 is a protein called 50S ribosomal protein L6.

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

- Molecule 37 is a protein called 50S ribosomal protein L9.

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

- Molecule 38 is a protein called 50S ribosomal protein L11.

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

- Molecule 39 is a protein called 50S ribosomal protein L13.

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

- Molecule 40 is a protein called 50S ribosomal protein L14.

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

- Molecule 41 is a protein called 50S ribosomal protein L15.

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

- Molecule 42 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CN	136	Total	C	N	O	S	0	0	0
			1075	686	205	178	6			
42	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 43 is a protein called 50S ribosomal protein L17.

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

- Molecule 44 is a protein called 50S ribosomal protein L18.

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

- Molecule 45 is a protein called 50S ribosomal protein L19.

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

- Molecule 46 is a protein called 50S ribosomal protein L20.

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

- Molecule 47 is a protein called 50S ribosomal protein L21.

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

- Molecule 48 is a protein called 50S ribosomal protein L22.

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

- Molecule 49 is a protein called 50S ribosomal protein L23.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L25.

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

- Molecule 52 is a protein called 50S ribosomal protein L27.

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

- Molecule 53 is a protein called 50S ribosomal protein L28.

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

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

- Molecule 54 is a protein called 50S ribosomal protein L29.

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

- Molecule 55 is a protein called 50S ribosomal protein L10.

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

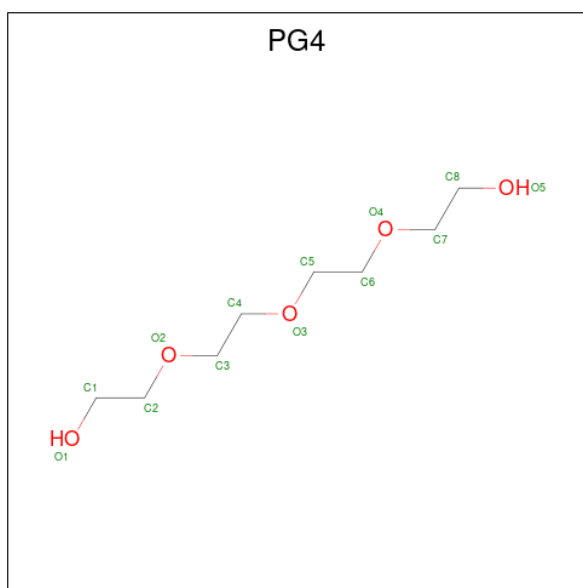
There are 2 discrepancies between the modelled and reference sequences:

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

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

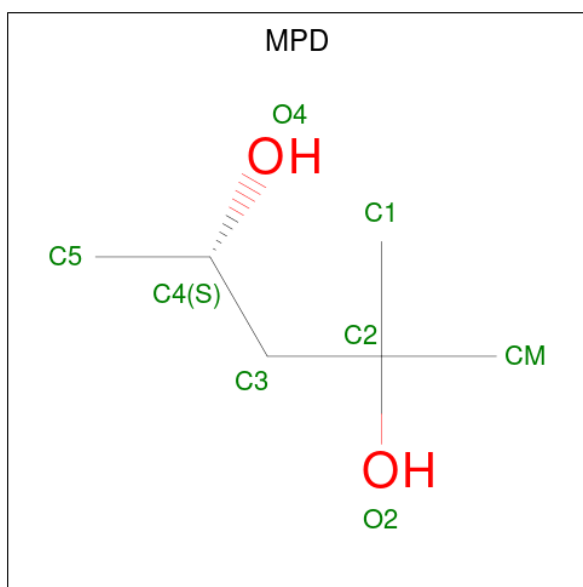
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	70	Total	Mg	0	0
			70	70		
56	BA	41	Total	Mg	0	0
			41	41		
56	CB	3	Total	Mg	0	0
			3	3		
56	CA	156	Total	Mg	0	0
			156	156		
56	DB	9	Total	Mg	0	0
			9	9		
56	DD	2	Total	Mg	0	0
			2	2		
56	DA	183	Total	Mg	0	0
			183	183		
56	DR	2	Total	Mg	0	0
			2	2		

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



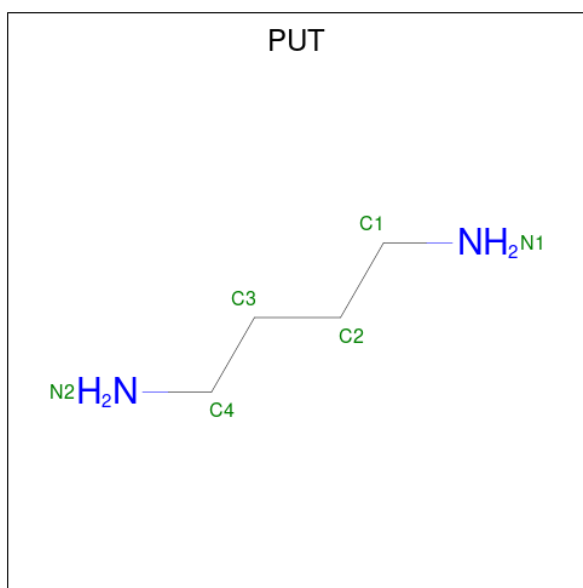
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			13	8	5		
57	BA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DQ	1	Total	C	O	0	0
			13	8	5		
57	DR	1	Total	C	O	0	0
			13	8	5		
57	DS	1	Total	C	O	0	0
			13	8	5		

- 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 8	C 6	O 2	0	0
58	AA	1	Total 8	C 6	O 2	0	0
58	DA	1	Total 8	C 6	O 2	0	0
58	DA	1	Total 8	C 6	O 2	0	0
58	DA	1	Total 8	C 6	O 2	0	0
58	DA	1	Total 8	C 6	O 2	0	0
58	DA	1	Total 8	C 6	O 2	0	0
58	DA	1	Total 8	C 6	O 2	0	0
58	DA	1	Total 8	C 6	O 2	0	0
58	DE	1	Total 8	C 6	O 2	0	0
58	DE	1	Total 8	C 6	O 2	0	0
58	DK	1	Total 8	C 6	O 2	0	0
58	DN	1	Total 8	C 6	O 2	0	0
58	DS	1	Total 8	C 6	O 2	0	0
58	DT	1	Total 8	C 6	O 2	0	0

- 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		
59	DA	1	Total	C	N	0	0
			6	4	2		

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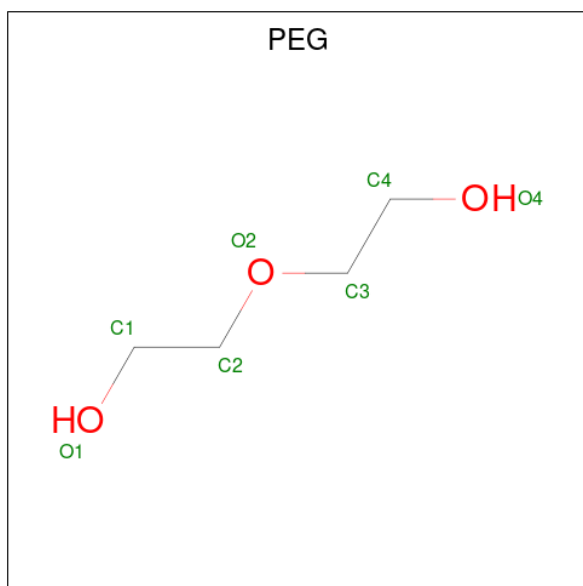
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		

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

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

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



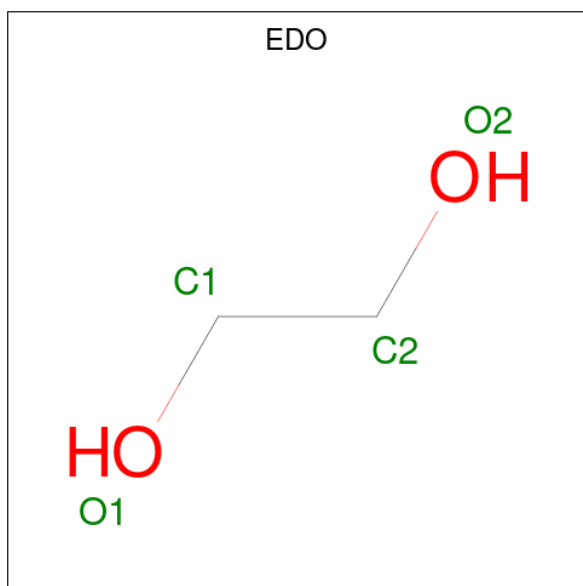
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	D1	1	Total	C	O	0	0
			7	4	3		
61	D3	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 62 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



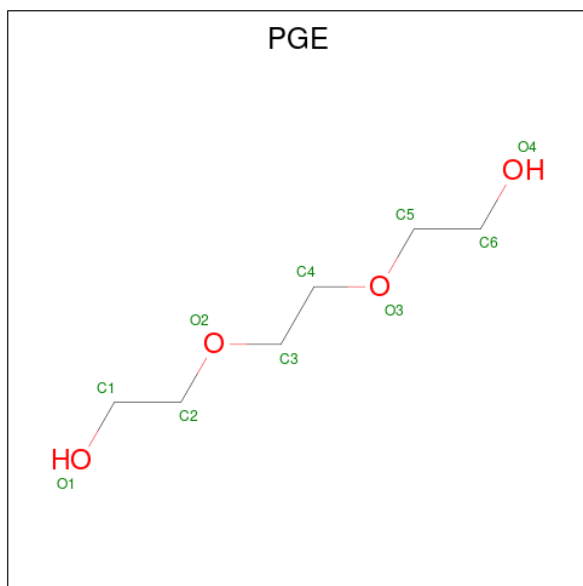
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	D1	1	Total C O 4 2 2	0	0
62	D0	1	Total C O 4 2 2	0	0
62	DB	1	Total C O 4 2 2	0	0

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

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



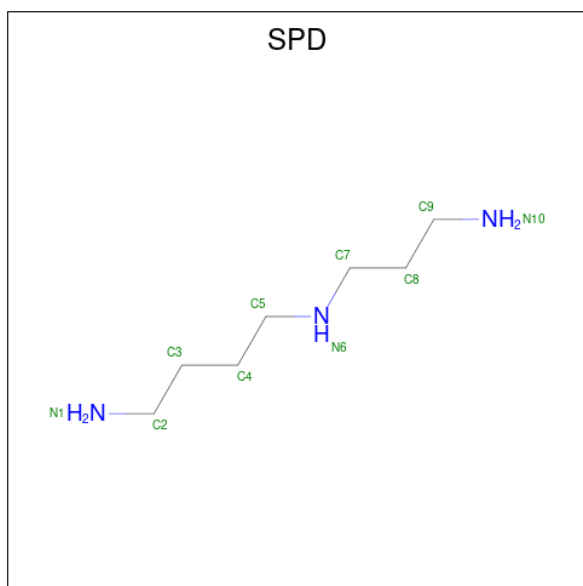
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D3	1	Total	C	O	0	0
			10	6	4		
63	DD	1	Total	C	O	0	0
			10	6	4		

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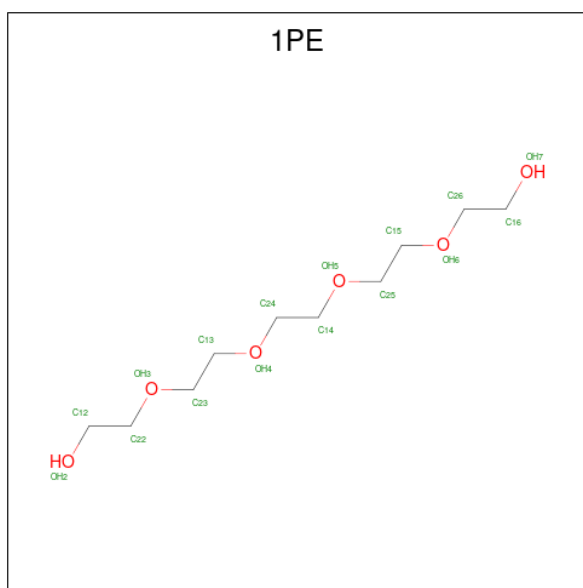
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DS	1	Total	C	O	0	0
			10	6	4		
63	DT	1	Total	C	O	0	0
			10	6	4		
63	DU	1	Total	C	O	0	0
			10	6	4		

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



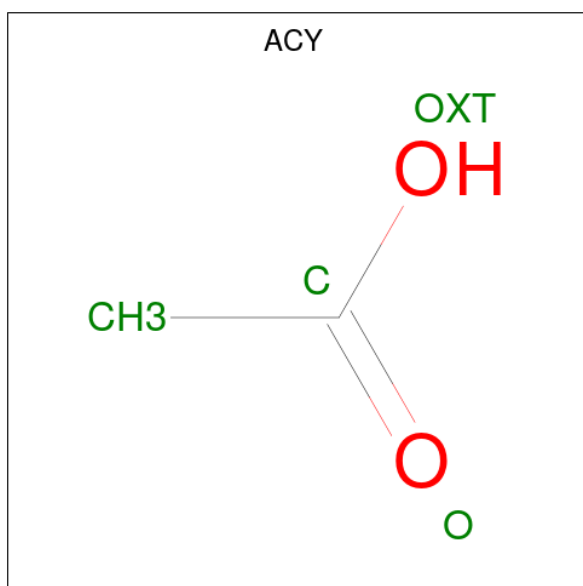
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		

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



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

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



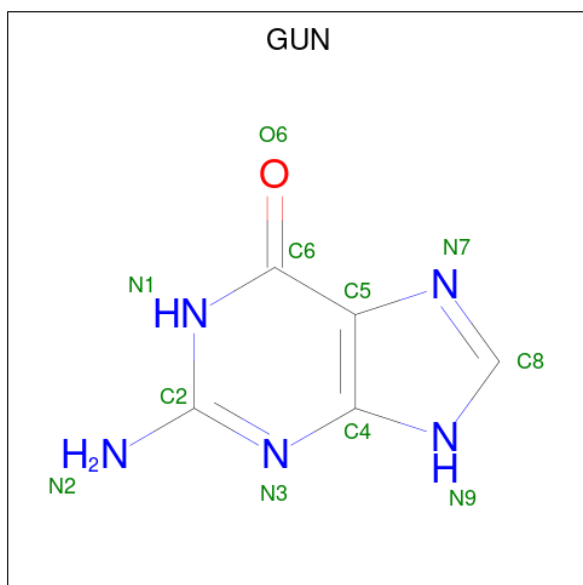
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		

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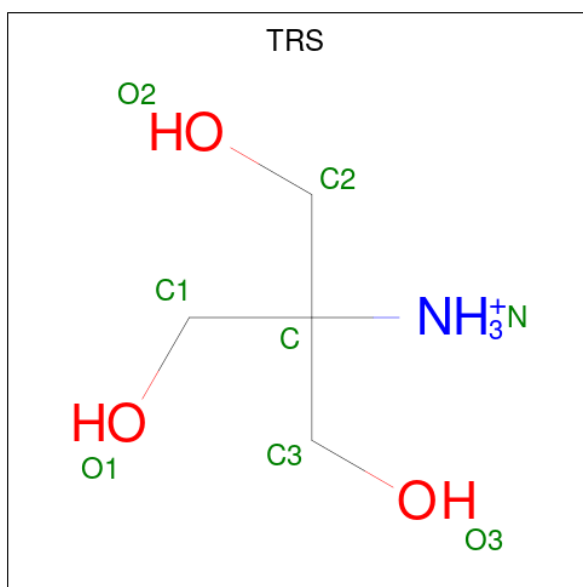
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		

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



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

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



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

- Molecule 69 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AA	507	Total	O	0	0
			507	507		
69	AC	4	Total	O	0	0
			4	4		
69	AD	3	Total	O	0	0
			3	3		
69	AE	5	Total	O	0	0
			5	5		
69	AF	1	Total	O	0	0
			1	1		
69	AG	1	Total	O	0	0
			1	1		
69	AJ	2	Total	O	0	0
			2	2		
69	AK	7	Total	O	0	0
			7	7		
69	AL	10	Total	O	0	0
			10	10		
69	AM	4	Total	O	0	0
			4	4		
69	AN	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AO	2	Total	O	0	0
			2	2		
69	AP	2	Total	O	0	0
			2	2		
69	AR	1	Total	O	0	0
			1	1		
69	AS	1	Total	O	0	0
			1	1		
69	AT	3	Total	O	0	0
			3	3		
69	AU	3	Total	O	0	0
			3	3		
69	C3	3	Total	O	0	0
			3	3		
69	C4	1	Total	O	0	0
			1	1		
69	C5	1	Total	O	0	0
			1	1		
69	BA	291	Total	O	0	0
			291	291		
69	BD	11	Total	O	0	0
			11	11		
69	BE	1	Total	O	0	0
			1	1		
69	BF	1	Total	O	0	0
			1	1		
69	BK	2	Total	O	0	0
			2	2		
69	BL	2	Total	O	0	0
			2	2		
69	BN	2	Total	O	0	0
			2	2		
69	BO	1	Total	O	0	0
			1	1		
69	BP	3	Total	O	0	0
			3	3		
69	BR	1	Total	O	0	0
			1	1		
69	BT	4	Total	O	0	0
			4	4		
69	BU	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	D1	42	Total 42	O 42	0	0
69	D2	7	Total 7	O 7	0	0
69	D3	28	Total 28	O 28	0	0
69	D4	39	Total 39	O 39	0	0
69	D5	9	Total 9	O 9	0	0
69	D0	21	Total 21	O 21	0	0
69	CB	13	Total 13	O 13	0	0
69	CC	10	Total 10	O 10	0	0
69	CD	6	Total 6	O 6	0	0
69	CA	692	Total 692	O 692	0	0
69	DB	199	Total 199	O 199	0	0
69	DC	98	Total 98	O 98	0	0
69	DD	95	Total 95	O 95	0	0
69	DA	4834	Total 4834	O 4834	0	0
69	CE	7	Total 7	O 7	0	0
69	CL	1	Total 1	O 1	0	0
69	CM	3	Total 3	O 3	0	0
69	CO	1	Total 1	O 1	0	0
69	CU	2	Total 2	O 2	0	0
69	CV	1	Total 1	O 1	0	0
69	CW	1	Total 1	O 1	0	0

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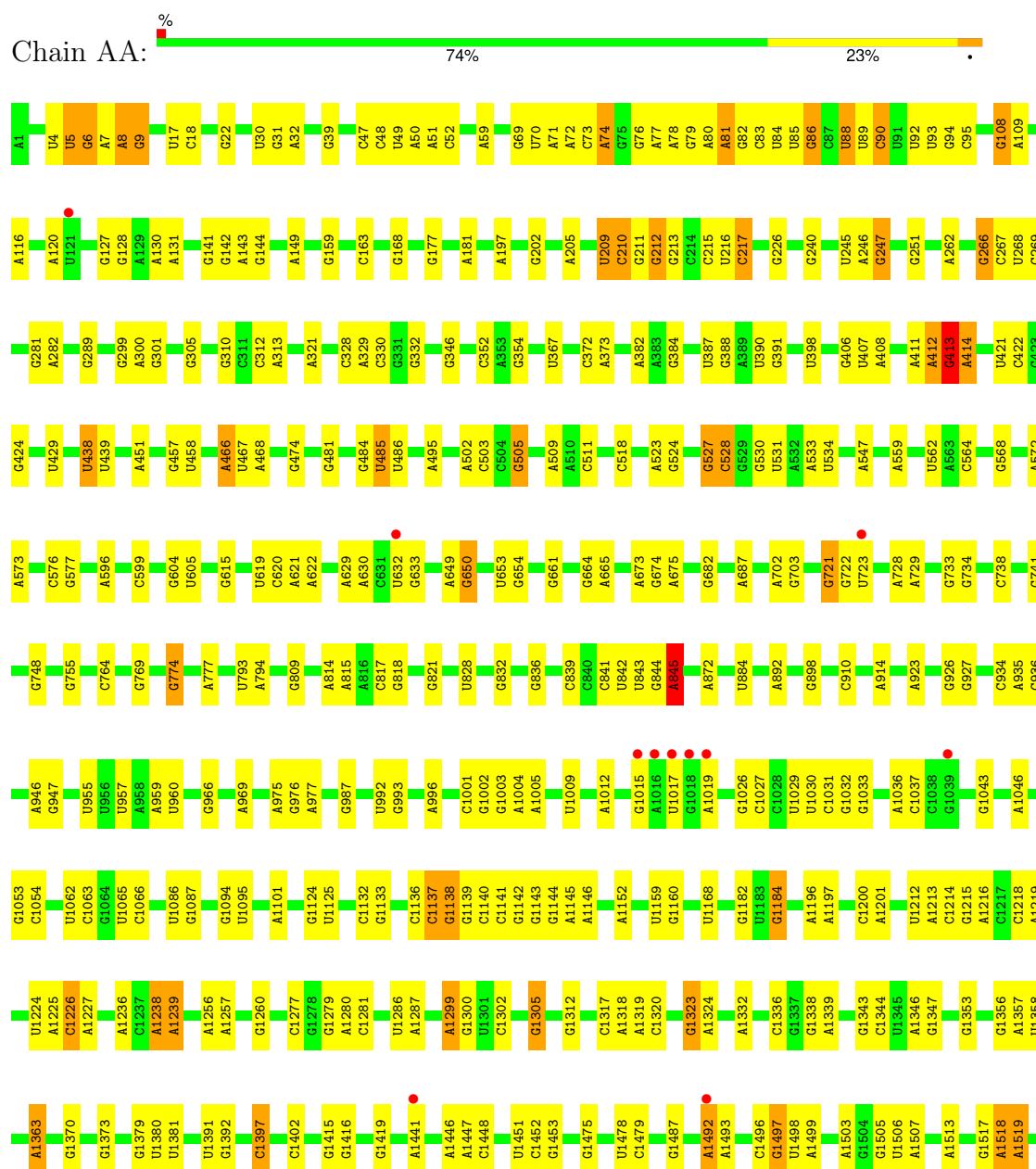
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	CY	1	Total 1	O 1	0	0
69	DE	63	Total 63	O 63	0	0
69	DF	15	Total 15	O 15	0	0
69	DG	7	Total 7	O 7	0	0
69	DH	1	Total 1	O 1	0	0
69	DK	65	Total 65	O 65	0	0
69	DL	52	Total 52	O 52	0	0
69	DM	62	Total 62	O 62	0	0
69	DN	64	Total 64	O 64	0	0
69	DO	48	Total 48	O 48	0	0
69	DP	44	Total 44	O 44	0	0
69	DQ	33	Total 33	O 33	0	0
69	DR	68	Total 68	O 68	0	0
69	DS	48	Total 48	O 48	0	0
69	DT	62	Total 62	O 62	0	0
69	DU	22	Total 22	O 22	0	0
69	DV	18	Total 18	O 18	0	0
69	DW	34	Total 34	O 34	0	0
69	DX	31	Total 31	O 31	0	0
69	DY	10	Total 10	O 10	0	0
69	DZ	5	Total 5	O 5	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.

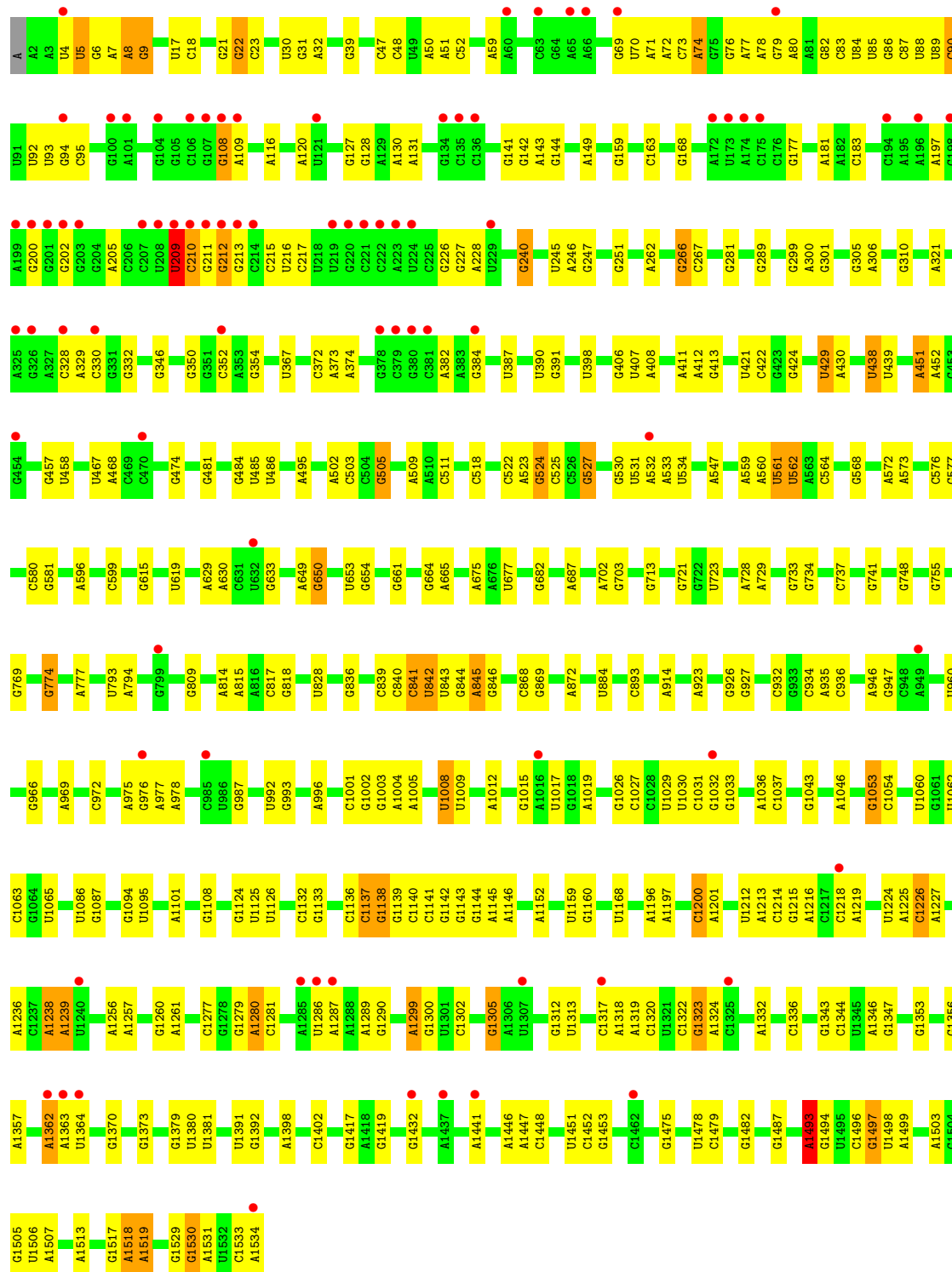
• Molecule 1: 16S rRNA



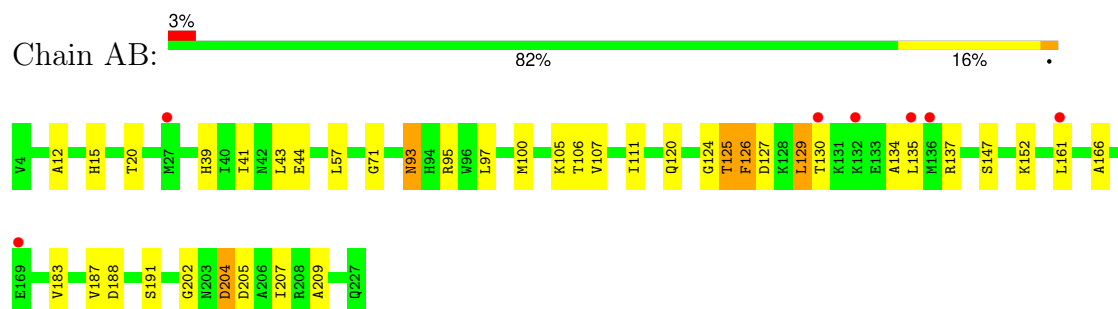
G1529
G1530
A1531
U1532
C1533
A1534

• Molecule 1: 16S rRNA

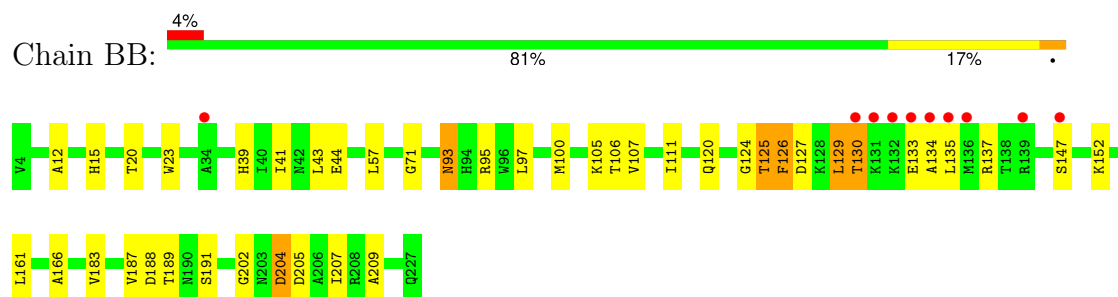
Chain BA:  5% 74% 23%



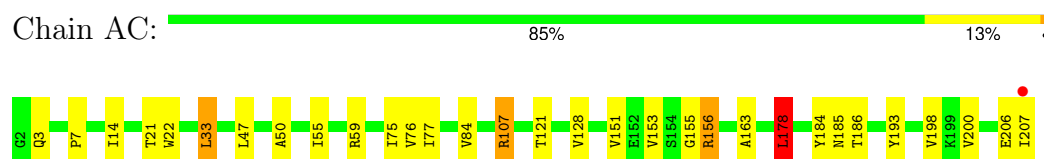
- Molecule 2: 30S ribosomal protein S2



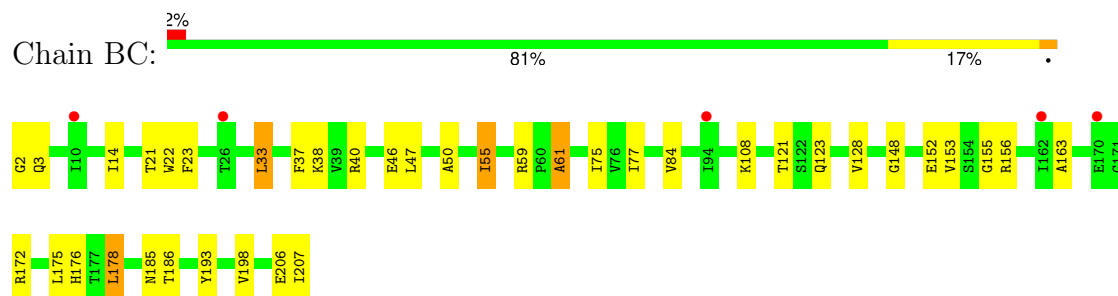
- Molecule 2: 30S ribosomal protein S2



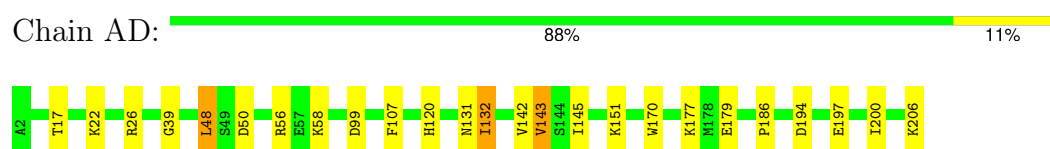
- Molecule 3: 30S ribosomal protein S3



- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4

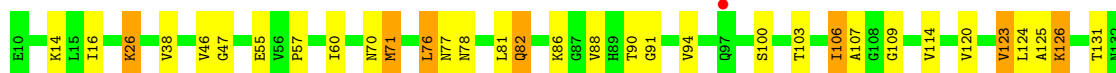
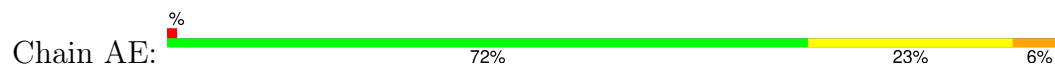


- Molecule 4: 30S ribosomal protein S4

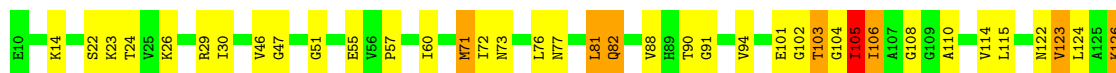




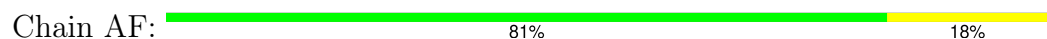
- Molecule 5: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S5



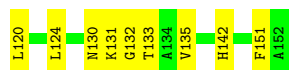
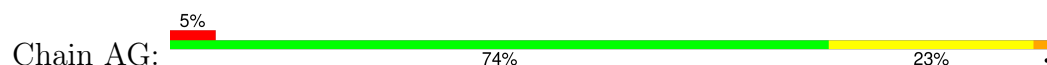
- Molecule 6: 30S ribosomal protein S6



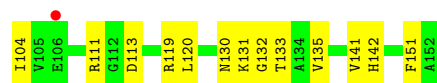
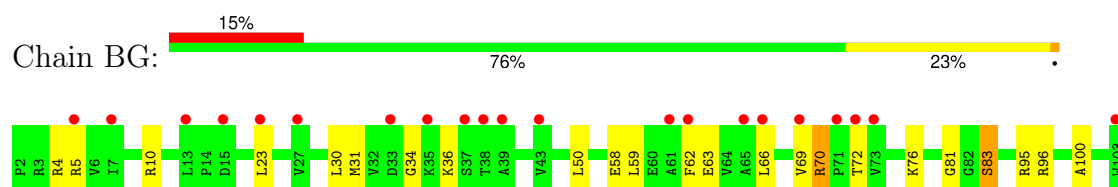
- Molecule 6: 30S ribosomal protein S6



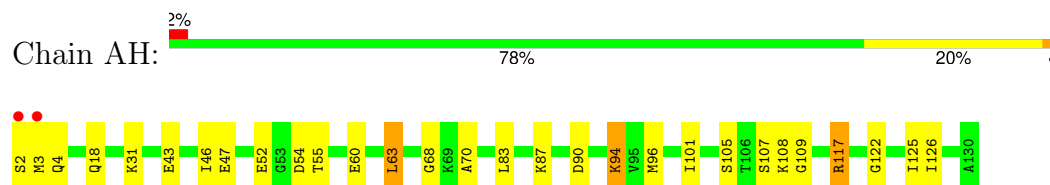
- Molecule 7: 30S ribosomal protein S7



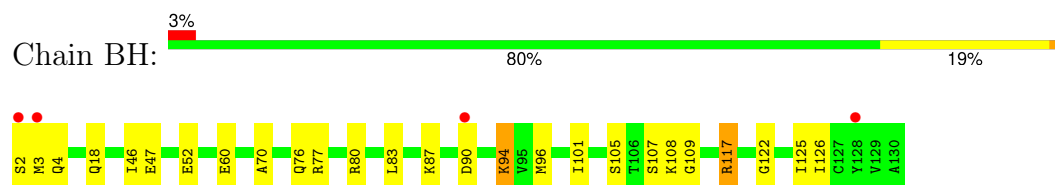
- Molecule 7: 30S ribosomal protein S7



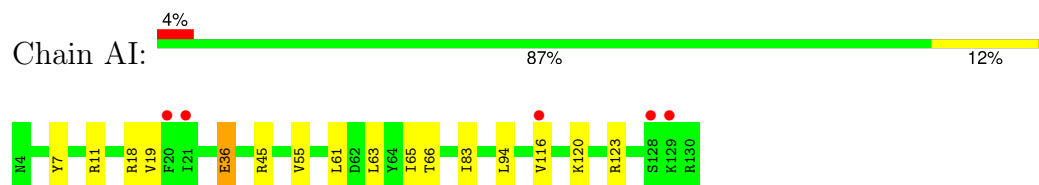
- Molecule 8: 30S ribosomal protein S8



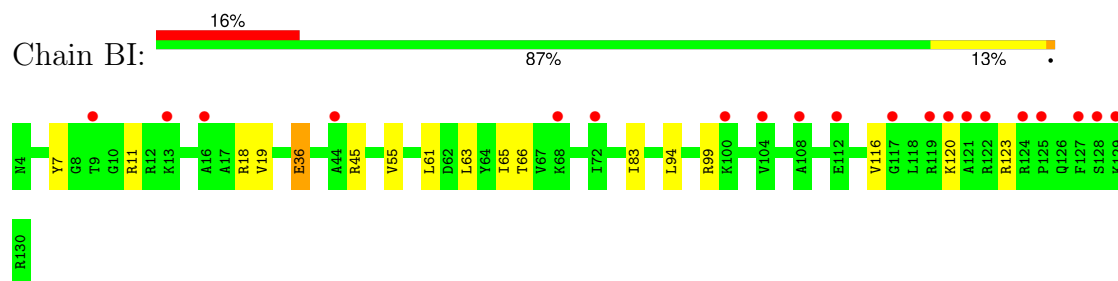
- Molecule 8: 30S ribosomal protein S8



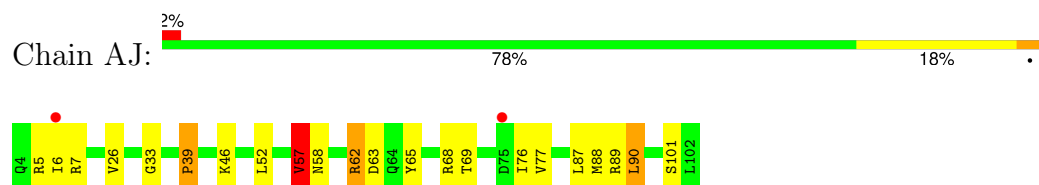
- Molecule 9: 30S ribosomal protein S9



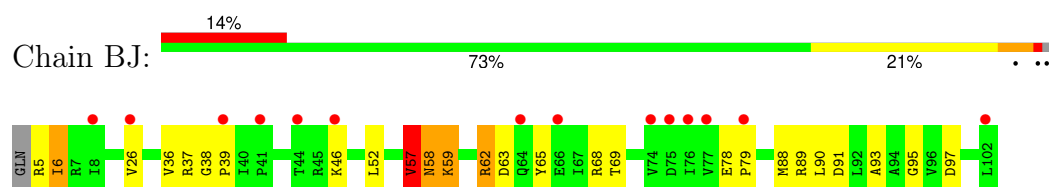
- Molecule 9: 30S ribosomal protein S9



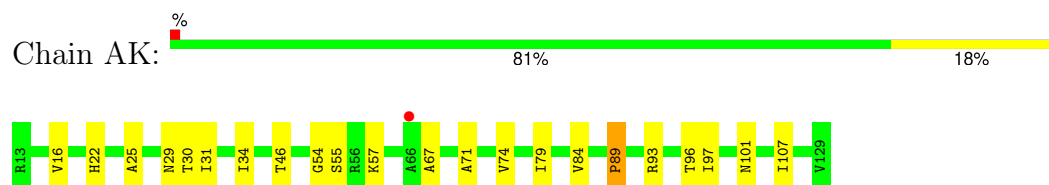
- Molecule 10: 30S ribosomal protein S10



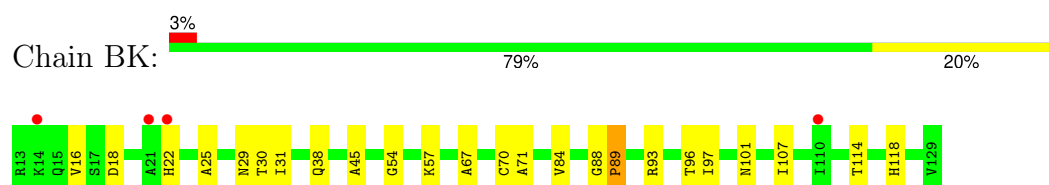
- Molecule 10: 30S ribosomal protein S10



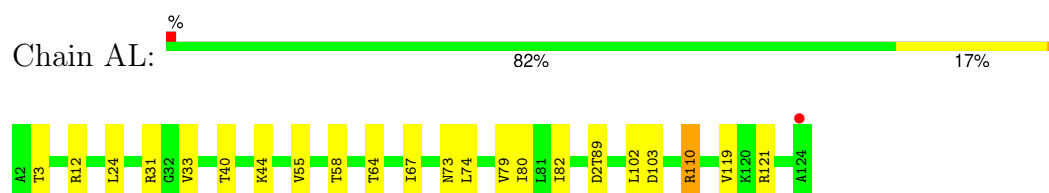
- Molecule 11: 30S ribosomal protein S11



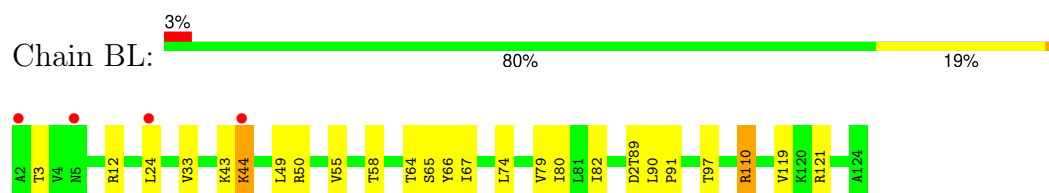
- Molecule 11: 30S ribosomal protein S11



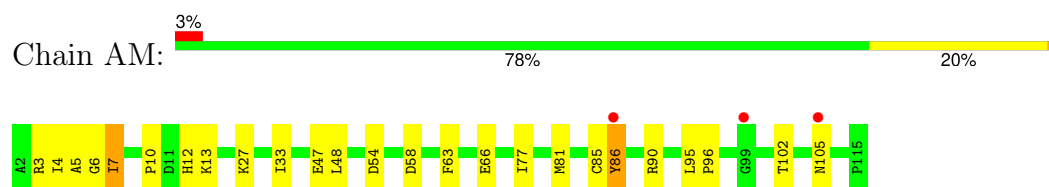
- Molecule 12: 30S ribosomal protein S12



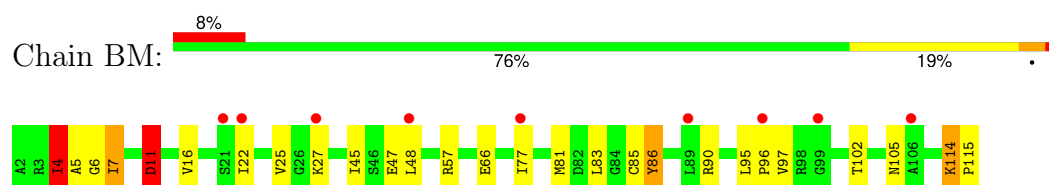
- Molecule 12: 30S ribosomal protein S12



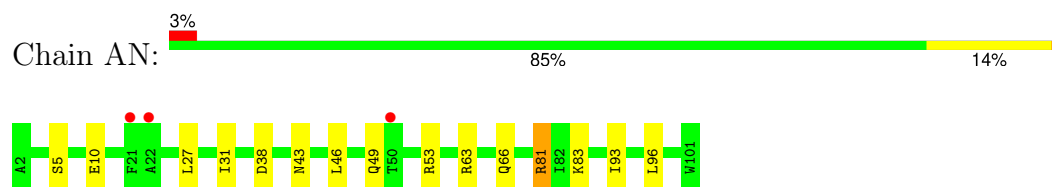
- Molecule 13: 30S ribosomal protein S13



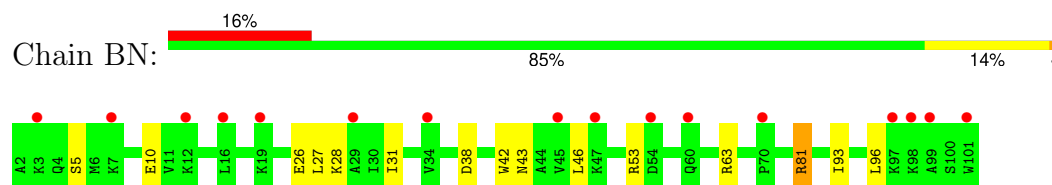
- Molecule 13: 30S ribosomal protein S13



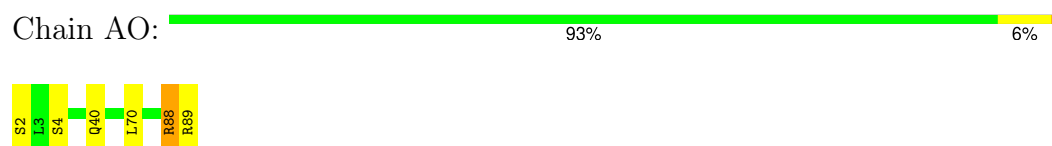
- Molecule 14: 30S ribosomal protein S14



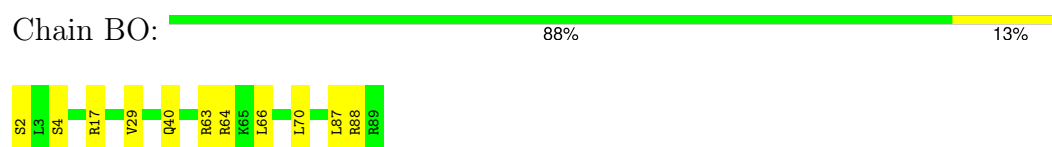
- Molecule 14: 30S ribosomal protein S14



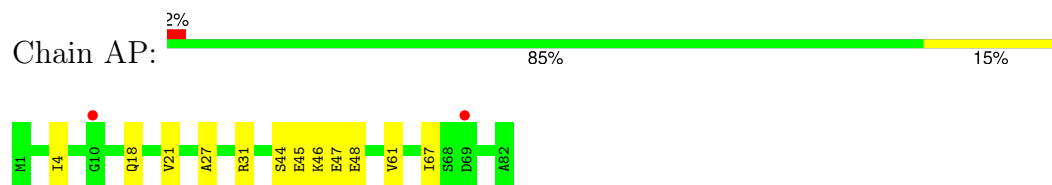
- Molecule 15: 30S ribosomal protein S15



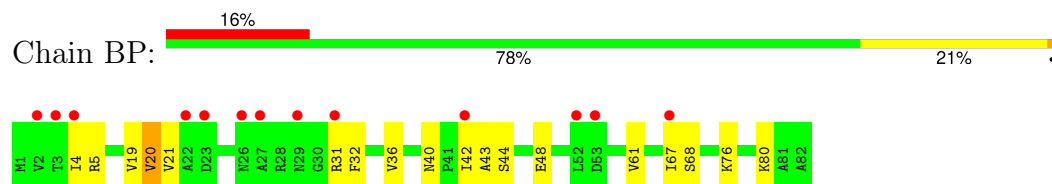
- Molecule 15: 30S ribosomal protein S15



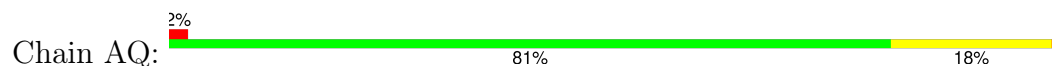
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16

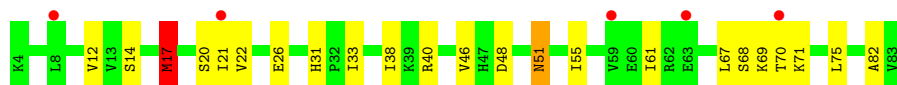
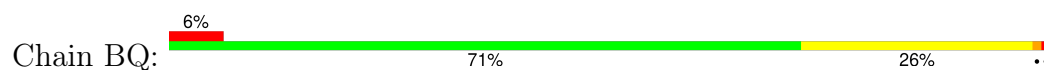


- Molecule 17: 30S ribosomal protein S17





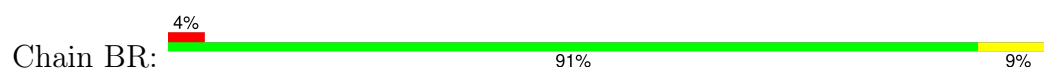
- Molecule 17: 30S ribosomal protein S17



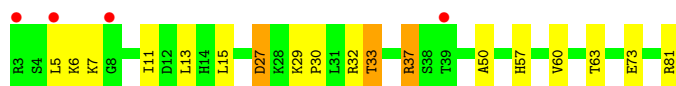
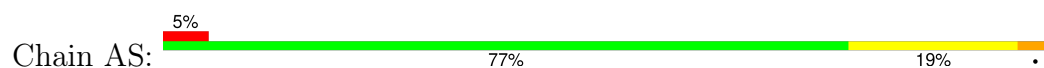
- Molecule 18: 30S ribosomal protein S18



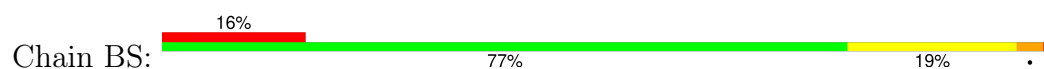
- Molecule 18: 30S ribosomal protein S18



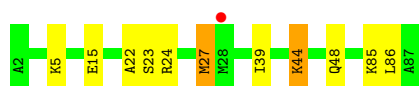
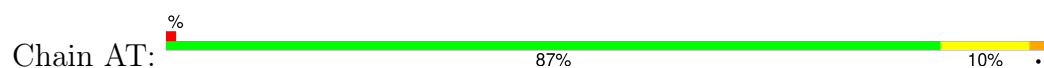
- Molecule 19: 30S ribosomal protein S19



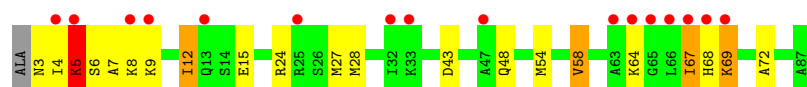
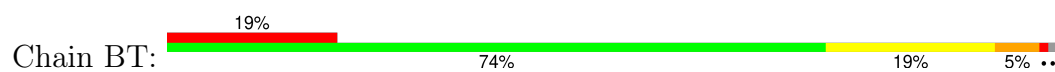
- Molecule 19: 30S ribosomal protein S19



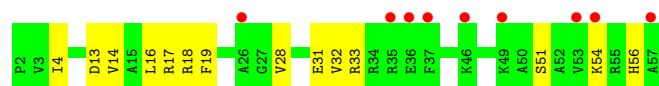
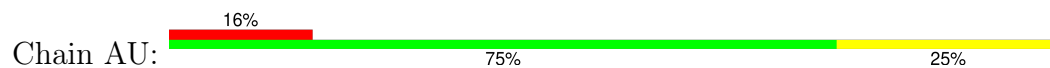
- Molecule 20: 30S ribosomal protein S20



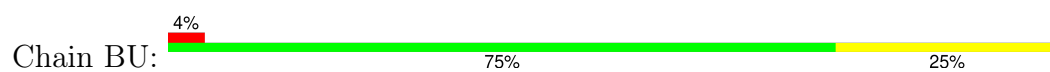
- Molecule 20: 30S ribosomal protein S20



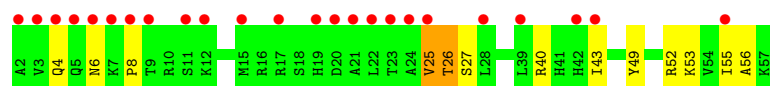
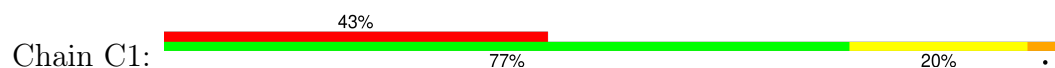
- Molecule 21: 30S ribosomal protein S21



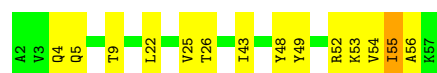
- Molecule 21: 30S ribosomal protein S21



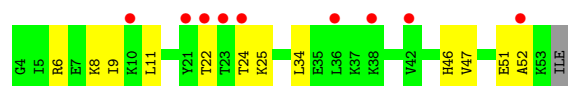
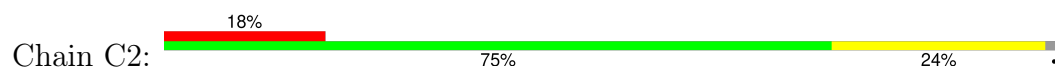
- Molecule 22: 50S ribosomal protein L32



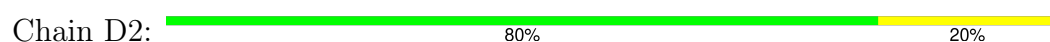
- Molecule 22: 50S ribosomal protein L32



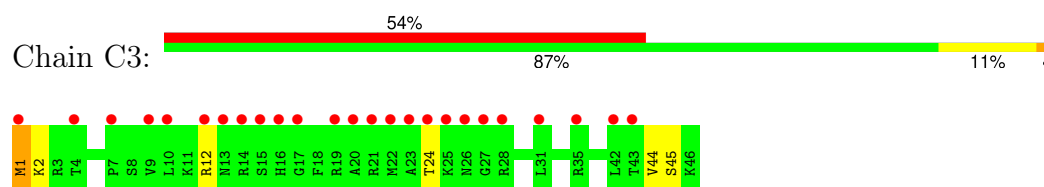
- Molecule 23: 50S ribosomal protein L33



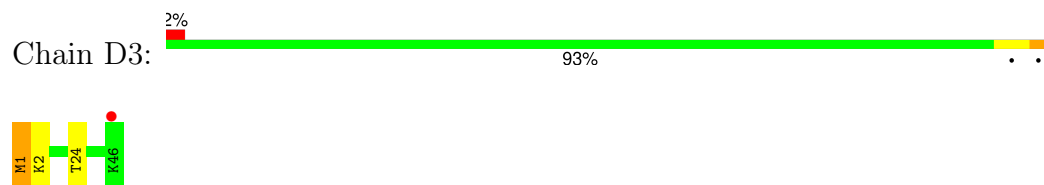
- Molecule 23: 50S ribosomal protein L33



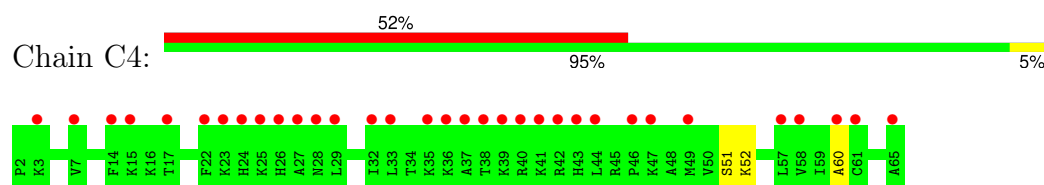
- Molecule 24: 50S ribosomal protein L34



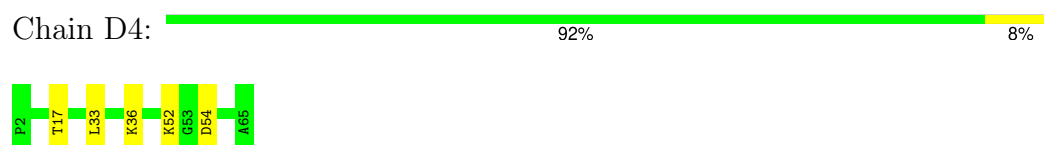
- Molecule 24: 50S ribosomal protein L34



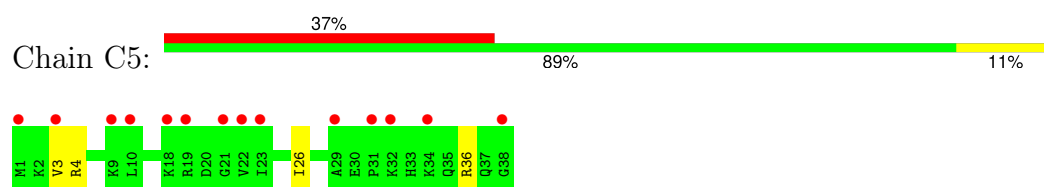
- Molecule 25: 50S ribosomal protein L35



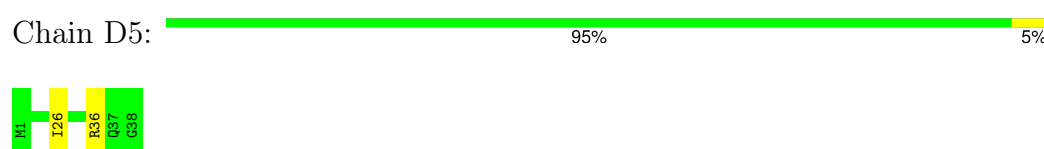
- Molecule 25: 50S ribosomal protein L35



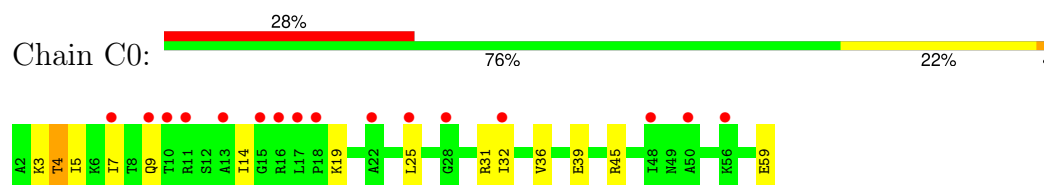
- Molecule 26: 50S ribosomal protein L36



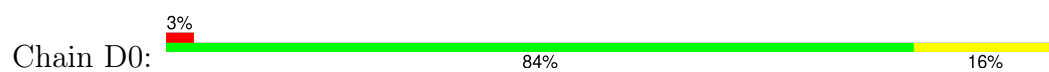
- Molecule 26: 50S ribosomal protein L36



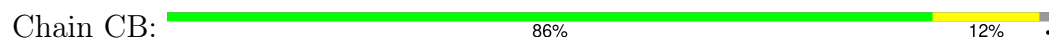
- Molecule 27: 50S ribosomal protein L30



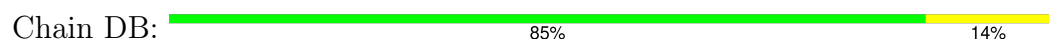
- Molecule 27: 50S ribosomal protein L30



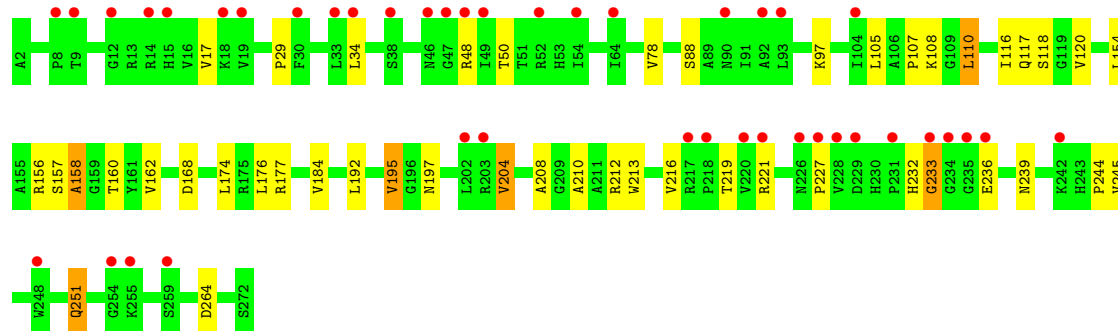
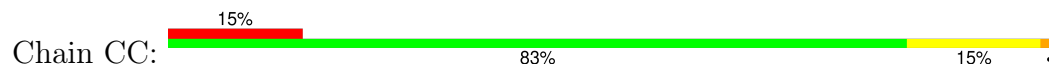
- Molecule 28: 5S rRNA



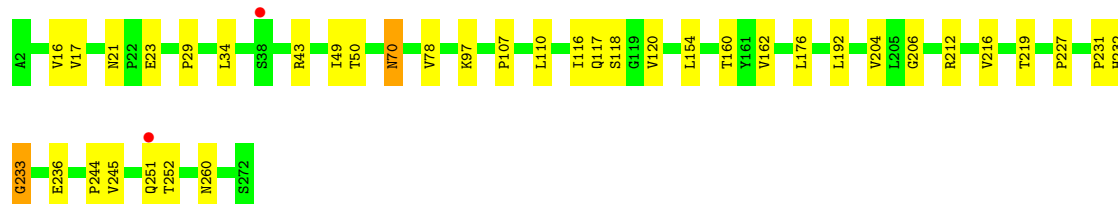
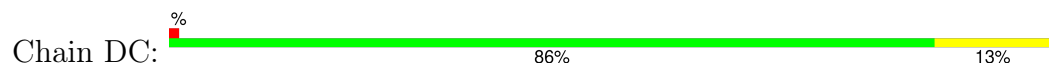
- Molecule 28: 5S rRNA



- Molecule 29: 50S ribosomal protein L2

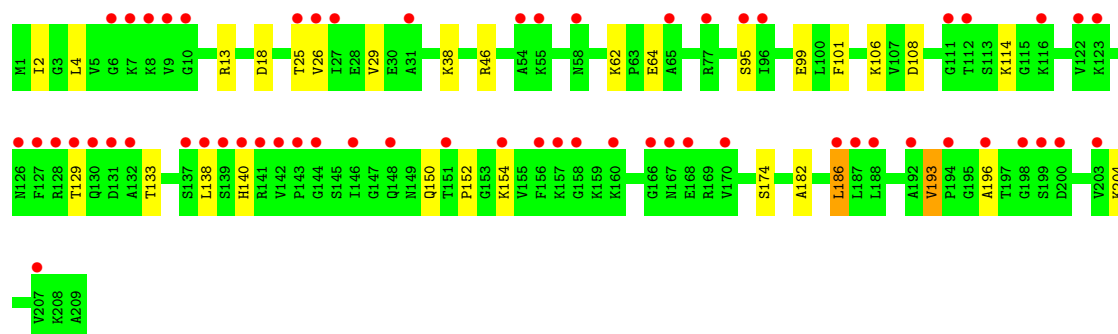


- Molecule 29: 50S ribosomal protein L2

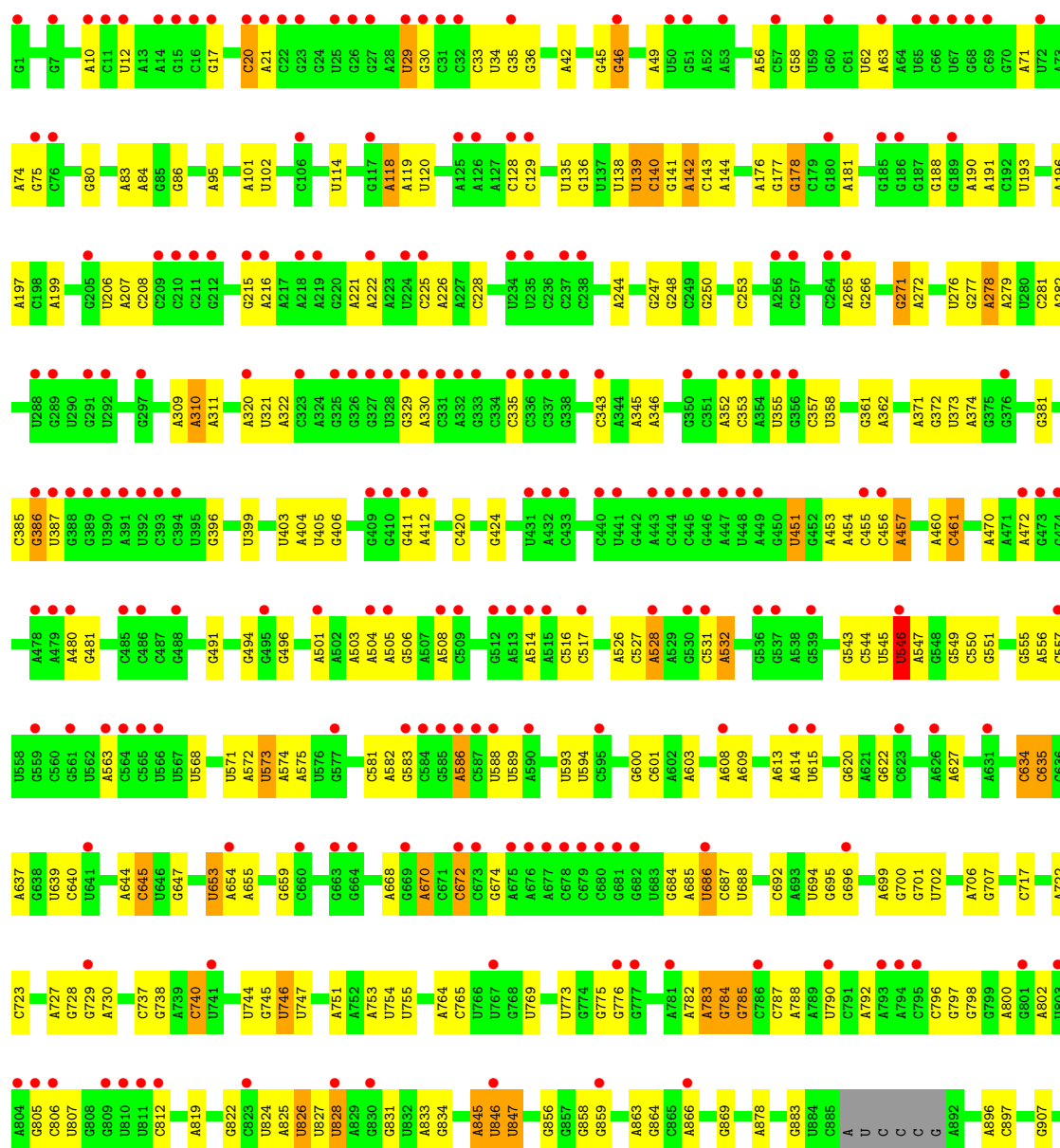


- Molecule 30: 50S ribosomal protein L3

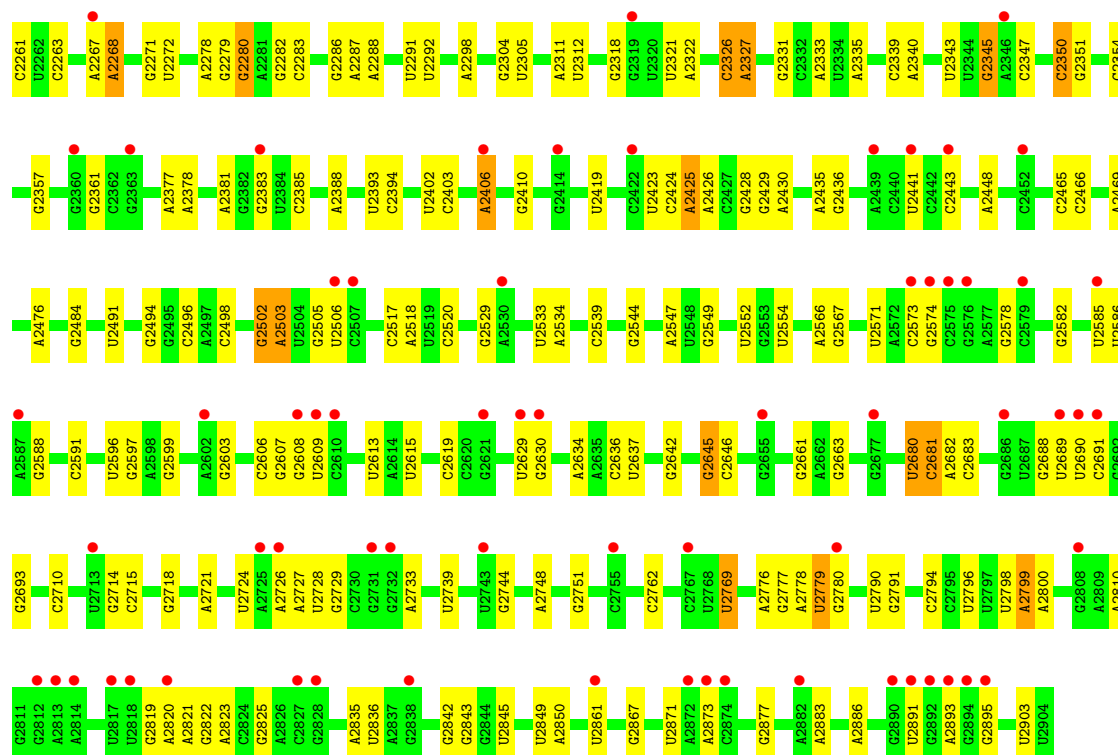




• Molecule 31: 23S rRNA







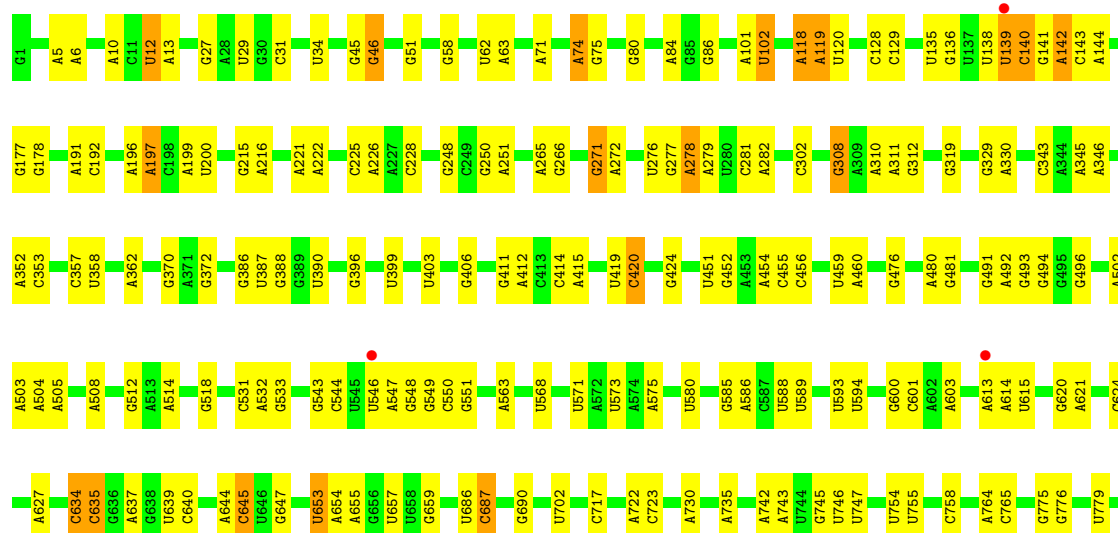
• Molecule 32: 50S ribosomal protein L3

Chain DD: 87% 11%

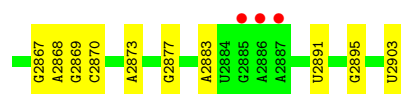


• Molecule 33: 23S rRNA

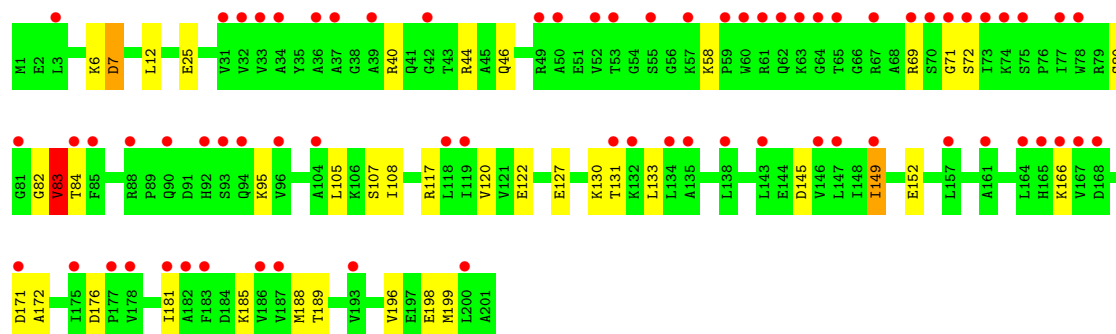
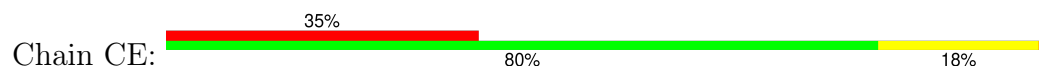
Chain DA: 2% 75% 22%



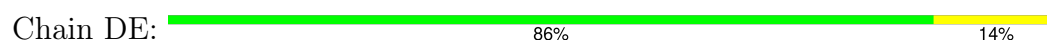




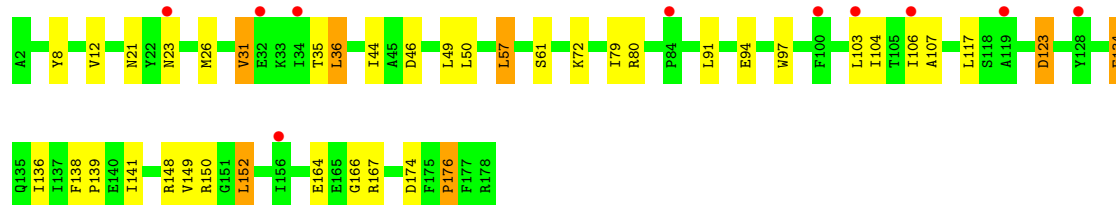
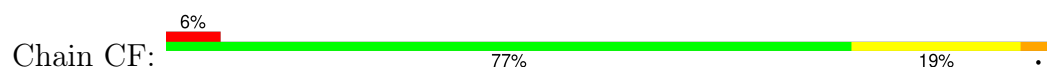
- Molecule 34: 50S ribosomal protein L4



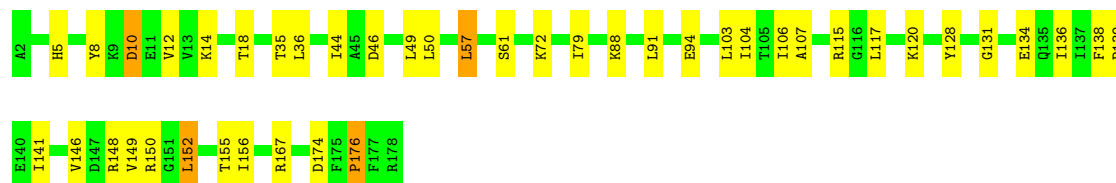
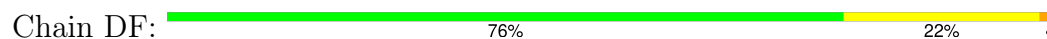
- Molecule 34: 50S ribosomal protein L4



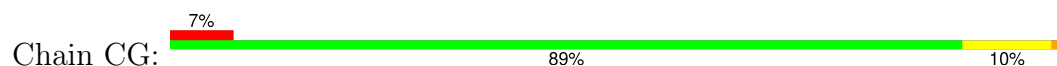
- Molecule 35: 50S ribosomal protein L5



- Molecule 35: 50S ribosomal protein L5

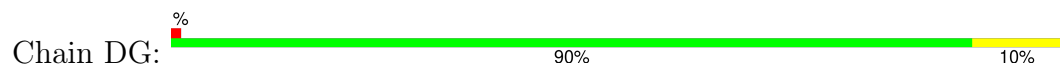


- Molecule 36: 50S ribosomal protein L6

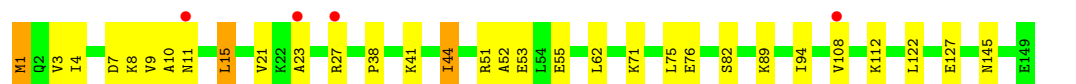
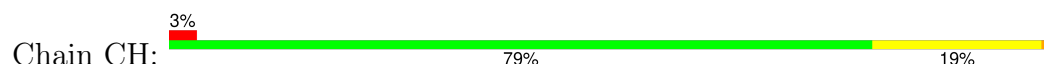




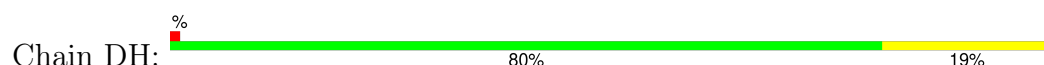
- Molecule 36: 50S ribosomal protein L6



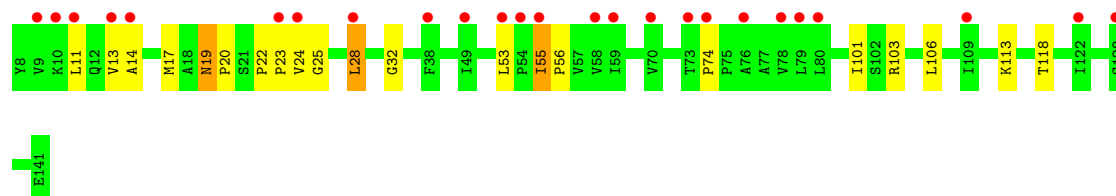
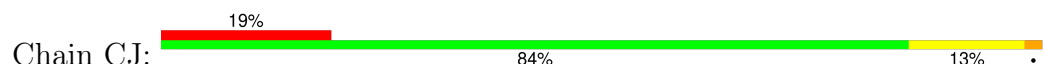
- Molecule 37: 50S ribosomal protein L9



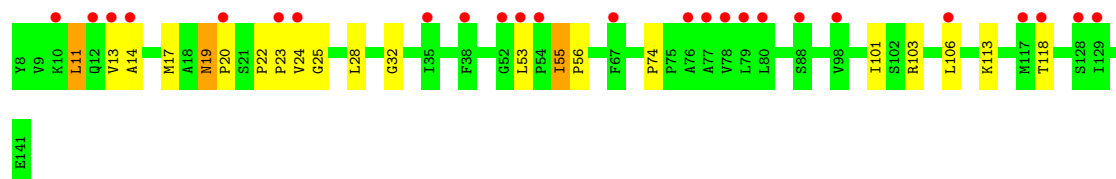
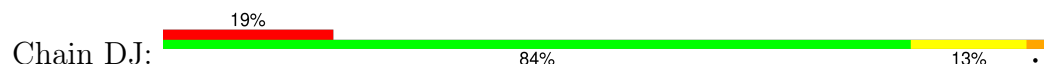
- Molecule 37: 50S ribosomal protein L9



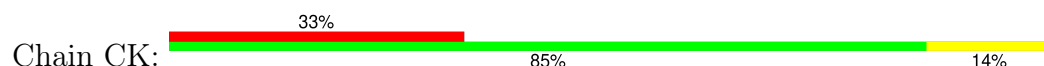
- Molecule 38: 50S ribosomal protein L11

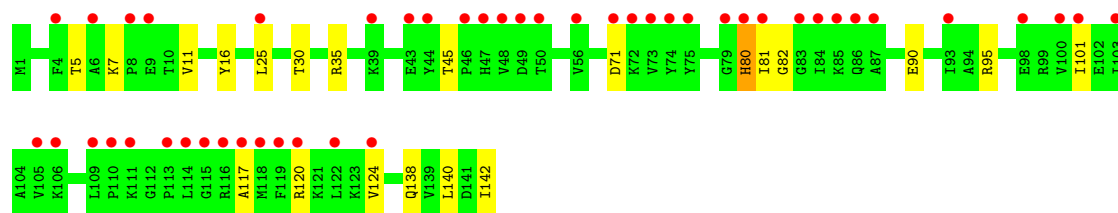


- Molecule 38: 50S ribosomal protein L11



- Molecule 39: 50S ribosomal protein L13





- Molecule 39: 50S ribosomal protein L13

Chain DK: 91% 9%



- Molecule 40: 50S ribosomal protein L14

Chain CL: 8% 80% 17% ...



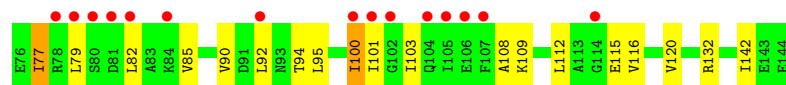
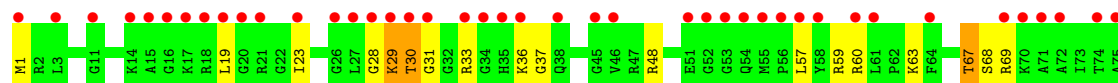
- Molecule 40: 50S ribosomal protein L14

Chain DL: 81% 17% .



- Molecule 41: 50S ribosomal protein L15

Chain CM: 40% 74% 22% .



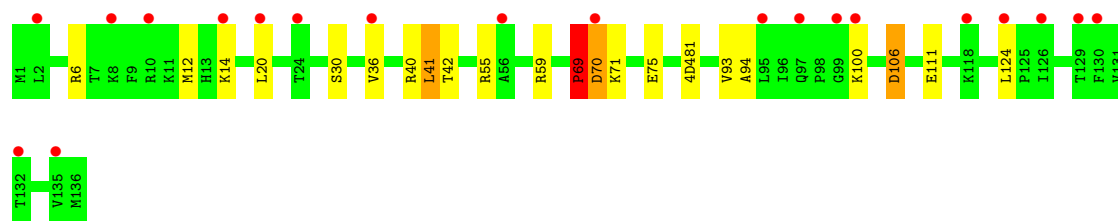
- Molecule 41: 50S ribosomal protein L15

Chain DM: 88% 12% .



- Molecule 42: 50S ribosomal protein L16

Chain CN: 15% 84% 13% ..



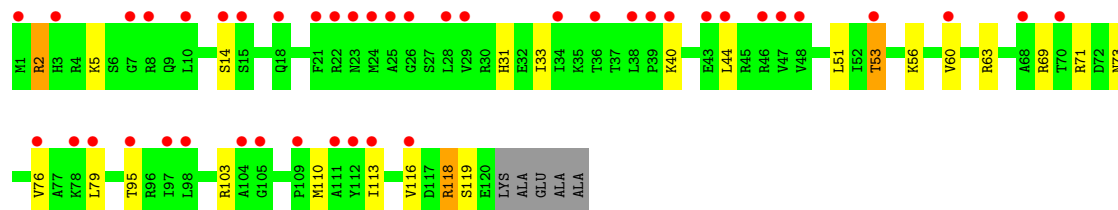
- Molecule 42: 50S ribosomal protein L16

Chain DN: 87% 12%



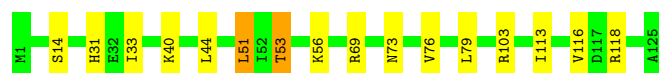
- Molecule 43: 50S ribosomal protein L17

Chain CO: 34% 77% 17%



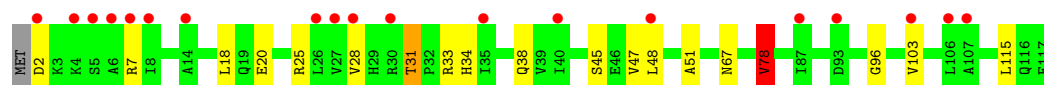
- Molecule 43: 50S ribosomal protein L17

Chain DO: 87% 11%



- Molecule 44: 50S ribosomal protein L18

Chain CP: 16% 83% 15%



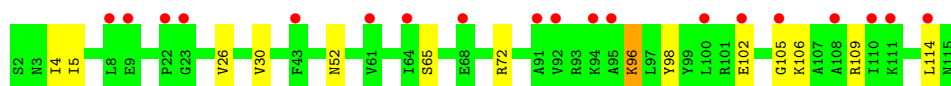
- Molecule 44: 50S ribosomal protein L18

Chain DP: 86% 11%



- Molecule 45: 50S ribosomal protein L19

Chain CQ: 17% 88% 11%



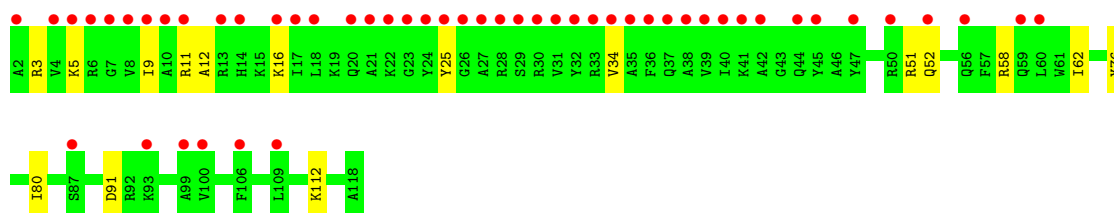
- Molecule 45: 50S ribosomal protein L19

Chain DQ: 88% 11% .



- Molecule 46: 50S ribosomal protein L20

Chain CR: 44% 86% 14% .



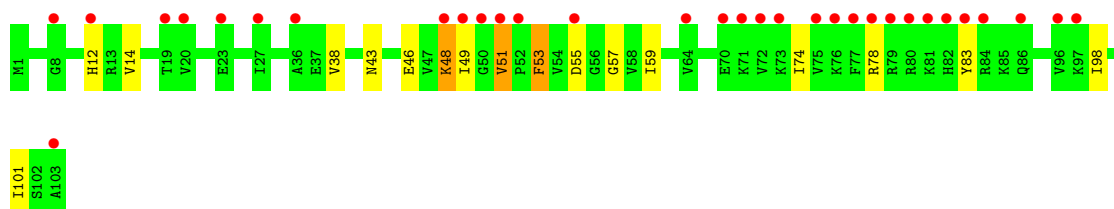
- Molecule 46: 50S ribosomal protein L20

Chain DR: 88% 11% .



- Molecule 47: 50S ribosomal protein L21

Chain CS: 31% 83% 14% .



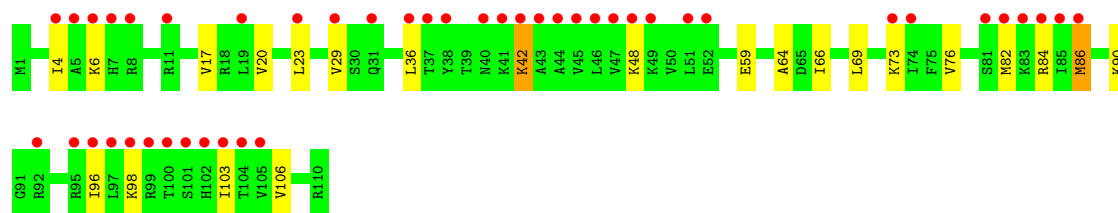
- Molecule 47: 50S ribosomal protein L21

Chain DS: 87% 12% .



- Molecule 48: 50S ribosomal protein L22

Chain CT: 41% 79% 19% .



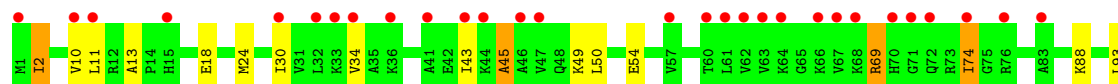
- Molecule 48: 50S ribosomal protein L22

Chain DT: 79% 21%



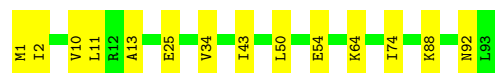
- Molecule 49: 50S ribosomal protein L23

Chain CU: 31% 82% 14%



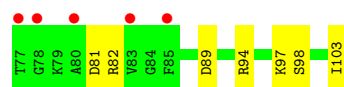
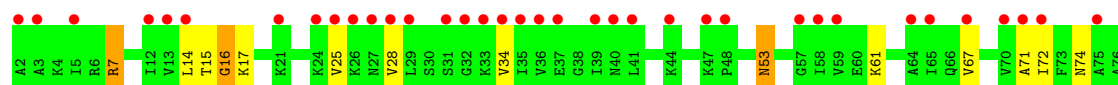
- Molecule 49: 50S ribosomal protein L23

Chain DU: 85% 15%



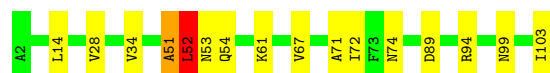
- Molecule 50: 50S ribosomal protein L24

Chain CV: 40% 79% 18%



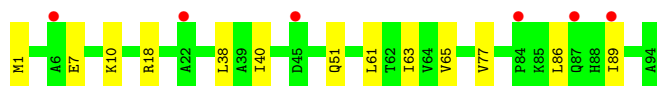
- Molecule 50: 50S ribosomal protein L24

Chain DV: 84% 14%

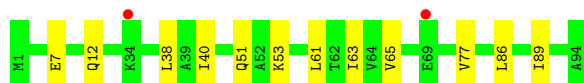
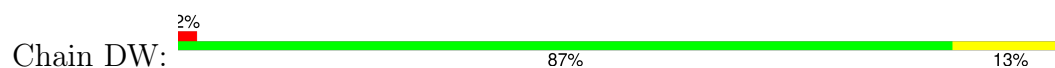


- Molecule 51: 50S ribosomal protein L25

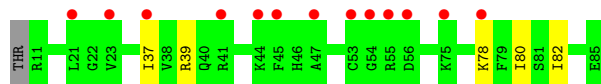
Chain CW: 6% 86% 14%



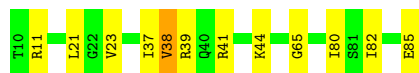
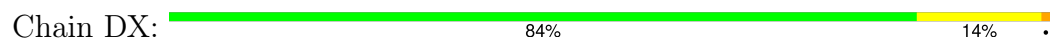
- Molecule 51: 50S ribosomal protein L25



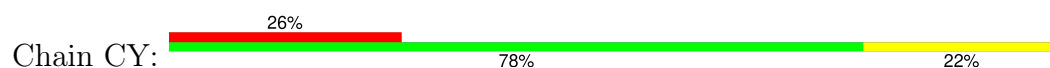
- Molecule 52: 50S ribosomal protein L27



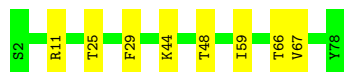
- Molecule 52: 50S ribosomal protein L27



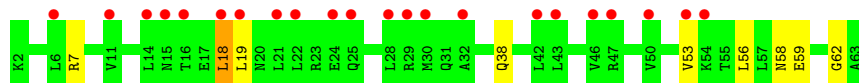
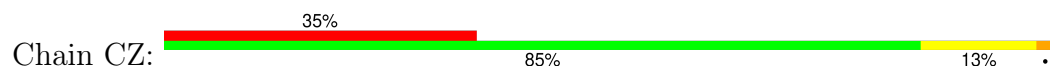
- Molecule 53: 50S ribosomal protein L28



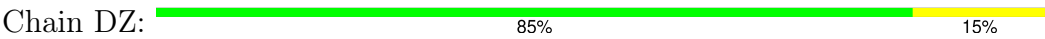
- Molecule 53: 50S ribosomal protein L28



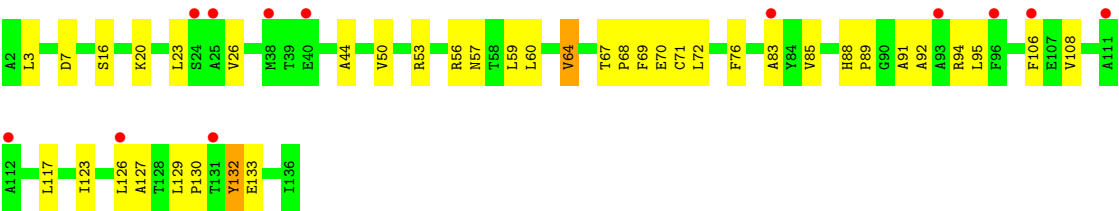
- Molecule 54: 50S ribosomal protein L29



- Molecule 54: 50S ribosomal protein L29



● Molecule 55: 50S ribosomal protein L10



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.92Å 434.36Å 623.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.19 – 3.12 47.19 – 3.12	Depositor EDS
% Data completeness (in resolution range)	82.3 (47.19-3.12) 82.3 (47.19-3.12)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	22.94 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.190 , 0.220 0.207 , 0.240	Depositor DCC
R_{free} test set	3316 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 100.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	295125	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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: 2MA, UR3, PSU, H2U, 4OC, OMG, EDO, 5MU, 4D4, PG4, 1MG, ZN, 6MZ, TRS, 3TD, PGE, 5MC, ACY, MEQ, OMC, D2T, SPD, PUT, PEG, GUN, MA6, 1PE, 2MG, G7M, MG, MPD, OMU

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	0.68	9/36593 (0.0%)	0.66	1/57081 (0.0%)
1	BA	0.68	9/36568 (0.0%)	0.66	1/57042 (0.0%)
2	AB	0.80	0/1784	1.38	5/2403 (0.2%)
2	BB	0.79	0/1784	1.38	5/2403 (0.2%)
3	AC	0.77	0/1652	1.28	4/2225 (0.2%)
3	BC	0.77	0/1652	1.29	6/2225 (0.3%)
4	AD	0.72	0/1665	1.36	5/2227 (0.2%)
4	BD	0.71	0/1665	1.36	5/2227 (0.2%)
5	AE	0.78	0/1157	1.35	10/1557 (0.6%)
5	BE	0.77	0/1118	1.36	5/1504 (0.3%)
6	AF	0.75	0/881	1.27	4/1189 (0.3%)
6	BF	0.79	0/835	1.40	10/1128 (0.9%)
7	AG	0.77	0/1196	1.38	3/1602 (0.2%)
7	BG	0.78	0/1196	1.37	3/1602 (0.2%)
8	AH	0.72	0/989	1.33	3/1326 (0.2%)
8	BH	0.73	0/989	1.32	3/1326 (0.2%)
9	AI	0.75	0/1034	1.29	0/1375
9	BI	0.74	0/1034	1.28	2/1375 (0.1%)
10	AJ	0.77	1/806 (0.1%)	1.26	2/1089 (0.2%)
10	BJ	0.86	1/797 (0.1%)	1.30	4/1077 (0.4%)
11	AK	0.75	0/893	1.24	2/1205 (0.2%)
11	BK	0.74	0/893	1.27	3/1205 (0.2%)
12	AL	0.73	0/960	1.22	2/1286 (0.2%)
12	BL	0.72	0/960	1.23	1/1286 (0.1%)
13	AM	0.84	0/893	1.50	5/1193 (0.4%)
13	BM	0.86	0/893	1.52	9/1193 (0.8%)
14	AN	0.79	0/817	1.34	0/1088
14	BN	0.76	0/817	1.33	0/1088
15	AO	0.73	0/722	1.47	1/964 (0.1%)
15	BO	0.73	0/722	1.51	0/964
16	AP	0.81	0/659	1.32	4/884 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BP	0.83	0/659	1.41	3/884 (0.3%)
17	AQ	0.77	0/658	1.22	2/881 (0.2%)
17	BQ	0.83	0/658	1.30	2/881 (0.2%)
18	AR	0.81	0/463	1.40	4/621 (0.6%)
18	BR	0.82	0/463	1.36	3/621 (0.5%)
19	AS	0.82	0/653	1.21	1/877 (0.1%)
19	BS	0.82	0/653	1.19	0/877
20	AT	0.74	0/676	1.55	4/895 (0.4%)
20	BT	0.82	0/671	1.61	2/888 (0.2%)
21	AU	0.75	0/472	1.36	2/627 (0.3%)
21	BU	0.72	0/472	1.35	2/627 (0.3%)
22	C1	0.81	0/450	1.31	2/599 (0.3%)
22	D1	0.79	0/450	1.33	0/599
23	C2	0.85	0/416	1.32	0/554
23	D2	0.82	0/421	1.28	0/561
24	C3	0.79	0/380	1.50	0/498
24	D3	0.86	0/380	1.53	0/498
25	C4	0.75	0/513	1.30	0/676
25	D4	0.82	0/513	1.33	2/676 (0.3%)
26	C5	0.77	0/303	1.13	0/397
26	D5	0.82	0/303	1.15	0/397
27	C0	0.90	0/453	1.38	0/605
27	D0	0.86	0/467	1.31	0/623
28	CB	0.68	0/2828	0.66	0/4410
28	DB	0.73	1/2872 (0.0%)	0.68	0/4478
29	CC	0.73	0/2122	1.28	6/2852 (0.2%)
29	DC	0.74	0/2122	1.25	4/2852 (0.1%)
30	CD	0.76	1/1586 (0.1%)	1.22	4/2134 (0.2%)
31	CA	0.71	53/69165 (0.1%)	0.67	5/107896 (0.0%)
32	DD	0.80	0/1576	1.22	5/2119 (0.2%)
33	DA	0.73	20/69364 (0.0%)	0.71	2/108207 (0.0%)
34	CE	0.77	0/1571	1.36	4/2113 (0.2%)
34	DE	0.78	0/1571	1.31	4/2113 (0.2%)
35	CF	0.74	0/1435	1.34	11/1926 (0.6%)
35	DF	0.75	0/1435	1.32	7/1926 (0.4%)
36	CG	0.75	0/1343	1.28	6/1816 (0.3%)
36	DG	0.73	0/1343	1.24	4/1816 (0.2%)
37	CH	0.83	0/1121	1.36	4/1515 (0.3%)
37	DH	0.83	0/1121	1.36	4/1515 (0.3%)
38	CJ	0.96	0/993	1.35	3/1341 (0.2%)
38	DJ	0.96	0/993	1.35	3/1341 (0.2%)
39	CK	0.69	0/1152	1.33	3/1551 (0.2%)
39	DK	0.78	0/1152	1.31	3/1551 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
40	CL	0.82	0/947	1.18	1/1268 (0.1%)
40	DL	0.83	0/955	1.17	1/1279 (0.1%)
41	CM	0.78	1/1062 (0.1%)	1.37	12/1413 (0.8%)
41	DM	0.74	0/1062	1.30	5/1413 (0.4%)
42	CN	0.74	1/1081 (0.1%)	1.29	6/1443 (0.4%)
42	DN	0.78	0/1092	1.28	2/1457 (0.1%)
43	CO	0.75	0/973	1.31	0/1301
43	DO	0.81	0/1006	1.34	0/1345
44	CP	0.74	0/902	1.44	5/1209 (0.4%)
44	DP	0.75	0/910	1.42	2/1219 (0.2%)
45	CQ	0.72	0/929	1.17	0/1242
45	DQ	0.74	0/929	1.14	0/1242
46	CR	0.76	0/960	1.43	3/1278 (0.2%)
46	DR	0.85	0/960	1.40	1/1278 (0.1%)
47	CS	0.76	0/829	1.17	2/1107 (0.2%)
47	DS	0.79	0/829	1.19	0/1107
48	CT	0.76	0/864	1.37	1/1156 (0.1%)
48	DT	0.80	0/864	1.35	3/1156 (0.3%)
49	CU	0.79	0/745	1.30	3/994 (0.3%)
49	DU	0.77	0/745	1.30	5/994 (0.5%)
50	CV	0.85	0/788	1.31	4/1051 (0.4%)
50	DV	0.78	0/788	1.27	4/1051 (0.4%)
51	CW	0.73	0/766	1.23	0/1025
51	DW	0.79	0/766	1.24	0/1025
52	CX	0.70	0/576	1.16	0/762
52	DX	0.75	0/598	1.17	1/790 (0.1%)
53	CY	0.66	0/635	1.35	1/848 (0.1%)
53	DY	0.72	0/635	1.33	0/848
54	CZ	0.73	0/502	1.53	0/667
54	DZ	0.73	0/502	1.52	0/667
55	DI	0.89	0/1037	1.46	8/1402 (0.6%)
All	All	0.73	97/309273 (0.0%)	0.90	289/462210 (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
1	AA	0	1
33	DA	0	15
42	CN	0	1
All	All	0	17

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2095	A	O5'-C5'	-8.52	1.29	1.42
33	DA	2585	U	C1'-N1	7.86	1.59	1.47
31	CA	769	U	C1'-N1	7.59	1.59	1.48
1	BA	5	U	C1'-N1	7.59	1.59	1.48
33	DA	2097	A	O5'-C5'	-7.29	1.31	1.42
33	DA	12	U	C1'-N1	7.07	1.59	1.48
31	CA	1788	C	C1'-N1	7.01	1.58	1.48
31	CA	1825	U	C1'-N1	6.78	1.58	1.48
1	AA	5	U	C1'-N1	6.66	1.58	1.48
33	DA	140	C	C1'-N1	6.61	1.57	1.47
33	DA	790	U	C1'-N1	6.49	1.57	1.47
1	BA	1493	A	C3'-O3'	6.40	1.51	1.42
31	CA	1658	C	C1'-N1	6.39	1.58	1.48
31	CA	1777	U	C1'-N1	6.37	1.57	1.48
1	BA	1008	U	O5'-C5'	-6.33	1.32	1.42
31	CA	1656	C	C1'-N1	6.29	1.57	1.48
31	CA	995	C	O5'-C5'	-6.28	1.33	1.42
1	BA	209	U	C1'-N1	6.24	1.57	1.48
31	CA	1994	C	C1'-N1	6.19	1.57	1.48
31	CA	2225	A	C3'-O3'	6.15	1.52	1.43
31	CA	12	U	C1'-N1	6.15	1.57	1.48
31	CA	2586	U	C1'-N1	6.03	1.57	1.48
1	AA	1498	UR3	O3'-P	6.01	1.62	1.56
31	CA	253	C	C1'-N1	5.99	1.57	1.48
31	CA	1314	C	C1'-N1	5.98	1.57	1.48
31	CA	688	U	C1'-N1	5.97	1.57	1.48
1	AA	1397	C	C1'-N1	5.95	1.56	1.47
31	CA	2619	C	C1'-N1	5.87	1.57	1.48
31	CA	2232	C	C1'-N1	5.86	1.57	1.48
1	AA	527	G7M	O3'-P	5.85	1.62	1.56
31	CA	826	U	C1'-N1	5.79	1.57	1.48
31	CA	1352	U	C1'-N1	5.75	1.57	1.48
31	CA	1730	C	C1'-N1	5.75	1.56	1.47
1	AA	485	U	C1'-N1	5.73	1.56	1.47
31	CA	2263	C	C1'-N1	5.71	1.57	1.48
31	CA	451	U	C1'-N1	5.69	1.56	1.48
31	CA	20	C	C1'-N1	5.65	1.56	1.48
33	DA	1170	C	C1'-N1	5.65	1.56	1.48
31	CA	692	C	C1'-N1	5.62	1.56	1.48
33	DA	1174	U	C1'-N1	5.60	1.56	1.48
1	AA	845	A	O5'-C5'	5.57	1.50	1.42
31	CA	2069	G7M	O3'-P	5.56	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	932	C	C1'-N1	5.55	1.56	1.48
31	CA	546	U	C1'-N1	5.52	1.56	1.48
31	CA	2055	C	C1'-N1	5.52	1.56	1.48
33	DA	653	U	C1'-N1	5.51	1.56	1.48
33	DA	1730	C	C1'-N1	5.50	1.55	1.47
31	CA	2215	C	C1'-N1	5.46	1.56	1.48
33	DA	2767	C	C1'-N1	5.46	1.56	1.48
33	DA	1306	C	C1'-N1	5.45	1.56	1.48
33	DA	2127	G	C3'-O3'	5.45	1.50	1.42
31	CA	2779	U	C1'-N1	5.43	1.55	1.47
31	CA	2591	C	C1'-N1	5.42	1.56	1.48
28	DB	70	C	C1'-N1	5.40	1.56	1.48
31	CA	140	C	C1'-N1	5.39	1.55	1.47
31	CA	1793	C	C1'-N1	5.37	1.56	1.48
31	CA	2715	C	C1'-N1	5.34	1.56	1.48
1	BA	183	C	C1'-N1	5.34	1.55	1.47
31	CA	1306	C	C1'-N1	5.33	1.56	1.48
33	DA	2506	U	C1'-N1	5.31	1.56	1.48
33	DA	139	U	C1'-N1	5.30	1.55	1.47
31	CA	355	U	C1'-N1	5.29	1.56	1.48
33	DA	1534	U	C1'-N1	5.28	1.56	1.48
31	CA	29	U	C1'-N1	5.26	1.56	1.48
31	CA	2443	C	C1'-N1	5.25	1.56	1.48
1	BA	1498	UR3	O3'-P	5.24	1.61	1.56
31	CA	635	C	C1'-N1	5.24	1.56	1.48
31	CA	2017	U	C1'-N1	5.23	1.56	1.48
30	CD	193	VAL	CA-C	5.21	1.56	1.52
33	DA	29	U	C1'-N1	5.21	1.56	1.48
41	CM	77	ILE	CG1-CD1	-5.21	1.31	1.51
31	CA	2769	U	C1'-N1	5.21	1.56	1.48
33	DA	635	C	C1'-N1	5.20	1.56	1.48
33	DA	998	C	C1'-N1	5.20	1.56	1.48
1	BA	893	C	C1'-N1	5.18	1.56	1.48
1	BA	737	C	C1'-N1	5.18	1.56	1.48
31	CA	790	U	C1'-N1	5.16	1.56	1.48
1	AA	632	U	C1'-N1	5.16	1.56	1.48
31	CA	557	C	C1'-N1	5.14	1.56	1.48
10	AJ	57	VAL	CA-C	5.12	1.59	1.52
31	CA	2691	C	C1'-N1	5.11	1.56	1.48
31	CA	653	U	C1'-N1	5.10	1.56	1.48
10	BJ	57	VAL	CA-C	5.09	1.59	1.52
33	DA	2016	U	C1'-N1	5.08	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	672	C	C1'-N1	5.08	1.56	1.48
31	CA	2506	U	C1'-N1	5.07	1.56	1.48
31	CA	1920	C	C1'-N1	5.07	1.56	1.48
42	CN	70	ASP	CA-C	5.06	1.59	1.52
33	DA	1958	C	C1'-N1	5.05	1.56	1.48
31	CA	828	U	C1'-N1	5.04	1.56	1.48
1	AA	955	U	C1'-N1	5.03	1.55	1.48
31	CA	1629	U	C1'-N1	5.03	1.55	1.48
1	AA	217	C	C1'-N1	5.03	1.55	1.48
31	CA	2871	U	C1'-N1	5.03	1.55	1.48
31	CA	2425	A	C3'-O3'	5.02	1.50	1.43
31	CA	461	C	C1'-N1	5.01	1.55	1.48
31	CA	1704	C	C1'-N1	5.01	1.55	1.48

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DI	132	TYR	CA-C-N	9.80	139.35	121.70
55	DI	132	TYR	C-N-CA	9.80	139.35	121.70
35	DF	10	ASP	CA-CB-CG	8.61	121.21	112.60
20	BT	6	SER	N-CA-C	-8.06	103.44	113.28
35	CF	134	GLU	CB-CG-CD	7.48	125.31	112.60
33	DA	271	G	C2'-C3'-O3'	7.41	120.61	109.50
20	BT	43	ASP	CA-CB-CG	7.36	119.96	112.60
41	CM	68	SER	N-CA-C	7.23	118.80	111.07
6	BF	90	MET	CA-C-N	7.15	131.32	120.82
6	BF	90	MET	C-N-CA	7.15	131.32	120.82
55	DI	106	PHE	CA-CB-CG	7.14	120.94	113.80
34	CE	7	ASP	CA-CB-CG	7.11	119.71	112.60
35	DF	46	ASP	CA-CB-CG	7.06	119.66	112.60
4	AD	99	ASP	CA-CB-CG	7.03	119.63	112.60
2	BB	126	PHE	CA-CB-CG	6.98	120.78	113.80
2	AB	126	PHE	CA-CB-CG	6.91	120.71	113.80
48	DT	65	ASP	CA-CB-CG	6.80	119.40	112.60
29	DC	260	ASN	CA-C-N	6.78	130.28	120.38
29	DC	260	ASN	C-N-CA	6.78	130.28	120.38
4	BD	99	ASP	CA-CB-CG	6.75	119.35	112.60
4	AD	131	ASN	CA-CB-CG	6.74	119.34	112.60
35	CF	46	ASP	CA-CB-CG	6.68	119.28	112.60
34	CE	171	ASP	CA-CB-CG	6.65	119.25	112.60
36	CG	175	LYS	CA-C-N	6.63	134.21	121.54
36	CG	175	LYS	C-N-CA	6.63	134.21	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	BF	79	ARG	CA-C-N	6.62	129.48	120.54
6	BF	79	ARG	C-N-CA	6.62	129.48	120.54
36	DG	80	THR	CA-C-N	6.57	128.99	120.44
36	DG	80	THR	C-N-CA	6.57	128.99	120.44
11	BK	71	ALA	N-CA-C	-6.57	104.30	112.90
37	CH	8	LYS	CA-C-N	6.53	133.73	121.97
37	CH	8	LYS	C-N-CA	6.53	133.73	121.97
48	DT	42	LYS	N-CA-C	-6.52	104.18	111.28
7	AG	151	PHE	CA-CB-CG	6.51	120.31	113.80
31	CA	2425	A	C4'-C3'-O3'	6.48	119.12	109.40
5	AE	55	GLU	CA-C-N	6.43	126.61	120.43
5	AE	55	GLU	C-N-CA	6.43	126.61	120.43
3	BC	61	ALA	CA-C-N	6.36	131.18	122.34
3	BC	61	ALA	C-N-CA	6.36	131.18	122.34
8	AH	109	GLY	N-CA-C	6.34	118.50	112.04
17	AQ	48	ASP	CA-CB-CG	6.32	118.92	112.60
6	BF	55	HIS	N-CA-C	-6.32	98.07	108.76
18	AR	34	THR	CA-C-N	6.31	129.02	120.38
18	AR	34	THR	C-N-CA	6.31	129.02	120.38
42	CN	69	PRO	CA-C-N	6.29	133.56	121.54
42	CN	69	PRO	C-N-CA	6.29	133.56	121.54
13	BM	11	ASP	CA-C-N	6.29	131.51	122.40
13	BM	11	ASP	C-N-CA	6.29	131.51	122.40
8	BH	109	GLY	N-CA-C	6.28	118.44	112.04
6	BF	98	GLU	CA-C-N	6.27	133.52	121.54
6	BF	98	GLU	C-N-CA	6.27	133.52	121.54
41	CM	68	SER	CA-C-N	6.23	133.44	121.54
41	CM	68	SER	C-N-CA	6.23	133.44	121.54
13	BM	96	PRO	CA-C-N	6.23	128.53	120.56
13	BM	96	PRO	C-N-CA	6.23	128.53	120.56
6	AF	79	ARG	CA-C-N	6.23	128.53	120.44
6	AF	79	ARG	C-N-CA	6.23	128.53	120.44
13	AM	96	PRO	CA-C-N	6.22	128.52	120.56
13	AM	96	PRO	C-N-CA	6.22	128.52	120.56
44	DP	78	VAL	N-CA-CB	6.20	117.81	110.55
3	BC	178	LEU	CA-C-N	6.17	129.16	120.28
3	BC	178	LEU	C-N-CA	6.17	129.16	120.28
36	CG	80	THR	CA-C-N	6.15	128.43	120.44
36	CG	80	THR	C-N-CA	6.15	128.43	120.44
6	AF	55	HIS	N-CA-C	-6.09	98.46	108.76
13	AM	86	TYR	CA-C-N	6.07	128.41	120.28
13	AM	86	TYR	C-N-CA	6.07	128.41	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	CF	21	ASN	CA-CB-CG	6.05	118.65	112.60
41	CM	67	THR	CA-C-N	6.05	128.30	120.44
41	CM	67	THR	C-N-CA	6.05	128.30	120.44
5	BE	55	GLU	CA-C-N	6.05	126.23	120.43
5	BE	55	GLU	C-N-CA	6.05	126.23	120.43
48	CT	42	LYS	N-CA-C	-6.01	104.73	111.28
39	CK	80	HIS	CA-C-N	6.00	132.76	121.97
39	CK	80	HIS	C-N-CA	6.00	132.76	121.97
44	CP	78	VAL	N-CA-CB	5.99	117.56	110.55
48	DT	69	LEU	N-CA-C	5.99	118.94	109.96
3	AC	178	LEU	CA-C-N	5.96	128.86	120.28
3	AC	178	LEU	C-N-CA	5.96	128.86	120.28
13	BM	86	TYR	CA-C-N	5.94	128.24	120.28
13	BM	86	TYR	C-N-CA	5.94	128.24	120.28
42	CN	69	PRO	CA-C-O	-5.93	109.80	120.60
55	DI	7	ASP	CA-CB-CG	5.93	118.53	112.60
50	DV	53	ASN	CA-C-N	5.91	128.59	120.67
50	DV	53	ASN	C-N-CA	5.91	128.59	120.67
16	BP	42	ILE	CA-C-N	5.90	129.67	120.82
16	BP	42	ILE	C-N-CA	5.90	129.67	120.82
21	AU	33	ARG	CA-C-N	5.86	128.13	120.28
21	AU	33	ARG	C-N-CA	5.86	128.13	120.28
10	BJ	37	ARG	CA-C-N	5.83	131.03	121.87
10	BJ	37	ARG	C-N-CA	5.83	131.03	121.87
37	DH	8	LYS	CA-C-N	5.80	130.74	123.14
37	DH	8	LYS	C-N-CA	5.80	130.74	123.14
42	DN	36	VAL	N-CA-C	-5.79	107.17	112.96
29	DC	70	ASN	CA-CB-CG	5.79	118.39	112.60
38	CJ	22	PRO	N-CA-C	5.77	117.74	110.70
29	CC	264	ASP	CA-C-N	5.76	128.28	120.38
29	CC	264	ASP	C-N-CA	5.76	128.28	120.38
38	DJ	22	PRO	N-CA-C	5.74	117.71	110.70
47	CS	53	PHE	CA-C-N	5.74	128.19	120.50
47	CS	53	PHE	C-N-CA	5.74	128.19	120.50
17	BQ	51	ASN	CA-CB-CG	5.74	118.34	112.60
37	DH	26	ALA	CA-C-N	5.73	128.53	120.28
37	DH	26	ALA	C-N-CA	5.73	128.53	120.28
10	AJ	76	ILE	CA-C-N	5.70	128.51	120.42
10	AJ	76	ILE	C-N-CA	5.70	128.51	120.42
18	BR	67	LEU	N-CA-C	-5.69	106.34	113.28
33	DA	271	G	P-O3'-C3'	5.68	128.73	120.20
40	DL	12	ASP	CA-CB-CG	5.65	118.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	DK	71	ASP	CA-CB-CG	5.63	118.23	112.60
15	AO	88	ARG	N-CA-C	-5.61	100.04	108.96
21	BU	33	ARG	CA-C-N	5.59	127.77	120.28
21	BU	33	ARG	C-N-CA	5.59	127.77	120.28
12	BL	64	THR	CB-CA-C	5.58	118.73	109.53
3	BC	206	GLU	CA-C-N	5.57	131.72	121.70
3	BC	206	GLU	C-N-CA	5.57	131.72	121.70
18	AR	72	ASP	CA-CB-CG	5.56	118.16	112.60
46	CR	12	ALA	CA-C-N	5.55	127.98	120.38
46	CR	12	ALA	C-N-CA	5.55	127.98	120.38
38	DJ	118	THR	CA-C-N	5.54	125.37	120.10
38	DJ	118	THR	C-N-CA	5.54	125.37	120.10
38	CJ	118	THR	CA-C-N	5.53	125.35	120.10
38	CJ	118	THR	C-N-CA	5.53	125.35	120.10
5	AE	86	LYS	CA-C-N	5.53	125.41	121.65
5	AE	86	LYS	C-N-CA	5.53	125.41	121.65
41	CM	101	ILE	CA-C-N	5.51	125.58	120.34
41	CM	101	ILE	C-N-CA	5.51	125.58	120.34
42	CN	106	ASP	CA-CB-CG	5.51	118.11	112.60
49	DU	92	ASN	CA-C-N	5.48	131.57	121.70
49	DU	92	ASN	C-N-CA	5.48	131.57	121.70
19	AS	27	ASP	CA-CB-CG	5.46	118.06	112.60
7	AG	62	PHE	CA-C-N	5.44	127.58	120.28
7	AG	62	PHE	C-N-CA	5.44	127.58	120.28
39	CK	71	ASP	CA-CB-CG	5.44	118.04	112.60
50	CV	53	ASN	CA-C-N	5.44	126.53	120.06
50	CV	53	ASN	C-N-CA	5.44	126.53	120.06
7	BG	151	PHE	CA-CB-CG	5.42	119.22	113.80
30	CD	108	ASP	CA-CB-CG	5.42	118.03	112.60
35	DF	167	ARG	CA-C-N	5.40	127.78	120.38
35	DF	167	ARG	C-N-CA	5.40	127.78	120.38
52	DX	44	LYS	N-CA-C	-5.40	105.40	111.28
50	DV	51	ALA	CA-C-N	5.39	131.84	121.54
50	DV	51	ALA	C-N-CA	5.39	131.84	121.54
13	BM	4	ILE	CA-C-N	5.38	131.82	121.54
13	BM	4	ILE	C-N-CA	5.38	131.82	121.54
41	CM	23	ILE	CA-C-N	5.37	126.06	119.99
41	CM	23	ILE	C-N-CA	5.37	126.06	119.99
25	D4	17	THR	CA-C-N	5.37	126.06	119.99
25	D4	17	THR	C-N-CA	5.37	126.06	119.99
16	BP	19	VAL	N-CA-CB	5.37	116.96	110.95
3	AC	206	GLU	CA-C-N	5.36	131.34	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AC	206	GLU	C-N-CA	5.36	131.34	121.70
5	BE	105	ILE	N-CA-CB	5.35	120.05	111.23
17	BQ	48	ASP	CA-CB-CG	5.35	117.95	112.60
32	DD	32	ASN	CA-CB-CG	5.35	117.95	112.60
41	CM	37	GLY	CA-C-N	5.34	127.75	120.54
41	CM	37	GLY	C-N-CA	5.34	127.75	120.54
13	AM	54	ASP	CA-CB-CG	5.33	117.93	112.60
31	CA	2095	A	C5'-C4'-C3'	-5.33	108.00	116.00
34	CE	198	GLU	CA-C-N	5.33	127.37	120.44
34	CE	198	GLU	C-N-CA	5.33	127.37	120.44
4	AD	39	GLY	CA-C-N	5.33	127.42	120.28
4	AD	39	GLY	C-N-CA	5.33	127.42	120.28
41	DM	81	ASP	CA-CB-CG	5.32	117.92	112.60
20	AT	23	SER	CA-C-N	5.31	127.40	120.28
20	AT	23	SER	C-N-CA	5.31	127.40	120.28
2	AB	93	ASN	CA-CB-CG	5.30	117.90	112.60
44	CP	2	ASP	CA-C-N	5.30	129.61	121.19
44	CP	2	ASP	C-N-CA	5.30	129.61	121.19
46	CR	91	ASP	CA-CB-CG	5.30	117.90	112.60
35	CF	167	ARG	CA-C-N	5.29	127.38	120.28
35	CF	167	ARG	C-N-CA	5.29	127.38	120.28
42	CN	111	GLU	CB-CG-CD	5.29	121.60	112.60
12	AL	64	THR	CB-CA-C	5.29	118.26	109.53
7	BG	62	PHE	CA-C-N	5.28	127.36	120.28
7	BG	62	PHE	C-N-CA	5.28	127.36	120.28
31	CA	271	G	C2'-C3'-O3'	5.28	117.42	109.50
5	AE	160	SER	CA-C-N	5.28	131.20	121.70
5	AE	160	SER	C-N-CA	5.28	131.20	121.70
32	DD	108	ASP	CA-CB-CG	5.27	117.87	112.60
40	CL	12	ASP	CA-CB-CG	5.27	117.87	112.60
35	CF	23	ASN	CA-CB-CG	5.26	117.86	112.60
29	CC	208	ALA	CA-C-N	5.25	125.81	119.98
29	CC	208	ALA	C-N-CA	5.25	125.81	119.98
18	AR	67	LEU	N-CA-C	-5.25	106.89	113.72
36	CG	69	ARG	CA-C-N	5.25	127.57	120.38
36	CG	69	ARG	C-N-CA	5.25	127.57	120.38
32	DD	186	LEU	N-CA-C	5.25	118.11	109.72
5	BE	51	GLY	CA-C-N	5.24	130.82	122.59
5	BE	51	GLY	C-N-CA	5.24	130.82	122.59
8	AH	94	LYS	CA-C-N	5.23	127.51	120.50
8	AH	94	LYS	C-N-CA	5.23	127.51	120.50
34	DE	198	GLU	CA-C-N	5.22	127.23	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	DE	198	GLU	C-N-CA	5.22	127.23	120.44
49	DU	64	LYS	CA-C-N	5.22	124.93	119.92
49	DU	64	LYS	C-N-CA	5.22	124.93	119.92
6	BF	92	THR	CA-C-N	5.22	129.75	122.08
6	BF	92	THR	C-N-CA	5.22	129.75	122.08
41	DM	101	ILE	CA-C-N	5.21	125.29	120.34
41	DM	101	ILE	C-N-CA	5.21	125.29	120.34
8	BH	94	LYS	CA-C-N	5.21	127.48	120.50
8	BH	94	LYS	C-N-CA	5.21	127.48	120.50
44	CP	67	ASN	CA-CB-CG	5.21	117.81	112.60
4	BD	39	GLY	CA-C-N	5.20	127.25	120.28
4	BD	39	GLY	C-N-CA	5.20	127.25	120.28
29	CC	195	VAL	N-CA-CB	5.20	116.20	110.53
42	DN	106	ASP	CA-CB-CG	5.20	117.80	112.60
5	AE	123	VAL	N-CA-C	5.20	115.21	108.35
35	CF	123	ASP	CA-CB-CG	5.19	117.79	112.60
35	CF	166	GLY	CA-C-N	5.19	128.00	120.79
35	CF	166	GLY	C-N-CA	5.19	128.00	120.79
34	DE	64	GLY	N-CA-C	5.19	120.99	114.25
5	AE	161	VAL	CA-C-N	5.18	131.44	121.54
5	AE	161	VAL	C-N-CA	5.18	131.44	121.54
44	CP	34	HIS	N-CA-C	5.18	117.25	109.23
50	CV	74	ASN	CA-C-N	5.18	131.43	121.54
50	CV	74	ASN	C-N-CA	5.18	131.43	121.54
4	BD	80	ALA	CA-C-N	5.17	127.21	120.28
4	BD	80	ALA	C-N-CA	5.17	127.21	120.28
29	DC	252	THR	N-CA-C	-5.17	103.86	110.53
30	CD	186	LEU	N-CA-C	5.17	117.99	109.72
34	DE	122	GLU	CB-CG-CD	5.17	121.38	112.60
35	CF	164	GLU	CA-C-N	5.16	128.16	120.31
35	CF	164	GLU	C-N-CA	5.16	128.16	120.31
44	DP	34	HIS	N-CA-C	5.16	117.22	109.23
31	CA	2406	A	C5'-C4'-O4'	5.15	116.83	109.10
2	BB	124	GLY	CA-C-N	5.15	131.37	121.54
2	BB	124	GLY	C-N-CA	5.15	131.37	121.54
42	CN	36	VAL	N-CA-C	-5.15	107.81	112.96
11	AK	71	ALA	CA-C-N	5.14	127.48	120.54
11	AK	71	ALA	C-N-CA	5.14	127.48	120.54
2	AB	124	GLY	CA-C-N	5.14	131.36	121.54
2	AB	124	GLY	C-N-CA	5.14	131.36	121.54
6	BF	80	PHE	CA-CB-CG	5.14	118.94	113.80
31	CA	974	G	N9-C1'-C2'	5.14	121.71	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	DD	127	PHE	CA-C-N	5.13	128.63	121.24
32	DD	127	PHE	C-N-CA	5.13	128.63	121.24
41	DM	23	ILE	CA-C-N	5.12	125.78	119.99
41	DM	23	ILE	C-N-CA	5.12	125.78	119.99
6	AF	80	PHE	CA-CB-CG	5.12	118.92	113.80
36	DG	69	ARG	CA-C-N	5.12	127.45	120.54
36	DG	69	ARG	C-N-CA	5.12	127.45	120.54
29	CC	239	ASN	CA-CB-CG	5.11	117.71	112.60
13	BM	11	ASP	N-CA-C	5.10	116.56	108.96
53	CY	17	ASN	CA-CB-CG	5.10	117.70	112.60
1	BA	1362	A	C1'-O4'-C4'	-5.10	104.60	109.70
17	AQ	15	ASP	CA-CB-CG	5.09	117.69	112.60
2	BB	93	ASN	CA-CB-CG	5.09	117.69	112.60
35	DF	146	VAL	CA-C-N	5.09	127.37	120.44
35	DF	146	VAL	C-N-CA	5.09	127.37	120.44
16	AP	47	GLU	CA-C-N	5.09	131.27	121.54
16	AP	47	GLU	C-N-CA	5.09	131.27	121.54
35	DF	5	HIS	N-CA-C	-5.09	105.81	111.36
2	AB	204	ASP	CA-CB-CG	5.08	117.68	112.60
1	AA	413	G	C1'-O4'-C4'	-5.07	104.63	109.70
49	CU	45	ALA	CA-C-N	5.07	127.58	120.28
49	CU	45	ALA	C-N-CA	5.07	127.58	120.28
12	AL	73	ASN	CA-CB-CG	5.07	117.67	112.60
46	DR	91	ASP	CA-CB-CG	5.07	117.67	112.60
5	AE	70	ASN	CA-CB-CG	5.06	117.66	112.60
18	BR	34	THR	CA-C-N	5.06	127.32	120.38
18	BR	34	THR	C-N-CA	5.06	127.32	120.38
9	BI	99	ARG	CA-C-N	5.06	127.37	120.54
9	BI	99	ARG	C-N-CA	5.06	127.37	120.54
41	CM	30	THR	N-CA-CB	5.06	119.04	110.49
37	CH	52	ALA	CA-C-N	5.05	127.00	120.44
37	CH	52	ALA	C-N-CA	5.05	127.00	120.44
39	DK	91	GLU	CA-C-N	5.05	127.00	120.44
39	DK	91	GLU	C-N-CA	5.05	127.00	120.44
11	BK	118	HIS	CA-C-N	5.05	131.18	121.54
11	BK	118	HIS	C-N-CA	5.05	131.18	121.54
22	C1	55	ILE	CA-C-N	5.04	129.89	122.63
22	C1	55	ILE	C-N-CA	5.04	129.89	122.63
10	BJ	58	ASN	CA-C-N	5.04	127.45	120.29
10	BJ	58	ASN	C-N-CA	5.04	127.45	120.29
55	DI	7	ASP	CA-C-N	5.04	126.99	120.44
55	DI	7	ASP	C-N-CA	5.04	126.99	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	AP	27	ALA	CA-C-N	5.03	127.78	120.79
16	AP	27	ALA	C-N-CA	5.03	127.78	120.79
4	AD	143	VAL	N-CA-CB	5.03	116.20	110.72
2	BB	204	ASP	CA-CB-CG	5.02	117.62	112.60
49	CU	13	ALA	N-CA-C	5.02	114.58	108.11
55	DI	20	LYS	CA-C-N	5.01	125.40	119.94
55	DI	20	LYS	C-N-CA	5.01	125.40	119.94
20	AT	22	ALA	CA-C-N	5.01	127.26	120.65
20	AT	22	ALA	C-N-CA	5.01	127.26	120.65
30	CD	64	GLU	CA-C-N	5.01	126.99	120.28
30	CD	64	GLU	C-N-CA	5.01	126.99	120.28
49	DU	13	ALA	N-CA-C	5.00	114.56	108.11

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	898	G	Sidechain
42	CN	69	PRO	Mainchain
33	DA	1753	G	Sidechain
33	DA	1954	G	Sidechain
33	DA	2250	G	Sidechain
33	DA	2358	A	Sidechain
33	DA	2589	A	Sidechain
33	DA	2595	G	Sidechain
33	DA	2692	G	Sidechain
33	DA	27	G	Sidechain
33	DA	2848	G	Sidechain
33	DA	308	G	Sidechain
33	DA	452	G	Sidechain
33	DA	512	G	Sidechain
33	DA	690	G	Sidechain
33	DA	956	G	Sidechain
33	DA	980	A	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	32930	0	16591	87	0
1	BA	32908	0	16580	89	0
2	AB	1753	0	1780	13	0
2	BB	1753	0	1780	17	0
3	AC	1625	0	1696	12	0
3	BC	1625	0	1696	15	0
4	AD	1643	0	1707	9	0
4	BD	1643	0	1707	12	0
5	AE	1144	0	1185	15	0
5	BE	1105	0	1148	19	0
6	AF	862	0	864	7	0
6	BF	817	0	808	9	0
7	AG	1182	0	1238	14	0
7	BG	1182	0	1238	9	0
8	AH	979	0	1031	8	0
8	BH	979	0	1031	7	0
9	AI	1022	0	1070	7	0
9	BI	1022	0	1070	7	0
10	AJ	796	0	836	9	0
10	BJ	787	0	828	10	0
11	AK	877	0	887	11	0
11	BK	877	0	887	10	0
12	AL	957	0	1017	9	0
12	BL	957	0	1017	11	0
13	AM	884	0	941	9	0
13	BM	884	0	941	14	0
14	AN	805	0	844	10	0
14	BN	805	0	844	10	0
15	AO	714	0	734	0	0
15	BO	714	0	734	1	0
16	AP	649	0	666	4	0
16	BP	649	0	666	7	0
17	AQ	649	0	691	4	0
17	BQ	649	0	691	7	0
18	AR	456	0	478	3	0
18	BR	456	0	478	1	0
19	AS	638	0	665	6	0
19	BS	638	0	665	10	0
20	AT	670	0	719	4	0
20	BT	665	0	714	9	0
21	AU	465	0	491	5	0
21	BU	465	0	491	5	0
22	C1	444	0	458	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	D1	444	0	458	9	0
23	C2	409	0	440	4	0
23	D2	414	0	442	2	0
24	C3	377	0	418	4	0
24	D3	377	0	418	2	0
25	C4	504	0	572	1	0
25	D4	504	0	572	2	0
26	C5	302	0	340	5	0
26	D5	302	0	340	1	0
27	C0	449	0	488	2	0
27	D0	463	0	504	2	0
28	CB	2529	0	1281	2	0
28	DB	2569	0	1301	5	0
29	CC	2083	0	2154	20	0
29	DC	2083	0	2154	17	0
30	CD	1565	0	1616	14	0
31	CA	62229	0	31318	253	0
32	DD	1576	0	1627	16	0
33	DA	62423	0	31410	188	0
34	CE	1552	0	1619	15	0
34	DE	1552	0	1619	11	0
35	CF	1411	0	1444	12	0
35	DF	1411	0	1444	13	0
36	CG	1323	0	1371	8	0
36	DG	1323	0	1371	9	0
37	CH	1110	0	1148	10	0
37	DH	1110	0	1148	7	0
38	CJ	979	0	1028	7	0
38	DJ	979	0	1028	6	0
39	CK	1129	0	1162	8	0
39	DK	1129	0	1162	3	0
40	CL	938	0	1012	10	0
40	DL	946	0	1023	10	0
41	CM	1053	0	1129	21	0
41	DM	1053	0	1129	11	0
42	CN	1075	0	1154	7	0
42	DN	1092	0	1177	7	0
43	CO	960	0	1000	10	0
43	DO	993	0	1034	8	0
44	CP	892	0	923	5	0
44	DP	900	0	935	8	0
45	CQ	917	0	962	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	DQ	917	0	962	5	0
46	CR	947	0	1019	10	0
46	DR	947	0	1019	13	0
47	CS	816	0	839	8	0
47	DS	816	0	839	8	0
48	CT	857	0	922	14	0
48	DT	857	0	922	13	0
49	CU	739	0	807	7	0
49	DU	739	0	807	3	0
50	CV	780	0	831	8	0
50	DV	780	0	831	5	0
51	CW	753	0	780	4	0
51	DW	753	0	780	5	0
52	CX	569	0	581	1	0
52	DX	591	0	606	7	0
53	CY	625	0	652	7	0
53	DY	625	0	652	2	0
54	CZ	501	0	531	3	0
54	DZ	501	0	531	3	0
55	DI	1023	0	1052	15	0
56	AA	70	0	0	0	0
56	BA	41	0	0	0	0
56	CA	156	0	0	0	0
56	CB	3	0	0	0	0
56	DA	183	0	0	0	0
56	DB	9	0	0	0	0
56	DD	2	0	0	0	0
56	DR	2	0	0	0	0
57	AA	13	0	18	1	0
57	BA	13	0	18	1	0
57	DA	26	0	36	1	0
57	DQ	13	0	18	0	0
57	DR	13	0	18	3	0
57	DS	13	0	18	1	0
58	AA	16	0	28	1	0
58	DA	48	0	84	1	0
58	DE	16	0	28	1	0
58	DK	8	0	14	0	0
58	DN	8	0	14	0	0
58	DS	8	0	14	0	0
58	DT	8	0	14	0	0
59	AA	24	0	48	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	DA	72	0	144	2	0
60	AB	1	0	0	0	0
60	C5	1	0	0	0	0
60	D5	1	0	0	0	0
61	AL	7	0	10	0	0
61	D1	7	0	10	2	0
61	D3	7	0	10	0	0
61	DA	35	0	50	0	0
61	DL	7	0	10	0	0
61	DP	7	0	10	0	0
61	DQ	7	0	10	0	0
62	D0	4	0	6	0	0
62	D1	4	0	6	0	0
62	DA	32	0	48	1	0
62	DB	8	0	12	0	0
63	D3	10	0	14	0	0
63	DA	40	0	56	2	0
63	DD	10	0	14	0	0
63	DS	10	0	14	2	0
63	DT	10	0	14	0	0
63	DU	10	0	14	0	0
64	DA	40	0	76	0	0
65	DA	32	0	44	1	0
66	DA	12	0	9	0	0
67	DA	11	0	5	0	0
68	DA	8	0	12	1	0
69	AA	507	0	0	1	0
69	AC	4	0	0	0	0
69	AD	3	0	0	0	0
69	AE	5	0	0	0	0
69	AF	1	0	0	0	0
69	AG	1	0	0	0	0
69	AJ	2	0	0	0	0
69	AK	7	0	0	0	0
69	AL	10	0	0	0	0
69	AM	4	0	0	1	0
69	AN	7	0	0	2	0
69	AO	2	0	0	0	0
69	AP	2	0	0	0	0
69	AR	1	0	0	0	0
69	AS	1	0	0	0	0
69	AT	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	AU	3	0	0	0	0
69	BA	291	0	0	1	0
69	BD	11	0	0	0	0
69	BE	1	0	0	0	0
69	BF	1	0	0	0	0
69	BK	2	0	0	0	0
69	BL	2	0	0	0	0
69	BN	2	0	0	0	0
69	BO	1	0	0	0	0
69	BP	3	0	0	2	0
69	BR	1	0	0	0	0
69	BT	4	0	0	0	0
69	BU	1	0	0	0	0
69	C3	3	0	0	0	0
69	C4	1	0	0	0	0
69	C5	1	0	0	0	0
69	CA	692	0	0	5	0
69	CB	13	0	0	0	0
69	CC	10	0	0	0	0
69	CD	6	0	0	0	0
69	CE	7	0	0	0	0
69	CL	1	0	0	0	0
69	CM	3	0	0	0	0
69	CO	1	0	0	0	0
69	CU	2	0	0	0	0
69	CV	1	0	0	0	0
69	CW	1	0	0	0	0
69	CY	1	0	0	0	0
69	D0	21	0	0	0	0
69	D1	42	0	0	0	0
69	D2	7	0	0	0	0
69	D3	28	0	0	0	0
69	D4	39	0	0	0	0
69	D5	9	0	0	0	0
69	DA	4834	0	0	14	0
69	DB	199	0	0	2	0
69	DC	98	0	0	1	0
69	DD	95	0	0	0	0
69	DE	63	0	0	1	0
69	DF	15	0	0	0	0
69	DG	7	0	0	0	0
69	DH	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	DK	65	0	0	1	0
69	DL	52	0	0	0	0
69	DM	62	0	0	0	0
69	DN	64	0	0	0	0
69	DO	48	0	0	0	0
69	DP	44	0	0	1	0
69	DQ	33	0	0	0	0
69	DR	68	0	0	1	0
69	DS	48	0	0	0	0
69	DT	62	0	0	1	0
69	DU	22	0	0	0	0
69	DV	18	0	0	0	0
69	DW	34	0	0	2	0
69	DX	31	0	0	0	0
69	DY	10	0	0	0	0
69	DZ	5	0	0	1	0
All	All	295125	0	194409	1259	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (1259) 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)
47:CS:14:VAL:HG21	47:CS:98:ILE:HG13	1.20	1.10
33:DA:1847:A:HO2'	33:DA:1848:A:H8	1.02	0.98
2:BB:20:THR:HA	2:BB:39:HIS:CE1	1.98	0.98
47:CS:14:VAL:CG2	47:CS:98:ILE:HG13	1.96	0.96
31:CA:1847:A:HO2'	31:CA:1848:A:H8	1.04	0.94
46:DR:20:GLN:HG3	57:DR:203:PG4:H42	1.50	0.91
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.52	0.91
26:C5:3:VAL:HG11	31:CA:2539:C:H5'	1.54	0.90
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.51	0.90
31:CA:1005:C:O2'	39:CK:30:THR:HG21	1.71	0.89
1:BA:841:C:H3'	1:BA:842:U:H5''	1.54	0.89
14:AN:66:GLN:HB2	69:AN:207:HOH:O	1.73	0.87
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.56	0.87
41:CM:77:ILE:HD11	41:CM:108:ALA:HB1	1.54	0.87
31:CA:1936:A:N6	31:CA:1963:U:H3	1.73	0.86
48:CT:86:MET:HB2	48:CT:96:ILE:HD11	1.58	0.86
1:AA:1492:A:H5''	12:AL:44:LYS:HG2	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.58	0.85
13:BM:6:GLY:HA3	13:BM:66:GLU:HG3	1.58	0.85
31:CA:2728:U:HO2'	31:CA:2729:G:H8	1.25	0.84
31:CA:1936:A:H2	31:CA:1943:U:H3	1.26	0.83
13:BM:114:LYS:HB3	13:BM:115:PRO:HD3	1.60	0.83
31:CA:2428:G:N2	41:CM:60:ARG:HH21	1.77	0.82
33:DA:2428:G:N2	41:DM:60:ARG:HH21	1.77	0.81
1:AA:664:G:H22	1:AA:741:G:H1	1.29	0.79
32:DD:4:LEU:HD12	32:DD:101:PHE:CE2	2.18	0.79
11:BK:88:GLY:H	11:BK:114:THR:HG22	1.48	0.78
1:BA:664:G:H22	1:BA:741:G:H1	1.29	0.76
29:CC:17:VAL:HB	29:CC:204:VAL:HG13	1.69	0.74
34:CE:149:ILE:HG12	34:CE:188:MET:HG2	1.68	0.74
8:BH:87:LYS:HB2	8:BH:125:ILE:HD11	1.69	0.74
1:BA:841:C:H3'	1:BA:842:U:C5'	2.16	0.74
24:C3:12:ARG:HD2	24:C3:44:VAL:HG11	1.71	0.73
48:CT:73:LYS:HB2	48:CT:106:VAL:HB	1.71	0.73
33:DA:580:U:O3'	46:DR:31:VAL:HG13	1.89	0.73
33:DA:2127:G:H4'	33:DA:2128:G:OP1	1.88	0.72
1:BA:1305:G:H21	1:BA:1332:A:H2	1.38	0.72
58:DA:3190:MPD:H12	34:DE:33:VAL:HG22	1.71	0.72
4:BD:197:GLU:HA	4:BD:200:ILE:HD12	1.71	0.72
1:AA:1305:G:H21	1:AA:1332:A:H2	1.38	0.72
31:CA:528:A:C2	31:CA:2043:C:H4'	2.25	0.72
8:AH:87:LYS:HB2	8:AH:125:ILE:HD11	1.72	0.71
4:AD:197:GLU:HA	4:AD:200:ILE:HD12	1.70	0.71
47:CS:14:VAL:HG21	47:CS:98:ILE:CG1	2.11	0.71
13:BM:22:ILE:HB	13:BM:25:VAL:CG1	2.19	0.71
31:CA:1394:U:H4'	31:CA:1603:A:H4'	1.72	0.71
31:CA:532:A:N1	31:CA:2020:A:H1'	2.05	0.71
1:AA:1358:U:H3	1:AA:1363:A:H62	1.38	0.70
31:CA:206:U:H2'	31:CA:207:A:H8	1.56	0.70
48:DT:73:LYS:HB2	48:DT:106:VAL:HB	1.72	0.70
33:DA:2262:U:H5''	52:DX:41[A]:ARG:HH12	1.57	0.69
39:DK:46:PRO:HD2	69:DK:363:HOH:O	1.91	0.69
3:BC:123:GLN:HB3	3:BC:128:VAL:HG21	1.74	0.69
33:DA:135:U:H3	33:DA:144:A:H61	1.39	0.69
33:DA:2591:C:H2'	33:DA:2592:G:C8	2.27	0.69
36:CG:80:THR:HG23	36:CG:81:GLU:H	1.57	0.69
22:C1:43:ILE:HG22	22:C1:49:TYR:HB2	1.75	0.69
30:CD:133:THR:HG22	31:CA:1993:U:H4'	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.75	0.69
19:BS:6:LYS:HD2	19:BS:7:LYS:H	1.58	0.69
33:DA:494:G:H4'	48:DT:6:LYS:HB2	1.74	0.69
33:DA:568:U:H1'	33:DA:2030:6MZ:H9C1	1.75	0.69
31:CA:1936:A:H61	31:CA:1963:U:H3	1.40	0.68
31:CA:135:U:H3	31:CA:144:A:H61	1.39	0.68
33:DA:2033:A:H5'	69:DA:3669:HOH:O	1.93	0.68
30:CD:4:LEU:HD12	30:CD:101:PHE:CE2	2.29	0.68
31:CA:846:U:H1'	31:CA:847:U:H5	1.58	0.68
22:D1:43:ILE:HG22	22:D1:49:TYR:HB2	1.76	0.68
48:CT:82:MET:HB2	48:CT:98:LYS:HB2	1.76	0.68
33:DA:1853:A:N1	33:DA:2087:G:H1'	2.09	0.68
1:AA:81:A:H61	1:AA:86:G:H1	1.42	0.67
43:CO:73:ASN:HA	43:CO:76:VAL:HG22	1.76	0.67
31:CA:17:G:H4'	46:CR:25:TYR:HE2	1.59	0.67
33:DA:2128:G:H1	33:DA:2160:C:H42	1.42	0.67
6:BF:38:ARG:HH12	6:BF:99:ALA:HB3	1.60	0.67
48:DT:82:MET:HB2	48:DT:98:LYS:HB2	1.77	0.67
3:BC:40:ARG:HH11	3:BC:55:ILE:HG23	1.59	0.66
50:CV:7:ARG:O	50:CV:25:VAL:HB	1.95	0.66
6:AF:102:MET:HE1	18:AR:24:LYS:HB3	1.76	0.66
3:BC:77:ILE:HA	3:BC:84:VAL:HG23	1.77	0.66
46:DR:20:GLN:CG	57:DR:203:PG4:H42	2.26	0.66
13:BM:83:LEU:HD21	19:BS:65:GLU:HB2	1.76	0.66
41:CM:82:LEU:HD11	41:CM:116:VAL:HG23	1.78	0.66
1:BA:451:A:H2'	69:BA:1701:HOH:O	1.96	0.66
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.77	0.66
33:DA:1913:A:H4'	33:DA:1913:A:OP1	1.96	0.65
10:AJ:7:ARG:HB3	10:AJ:101:SER:HB2	1.77	0.65
31:CA:2428:G:N2	41:CM:60:ARG:NH2	2.44	0.65
31:CA:2728:U:O2'	31:CA:2729:G:H8	1.78	0.65
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.77	0.65
43:DO:73:ASN:HA	43:DO:76:VAL:HG22	1.77	0.65
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.78	0.65
20:BT:9:LYS:O	20:BT:12:ILE:HG13	1.97	0.65
46:DR:28:ARG:HD3	69:DR:318:HOH:O	1.96	0.65
31:CA:2074:U:H2'	31:CA:2075:U:C6	2.33	0.64
31:CA:2796:U:H3	31:CA:2799:A:H61	1.45	0.64
11:AK:31:ILE:HG12	11:AK:46:THR:HG22	1.79	0.64
33:DA:2796:U:H3	33:DA:2799:A:H61	1.44	0.64
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BK:88:GLY:N	11:BK:114:THR:HG22	2.13	0.64
31:CA:1105:U:H2'	31:CA:1106:G:H8	1.62	0.64
33:DA:1105:U:H2'	33:DA:1106:G:H8	1.63	0.64
33:DA:2428:G:H21	41:DM:60:ARG:HH21	1.44	0.64
52:CX:37:ILE:HG21	52:CX:80:ILE:HG21	1.79	0.64
31:CA:783:A:H4'	31:CA:1779:U:O2	1.97	0.63
2:BB:23:TRP:HB3	2:BB:39:HIS:CE1	2.33	0.63
30:CD:129:THR:HG23	30:CD:140:HIS:O	1.98	0.63
31:CA:659:G:H4'	34:CE:95:LYS:HD3	1.81	0.63
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.35	0.62
13:AM:4:ILE:HD12	13:AM:10:PRO:HG2	1.80	0.62
1:BA:1218:C:H2'	1:BA:1219:A:C8	2.35	0.62
33:DA:2428:G:N2	41:DM:60:ARG:NH2	2.47	0.62
31:CA:740:C:H5'	31:CA:1784:A:H3'	1.82	0.62
69:DA:8015:HOH:O	42:DN:55:ARG:HG3	1.97	0.62
31:CA:699:A:H2'	31:CA:700:G:O4'	2.00	0.62
50:DV:52:LEU:HB3	50:DV:54:GLN:HB2	1.81	0.62
55:DI:64:VAL:HG22	55:DI:69:PHE:HB2	1.82	0.62
44:DP:31:THR:HG22	44:DP:33:ARG:H	1.64	0.62
31:CA:674:G:H1'	34:CE:69:ARG:HH11	1.65	0.62
5:BE:106:ILE:HD11	5:BE:124:LEU:HD23	1.81	0.61
6:BF:38:ARG:NH1	6:BF:99:ALA:HB3	2.15	0.61
20:BT:4:ILE:HA	20:BT:8:LYS:HE2	1.81	0.61
48:CT:17:VAL:HG11	48:CT:103:ILE:HG12	1.82	0.61
19:AS:15:LEU:HD13	19:AS:33:THR:HG21	1.82	0.61
12:BL:43:LYS:HD2	12:BL:91:PRO:HG3	1.81	0.61
13:BM:22:ILE:HB	13:BM:25:VAL:HG12	1.81	0.61
40:DL:43:ILE:HD12	40:DL:56:ASP:HB2	1.83	0.61
52:DX:37:ILE:HG21	52:DX:80:ILE:HG21	1.81	0.61
17:BQ:17:MET:HB3	17:BQ:20:SER:HB3	1.82	0.61
31:CA:2469:A:H4'	42:CN:55:ARG:HD3	1.82	0.61
5:BE:104:GLY:HA3	5:BE:122:ASN:HA	1.83	0.61
31:CA:2428:G:H21	41:CM:60:ARG:HH21	1.45	0.61
24:D3:1:MET:HE1	33:DA:1781:U:H5	1.65	0.61
4:BD:107:PHE:HB3	4:BD:145:ILE:HD11	1.83	0.60
41:CM:95:LEU:HD22	41:CM:100:ILE:HG12	1.81	0.60
36:DG:24:ILE:HD11	36:DG:43:VAL:HG11	1.82	0.60
48:DT:17:VAL:HG11	48:DT:103:ILE:HG12	1.83	0.60
1:AA:209:U:H4'	1:AA:210:C:OP2	2.01	0.60
31:CA:634:C:H2'	31:CA:635:C:C6	2.36	0.60
31:CA:2845:U:H5''	45:CQ:52:ASN:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1144:G:H21	1:AA:1146:A:H62	1.47	0.60
1:BA:1144:G:H21	1:BA:1146:A:H62	1.47	0.60
33:DA:1014:A:H1'	69:DA:6685:HOH:O	2.01	0.60
4:AD:107:PHE:HB3	4:AD:145:ILE:HD11	1.82	0.60
1:BA:1323:G:H2'	1:BA:1324:A:C8	2.36	0.60
36:CG:24:ILE:HD11	36:CG:43:VAL:HG11	1.82	0.60
40:CL:43:ILE:HD12	40:CL:56:ASP:HB2	1.82	0.60
31:CA:2394:C:H5''	41:CM:63:LYS:HE2	1.83	0.60
34:DE:131:THR:HG23	34:DE:160:ALA:O	2.02	0.60
1:AA:73:C:HO2'	1:AA:74:A:H8	1.50	0.60
2:AB:188:ASP:HB2	2:AB:204:ASP:OD2	2.02	0.60
1:BA:73:C:HO2'	1:BA:74:A:H8	1.48	0.60
1:BA:1226:C:H2'	13:BM:102:THR:HB	1.84	0.60
33:DA:1509:A:HO2'	33:DA:1510:G:H8	1.49	0.60
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.37	0.60
31:CA:784:G:H3'	69:CA:3484:HOH:O	2.01	0.59
31:CA:2680:U:H2'	31:CA:2681:C:C6	2.37	0.59
31:CA:1105:U:H2'	31:CA:1106:G:C8	2.37	0.59
35:CF:36:LEU:HD21	35:CF:91:LEU:CD1	2.32	0.59
48:DT:4:ILE:HG12	48:DT:106:VAL:HG22	1.84	0.59
44:CP:31:THR:HG22	44:CP:33:ARG:H	1.66	0.59
12:BL:33:VAL:HG22	12:BL:79:VAL:HG22	1.85	0.59
31:CA:2291:U:H2'	31:CA:2292:U:C6	2.38	0.59
31:CA:1447:C:H2'	31:CA:1448:G:C8	2.38	0.59
48:CT:59:GLU:HA	48:CT:64:ALA:HA	1.84	0.59
1:AA:1226:C:H2'	13:AM:102:THR:HB	1.85	0.58
46:CR:58:ARG:NH1	46:CR:62:ILE:HD11	2.19	0.58
6:BF:3:HIS:H	6:BF:92:THR:HG23	1.67	0.58
32:DD:114:LYS:HE2	33:DA:2681:C:OP2	2.03	0.58
1:BA:209:U:H4'	1:BA:210:C:OP2	2.03	0.58
1:AA:6:G:H1	5:AE:103:THR:HG21	1.68	0.58
35:CF:36:LEU:HD21	35:CF:91:LEU:HD12	1.84	0.58
1:AA:1277:C:HO2'	1:AA:1279:G:H8	1.50	0.58
2:AB:129:LEU:HD13	2:AB:134:ALA:HB2	1.86	0.58
8:AH:94:LYS:HB3	8:AH:117:ARG:HH22	1.68	0.58
31:CA:17:G:H4'	46:CR:25:TYR:CE2	2.37	0.58
31:CA:1311:G:H21	31:CA:1603:A:H62	1.50	0.58
2:BB:188:ASP:HB2	2:BB:204:ASP:OD2	2.03	0.58
33:DA:5:A:H2'	33:DA:6:A:C8	2.39	0.58
5:AE:106:ILE:HD11	5:AE:124:LEU:HD23	1.86	0.58
2:BB:129:LEU:HD13	2:BB:134:ALA:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:CL:77:ILE:HG12	45:CQ:72:ARG:HG3	1.86	0.58
22:D1:53:LYS:HE3	22:D1:56:ALA:HA	1.86	0.58
33:DA:1105:U:H2'	33:DA:1106:G:C8	2.38	0.58
35:DF:106:ILE:HD12	35:DF:139:PRO:HG2	1.85	0.58
5:AE:38:VAL:HG11	5:AE:114:VAL:HG22	1.86	0.57
12:AL:33:VAL:HG22	12:AL:79:VAL:HG22	1.85	0.57
1:BA:522:C:H5	12:BL:50:ARG:HH12	1.52	0.57
50:CV:82:ARG:HB2	50:CV:97:LYS:HG3	1.86	0.57
1:AA:774:G:H21	57:AA:1670:PG4:H51	1.69	0.57
48:CT:4:ILE:HG12	48:CT:106:VAL:HG22	1.86	0.57
20:BT:58:VAL:HG13	20:BT:72:ALA:HB1	1.85	0.57
33:DA:1645:G:H5''	33:DA:1646:C:H5'	1.86	0.57
33:DA:1182:G:H2'	33:DA:1183:U:O4'	2.05	0.57
38:CJ:14:ALA:HB3	38:CJ:17:MET:HB2	1.87	0.57
55:DI:69:PHE:HB3	55:DI:72:LEU:HD12	1.87	0.57
11:BK:89:PRO:HG3	21:BU:32:VAL:HG11	1.85	0.57
35:CF:106:ILE:HD12	35:CF:139:PRO:HG2	1.85	0.57
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.86	0.57
33:DA:31:C:O3'	33:DA:1238:G:H5''	2.05	0.57
44:DP:7:ARG:HG3	44:DP:96:GLY:HA3	1.86	0.57
38:DJ:14:ALA:HB3	38:DJ:17:MET:HB2	1.87	0.57
41:DM:57:LEU:HA	41:DM:60:ARG:HE	1.70	0.57
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.87	0.56
7:BG:113:ASP:HB2	7:BG:119:ARG:HG3	1.87	0.56
29:CC:219:THR:O	31:CA:1789:A:H5''	2.05	0.56
31:CA:118:A:N3	31:CA:178:G:H1'	2.20	0.56
40:CL:38:ILE:HD11	40:CL:112:PHE:HZ	1.68	0.56
20:BT:28:MET:HE1	20:BT:67:ILE:HG12	1.87	0.56
3:AC:151:VAL:HG12	3:AC:200:VAL:HG22	1.87	0.56
31:CA:1636:U:H2'	31:CA:1637:A:C8	2.39	0.56
41:CM:57:LEU:HB2	41:CM:60:ARG:HH11	1.70	0.56
41:DM:57:LEU:HB2	41:DM:60:ARG:HH11	1.69	0.56
6:AF:45:ARG:O	6:AF:56:LYS:HA	2.05	0.56
33:DA:2529:G:H4'	36:DG:175:LYS:HG3	1.87	0.56
55:DI:132:TYR:H	55:DI:133:GLU:HB2	1.70	0.56
33:DA:1278:C:H2'	33:DA:1279:G:H8	1.70	0.56
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.87	0.56
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.88	0.56
22:C1:53:LYS:HE3	22:C1:56:ALA:HA	1.87	0.56
32:DD:99:GLU:HG2	32:DD:182:ALA:HB2	1.88	0.56
51:CW:38:LEU:HD21	51:CW:65:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:335:C:H5''	50:CV:82:ARG:HD3	1.87	0.56
6:BF:45:ARG:O	6:BF:56:LYS:HA	2.06	0.56
33:DA:1278:C:H2'	33:DA:1279:G:C8	2.40	0.56
47:DS:44:GLY:O	47:DS:45:GLU:HG2	2.06	0.55
31:CA:1509:A:HO2'	31:CA:1510:G:H8	1.52	0.55
31:CA:2036:C:H2'	31:CA:2037:A:C8	2.42	0.55
49:CU:18:GLU:H	49:CU:18:GLU:CD	2.15	0.55
47:DS:21:ARG:HH21	57:DS:202:PG4:H71	1.70	0.55
44:CP:7:ARG:HG3	44:CP:96:GLY:HA3	1.87	0.55
8:BH:94:LYS:HB3	8:BH:117:ARG:HH22	1.71	0.55
40:DL:38:ILE:HD11	40:DL:112:PHE:HZ	1.70	0.55
1:AA:412:A:H3'	1:AA:413:G:H5'	1.87	0.55
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.89	0.55
1:BA:769:G:H4'	1:BA:1513:A:H4'	1.88	0.55
26:C5:3:VAL:HG11	31:CA:2539:C:C5'	2.34	0.55
33:DA:396:G:H1'	53:DY:29:PHE:HB3	1.87	0.55
22:D1:5:GLN:O	33:DA:2017:U:H4'	2.06	0.55
31:CA:457:A:N1	31:CA:470:A:H5''	2.22	0.55
65:DA:3183:1PE:H121	48:DT:73:LYS:HZ1	1.72	0.55
31:CA:1974:C:H3'	69:CA:3256:HOH:O	2.07	0.55
42:CN:69:PRO:HA	42:CN:94:ALA:HB2	1.89	0.54
17:BQ:14:SER:HB3	17:BQ:22:VAL:HG12	1.88	0.54
31:CA:784:G:H5'	31:CA:785:G:OP1	2.07	0.54
2:BB:20:THR:HA	2:BB:39:HIS:HE1	1.63	0.54
30:CD:99:GLU:HG2	30:CD:182:ALA:HB2	1.88	0.54
1:BA:209:U:H2'	1:BA:209:U:O2	2.06	0.54
31:CA:1794:A:H2'	31:CA:1795:C:C6	2.43	0.54
1:BA:946:A:H2'	1:BA:947:G:C8	2.43	0.54
31:CA:2019:A:H4'	46:CR:34:VAL:HG21	1.89	0.54
53:CY:11:ARG:HG2	53:CY:12:PRO:HD2	1.90	0.54
35:DF:138:PHE:HE2	35:DF:152:LEU:HD21	1.71	0.54
36:DG:19:ILE:HG12	36:DG:24:ILE:HG12	1.89	0.54
11:AK:84:VAL:HG21	11:AK:97:ILE:HG23	1.88	0.54
11:BK:84:VAL:HG21	11:BK:97:ILE:HG23	1.90	0.54
33:DA:644:A:H2'	33:DA:645:C:O4'	2.08	0.54
40:CL:24:VAL:HG13	40:CL:33:ALA:HB2	1.88	0.54
5:AE:107:ALA:HB2	5:AE:125:ALA:HB3	1.89	0.54
5:BE:105:ILE:HA	5:BE:123:VAL:HG23	1.90	0.54
37:CH:27:ARG:HH11	53:CY:60:ASP:HA	1.71	0.54
38:CJ:55:ILE:HD12	38:CJ:74:PRO:HD3	1.90	0.54
50:DV:94:ARG:HB3	50:DV:103:ILE:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:494:G:H4'	48:CT:6:LYS:HB2	1.89	0.54
21:AU:51:SER:HA	21:AU:54:LYS:HE3	1.90	0.54
1:AA:946:A:H2'	1:AA:947:G:C8	2.43	0.54
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.37	0.54
26:C5:3:VAL:CG1	31:CA:2539:C:H5'	2.35	0.54
31:CA:244:A:H5''	41:CM:67:THR:HG21	1.90	0.54
37:CH:3:VAL:HG12	37:CH:38:PRO:HA	1.90	0.54
41:CM:57:LEU:HA	41:CM:60:ARG:HE	1.72	0.54
34:DE:130:LYS:HB2	34:DE:133:LEU:HD12	1.89	0.54
1:BA:1432:G:H3'	45:CQ:106:LYS:HE2	1.89	0.53
33:DA:2327:A:H2'	33:DA:2328:A:C8	2.43	0.53
33:DA:2591:C:H2'	33:DA:2592:G:H8	1.72	0.53
51:DW:38:LEU:HD21	51:DW:65:VAL:HG11	1.88	0.53
31:CA:1645:G:H5''	31:CA:1646:C:H5'	1.89	0.53
59:DA:3210:PUT:H32	69:DA:6598:HOH:O	2.08	0.53
26:C5:36:ARG:HH22	31:CA:2539:C:H4'	1.72	0.53
1:BA:202:G:H1	1:BA:215:C:H42	1.56	0.53
23:C2:11:LEU:HD21	23:C2:34:LEU:HD23	1.91	0.53
2:BB:187:VAL:HG13	2:BB:191:SER:HB2	1.91	0.53
22:C1:4:GLN:HA	31:CA:2615:U:C2	2.43	0.53
26:C5:4:ARG:HB2	31:CA:2466:C:OP1	2.09	0.53
31:CA:373:U:H2'	31:CA:374:A:H8	1.73	0.53
33:DA:927:A:H2'	33:DA:928:A:C8	2.44	0.53
36:CG:19:ILE:HG12	36:CG:24:ILE:HG12	1.89	0.53
39:CK:117:ALA:HA	39:CK:120:ARG:HD2	1.90	0.53
51:DW:63:ILE:HG22	51:DW:65:VAL:HG23	1.90	0.53
1:BA:9:G:OP2	5:BE:126:LYS:HE2	2.08	0.53
31:CA:1476:U:H2'	31:CA:1477:A:H8	1.73	0.53
43:CO:2:ARG:HA	43:CO:5:LYS:HD2	1.91	0.53
49:CU:54:GLU:HB3	49:CU:88:LYS:HD2	1.90	0.53
13:BM:90:ARG:HH21	13:BM:95:LEU:HB3	1.74	0.53
38:DJ:55:ILE:HD12	38:DJ:74:PRO:HD3	1.90	0.53
10:BJ:5:ARG:HG2	10:BJ:79:PRO:HG3	1.91	0.53
30:CD:186:LEU:HD21	45:CQ:4:ILE:HG21	1.90	0.53
54:DZ:47:ARG:HD3	69:DZ:102:HOH:O	2.07	0.53
12:BL:110:ARG:HB2	12:BL:119:VAL:HG21	1.90	0.53
16:BP:61:VAL:HG21	16:BP:67:ILE:HD11	1.91	0.53
35:DF:36:LEU:HB2	35:DF:57:LEU:HD21	1.91	0.53
42:CN:41:LEU:HD21	42:CN:124:LEU:HD22	1.90	0.53
41:DM:85:VAL:HG21	41:DM:90:VAL:HG22	1.91	0.53
5:BE:77:ASN:HB2	5:BE:82:GLN:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BG:69:VAL:HG23	7:BG:100:ALA:HB1	1.91	0.52
16:BP:4:ILE:HG12	16:BP:21:VAL:HG22	1.90	0.52
31:CA:1779:U:C5	31:CA:1784:A:N7	2.77	0.52
32:DD:25:THR:HG21	32:DD:193:VAL:HG22	1.91	0.52
33:DA:45:G:H5''	33:DA:46:G:H5'	1.91	0.52
40:CL:58:LEU:HD11	40:CL:86:LEU:HD13	1.91	0.52
39:DK:117:ALA:HA	39:DK:120:ARG:HD2	1.91	0.52
1:BA:17:U:H2'	1:BA:18:C:C6	2.44	0.52
21:BU:14:VAL:HG22	21:BU:17:ARG:HH12	1.75	0.52
40:DL:24:VAL:HG13	40:DL:33:ALA:HB2	1.90	0.52
1:BA:9:G:H5'	5:BE:108:GLY:HA3	1.91	0.52
50:CV:94:ARG:HB3	50:CV:103:ILE:HD12	1.90	0.52
37:DH:3:VAL:HG12	37:DH:38:PRO:HA	1.92	0.52
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.38	0.52
14:BN:10:GLU:HG3	14:BN:63:ARG:HD2	1.92	0.52
1:AA:17:U:H2'	1:AA:18:C:C6	2.45	0.52
1:BA:1060:U:C5	3:BC:2:GLY:HA3	2.44	0.52
31:CA:176:A:O5'	31:CA:176:A:H8	1.93	0.52
2:AB:20:THR:HG22	2:AB:39:HIS:CE1	2.44	0.52
33:DA:2305:U:H5''	35:DF:131:GLY:HA3	1.90	0.52
38:CJ:103:ARG:HA	38:CJ:106:LEU:HD12	1.91	0.52
51:CW:63:ILE:HG22	51:CW:65:VAL:HG23	1.91	0.52
2:AB:15:HIS:HB3	2:AB:43:LEU:HD11	1.90	0.52
31:CA:1028:A:N6	31:CA:1125:G:H2'	2.25	0.52
1:AA:9:G:OP2	5:AE:126:LYS:HE2	2.10	0.52
1:AA:1492:A:C5'	12:AL:44:LYS:HG2	2.36	0.52
27:C0:9:GLN:HB3	27:C0:32:ILE:HA	1.92	0.52
31:CA:744:U:H4'	31:CA:1658:C:H4'	1.91	0.52
33:DA:1250:G:H5''	46:DR:6:ARG:HD3	1.92	0.52
52:DX:65:GLY:HA2	52:DX:85:GLU:HG2	1.92	0.52
30:CD:25:THR:HG21	30:CD:193:VAL:HG22	1.91	0.52
31:CA:1379:U:H4'	31:CA:1380:G:OP1	2.10	0.52
33:DA:839:U:H2'	33:DA:840:C:C6	2.44	0.52
34:CE:145:ASP:HA	34:CE:166:LYS:HB3	1.92	0.52
51:CW:77:VAL:HG23	51:CW:89:ILE:HG12	1.92	0.52
45:DQ:31:TRP:CE2	45:DQ:40:LEU:HD21	2.45	0.52
48:DT:41:LYS:HD2	69:DT:344:HOH:O	2.09	0.52
31:CA:310:A:H5''	50:CV:15:THR:HG23	1.92	0.52
32:DD:150[A]:MEQ:HE3	33:DA:2032:G:C8	2.45	0.52
33:DA:514:A:H5'	46:DR:11:ARG:HH12	1.74	0.52
33:DA:2800:A:C2	33:DA:2895:G:H1'	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:DL:58:LEU:HD11	40:DL:86:LEU:HD13	1.92	0.52
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.91	0.51
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	1.92	0.51
1:BA:1277:C:HO2'	1:BA:1279:G:H8	1.57	0.51
2:BB:97:LEU:H	2:BB:100:MET:HE3	1.75	0.51
31:CA:2533:U:H2'	31:CA:2534:A:O4'	2.10	0.51
33:DA:639:U:H2'	33:DA:640:C:C6	2.45	0.51
31:CA:796:C:H2'	31:CA:797:G:C8	2.45	0.51
31:CA:1651:G:OP1	43:CO:40:LYS:HE3	2.10	0.51
33:DA:1935:G:H1'	33:DA:1964:G:N2	2.25	0.51
35:DF:61:SER:HB2	35:DF:91:LEU:HD21	1.92	0.51
36:DG:95:ARG:HG2	36:DG:128:GLN:HB3	1.93	0.51
5:AE:77:ASN:HB2	5:AE:82:GLN:NE2	2.25	0.51
1:BA:1062:U:H2'	1:BA:1063:C:C6	2.46	0.51
31:CA:1936:A:N6	31:CA:1963:U:N3	2.53	0.51
33:DA:2262:U:H5''	52:DX:41[A]:ARG:NH1	2.22	0.51
44:DP:39:VAL:HB	44:DP:49:VAL:HG23	1.91	0.51
52:DX:21:LEU:HD11	52:DX:41[A]:ARG:HE	1.75	0.51
1:AA:1238:A:H5'	1:AA:1336:C:H41	1.75	0.51
23:C2:22:THR:HG21	31:CA:2419:U:H5''	1.93	0.51
2:BB:15:HIS:HB3	2:BB:43:LEU:HD11	1.92	0.51
9:BI:7:TYR:HE1	9:BI:18:ARG:HB2	1.74	0.51
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.76	0.51
31:CA:581:C:H2'	31:CA:582:A:C8	2.46	0.51
31:CA:806:C:H2'	31:CA:807:U:C6	2.46	0.51
12:AL:110:ARG:HB2	12:AL:119:VAL:HG21	1.92	0.51
14:AN:10:GLU:HG3	14:AN:63:ARG:HD2	1.92	0.51
31:CA:674:G:H1'	34:CE:69:ARG:HD2	1.92	0.51
33:DA:1026:G:H2'	33:DA:1027:A:C8	2.46	0.51
54:DZ:18:LEU:HB2	54:DZ:53:VAL:HG11	1.93	0.51
2:BB:120:GLN:HE22	2:BB:137:ARG:HE	1.58	0.51
28:CB:55:U:H1'	35:CF:26:MET:HG3	1.93	0.51
41:CM:85:VAL:HG11	41:CM:90:VAL:HG22	1.92	0.51
1:AA:202:G:H1	1:AA:215:C:H42	1.58	0.51
13:AM:33:ILE:HD11	13:AM:63:PHE:HE1	1.75	0.51
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.74	0.51
21:AU:14:VAL:HG22	21:AU:17:ARG:HH12	1.76	0.51
23:D2:11:LEU:HD21	23:D2:34:LEU:HD23	1.92	0.51
33:DA:1250:G:C5'	46:DR:6:ARG:HD3	2.41	0.51
37:CH:82:SER:HB2	37:CH:94:ILE:HD11	1.93	0.51
36:DG:164:TYR:HB2	36:DG:167:GLU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:DM:85:VAL:HB	41:DM:94:THR:HG22	1.92	0.51
31:CA:309:A:O3'	50:CV:16:GLY:HA2	2.10	0.51
32:DD:150[A]:MEQ:HG2	69:DA:4147:HOH:O	2.11	0.51
33:DA:1101:U:H2'	33:DA:1102:C:C6	2.46	0.51
33:DA:2409:G:H2'	33:DA:2410:G:O4'	2.11	0.51
2:AB:120:GLN:HE22	2:AB:137:ARG:HE	1.57	0.51
2:AB:187:VAL:HG13	2:AB:191:SER:HB2	1.92	0.51
31:CA:2261:C:C2	31:CA:2280:G:N2	2.79	0.51
34:CE:130:LYS:HB2	34:CE:133:LEU:HD12	1.93	0.51
37:DH:82:SER:HB2	37:DH:94:ILE:HD11	1.93	0.51
38:DJ:103:ARG:HA	38:DJ:106:LEU:HD12	1.91	0.51
13:AM:77:ILE:HG22	13:AM:81:MET:HE2	1.93	0.51
33:DA:2243:U:H2'	33:DA:2244:U:C6	2.47	0.51
69:DA:7302:HOH:O	46:DR:6:ARG:HG2	2.11	0.51
2:AB:97:LEU:H	2:AB:100:MET:HE3	1.76	0.50
29:CC:232:HIS:NE2	29:CC:244:PRO:HA	2.26	0.50
31:CA:45:G:H5''	31:CA:46:G:H5'	1.92	0.50
31:CA:571:U:H4'	31:CA:573:U:H5	1.76	0.50
31:CA:1662:U:H3	31:CA:1998:A:H61	1.59	0.50
33:DA:1794:A:H2'	33:DA:1795:C:C6	2.46	0.50
33:DA:2845:U:H5''	45:DQ:52:ASN:O	2.11	0.50
34:DE:145:ASP:HA	34:DE:166:LYS:HB3	1.92	0.50
7:AG:69:VAL:HG21	7:AG:104:ILE:HD11	1.92	0.50
7:AG:70:ARG:HG2	7:AG:96:ARG:HG2	1.91	0.50
10:AJ:5:ARG:HE	10:AJ:77:VAL:HG22	1.76	0.50
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.77	0.50
31:CA:2189:U:H2'	31:CA:2190:G:H8	1.75	0.50
33:DA:979:A:H2'	33:DA:982:C:H42	1.75	0.50
35:CF:36:LEU:HB2	35:CF:57:LEU:HD21	1.92	0.50
38:CJ:19:ASN:H	38:CJ:20:PRO:HD2	1.77	0.50
1:AA:845:A:O4'	1:AA:845:A:P	2.69	0.50
17:BQ:46:VAL:HG11	17:BQ:61:ILE:CG2	2.41	0.50
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.75	0.50
12:AL:55:VAL:HG21	12:AL:80:ILE:HD11	1.94	0.50
31:CA:608:A:H2'	31:CA:609:A:C8	2.47	0.50
31:CA:917:A:H5''	31:CA:2268:A:H61	1.76	0.50
33:DA:1651:G:H3'	69:DA:5545:HOH:O	2.12	0.50
35:CF:61:SER:HB2	35:CF:91:LEU:HD21	1.93	0.50
36:CG:164:TYR:HB2	36:CG:167:GLU:HB2	1.92	0.50
3:AC:156:ARG:HD3	3:AC:193:TYR:O	2.12	0.50
51:DW:77:VAL:HG23	51:DW:89:ILE:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DI:50:VAL:HG11	55:DI:92:ALA:HB2	1.94	0.50
1:AA:79:G:H22	1:AA:90:C:H42	1.60	0.50
7:BG:70:ARG:HG2	7:BG:96:ARG:HG2	1.92	0.50
11:BK:29:ASN:HB2	11:BK:57:LYS:HE3	1.94	0.50
13:BM:77:ILE:HG22	13:BM:81:MET:HE2	1.93	0.50
31:CA:910:A:H62	42:CN:12:MET:HA	1.77	0.50
31:CA:1665:A:H2'	31:CA:1666:G:O4'	2.10	0.50
31:CA:1779:U:H5	31:CA:1784:A:N7	2.09	0.50
31:CA:2028:U:H2'	31:CA:2029:G:C8	2.46	0.50
49:CU:45:ALA:O	49:CU:49:LYS:HG2	2.11	0.50
38:DJ:19:ASN:H	38:DJ:20:PRO:HD2	1.77	0.50
1:AA:1478:U:H2'	1:AA:1479:C:C6	2.46	0.50
16:AP:61:VAL:HG21	16:AP:67:ILE:HD11	1.92	0.50
31:CA:1101:U:H2'	31:CA:1102:C:C6	2.46	0.50
49:DU:54:GLU:HB3	49:DU:88:LYS:HD2	1.93	0.50
1:BA:1478:U:H2'	1:BA:1479:C:C6	2.47	0.50
5:BE:72:ILE:HG12	5:BE:145:GLU:HG3	1.94	0.50
11:BK:45:ALA:HB3	11:BK:70:CYS:HB2	1.94	0.50
19:BS:15:LEU:HD13	19:BS:33:THR:HG21	1.93	0.50
31:CA:1638:C:H5''	31:CA:2710:C:O2'	2.12	0.50
36:CG:95:ARG:HG2	36:CG:128:GLN:HB3	1.93	0.50
46:CR:76:TYR:CZ	46:CR:80:ILE:HG13	2.46	0.50
1:AA:412:A:H3'	1:AA:413:G:C5'	2.42	0.49
24:C3:2:LYS:HE2	31:CA:687:C:H5''	1.94	0.49
29:CC:154:LEU:HD13	29:CC:176:LEU:HD21	1.93	0.49
31:CA:639:U:H2'	31:CA:640:C:C6	2.46	0.49
31:CA:1936:A:H2	31:CA:1943:U:N3	2.02	0.49
31:CA:2267:A:H5''	31:CA:2268:A:H5'	1.94	0.49
31:CA:2350:C:H2'	31:CA:2351:G:O4'	2.12	0.49
33:DA:1171:G:H1'	33:DA:1179:G:N2	2.27	0.49
33:DA:1268:A:H2'	33:DA:1269:A:O4'	2.11	0.49
9:BI:19:VAL:HG22	9:BI:65:ILE:HG22	1.94	0.49
46:CR:112:LYS:HD3	47:CS:48:LYS:HG3	1.92	0.49
46:DR:76:TYR:CZ	46:DR:80:ILE:HG13	2.47	0.49
1:AA:299:G:H2'	1:AA:300:A:C8	2.46	0.49
14:AN:43:ASN:HA	14:AN:46:LEU:HD12	1.94	0.49
9:BI:120:LYS:HB2	9:BI:123:ARG:HB3	1.94	0.49
31:CA:574:A:C6	31:CA:2033:A:H5'	2.48	0.49
32:DD:186:LEU:HD21	45:DQ:4:ILE:HG21	1.93	0.49
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	1.94	0.49
16:BP:68:SER:HB3	69:BP:101:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:160:THR:HG22	29:CC:177:ARG:HG2	1.93	0.49
31:CA:727:A:H2'	31:CA:728:G:C8	2.48	0.49
33:DA:858:G:H3'	33:DA:859:G:C8	2.47	0.49
2:AB:12:ALA:HB1	2:AB:209:ALA:HA	1.95	0.49
6:AF:46:GLN:HA	6:AF:56:LYS:HG2	1.95	0.49
9:AI:19:VAL:HG22	9:AI:65:ILE:HG22	1.94	0.49
1:BA:1496:C:H2'	1:BA:1497:G:O4'	2.12	0.49
3:BC:47:LEU:HB3	3:BC:50:ALA:HB3	1.95	0.49
17:BQ:68:SER:OG	17:BQ:71:LYS:HB3	2.11	0.49
29:DC:29:PRO:HG2	29:DC:34:LEU:HD11	1.95	0.49
33:DA:102:U:H2'	33:DA:102:U:O2	2.13	0.49
33:DA:585:G:N7	46:DR:6:ARG:NH1	2.60	0.49
33:DA:2779:U:H5'	33:DA:2781:A:O4'	2.12	0.49
34:CE:46:GLN:HB3	34:CE:83:VAL:HG11	1.95	0.49
11:AK:29:ASN:HB2	11:AK:57:LYS:HE3	1.93	0.49
12:BL:55:VAL:HG21	12:BL:80:ILE:HD11	1.95	0.49
31:CA:2190:G:H2'	31:CA:2191:A:H8	1.78	0.49
33:DA:1223:G:P	47:DS:68:ARG:HH22	2.35	0.49
35:CF:44:ILE:HG21	35:CF:79:ILE:HG22	1.95	0.49
14:BN:43:ASN:HA	14:BN:46:LEU:HD12	1.93	0.49
69:DA:6392:HOH:O	43:DO:103:ARG:HA	2.13	0.49
40:CL:103:VAL:O	40:CL:122:VAL:HB	2.12	0.49
5:AE:133:PRO:O	5:AE:137:VAL:HG13	2.11	0.49
12:AL:31:ARG:O	12:AL:58:THR:HG23	2.12	0.49
13:AM:12:HIS:HB3	69:AM:303:HOH:O	2.12	0.49
33:DA:1430:G:H2'	33:DA:1431:A:O4'	2.12	0.49
33:DA:2273:A:H2'	33:DA:2274:A:C8	2.47	0.49
54:CZ:18:LEU:HB2	54:CZ:53:VAL:HG11	1.94	0.49
40:DL:113:MET:HE1	40:DL:116:ILE:HD11	1.95	0.49
55:DI:26:VAL:HB	55:DI:83:ALA:HB3	1.93	0.49
6:BF:46:GLN:HA	6:BF:56:LYS:HG2	1.94	0.49
50:DV:74:ASN:HD21	50:DV:99:ASN:ND2	2.11	0.49
7:BG:69:VAL:HG21	7:BG:104:ILE:HD11	1.93	0.49
33:DA:1999:C:H4'	33:DA:2723:C:O2	2.13	0.49
33:DA:2728:U:O2'	33:DA:2729:G:H5''	2.12	0.49
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	1.94	0.48
24:C3:1:MET:HE1	31:CA:1781:U:H5	1.78	0.48
31:CA:2718:G:OP1	45:CQ:98:TYR:HD2	1.96	0.48
1:BA:1493:A:H1'	31:CA:1913:A:H61	1.78	0.48
29:CC:105:LEU:H	29:CC:105:LEU:HD12	1.78	0.48
33:DA:784:G:O2'	33:DA:785:G:H5''	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:CE:58:LYS:HG3	34:CE:71:GLY:HA2	1.95	0.48
13:AM:85:CYS:HB2	19:AS:73:GLU:HB3	1.95	0.48
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.94	0.48
23:C2:25:LYS:HD2	23:C2:52:ALA:HB1	1.94	0.48
1:BA:299:G:H2'	1:BA:300:A:C8	2.47	0.48
1:BA:1238:A:H5'	1:BA:1336:C:H41	1.76	0.48
29:CC:29:PRO:HG2	29:CC:34:LEU:HD11	1.94	0.48
31:CA:20:C:H2'	31:CA:21:A:H8	1.78	0.48
31:CA:833:A:H2'	31:CA:834:G:C8	2.48	0.48
33:DA:1651:G:OP1	43:DO:40:LYS:HE3	2.14	0.48
34:CE:105:LEU:HD23	34:CE:108:ILE:HD11	1.95	0.48
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.48	0.48
17:AQ:17:MET:HG2	17:AQ:20:SER:HB2	1.96	0.48
13:BM:85:CYS:HB2	19:BS:73:GLU:HB3	1.96	0.48
31:CA:2636:C:H2'	31:CA:2637:U:C6	2.48	0.48
47:CS:49:ILE:HB	47:CS:51:VAL:O	2.13	0.48
55:DI:57:ASN:HD22	55:DI:76:PHE:C	2.22	0.48
1:BA:212:G:H2'	1:BA:213:G:C8	2.49	0.48
32:DD:114:LYS:HD3	32:DD:196:ALA:HB2	1.95	0.48
6:BF:81:ASN:HB3	6:BF:84:VAL:HG12	1.96	0.48
31:CA:1935:G:H1'	31:CA:1964:G:N2	2.28	0.48
6:BF:99:ALA:O	6:BF:100:SER:HB3	2.14	0.48
31:CA:694:U:OP1	31:CA:1569:A:H1'	2.13	0.48
29:DC:232:HIS:NE2	29:DC:244:PRO:HA	2.28	0.48
32:DD:150[B]:MEQ:HG3	33:DA:2032:G:N3	2.28	0.48
48:CT:84:ARG:HB2	48:CT:96:ILE:HB	1.96	0.48
31:CA:668:A:H2'	31:CA:670:A:H62	1.78	0.48
31:CA:1931:U:H2'	31:CA:1932:A:H8	1.79	0.48
1:BA:79:G:H22	1:BA:90:C:H42	1.61	0.48
1:BA:1003:G:H21	1:BA:1005:A:H5'	1.79	0.48
33:DA:1720:U:H2'	33:DA:1721:G:O4'	2.13	0.48
33:DA:2314:A:H1'	35:DF:155:THR:HG21	1.96	0.48
34:CE:149:ILE:HD12	34:CE:172:ALA:HA	1.95	0.48
37:CH:15:LEU:HD22	37:CH:15:LEU:H	1.79	0.48
1:AA:1277:C:O2'	1:AA:1279:G:H8	1.97	0.48
5:AE:157:ARG:HD2	8:AH:43:GLU:O	2.14	0.48
7:AG:72:THR:HG23	7:AG:73:VAL:HG22	1.95	0.48
10:AJ:52:LEU:HB2	14:AN:81:ARG:HD2	1.96	0.48
1:BA:76:G:H1	1:BA:93:U:H3	1.62	0.48
44:CP:18:LEU:HD23	44:CP:25:ARG:HD3	1.96	0.48
31:CA:1677:A:H5''	69:CA:3685:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1783:A:C2	31:CA:2588:G:O4'	2.67	0.47
29:DC:231:PRO:HA	69:DC:304:HOH:O	2.14	0.47
11:AK:25:ALA:HA	11:AK:30:THR:HG22	1.96	0.47
1:BA:1277:C:O2'	1:BA:1279:G:H8	1.97	0.47
35:CF:103:LEU:HA	35:CF:107:ALA:HB3	1.96	0.47
22:C1:25:VAL:HG13	22:C1:26:THR:H	1.80	0.47
2:BB:12:ALA:HB1	2:BB:209:ALA:HA	1.95	0.47
2:BB:166:ALA:HB3	2:BB:191:SER:HB3	1.96	0.47
31:CA:831:G:O5'	31:CA:831:G:H8	1.97	0.47
31:CA:1716:U:H2'	31:CA:1717:A:H8	1.78	0.47
31:CA:1775:U:H2'	31:CA:1776:G:O4'	2.14	0.47
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.49	0.47
28:DB:90:C:H5'	42:DN:18[B]:ARG:HG3	1.96	0.47
33:DA:2128:G:H1	33:DA:2160:C:N4	2.11	0.47
1:AA:673:A:H2'	1:AA:674:G:C8	2.49	0.47
6:AF:38:ARG:HE	6:AF:63:ASN:ND2	2.13	0.47
9:AI:120:LYS:HB2	9:AI:123:ARG:HB3	1.95	0.47
12:BL:50:ARG:HB3	12:BL:66:TYR:HE1	1.80	0.47
29:CC:174:LEU:CD2	29:CC:184:VAL:HB	2.44	0.47
31:CA:20:C:H2'	31:CA:21:A:C8	2.48	0.47
31:CA:1447:C:H2'	31:CA:1448:G:H8	1.80	0.47
31:CA:2428:G:H22	41:CM:60:ARG:NH2	2.12	0.47
29:DC:154:LEU:HD13	29:DC:176:LEU:HD21	1.95	0.47
35:DF:128:TYR:HD2	35:DF:156:ILE:HD12	1.79	0.47
2:AB:166:ALA:HB3	2:AB:191:SER:HB3	1.96	0.47
22:D1:4:GLN:HA	33:DA:2615:U:C2	2.48	0.47
31:CA:2718:G:O2'	45:CQ:96:LYS:HG3	2.15	0.47
33:DA:659:G:H4'	34:DE:95:LYS:HD3	1.95	0.47
33:DA:2291:U:H2'	33:DA:2292:U:C6	2.49	0.47
1:BA:562:U:H1'	12:BL:12:ARG:HD2	1.97	0.47
3:BC:22:TRP:HB3	3:BC:59:ARG:H	1.79	0.47
3:BC:33:LEU:HD21	14:BN:93:ILE:HG12	1.96	0.47
35:DF:103:LEU:HA	35:DF:107:ALA:HB3	1.97	0.47
1:AA:216:U:H2'	1:AA:217:C:C6	2.49	0.47
1:AA:1003:G:H21	1:AA:1005:A:H5'	1.79	0.47
58:AA:1671:MPD:H31	20:AT:24:ARG:NH1	2.29	0.47
1:BA:216:U:H2'	1:BA:217:C:C6	2.50	0.47
3:BC:23:PHE:CD2	10:BJ:97:ASP:HB2	2.49	0.47
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	1.97	0.47
31:CA:381:G:OP1	53:CY:18:ARG:HD3	2.15	0.47
31:CA:1154:G:OP1	46:CR:58:ARG:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DA:476:G:H4'	33:DA:502:A:N1	2.30	0.47
33:DA:1187:G:H5''	47:DS:83:TYR:CE1	2.49	0.47
33:DA:2133:G:H21	33:DA:2158:A:N6	2.13	0.47
33:DA:2328:A:H2'	33:DA:2329:U:C6	2.49	0.47
33:DA:2547:A:H4'	40:DL:29:HIS:NE2	2.30	0.47
33:DA:2636:C:H2'	33:DA:2637:U:C6	2.48	0.47
40:CL:42:THR:HG23	40:CL:44:LYS:HE2	1.97	0.47
42:CN:40:ARG:HD3	42:CN:93:VAL:HG21	1.97	0.47
34:DE:58:LYS:HG3	34:DE:71:GLY:HA2	1.95	0.47
55:DI:126:LEU:HA	55:DI:129:LEU:HD12	1.96	0.47
1:AA:1496:C:H2'	1:AA:1497:G:O4'	2.14	0.47
8:AH:2:SER:HB2	8:AH:4:GLN:HE21	1.79	0.47
10:AJ:87:LEU:HA	10:AJ:90:LEU:HD12	1.95	0.47
27:D0:45:ARG:HH12	27:D0:59:GLU:CD	2.22	0.47
31:CA:1405:U:H2'	31:CA:1406:U:C6	2.49	0.47
33:DA:1716:U:H2'	33:DA:1717:A:H8	1.78	0.47
35:DF:44:ILE:HG21	35:DF:79:ILE:HG22	1.95	0.47
55:DI:23:LEU:HD13	55:DI:89:PRO:HD3	1.97	0.47
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	1.95	0.47
10:BJ:52:LEU:HB2	14:BN:81:ARG:HD2	1.97	0.47
31:CA:1703:G:H2'	31:CA:1704:C:C6	2.50	0.47
23:C2:6:ARG:HG2	23:C2:24:THR:HB	1.97	0.47
3:BC:148:GLY:HA3	3:BC:172:ARG:O	2.15	0.47
21:BU:51:SER:HA	21:BU:54:LYS:HE3	1.97	0.47
31:CA:396:G:H1'	53:CY:29:PHE:HB3	1.97	0.47
33:DA:1754:A:C8	45:DQ:94:LYS:HE2	2.50	0.47
34:CE:108:ILE:HG22	41:CM:1:MET:SD	2.55	0.47
47:CS:38:VAL:HG22	47:CS:57:GLY:HA3	1.97	0.47
35:DF:104:ILE:HG23	35:DF:176:PRO:HD3	1.97	0.47
50:DV:51:ALA:O	50:DV:52:LEU:HB2	2.15	0.47
21:AU:4:ILE:HG13	21:AU:19:PHE:HA	1.97	0.46
22:D1:25:VAL:HG11	48:DT:38:TYR:HB2	1.97	0.46
31:CA:644:A:H2'	31:CA:645:C:O4'	2.15	0.46
32:DD:38:LYS:O	32:DD:46:ARG:HA	2.15	0.46
35:CF:8:TYR:HA	35:CF:12:VAL:HB	1.97	0.46
39:CK:35:ARG:HH21	39:CK:140:LEU:HD11	1.79	0.46
40:DL:15:GLY:HA2	40:DL:47:ILE:HG12	1.97	0.46
20:AT:39:ILE:HG23	20:AT:86:LEU:HD11	1.97	0.46
11:BK:25:ALA:HA	11:BK:30:THR:HG22	1.97	0.46
31:CA:139:U:H3	49:CU:2:ILE:HG21	1.80	0.46
33:DA:1794:A:H2'	33:DA:1795:C:H6	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:58:LYS:HA	4:AD:200:ILE:HG12	1.97	0.46
1:BA:845:A:O5'	1:BA:845:A:H8	1.98	0.46
17:BQ:31:HIS:HE1	17:BQ:33:ILE:HD12	1.80	0.46
23:D2:6:ARG:HG2	23:D2:24:THR:HB	1.96	0.46
31:CA:320:A:H4'	31:CA:322:A:N7	2.29	0.46
31:CA:845:A:H61	31:CA:932:U:H3	1.63	0.46
32:DD:152:PRO:HB2	32:DD:154:LYS:HG2	1.97	0.46
33:DA:1190:G:H5''	41:DM:32:GLY:HA2	1.97	0.46
50:DV:14:LEU:HD11	50:DV:71:ALA:HB2	1.98	0.46
22:C1:8:PRO:HG2	31:CA:1264:A:H5'	1.97	0.46
27:C0:31:ARG:HD3	31:CA:1158:C:H5''	1.97	0.46
31:CA:2596:U:H2'	31:CA:2597:G:C8	2.51	0.46
41:CM:28:GLY:O	41:CM:29:LYS:C	2.58	0.46
36:DG:24:ILE:HD13	36:DG:72:LEU:HD21	1.97	0.46
31:CA:965:C:H5''	69:CA:3770:HOH:O	2.15	0.46
43:CO:103:ARG:HD3	43:CO:110:MET:SD	2.56	0.46
1:AA:202:G:H21	1:AA:466:A:H61	1.64	0.46
1:BA:1391:U:H2'	1:BA:1392:G:C8	2.51	0.46
5:BE:72:ILE:HG13	5:BE:73:ASN:N	2.30	0.46
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	1.96	0.46
31:CA:751:A:H5'	48:CT:90:LYS:HA	1.98	0.46
33:DA:278:A:N3	33:DA:278:A:H2'	2.31	0.46
33:DA:1509:A:O2'	33:DA:1510:G:H8	1.99	0.46
33:DA:2849:U:H4'	33:DA:2868:A:C2	2.51	0.46
35:CF:104:ILE:HG23	35:CF:176:PRO:HD3	1.97	0.46
42:CN:71:LYS:HB3	42:CN:93:VAL:O	2.16	0.46
9:AI:55:VAL:HG22	9:AI:94:LEU:HD22	1.96	0.46
1:BA:390:U:H2'	1:BA:391:G:C8	2.50	0.46
21:BU:4:ILE:HG13	21:BU:19:PHE:HA	1.98	0.46
29:CC:88:SER:HB2	29:CC:158:ALA:HB2	1.96	0.46
30:CD:114:LYS:HD3	30:CD:196:ALA:HB2	1.97	0.46
31:CA:1838:C:N4	31:CA:1898:U:H2'	2.30	0.46
31:CA:2185:U:H2'	31:CA:2186:G:C8	2.51	0.46
31:CA:2642:G:H5'	39:CK:80:HIS:CG	2.51	0.46
49:CU:69:ARG:HB2	49:CU:74:ILE:HG22	1.97	0.46
40:DL:42:THR:HG23	40:DL:44:LYS:HE2	1.98	0.46
1:AA:108:G:H5'	1:AA:109:A:H5''	1.98	0.46
8:BH:2:SER:HB2	8:BH:4:GLN:HE21	1.81	0.46
10:BJ:26:VAL:HG21	10:BJ:39:PRO:HD3	1.97	0.46
33:DA:1532:A:H5''	33:DA:1532:A:H8	1.81	0.46
3:AC:33:LEU:HD21	14:AN:93:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:177:LYS:HB3	4:AD:179:GLU:HG2	1.98	0.46
9:BI:116:VAL:HG21	10:BJ:62:ARG:HB2	1.98	0.46
31:CA:2025:C:H2'	31:CA:2026:U:C6	2.50	0.46
29:DC:17:VAL:HB	29:DC:204:VAL:HB	1.97	0.46
33:DA:2629:U:C5	59:DA:3193:PUT:H12	2.51	0.46
1:AA:505:G:H5'	1:AA:534:U:C2	2.51	0.46
2:AB:129:LEU:H	2:AB:129:LEU:HG	1.56	0.46
4:BD:48:LEU:HD21	4:BD:56:ARG:HG3	1.97	0.46
4:BD:177:LYS:HB3	4:BD:179:GLU:HG2	1.96	0.46
31:CA:278:A:N3	31:CA:278:A:H2'	2.31	0.46
33:DA:250:G:H2'	33:DA:251:A:C8	2.51	0.46
37:CH:27:ARG:HH12	37:CH:38:PRO:HG3	1.81	0.46
55:DI:44:ALA:HB1	55:DI:95:LEU:HD11	1.98	0.46
1:AA:562:U:H1'	12:AL:12:ARG:HD2	1.96	0.45
1:AA:1343:G:H2'	1:AA:1344:C:C6	2.51	0.45
4:BD:85:ASN:HA	5:BE:102:GLY:CA	2.35	0.45
31:CA:1380:G:H2'	31:CA:1381:G:H8	1.81	0.45
31:CA:2010:G:H5''	48:CT:42:LYS:HB2	1.98	0.45
35:DF:8:TYR:HA	35:DF:12:VAL:HB	1.97	0.45
47:DS:24:LYS:HD2	63:DS:201:PGE:H22	1.97	0.45
17:AQ:31:HIS:HE1	17:AQ:33:ILE:HD12	1.81	0.45
31:CA:1454:C:H1'	43:CO:60:VAL:HG13	1.97	0.45
31:CA:1794:A:H2'	31:CA:1795:C:H6	1.81	0.45
28:DB:49:C:H3'	69:DB:353:HOH:O	2.17	0.45
33:DA:1028:A:N6	33:DA:1125:G:H2'	2.31	0.45
40:CL:15:GLY:HA2	40:CL:47:ILE:HG12	1.97	0.45
49:DU:34:VAL:HG11	49:DU:43:ILE:HG12	1.99	0.45
1:BA:407:U:H2'	1:BA:408:A:C8	2.51	0.45
33:DA:388:G:N7	33:DA:390:U:H2'	2.31	0.45
33:DA:624:C:O2'	33:DA:657:U:H5''	2.16	0.45
33:DA:783:A:N3	33:DA:783:A:H2'	2.30	0.45
33:DA:811:U:H2'	41:DM:21:ARG:HA	1.97	0.45
33:DA:1756:G:H1'	69:DA:6693:HOH:O	2.16	0.45
33:DA:2751:G:H2'	69:DA:5074:HOH:O	2.15	0.45
55:DI:3:LEU:HD12	55:DI:56:ARG:CZ	2.46	0.45
1:AA:6:G:H22	5:AE:103:THR:CG2	2.30	0.45
5:AE:57:PRO:O	5:AE:60:ILE:HG13	2.16	0.45
1:BA:310:G:H5''	16:BP:31:ARG:HB2	1.97	0.45
1:BA:1012:A:H61	1:BA:1017:U:H3	1.64	0.45
31:CA:1357:C:H2'	31:CA:1358:G:O4'	2.15	0.45
37:CH:4:ILE:HD11	37:CH:44:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:CK:16:TYR:HE1	39:CK:138:GLN:HE21	1.63	0.45
2:AB:41:ILE:HD13	2:AB:202:GLY:HA2	1.98	0.45
1:BA:73:C:O2'	1:BA:74:A:H8	1.98	0.45
2:BB:41:ILE:HD13	2:BB:202:GLY:HA2	1.98	0.45
27:D0:9:GLN:HB2	27:D0:29:LEU:HD22	1.98	0.45
31:CA:309:A:H4'	50:CV:16:GLY:HA2	1.99	0.45
31:CA:2251:OMG:HM23	31:CA:2251:OMG:H1'	1.84	0.45
30:CD:26:VAL:HG21	45:CQ:5:ILE:HG12	1.99	0.45
31:CA:136:G:H1	31:CA:143:C:H42	1.65	0.45
31:CA:2842:G:H2'	31:CA:2843:G:O4'	2.16	0.45
28:DB:111:U:H2'	28:DB:112:G:H8	1.82	0.45
33:DA:2262:U:H2'	33:DA:2263:C:H6	1.81	0.45
1:AA:1012:A:H61	1:AA:1017:U:H3	1.64	0.45
9:AI:116:VAL:HG21	10:AJ:62:ARG:HB2	1.99	0.45
25:C4:60:ALA:O	41:CM:48:ARG:HD2	2.17	0.45
31:CA:1783:A:H5'	31:CA:2608:G:H4'	1.99	0.45
31:CA:2339:C:H2'	31:CA:2340:A:C8	2.52	0.45
33:DA:2313:C:H5''	35:DF:88:LYS:HD3	1.99	0.45
48:DT:84:ARG:HB2	48:DT:96:ILE:HB	1.99	0.45
1:BA:518:C:H2'	1:BA:530:G:C8	2.51	0.45
1:BA:1347:G:N2	1:BA:1373:G:H2'	2.32	0.45
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	1.99	0.45
4:BD:58:LYS:HA	4:BD:200:ILE:HG12	1.97	0.45
7:BG:111:ARG:HB3	7:BG:119:ARG:HG2	1.99	0.45
33:DA:136:G:H1	33:DA:143:C:H42	1.65	0.45
1:AA:73:C:O2'	1:AA:74:A:H8	1.98	0.45
1:BA:649:A:H2'	1:BA:650:G:O4'	2.17	0.45
29:CC:162:VAL:HG22	29:CC:176:LEU:HA	1.99	0.45
31:CA:706:A:H2'	31:CA:707:G:O4'	2.17	0.45
31:CA:863:A:H2'	31:CA:864:G:C8	2.52	0.45
33:DA:833:A:H2'	33:DA:834:G:C8	2.52	0.45
33:DA:1141:U:H4'	33:DA:1142:A:O4'	2.17	0.45
44:DP:41:ALA:HB2	44:DP:48:LEU:HD21	1.99	0.45
1:AA:1347:G:N2	1:AA:1373:G:H2'	2.32	0.45
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.52	0.45
7:AG:111:ARG:HB3	7:AG:119:ARG:HG2	1.99	0.45
5:BE:57:PRO:O	5:BE:60:ILE:HG13	2.17	0.45
22:D1:9:THR:CG2	33:DA:2020:A:H5'	2.46	0.45
29:CC:212:ARG:HD2	29:CC:216:VAL:O	2.17	0.45
31:CA:1788:C:H6	31:CA:1788:C:O5'	2.00	0.45
47:DS:26:ASP:HA	63:DS:201:PGE:H52	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:523:A:H61	12:AL:89:D2T:CG	2.31	0.44
1:BA:350:G:H5''	20:BT:3:ASN:HD22	1.82	0.44
1:BA:505:G:H5'	1:BA:534:U:C2	2.51	0.44
1:BA:523:A:H61	12:BL:89:D2T:CG	2.30	0.44
5:BE:90:THR:HG22	5:BE:91:GLY:H	1.82	0.44
16:BP:20:VAL:HG13	16:BP:32:PHE:HB2	1.99	0.44
31:CA:822:G:O6	31:CA:943:A:H2	1.99	0.44
33:DA:2086:U:H2'	33:DA:2087:G:C8	2.52	0.44
42:CN:30:SER:H	42:CN:106:ASP:HB3	1.82	0.44
1:AA:619:U:C2	4:AD:132:ILE:HD11	2.52	0.44
1:BA:8:A:C6	4:BD:206:LYS:HB3	2.52	0.44
1:BA:774:G:H21	57:BA:1642:PG4:H62	1.82	0.44
31:CA:193:U:H5	69:CA:3405:HOH:O	2.01	0.44
31:CA:1121:C:H2'	31:CA:1122:G:O4'	2.17	0.44
31:CA:1532:A:H8	31:CA:1532:A:H5''	1.83	0.44
33:DA:1357:C:H2'	33:DA:1358:G:O4'	2.17	0.44
36:DG:52:PHE:CD1	36:DG:52:PHE:N	2.85	0.44
1:AA:212:G:H2'	1:AA:213:G:C8	2.52	0.44
1:AA:390:U:H2'	1:AA:391:G:C8	2.53	0.44
16:BP:5:ARG:HB3	69:BP:101:HOH:O	2.16	0.44
30:CD:62:LYS:HE2	31:CA:2810:A:H5''	1.99	0.44
31:CA:247:G:H4'	31:CA:386:G:C5	2.52	0.44
33:DA:2339:C:H2'	33:DA:2340:A:C8	2.52	0.44
33:DA:2502:G:H5''	33:DA:2503:2MA:H5''	1.99	0.44
44:CP:51:ALA:HB3	44:CP:78:VAL:HG13	2.00	0.44
1:AA:77:A:H2'	1:AA:78:A:C8	2.53	0.44
8:AH:105:SER:HB2	8:AH:126:ILE:HD11	1.99	0.44
18:AR:36:SER:HA	18:AR:72:ASP:HB3	1.98	0.44
6:BF:91:ARG:HD2	18:BR:61:ARG:HH22	1.83	0.44
29:CC:50:THR:O	31:CA:1805:A:H1'	2.18	0.44
31:CA:729:G:H2'	31:CA:1775:U:H1'	2.00	0.44
31:CA:1182:G:H2'	31:CA:1183:U:O4'	2.17	0.44
31:CA:1681:G:O2'	31:CA:1762:A:H2'	2.18	0.44
28:DB:28:C:P	44:DP:31:THR:HG21	2.57	0.44
29:DC:49:ILE:HD11	33:DA:779:U:H5''	1.99	0.44
33:DA:634:C:H2'	33:DA:635:C:C6	2.53	0.44
36:CG:24:ILE:HG21	36:CG:72:LEU:HD21	1.99	0.44
36:DG:145:ALA:HB1	36:DG:164:TYR:HE1	1.82	0.44
48:DT:20:VAL:HA	48:DT:23:LEU:HD12	1.98	0.44
1:AA:76:G:H1	1:AA:93:U:H3	1.64	0.44
1:AA:407:U:H2'	1:AA:408:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:649:A:H2'	1:AA:650:G:O4'	2.17	0.44
2:AB:111:ILE:HD12	2:AB:152:LYS:HA	1.99	0.44
3:AC:22:TRP:HB3	3:AC:59:ARG:H	1.82	0.44
11:AK:89:PRO:HA	11:AK:93:ARG:HD2	2.00	0.44
14:AN:83:LYS:HG3	69:AN:207:HOH:O	2.16	0.44
20:BT:69:LYS:H	20:BT:69:LYS:HG3	1.55	0.44
31:CA:281:C:H2'	31:CA:282:A:C8	2.53	0.44
31:CA:962:G:H4'	31:CA:2496:C:O2'	2.18	0.44
31:CA:2006:C:H2'	31:CA:2007:U:C6	2.52	0.44
31:CA:2544:G:H5'	31:CA:2645:G:C2	2.53	0.44
31:CA:2800:A:C2	31:CA:2895:G:H1'	2.52	0.44
29:DC:16:VAL:HG22	29:DC:206:GLY:HA3	2.00	0.44
29:DC:162:VAL:HG22	29:DC:176:LEU:HA	1.99	0.44
36:CG:145:ALA:HB1	36:CG:164:TYR:HE1	1.83	0.44
43:DO:31:HIS:C	43:DO:33:ILE:H	2.25	0.44
7:AG:81:GLY:C	7:AG:83:SER:H	2.25	0.44
5:BE:105:ILE:H	5:BE:123:VAL:H	1.64	0.44
13:BM:6:GLY:O	13:BM:7:ILE:HG13	2.18	0.44
26:D5:36:ARG:HH22	33:DA:2539:C:H4'	1.83	0.44
30:CD:152:PRO:HB2	30:CD:154:LYS:HG2	1.99	0.44
31:CA:321:U:H5''	34:CE:131:THR:HG23	1.99	0.44
33:DA:1168:G:H2'	33:DA:1169:A:O4'	2.17	0.44
33:DA:2298:A:H61	33:DA:2318:G:H1'	1.83	0.44
48:CT:20:VAL:HA	48:CT:23:LEU:HD12	1.99	0.44
40:DL:70:ARG:HD3	40:DL:76:VAL:HG22	2.00	0.44
1:BA:21:G:H2'	1:BA:22:G:C8	2.52	0.44
9:BI:55:VAL:HG22	9:BI:94:LEU:HD22	1.99	0.44
14:BN:53:ARG:HH21	19:BS:37:ARG:HH22	1.65	0.44
29:DC:212:ARG:HD2	29:DC:216:VAL:O	2.18	0.44
33:DA:722:A:H2'	33:DA:723:C:O4'	2.18	0.44
33:DA:1928:A:H2'	33:DA:1929:G:O4'	2.18	0.44
57:DA:3191:PG4:H12	52:DX:11:ARG:HG2	1.99	0.44
1:AA:518:C:H2'	1:AA:530:G:C8	2.52	0.44
1:AA:738:C:H5''	6:AF:68:GLN:HG2	2.00	0.44
7:AG:50:LEU:HD22	7:AG:124:LEU:HD13	1.99	0.44
10:AJ:46:LYS:HG2	10:AJ:68:ARG:HG2	1.99	0.44
1:BA:240:G:H4'	1:BA:240:G:OP1	2.17	0.44
1:BA:972:C:H4'	10:BJ:59:LYS:HG2	2.00	0.44
8:BH:105:SER:HB2	8:BH:126:ILE:HD11	2.00	0.44
11:BK:89:PRO:HA	11:BK:93:ARG:HD2	1.99	0.44
19:BS:33:THR:HG22	19:BS:35:SER:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BT:5:LYS:HB3	20:BT:7:ALA:H	1.82	0.44
31:CA:225:C:H2'	31:CA:226:A:O4'	2.18	0.44
31:CA:2607:G:H2'	31:CA:2608:G:O4'	2.17	0.44
36:CG:24:ILE:HD13	36:CG:72:LEU:HD21	1.99	0.44
42:DN:42:THR:HG22	42:DN:93:VAL:HG12	2.00	0.44
5:AE:90:THR:HG22	5:AE:91:GLY:H	1.83	0.44
7:AG:31:MET:HE3	7:AG:34:GLY:HA2	2.00	0.44
14:BN:31:ILE:HG23	14:BN:42:TRP:HZ2	1.83	0.44
61:D1:102:PEG:H12	33:DA:2008:C:H5''	1.99	0.44
31:CA:1326:U:H2'	31:CA:1327:A:H8	1.83	0.44
29:DC:78:VAL:HG21	29:DC:110:LEU:HD21	2.00	0.44
33:DA:74:A:H5''	33:DA:74:A:N3	2.33	0.44
3:BC:14:ILE:HG21	3:BC:178:LEU:HB3	2.00	0.43
7:BG:31:MET:HE3	7:BG:34:GLY:HA2	2.00	0.43
28:CB:111:U:H2'	28:CB:112:G:H8	1.84	0.43
31:CA:2326:C:O2'	31:CA:2327:A:H8	2.02	0.43
37:DH:71:LYS:HB3	37:DH:108:VAL:HG22	2.00	0.43
45:DQ:106:LYS:HA	45:DQ:109:ARG:HD3	2.00	0.43
52:DX:23:VAL:HA	52:DX:38:VAL:HG23	1.99	0.43
1:AA:310:G:H5''	16:AP:31:ARG:HB2	1.99	0.43
3:AC:14:ILE:HG21	3:AC:178:LEU:HB3	2.00	0.43
11:BK:67:ALA:HB2	11:BK:96:THR:HG23	1.99	0.43
29:CC:48:ARG:HD3	31:CA:773:U:O2'	2.18	0.43
31:CA:1183:U:H2'	31:CA:1184:U:C6	2.53	0.43
31:CA:2298:A:H61	31:CA:2318:G:H1'	1.83	0.43
33:DA:142:A:H2'	33:DA:143:C:C6	2.52	0.43
33:DA:2741:A:H2'	33:DA:2742:G:O4'	2.18	0.43
20:AT:27:MET:HE2	20:AT:27:MET:HB3	1.93	0.43
1:BA:1001:C:H2'	1:BA:1002:G:H8	1.83	0.43
1:BA:1343:G:H2'	1:BA:1344:C:C6	2.52	0.43
31:CA:56:A:H61	31:CA:114:U:H3	1.66	0.43
31:CA:1434:A:H2'	31:CA:1435:G:C8	2.53	0.43
33:DA:281:C:H2'	33:DA:282:A:C8	2.53	0.43
33:DA:909:A:O2'	33:DA:910:A:H5'	2.18	0.43
11:AK:67:ALA:HB2	11:AK:96:THR:HG23	1.99	0.43
7:BG:81:GLY:C	7:BG:83:SER:H	2.26	0.43
30:CD:38:LYS:O	30:CD:46:ARG:HA	2.18	0.43
31:CA:373:U:H2'	31:CA:374:A:C8	2.53	0.43
33:DA:571:U:H3'	47:DS:80:ARG:NH2	2.33	0.43
1:BA:619:U:H3	4:BD:131:ASN:HB3	1.83	0.43
3:BC:40:ARG:HG2	3:BC:55:ILE:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:153:VAL:HG12	3:BC:198:VAL:HG22	2.00	0.43
31:CA:785:G:O2'	31:CA:1779:U:H5''	2.18	0.43
33:DA:1604:C:H5'	69:DA:5598:HOH:O	2.19	0.43
33:DA:1975:G:H21	63:DA:3222:PGE:C2	2.31	0.43
44:DP:102:ARG:HD2	69:DP:317:HOH:O	2.17	0.43
1:BA:108:G:H5'	1:BA:109:A:H5''	2.00	0.43
1:BA:1108:G:H5''	3:BC:176:HIS:CE1	2.54	0.43
10:BJ:46:LYS:HG2	10:BJ:68:ARG:HG2	1.99	0.43
24:D3:2:LYS:HE2	33:DA:687:C:H5''	1.99	0.43
31:CA:142:A:H2'	31:CA:143:C:C6	2.52	0.43
31:CA:787:C:H5''	31:CA:788:A:H5'	2.01	0.43
33:DA:191:A:H2'	33:DA:192:C:C6	2.54	0.43
33:DA:2028:U:H2'	33:DA:2029:G:O4'	2.19	0.43
33:DA:2255:G:H21	68:DA:3217:TRS:H12	1.84	0.43
43:CO:31:HIS:C	43:CO:33:ILE:H	2.27	0.43
36:DG:24:ILE:HG21	36:DG:72:LEU:HD21	1.98	0.43
44:DP:51:ALA:HB3	44:DP:78:VAL:HG13	2.00	0.43
1:BA:59:A:H5''	1:BA:387:U:H5''	1.99	0.43
2:BB:129:LEU:H	2:BB:129:LEU:HG	1.56	0.43
11:BK:101:ASN:HD22	11:BK:107:ILE:HG12	1.83	0.43
22:D1:48:TYR:CE1	22:D1:53:LYS:HD3	2.54	0.43
31:CA:95:A:H4'	54:CZ:38:GLN:O	2.19	0.43
31:CA:190:A:H2'	31:CA:191:A:O4'	2.18	0.43
31:CA:1509:A:O2'	31:CA:1510:G:H8	2.00	0.43
31:CA:2043:C:C6	31:CA:2043:C:H5''	2.54	0.43
33:DA:2097:A:H8	33:DA:2097:A:H5''	1.84	0.43
33:DA:2547:A:H2'	33:DA:2548:U:C6	2.53	0.43
40:CL:35:VAL:HB	40:CL:36:GLY:H	1.65	0.43
46:CR:58:ARG:HH11	46:CR:62:ILE:HD11	1.82	0.43
48:CT:36:LEU:HD13	48:CT:48:LYS:HA	2.00	0.43
49:CU:34:VAL:HG11	49:CU:43:ILE:HG12	2.00	0.43
51:CW:51:GLN:HG2	51:CW:86:LEU:HD11	2.00	0.43
43:DO:44:LEU:HD23	43:DO:113:ILE:HD13	1.99	0.43
1:AA:923:A:OP1	5:AE:26:LYS:HG2	2.18	0.43
12:AL:102:LEU:HB3	12:AL:103:ASP:H	1.65	0.43
21:AU:28:VAL:O	21:AU:32:VAL:HG23	2.18	0.43
5:BE:134:ILE:H	5:BE:134:ILE:HG13	1.68	0.43
12:BL:80:ILE:HD12	12:BL:97:THR:HG22	2.00	0.43
22:D1:22:LEU:HD23	61:D1:102:PEG:H31	2.01	0.43
31:CA:593:U:H2'	31:CA:594:U:C6	2.54	0.43
31:CA:1188:U:H2'	31:CA:1189:A:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1248:G:O2'	46:CR:3:ARG:HA	2.18	0.43
31:CA:1354:A:H2'	31:CA:1355:G:O4'	2.18	0.43
33:DA:1881:C:H2'	33:DA:1882:U:O4'	2.19	0.43
39:CK:35:ARG:HE	39:CK:140:LEU:HD21	1.83	0.43
38:DJ:11:LEU:HD22	38:DJ:24:VAL:HG23	2.01	0.43
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.84	0.43
1:AA:1416:G:H5''	69:AA:2080:HOH:O	2.18	0.43
4:AD:48:LEU:HD21	4:AD:56:ARG:HG3	2.00	0.43
1:BA:923:A:OP1	5:BE:26:LYS:HG2	2.19	0.43
31:CA:532:A:N3	31:CA:532:A:H2'	2.34	0.43
31:CA:588:U:H2'	31:CA:589:U:C6	2.53	0.43
31:CA:976:G:H2'	31:CA:977:G:H8	1.84	0.43
28:DB:77:U:H4'	69:DW:110:HOH:O	2.19	0.43
33:DA:735:A:H5''	69:DA:3598:HOH:O	2.19	0.43
33:DA:804:A:H2'	33:DA:806:C:C4	2.54	0.43
33:DA:1831:G:H1'	63:DA:3222:PGE:H22	2.01	0.43
33:DA:2869:G:H2'	33:DA:2870:C:O4'	2.19	0.43
41:CM:77:ILE:CD1	41:CM:108:ALA:HB1	2.39	0.43
51:DW:51:GLN:HG2	51:DW:86:LEU:HD11	2.01	0.43
54:DZ:56:LEU:HA	54:DZ:59:GLU:HG2	2.01	0.43
1:BA:77:A:H2'	1:BA:78:A:C8	2.54	0.43
31:CA:357:C:H2'	31:CA:358:U:C6	2.54	0.43
31:CA:1716:U:H2'	31:CA:1717:A:C8	2.54	0.43
33:DA:819:A:C4	33:DA:1189:A:C2	3.07	0.43
33:DA:1394:U:H4'	33:DA:1603:A:H4'	2.01	0.43
37:DH:41:LYS:HA	37:DH:44:ILE:HG12	2.00	0.43
39:DK:7:LYS:O	39:DK:11:VAL:HG23	2.18	0.43
55:DI:67:THR:CG2	55:DI:68:PRO:HA	2.48	0.43
1:AA:1137:C:H1'	1:AA:1138:G:N2	2.34	0.42
7:AG:59:LEU:H	7:AG:59:LEU:HG	1.65	0.42
14:AN:53:ARG:HH21	19:AS:37:ARG:HH22	1.66	0.42
1:BA:1137:C:H1'	1:BA:1138:G:N2	2.34	0.42
2:BB:100:MET:HA	2:BB:107:VAL:HG21	2.01	0.42
5:BE:47:GLY:HA3	5:BE:71:MET:HG2	2.01	0.42
29:CC:107:PRO:HD2	29:CC:110:LEU:HD22	2.01	0.42
31:CA:2822:G:H2'	31:CA:2823:A:H5''	2.00	0.42
37:CH:41:LYS:HA	37:CH:44:ILE:HG12	2.00	0.42
37:CH:71:LYS:HB3	37:CH:108:VAL:HG22	2.00	0.42
41:CM:19:LEU:HD23	41:CM:31:GLY:O	2.19	0.42
47:CS:59:ILE:HG12	47:CS:101:ILE:HD13	2.01	0.42
13:BM:11:ASP:HA	13:BM:45:ILE:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DA:419:U:H2'	33:DA:420:C:C6	2.53	0.42
33:DA:588:U:H2'	33:DA:589:U:C6	2.54	0.42
33:DA:1171:G:H1'	33:DA:1179:G:H22	1.83	0.42
54:CZ:56:LEU:HA	54:CZ:59:GLU:HG2	2.01	0.42
1:AA:246:A:N3	1:AA:247:G:H1'	2.33	0.42
5:AE:47:GLY:HA3	5:AE:71:MET:HG2	2.01	0.42
7:AG:132:GLY:H	7:AG:135:VAL:HG22	1.84	0.42
10:BJ:65:TYR:HB2	14:BN:96:LEU:HD11	2.02	0.42
33:DA:1680:U:H2'	33:DA:1681:G:O4'	2.19	0.42
33:DA:1746:A:H2'	33:DA:1747:U:C6	2.54	0.42
41:CM:77:ILE:HD12	41:CM:109:LYS:O	2.18	0.42
38:DJ:56:PRO:HD3	38:DJ:74:PRO:HA	2.01	0.42
47:DS:59:ILE:HG12	47:DS:101:ILE:HD13	2.01	0.42
49:DU:11:LEU:HD12	49:DU:50:LEU:HD12	2.01	0.42
55:DI:132:TYR:N	55:DI:133:GLU:HB2	2.33	0.42
19:AS:29:LYS:HB3	19:AS:30:PRO:HD2	2.02	0.42
1:BA:629:A:H2'	1:BA:630:A:O4'	2.19	0.42
7:BG:130:ASN:HA	7:BG:135:VAL:HG11	2.01	0.42
9:BI:19:VAL:HG11	9:BI:83:ILE:HA	2.01	0.42
29:CC:210:ALA:HA	29:CC:213:TRP:CE2	2.55	0.42
30:CD:13:ARG:NH1	31:CA:2683:C:H4'	2.35	0.42
31:CA:586:A:H5'	34:CE:84:THR:HG21	2.00	0.42
31:CA:1131:G:OP1	39:CK:82:GLY:HA2	2.19	0.42
31:CA:1454:C:H5'	43:CO:63:ARG:HH21	1.85	0.42
69:DB:321:HOH:O	44:DP:103:VAL:HG23	2.19	0.42
45:CQ:106:LYS:HA	45:CQ:109:ARG:HD3	2.01	0.42
53:DY:59:ILE:HG12	53:DY:67:VAL:HG21	2.01	0.42
1:AA:528:C:H5''	1:AA:528:C:H6	1.84	0.42
8:AH:18:GLN:HG2	8:AH:63:LEU:HD21	2.01	0.42
1:BA:524:G:H2'	1:BA:525:C:C6	2.54	0.42
5:BE:81:LEU:HB3	5:BE:147:MET:SD	2.59	0.42
7:BG:132:GLY:H	7:BG:135:VAL:HG22	1.84	0.42
12:BL:65:SER:HB2	12:BL:82:ILE:HD11	2.01	0.42
31:CA:128:C:H2'	31:CA:129:C:C6	2.55	0.42
31:CA:1881:C:H2'	31:CA:1882:U:O4'	2.20	0.42
32:DD:13:ARG:NH1	33:DA:2683:C:H4'	2.35	0.42
32:DD:121:THR:HB	32:DD:127:PHE:CD2	2.55	0.42
33:DA:1381:G:H1'	33:DA:1571:A:N1	2.35	0.42
33:DA:1716:U:H2'	33:DA:1717:A:C8	2.55	0.42
33:DA:2215:C:H2'	33:DA:2216:G:C8	2.54	0.42
47:CS:78:ARG:HB2	47:CS:83:TYR:HD1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:DN:30:SER:H	42:DN:106:ASP:HB3	1.84	0.42
1:BA:728:A:H2'	1:BA:729:A:C8	2.54	0.42
1:BA:1313:U:OP2	19:BS:6:LYS:HB3	2.19	0.42
31:CA:2271:G:H2'	31:CA:2272:U:C6	2.55	0.42
29:DC:227:PRO:HA	29:DC:233:GLY:HA2	2.01	0.42
32:DD:133:THR:HG21	33:DA:1676:A:H1'	2.02	0.42
33:DA:1938:A:H2'	69:DA:7933:HOH:O	2.19	0.42
33:DA:2577:A:H5''	33:DA:2578:G:H5'	2.00	0.42
62:DA:3206:EDO:H22	57:DR:203:PG4:H21	2.02	0.42
40:CL:35:VAL:CG1	40:CL:106:GLU:HG2	2.49	0.42
35:DF:14:LYS:O	35:DF:18:THR:HG22	2.19	0.42
1:AA:1182:G:H5'	1:AA:1184:G:H5'	2.02	0.42
3:AC:153:VAL:HG12	3:AC:198:VAL:HG22	2.00	0.42
1:BA:1530:G:H2'	1:BA:1531:A:C8	2.55	0.42
13:BM:86:TYR:CZ	13:BM:90:ARG:HD2	2.54	0.42
29:CC:78:VAL:HG21	29:CC:110:LEU:HD21	2.00	0.42
31:CA:1101:U:H2'	31:CA:1102:C:H6	1.85	0.42
31:CA:1434:A:H2'	31:CA:1435:G:H8	1.84	0.42
31:CA:2377:A:H2'	31:CA:2378:A:C8	2.55	0.42
29:DC:219:THR:O	33:DA:1789:A:H5''	2.20	0.42
33:DA:1425:G:H2'	33:DA:1426:G:O4'	2.20	0.42
38:CJ:11:LEU:HD22	38:CJ:24:VAL:HG23	2.02	0.42
50:CV:14:LEU:HD11	50:CV:71:ALA:HB2	2.01	0.42
34:DE:21:ARG:HD2	69:DE:417:HOH:O	2.18	0.42
1:AA:300:A:H2'	1:AA:301:G:O4'	2.20	0.42
4:BD:170:TRP:CD2	4:BD:186:PRO:HB3	2.54	0.42
5:BE:24:THR:HA	5:BE:29:ARG:HA	2.02	0.42
31:CA:686:U:H6	31:CA:788:A:N1	2.17	0.42
31:CA:722:A:H2'	31:CA:723:C:O4'	2.19	0.42
33:DA:832:U:H2'	33:DA:833:A:C8	2.55	0.42
53:CY:59:ILE:HG12	53:CY:67:VAL:HG21	2.02	0.42
40:DL:113:MET:CE	40:DL:116:ILE:HD11	2.49	0.42
16:AP:44:SER:C	16:AP:46:LYS:H	2.28	0.42
20:AT:44:LYS:H	20:AT:44:LYS:HG3	1.53	0.42
21:BU:28:VAL:O	21:BU:32:VAL:HG23	2.20	0.42
29:CC:174:LEU:HD21	29:CC:184:VAL:HB	2.02	0.42
31:CA:2345:G:N3	31:CA:2381:A:H2'	2.35	0.42
33:DA:118:A:C8	33:DA:119:A:C8	3.07	0.42
33:DA:514:A:H5'	46:DR:11:ARG:NH1	2.34	0.42
33:DA:593:U:H2'	33:DA:594:U:C6	2.55	0.42
69:DA:5611:HOH:O	34:DE:42:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:CJ:56:PRO:HD3	38:CJ:74:PRO:HA	2.01	0.42
1:AA:312:C:H2'	1:AA:313:A:C8	2.55	0.42
1:AA:1239:A:H62	1:AA:1299:A:H62	1.68	0.42
9:AI:19:VAL:HG11	9:AI:83:ILE:HA	2.02	0.42
14:AN:46:LEU:HA	14:AN:49:GLN:HE21	1.85	0.42
1:BA:300:A:H2'	1:BA:301:G:O4'	2.20	0.42
1:BA:1239:A:H62	1:BA:1299:A:H62	1.67	0.42
16:BP:40:ASN:O	16:BP:43:ALA:HB2	2.20	0.42
19:BS:29:LYS:HB3	19:BS:30:PRO:HD2	2.02	0.42
31:CA:825:A:H2'	31:CA:826:U:O4'	2.20	0.42
31:CA:1974:C:H2'	31:CA:1975:G:H8	1.85	0.42
33:DA:492:A:H2'	33:DA:493:G:O4'	2.20	0.42
33:DA:1101:U:H2'	33:DA:1102:C:H6	1.84	0.42
33:DA:1442:U:H2'	33:DA:1443:U:C6	2.54	0.42
33:DA:2678:C:H2'	33:DA:2679:A:O4'	2.19	0.42
43:CO:33:ILE:HB	43:CO:118:ARG:HD2	2.02	0.42
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.55	0.41
2:AB:100:MET:HA	2:AB:107:VAL:HG21	2.01	0.41
7:AG:130:ASN:HA	7:AG:135:VAL:HG11	2.01	0.41
14:BN:31:ILE:HG23	14:BN:42:TRP:CZ2	2.54	0.41
29:CC:227:PRO:HA	29:CC:233:GLY:HA2	2.02	0.41
30:CD:4:LEU:HD13	30:CD:29:VAL:HG11	2.02	0.41
31:CA:35:G:H2'	31:CA:36:G:O4'	2.19	0.41
31:CA:586:A:H1'	31:CA:672:C:H1'	2.02	0.41
31:CA:2101:A:H2'	31:CA:2102:G:H8	1.84	0.41
31:CA:2298:A:C2	31:CA:2321:U:N3	2.87	0.41
31:CA:2502:G:H5''	31:CA:2503:2MA:H5''	2.02	0.41
33:DA:2123:G:H1	33:DA:2175:C:H42	1.68	0.41
33:DA:2193:G:H2'	33:DA:2194:U:C6	2.55	0.41
35:CF:31:VAL:CG1	35:CF:97:TRP:CH2	3.03	0.41
34:DE:126:VAL:HA	58:DE:301:MPD:H13	2.01	0.41
42:DN:33:LEU:HD13	42:DN:117:PHE:HB3	2.02	0.41
48:DT:36:LEU:HD13	48:DT:48:LYS:HA	2.00	0.41
1:AA:8:A:C6	4:AD:206:LYS:HB3	2.55	0.41
1:AA:728:A:H2'	1:AA:729:A:C8	2.56	0.41
13:AM:86:TYR:CZ	13:AM:90:ARG:HD2	2.54	0.41
1:BA:227:G:H2'	1:BA:228:A:O4'	2.20	0.41
1:BA:677:U:H3	1:BA:713:G:H22	1.68	0.41
5:BE:23:LYS:HB3	5:BE:30:ILE:HG23	2.02	0.41
20:BT:67:ILE:O	20:BT:68:HIS:HB2	2.19	0.41
31:CA:514:A:H4'	46:CR:11:ARG:HH12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1310:G:H2'	31:CA:1311:G:O4'	2.21	0.41
31:CA:1442:U:H2'	31:CA:1443:U:C6	2.55	0.41
35:CF:138:PHE:HE1	35:CF:152:LEU:HD21	1.85	0.41
1:AA:620:C:H2'	1:AA:621:A:O4'	2.20	0.41
4:AD:170:TRP:CD2	4:AD:186:PRO:HB3	2.54	0.41
11:AK:34:ILE:HB	11:AK:74:VAL:HG11	2.02	0.41
31:CA:737:C:H2'	31:CA:738:G:O4'	2.20	0.41
33:DA:357:C:H2'	33:DA:358:U:C6	2.55	0.41
33:DA:1590:A:H2'	33:DA:1591:A:C8	2.55	0.41
53:CY:37:ARG:HG2	53:CY:48:THR:HG22	2.01	0.41
55:DI:94:ARG:HG2	55:DI:127:ALA:HA	2.02	0.41
1:AA:1216:A:H5''	14:AN:5:SER:HB3	2.03	0.41
1:BA:522:C:H41	12:BL:50:ARG:NH2	2.18	0.41
1:BA:1417:G:C6	1:BA:1482:G:C6	3.08	0.41
29:CC:245:VAL:HG12	29:CC:251:GLN:HA	2.02	0.41
30:CD:106:LYS:HD3	30:CD:174:SER:HB3	2.01	0.41
31:CA:1196:C:H1'	31:CA:1226:A:C4	2.55	0.41
31:CA:1274:A:N3	31:CA:1297:C:H1'	2.35	0.41
31:CA:1808:A:N1	53:CY:28:ARG:HD2	2.36	0.41
31:CA:1957:C:H5'	31:CA:1984:G:O2'	2.21	0.41
31:CA:2304:G:H22	31:CA:2312:U:H3	1.68	0.41
33:DA:1011:G:OP1	46:DR:75:SER:HB2	2.20	0.41
33:DA:2026:U:H2'	33:DA:2027:G:O4'	2.20	0.41
33:DA:2101:A:H2'	33:DA:2102:G:H8	1.86	0.41
38:CJ:24:VAL:HG22	38:CJ:28:LEU:HD22	2.03	0.41
39:CK:7:LYS:O	39:CK:11:VAL:HG23	2.21	0.41
41:CM:28:GLY:O	41:CM:29:LYS:O	2.39	0.41
48:DT:29:VAL:HB	48:DT:55:ILE:HD11	2.02	0.41
1:AA:413:G:H5''	1:AA:414:A:H5'	2.01	0.41
10:AJ:65:TYR:HB2	14:AN:96:LEU:HD11	2.01	0.41
11:AK:101:ASN:HD22	11:AK:107:ILE:HG12	1.84	0.41
8:BH:87:LYS:HB2	8:BH:125:ILE:CD1	2.45	0.41
13:BM:4:ILE:HA	13:BM:57:ARG:HG2	2.03	0.41
31:CA:188:G:H1	31:CA:208:C:H42	1.68	0.41
31:CA:582:A:H2'	31:CA:583:G:C8	2.55	0.41
31:CA:1835:2MG:HM23	31:CA:1836:C:H1'	2.02	0.41
29:DC:245:VAL:HG12	29:DC:251:GLN:HA	2.03	0.41
33:DA:1482:G:H1'	33:DA:1509:A:H61	1.85	0.41
33:DA:2428:G:H22	41:DM:60:ARG:NH2	2.15	0.41
33:DA:2633:G:H2'	33:DA:2634:A:O4'	2.21	0.41
43:DO:51:LEU:HD22	43:DO:51:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DI:50:VAL:HG13	55:DI:85:VAL:HG22	2.02	0.41
1:AA:910:C:O5'	1:AA:910:C:H6	2.04	0.41
5:AE:76:LEU:HD11	5:AE:120:VAL:HG22	2.03	0.41
25:D4:54:ASP:HB3	41:DM:57:LEU:HD22	2.02	0.41
31:CA:460:A:H2'	31:CA:461:C:O4'	2.20	0.41
31:CA:1587:G:H2'	31:CA:1588:G:H8	1.86	0.41
31:CA:1785:A:H2'	31:CA:1787:A:N7	2.35	0.41
31:CA:2114:A:N6	31:CA:2119:A:H62	2.18	0.41
41:CM:79:LEU:HD11	41:CM:112:LEU:HD12	2.01	0.41
37:DH:104:THR:HG22	37:DH:109:GLU:HA	2.02	0.41
1:AA:268:U:H2'	1:AA:269:C:C6	2.56	0.41
7:AG:57:SER:HB3	7:AG:60:GLU:HB2	2.03	0.41
1:BA:599:C:H4'	8:BH:122:GLY:C	2.46	0.41
1:BA:1053:G:N7	1:BA:1200:C:H5''	2.36	0.41
1:BA:1216:A:H5''	14:BN:5:SER:HB3	2.03	0.41
9:BI:36:GLU:HA	9:BI:45:ARG:HE	1.85	0.41
20:BT:24:ARG:O	20:BT:27:MET:HG3	2.20	0.41
22:D1:54:VAL:HG23	22:D1:55:ILE:HG12	2.03	0.41
31:CA:453:A:H4'	31:CA:472:A:H62	1.85	0.41
31:CA:1590:A:H2'	31:CA:1591:A:C8	2.56	0.41
31:CA:2688:G:H1'	31:CA:2721:A:H61	1.85	0.41
29:DC:50:THR:O	33:DA:1805:A:H1'	2.21	0.41
33:DA:118:A:N3	33:DA:178:G:H1'	2.36	0.41
43:CO:53:THR:HA	43:CO:56:LYS:HD2	2.01	0.41
1:AA:438:U:H5'	4:AD:120:HIS:HB3	2.03	0.41
1:AA:604:G:H2'	1:AA:605:U:O4'	2.21	0.41
1:AA:1338:G:H2'	1:AA:1339:A:C8	2.56	0.41
1:BA:23:C:H5	1:BA:561:U:O4	2.04	0.41
1:BA:429:U:H1'	1:BA:430:A:H5''	2.03	0.41
31:CA:754:U:H2'	31:CA:755:U:C6	2.56	0.41
33:DA:225:C:H2'	33:DA:226:A:O4'	2.20	0.41
33:DA:1172:C:C5	33:DA:1173:U:H1'	2.56	0.41
44:CP:28:VAL:HG11	44:CP:103:VAL:HG13	2.03	0.41
42:DN:63:ILE:HG12	42:DN:105:MET:HG3	2.03	0.41
51:DW:12:GLN:HB3	69:DW:126:HOH:O	2.20	0.41
1:AA:599:C:H4'	8:AH:122:GLY:C	2.46	0.41
1:AA:721:G:H4'	1:AA:722:G:O4'	2.20	0.41
7:AG:22:LEU:HD12	7:AG:62:PHE:HE2	1.86	0.41
17:AQ:15:ASP:HA	17:AQ:21:ILE:HG22	2.03	0.41
22:C1:6:ASN:ND2	31:CA:2020:A:H62	2.18	0.41
1:BA:374:A:H5''	1:BA:452:A:N1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:438:U:H5'	4:BD:120:HIS:HB3	2.02	0.41
1:BA:978:A:O2'	1:BA:1322:C:H5	2.04	0.41
2:BB:39:HIS:HB2	2:BB:189:THR:HG21	2.03	0.41
31:CA:600:G:H2'	31:CA:601:C:O4'	2.20	0.41
31:CA:1998:A:O3'	31:CA:2724:U:H4'	2.20	0.41
31:CA:2182:U:H2'	31:CA:2183:A:C8	2.56	0.41
31:CA:2798:U:H4'	31:CA:2799:A:H5'	2.02	0.41
29:DC:107:PRO:HD2	29:DC:110:LEU:HD22	2.03	0.41
32:DD:56:LYS:O	32:DD:60:VAL:HG23	2.20	0.41
33:DA:128:C:H2'	33:DA:129:C:C6	2.55	0.41
34:CE:108:ILE:HG21	34:CE:181:ILE:HD11	2.02	0.41
34:CE:117:ARG:HA	34:CE:185:LYS:HD3	2.03	0.41
49:CU:11:LEU:HD12	49:CU:50:LEU:HD12	2.03	0.41
43:DO:33:ILE:HB	43:DO:118:ARG:HD2	2.02	0.41
43:DO:53:THR:HA	43:DO:56:LYS:HD2	2.03	0.41
10:AJ:26:VAL:HG21	10:AJ:39:PRO:HD3	2.01	0.41
11:AK:34:ILE:HG21	11:AK:74:VAL:HG21	2.02	0.41
1:BA:502:A:H2'	1:BA:503:C:O4'	2.21	0.41
1:BA:580:C:H2'	1:BA:581:G:O4'	2.21	0.41
2:BB:130:THR:H	2:BB:133:GLU:HB2	1.85	0.41
19:BS:32:ARG:HA	19:BS:50:ALA:HB3	2.03	0.41
33:DA:1957:C:H5'	33:DA:1984:G:O2'	2.21	0.41
33:DA:2182:U:H2'	33:DA:2183:A:C8	2.56	0.41
9:AI:36:GLU:HA	9:AI:45:ARG:HE	1.86	0.40
1:BA:1356:G:H2'	1:BA:1357:A:C8	2.55	0.40
4:BD:91:LEU:HD21	4:BD:195:ILE:HG21	2.03	0.40
31:CA:2819:G:H2'	31:CA:2821:A:N7	2.36	0.40
29:DC:160:THR:HG21	33:DA:1819:A:H5''	2.03	0.40
33:DA:600:G:H2'	33:DA:601:C:O4'	2.20	0.40
33:DA:754:U:H2'	33:DA:755:U:C6	2.57	0.40
33:DA:839:U:H1'	33:DA:1191:G:H1'	2.02	0.40
43:CO:44:LEU:HD23	43:CO:113:ILE:HD13	2.02	0.40
1:AA:59:A:H5''	1:AA:387:U:H5''	2.03	0.40
1:AA:81:A:H2	1:AA:88:U:H3	1.69	0.40
3:AC:7:PRO:HD2	3:AC:184:TYR:CD1	2.56	0.40
6:AF:74:LEU:O	6:AF:77:THR:HG22	2.21	0.40
1:BA:868:C:H2'	1:BA:869:G:O4'	2.21	0.40
17:BQ:12:VAL:HG12	17:BQ:55:ILE:HA	2.04	0.40
31:CA:545:U:H2'	31:CA:546:U:O3'	2.20	0.40
31:CA:1556:C:H2'	31:CA:1557:C:C6	2.56	0.40
31:CA:1810:A:H2'	31:CA:1811:G:O4'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2193:G:H2'	31:CA:2194:U:C6	2.56	0.40
33:DA:414:C:H2'	33:DA:415:A:C8	2.56	0.40
33:DA:1169:A:H2'	33:DA:1170:C:O4'	2.22	0.40
33:DA:2544:G:H2'	33:DA:2545:G:O4'	2.20	0.40
48:CT:66:ILE:HA	48:CT:69:LEU:HD22	2.04	0.40
37:DH:4:ILE:HD11	37:DH:44:ILE:HG22	2.03	0.40
42:DN:57:VAL:HA	42:DN:112:LEU:HD21	2.03	0.40
48:DT:17:VAL:HB	48:DT:76:VAL:HG11	2.03	0.40
1:AA:502:A:H2'	1:AA:503:C:O4'	2.21	0.40
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.56	0.40
3:AC:47:LEU:HD22	3:AC:76:VAL:HG22	2.04	0.40
10:BJ:6:ILE:HD11	10:BJ:79:PRO:HB3	2.02	0.40
13:BM:90:ARG:HD3	13:BM:97:VAL:HA	2.03	0.40
25:D4:33:LEU:HD23	25:D4:36:LYS:HD2	2.03	0.40
31:CA:796:C:H2'	31:CA:797:G:H8	1.86	0.40
31:CA:1430:G:H2'	31:CA:1431:A:O4'	2.21	0.40
33:DA:742:A:H2'	33:DA:743:A:C8	2.57	0.40
33:DA:2377:A:H2'	33:DA:2378:A:C8	2.56	0.40
41:CM:132:ARG:HG3	41:CM:142:ILE:HD13	2.04	0.40
48:CT:17:VAL:HB	48:CT:76:VAL:HG11	2.03	0.40
37:DH:50:ARG:HD3	37:DH:53:GLU:HG2	2.03	0.40
1:AA:621:A:H2'	1:AA:622:A:O4'	2.21	0.40
1:AA:957:U:O2	1:AA:959:A:H8	2.05	0.40
5:AE:16:ILE:HD13	5:AE:137:VAL:HG11	2.03	0.40
11:AK:16:VAL:HG23	11:AK:79:ILE:HG13	2.02	0.40
24:C3:1:MET:HG2	31:CA:753:A:OP1	2.21	0.40
1:BA:1126:U:O2	1:BA:1280:A:H5'	2.22	0.40
1:BA:1289:A:H3'	1:BA:1290:G:H8	1.86	0.40
15:BO:29:VAL:HG13	15:BO:63:ARG:HG3	2.04	0.40
29:CC:158:ALA:HB3	31:CA:1820:U:O2'	2.21	0.40
31:CA:29:U:H2'	31:CA:30:G:C8	2.56	0.40
31:CA:942:G:H4'	31:CA:1190:G:H5'	2.02	0.40
1:AA:629:A:H2'	1:AA:630:A:O4'	2.22	0.40
1:AA:892:A:O2'	1:AA:1415:G:H4'	2.21	0.40
8:AH:18:GLN:CD	8:AH:70:ALA:HB1	2.45	0.40
19:AS:32:ARG:HA	19:AS:50:ALA:HB3	2.02	0.40
8:BH:18:GLN:CD	8:BH:70:ALA:HB1	2.46	0.40
31:CA:516:C:H1'	31:CA:1261:C:O2'	2.21	0.40
31:CA:634:C:H2'	31:CA:635:C:H6	1.86	0.40
31:CA:824:U:H3	31:CA:833:A:H61	1.69	0.40
31:CA:2552:OMU:O5'	31:CA:2552:OMU:H6	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2571:U:C4	31:CA:2574:G:C8	3.10	0.40
29:DC:21:ASN:OD1	29:DC:23:GLU:HB2	2.22	0.40
32:DD:3:GLY:HA3	32:DD:204:LYS:HG2	2.04	0.40
33:DA:319:G:OP2	34:DE:132:LYS:HE2	2.22	0.40
33:DA:1125:G:C6	33:DA:1126:A:N6	2.90	0.40
33:DA:1759:A:H2'	33:DA:1760:C:C6	2.56	0.40
37:CH:1:MET:HE3	37:CH:23:ALA:HA	2.03	0.40
37:CH:27:ARG:HD3	37:CH:27:ARG:HA	1.82	0.40
34:DE:117:ARG:HA	34:DE:185:LYS:HD3	2.03	0.40
46:DR:90:ILE:HG22	46:DR:95:LEU:HG	2.04	0.40
55:DI:69:PHE:C	55:DI:71:CYS:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	209 (94%)	8 (4%)	5 (2%)	5	21
2	BB	222/224 (99%)	209 (94%)	8 (4%)	5 (2%)	5	21
3	AC	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	12	39
3	BC	204/206 (99%)	193 (95%)	8 (4%)	3 (2%)	8	30
4	AD	203/205 (99%)	192 (95%)	11 (5%)	0	100	100
4	BD	203/205 (99%)	193 (95%)	10 (5%)	0	100	100
5	AE	153/155 (99%)	144 (94%)	7 (5%)	2 (1%)	9	33
5	BE	148/155 (96%)	130 (88%)	15 (10%)	3 (2%)	6	24
6	AF	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
6	BF	98/106 (92%)	89 (91%)	7 (7%)	2 (2%)	6	24
7	AG	149/151 (99%)	135 (91%)	13 (9%)	1 (1%)	18	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	BG	149/151 (99%)	139 (93%)	10 (7%)	0	100	100
8	AH	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	45
8	BH	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
9	AI	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
9	BI	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
10	AJ	97/99 (98%)	89 (92%)	5 (5%)	3 (3%)	3	17
10	BJ	96/99 (97%)	76 (79%)	14 (15%)	6 (6%)	1	6
11	AK	115/117 (98%)	103 (90%)	10 (9%)	2 (2%)	7	28
11	BK	115/117 (98%)	103 (90%)	10 (9%)	2 (2%)	7	28
12	AL	120/123 (98%)	116 (97%)	3 (2%)	1 (1%)	16	45
12	BL	120/123 (98%)	114 (95%)	4 (3%)	2 (2%)	7	28
13	AM	112/114 (98%)	101 (90%)	7 (6%)	4 (4%)	2	14
13	BM	112/114 (98%)	100 (89%)	6 (5%)	6 (5%)	1	8
14	AN	98/100 (98%)	88 (90%)	8 (8%)	2 (2%)	6	24
14	BN	98/100 (98%)	90 (92%)	6 (6%)	2 (2%)	6	24
15	AO	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
15	BO	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	10	34
16	AP	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	9	33
16	BP	80/82 (98%)	68 (85%)	10 (12%)	2 (2%)	4	20
17	AQ	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	9	33
17	BQ	78/80 (98%)	73 (94%)	2 (3%)	3 (4%)	2	13
18	AR	53/55 (96%)	53 (100%)	0	0	100	100
18	BR	53/55 (96%)	51 (96%)	1 (2%)	1 (2%)	6	25
19	AS	77/79 (98%)	68 (88%)	8 (10%)	1 (1%)	9	33
19	BS	77/79 (98%)	65 (84%)	11 (14%)	1 (1%)	9	33
20	AT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
20	BT	83/86 (96%)	79 (95%)	3 (4%)	1 (1%)	10	34
21	AU	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
21	BU	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
22	C1	54/56 (96%)	48 (89%)	3 (6%)	3 (6%)	1	8
22	D1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	C2	48/51 (94%)	42 (88%)	5 (10%)	1 (2%)	5	23
23	D2	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
24	C3	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	5	21
24	D3	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
25	C4	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
25	D4	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
26	C5	36/38 (95%)	36 (100%)	0	0	100	100
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	2	14
27	D0	57/58 (98%)	55 (96%)	2 (4%)	0	100	100
29	CC	269/271 (99%)	250 (93%)	14 (5%)	5 (2%)	6	25
29	DC	269/271 (99%)	253 (94%)	15 (6%)	1 (0%)	30	60
30	CD	207/209 (99%)	193 (93%)	14 (7%)	0	100	100
32	DD	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
34	CE	199/201 (99%)	187 (94%)	9 (4%)	3 (2%)	8	30
34	DE	199/201 (99%)	191 (96%)	7 (4%)	1 (0%)	24	55
35	CF	175/177 (99%)	165 (94%)	9 (5%)	1 (1%)	21	50
35	DF	175/177 (99%)	164 (94%)	10 (6%)	1 (1%)	21	50
36	CG	174/176 (99%)	158 (91%)	12 (7%)	4 (2%)	5	21
36	DG	174/176 (99%)	160 (92%)	13 (8%)	1 (1%)	21	50
37	CH	147/149 (99%)	132 (90%)	11 (8%)	4 (3%)	4	19
37	DH	147/149 (99%)	135 (92%)	10 (7%)	2 (1%)	9	31
38	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	3	17
38	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	3	17
39	CK	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	5	23
39	DK	140/142 (99%)	134 (96%)	4 (3%)	2 (1%)	9	31
40	CL	120/123 (98%)	112 (93%)	7 (6%)	1 (1%)	16	45
40	DL	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
41	CM	142/144 (99%)	130 (92%)	8 (6%)	4 (3%)	4	19
41	DM	142/144 (99%)	136 (96%)	4 (3%)	2 (1%)	9	31
42	CN	133/136 (98%)	123 (92%)	9 (7%)	1 (1%)	16	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	DN	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
43	CO	118/125 (94%)	107 (91%)	8 (7%)	3 (2%)	4	20
43	DO	123/125 (98%)	113 (92%)	9 (7%)	1 (1%)	16	45
44	CP	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
44	DP	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
45	CQ	112/114 (98%)	104 (93%)	7 (6%)	1 (1%)	14	42
45	DQ	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	14	42
46	CR	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
46	DR	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
47	CS	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	3	17
47	DS	101/103 (98%)	95 (94%)	5 (5%)	1 (1%)	12	39
48	CT	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
48	DT	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
49	CU	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
49	DU	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
50	CV	100/102 (98%)	86 (86%)	10 (10%)	4 (4%)	2	12
50	DV	100/102 (98%)	95 (95%)	3 (3%)	2 (2%)	6	24
51	CW	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
51	DW	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
52	CX	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
52	DX	75/76 (99%)	72 (96%)	3 (4%)	0	100	100
53	CY	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
53	DY	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
54	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	28
54	DZ	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
55	DI	133/135 (98%)	114 (86%)	14 (10%)	5 (4%)	2	13
All	All	11407/11629 (98%)	10635 (93%)	633 (6%)	139 (1%)	10	34

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE
3	AC	156	ARG

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Mol	Chain	Res	Type
5	AE	162	GLU
13	AM	5	ALA
22	C1	25	VAL
27	C0	14	ILE
2	BB	126	PHE
3	BC	156	ARG
10	BJ	91	ASP
13	BM	7	ILE
13	BM	114	LYS
19	BS	6	LYS
20	BT	5	LYS
34	CE	83	VAL
36	CG	119	ALA
36	CG	175	LYS
36	CG	176	LYS
37	CH	10	ALA
38	CJ	19	ASN
39	CK	81	ILE
41	CM	29	LYS
42	CN	70	ASP
43	CO	118	ARG
50	CV	7	ARG
50	CV	16	GLY
50	CV	17	LYS
38	DJ	19	ASN
50	DV	52	LEU
55	DI	91	ALA
2	AB	95	ARG
5	AE	109	GLY
10	AJ	57	VAL
11	AK	54	GLY
13	AM	105	ASN
14	AN	38	ASP
17	AQ	82	ALA
2	BB	95	ARG
3	BC	61	ALA
5	BE	103	THR
5	BE	110	ALA
6	BF	98	GLU
10	BJ	38	GLY
10	BJ	57	VAL
11	BK	54	GLY

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Mol	Chain	Res	Type
12	BL	44	LYS
13	BM	5	ALA
13	BM	105	ASN
14	BN	38	ASP
16	BP	80	LYS
17	BQ	70	THR
17	BQ	82	ALA
29	CC	158	ALA
34	CE	82	GLY
36	CG	46	ALA
38	CJ	25	GLY
39	CK	25	LEU
39	CK	95	ARG
40	CL	35	VAL
41	CM	30	THR
41	CM	69	ARG
43	CO	119	SER
45	CQ	105	GLY
36	DG	46	ALA
37	DH	11	ASN
38	DJ	25	GLY
39	DK	95	ARG
45	DQ	105	GLY
47	DS	44	GLY
2	AB	127	ASP
7	AG	56	LYS
11	AK	89	PRO
19	AS	6	LYS
22	C1	26	THR
22	C1	27	SER
24	C3	45	SER
27	C0	4	THR
2	BB	127	ASP
6	BF	92	THR
10	BJ	36	VAL
11	BK	89	PRO
15	BO	88	ARG
29	CC	108	LYS
29	CC	197	ASN
37	CH	122	LEU
41	CM	36	LYS
37	DH	122	LEU

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Mol	Chain	Res	Type
39	DK	25	LEU
41	DM	29	LYS
41	DM	36	LYS
55	DI	70	GLU
55	DI	130	PRO
2	AB	125	THR
12	AL	74	LEU
13	AM	47	GLU
16	AP	45	GLU
23	C2	51	GLU
2	BB	125	THR
10	BJ	95	GLY
12	BL	74	LEU
13	BM	47	GLU
17	BQ	17	MET
37	CH	9	VAL
37	CH	11	ASN
38	CJ	23	PRO
47	CS	53	PHE
50	CV	89	ASP
38	DJ	23	PRO
50	DV	89	ASP
55	DI	88	HIS
10	AJ	33	GLY
13	AM	7	ILE
14	AN	81	ARG
13	BM	4	ILE
29	CC	233	GLY
34	CE	6	LYS
38	CJ	32	GLY
47	CS	55	ASP
34	DE	6	LYS
38	DJ	32	GLY
55	DI	108	VAL
3	AC	107	ARG
10	BJ	93	ALA
14	BN	81	ARG
16	BP	44	SER
18	BR	66	SER
29	CC	251	GLN
29	DC	233	GLY
47	CS	43	ASN

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Mol	Chain	Res	Type
35	DF	176	PRO
35	CF	176	PRO
43	CO	116	VAL
54	CZ	62	GLY
43	DO	116	VAL
8	AH	68	GLY
3	BC	108	LYS
5	BE	105	ILE
2	AB	71	GLY
2	BB	71	GLY
10	AJ	39	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/186 (100%)	172 (92%)	14 (8%)	12	38
2	BB	186/186 (100%)	172 (92%)	14 (8%)	12	38
3	AC	170/170 (100%)	158 (93%)	12 (7%)	13	39
3	BC	170/170 (100%)	155 (91%)	15 (9%)	9	31
4	AD	172/172 (100%)	162 (94%)	10 (6%)	18	46
4	BD	172/172 (100%)	162 (94%)	10 (6%)	18	46
5	AE	118/118 (100%)	96 (81%)	22 (19%)	1	7
5	BE	113/118 (96%)	90 (80%)	23 (20%)	1	5
6	AF	92/92 (100%)	83 (90%)	9 (10%)	7	28
6	BF	87/92 (95%)	77 (88%)	10 (12%)	5	21
7	AG	124/124 (100%)	107 (86%)	17 (14%)	3	15
7	BG	124/124 (100%)	103 (83%)	21 (17%)	2	10
8	AH	104/104 (100%)	88 (85%)	16 (15%)	2	12
8	BH	104/104 (100%)	89 (86%)	15 (14%)	3	13
9	AI	105/105 (100%)	100 (95%)	5 (5%)	23	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	BI	105/105 (100%)	100 (95%)	5 (5%)	23	52
10	AJ	87/87 (100%)	80 (92%)	7 (8%)	11	35
10	BJ	86/87 (99%)	77 (90%)	9 (10%)	6	25
11	AK	90/90 (100%)	88 (98%)	2 (2%)	45	68
11	BK	90/90 (100%)	85 (94%)	5 (6%)	19	47
12	AL	102/102 (100%)	95 (93%)	7 (7%)	14	40
12	BL	102/102 (100%)	93 (91%)	9 (9%)	9	31
13	AM	92/92 (100%)	86 (94%)	6 (6%)	15	42
13	BM	92/92 (100%)	88 (96%)	4 (4%)	26	55
14	AN	83/83 (100%)	81 (98%)	2 (2%)	43	67
14	BN	83/83 (100%)	81 (98%)	2 (2%)	43	67
15	AO	76/76 (100%)	70 (92%)	6 (8%)	11	35
15	BO	76/76 (100%)	68 (90%)	8 (10%)	6	25
16	AP	65/65 (100%)	63 (97%)	2 (3%)	35	62
16	BP	65/65 (100%)	61 (94%)	4 (6%)	16	44
17	AQ	74/74 (100%)	68 (92%)	6 (8%)	11	34
17	BQ	74/74 (100%)	66 (89%)	8 (11%)	6	23
18	AR	48/48 (100%)	46 (96%)	2 (4%)	26	56
18	BR	48/48 (100%)	47 (98%)	1 (2%)	47	69
19	AS	70/70 (100%)	60 (86%)	10 (14%)	3	13
19	BS	70/70 (100%)	62 (89%)	8 (11%)	5	22
20	AT	65/65 (100%)	59 (91%)	6 (9%)	8	30
20	BT	65/65 (100%)	56 (86%)	9 (14%)	3	14
21	AU	48/48 (100%)	43 (90%)	5 (10%)	7	25
21	BU	48/48 (100%)	43 (90%)	5 (10%)	7	25
22	C1	47/47 (100%)	45 (96%)	2 (4%)	26	55
22	D1	47/47 (100%)	44 (94%)	3 (6%)	16	42
23	C2	45/46 (98%)	41 (91%)	4 (9%)	9	31
23	D2	45/46 (98%)	39 (87%)	6 (13%)	4	16
24	C3	38/38 (100%)	36 (95%)	2 (5%)	20	49
24	D3	38/38 (100%)	36 (95%)	2 (5%)	20	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	C4	51/51 (100%)	49 (96%)	2 (4%)	28	58
25	D4	51/51 (100%)	50 (98%)	1 (2%)	48	70
26	C5	34/34 (100%)	33 (97%)	1 (3%)	37	63
26	D5	34/34 (100%)	33 (97%)	1 (3%)	37	63
27	C0	48/48 (100%)	38 (79%)	10 (21%)	1	5
27	D0	49/48 (102%)	44 (90%)	5 (10%)	7	26
29	CC	216/216 (100%)	202 (94%)	14 (6%)	15	42
29	DC	216/216 (100%)	207 (96%)	9 (4%)	26	56
30	CD	164/164 (100%)	158 (96%)	6 (4%)	30	59
32	DD	163/163 (100%)	158 (97%)	5 (3%)	35	62
34	CE	165/165 (100%)	147 (89%)	18 (11%)	6	23
34	DE	165/165 (100%)	156 (94%)	9 (6%)	19	47
35	CF	148/148 (100%)	129 (87%)	19 (13%)	4	17
35	DF	148/148 (100%)	130 (88%)	18 (12%)	5	19
36	CG	137/137 (100%)	132 (96%)	5 (4%)	31	59
36	DG	137/137 (100%)	132 (96%)	5 (4%)	31	59
37	CH	114/114 (100%)	99 (87%)	15 (13%)	4	16
37	DH	114/114 (100%)	99 (87%)	15 (13%)	4	16
38	CJ	104/104 (100%)	98 (94%)	6 (6%)	18	46
38	DJ	104/104 (100%)	97 (93%)	7 (7%)	15	41
39	CK	116/116 (100%)	110 (95%)	6 (5%)	21	49
39	DK	116/116 (100%)	112 (97%)	4 (3%)	32	60
40	CL	103/104 (99%)	95 (92%)	8 (8%)	11	36
40	DL	104/104 (100%)	97 (93%)	7 (7%)	15	41
41	CM	103/103 (100%)	95 (92%)	8 (8%)	11	36
41	DM	103/103 (100%)	96 (93%)	7 (7%)	14	40
42	CN	108/108 (100%)	100 (93%)	8 (7%)	13	38
42	DN	109/108 (101%)	105 (96%)	4 (4%)	30	59
43	CO	100/102 (98%)	92 (92%)	8 (8%)	11	35
43	DO	102/102 (100%)	97 (95%)	5 (5%)	22	51
44	CP	86/87 (99%)	78 (91%)	8 (9%)	8	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	DP	87/87 (100%)	81 (93%)	6 (7%)	14	40
45	CQ	99/99 (100%)	93 (94%)	6 (6%)	17	44
45	DQ	99/99 (100%)	92 (93%)	7 (7%)	13	39
46	CR	89/89 (100%)	84 (94%)	5 (6%)	19	47
46	DR	89/89 (100%)	85 (96%)	4 (4%)	24	54
47	CS	84/84 (100%)	79 (94%)	5 (6%)	17	45
47	DS	84/84 (100%)	81 (96%)	3 (4%)	31	59
48	CT	93/93 (100%)	91 (98%)	2 (2%)	45	68
48	DT	93/93 (100%)	92 (99%)	1 (1%)	65	76
49	CU	80/80 (100%)	73 (91%)	7 (9%)	9	31
49	DU	80/80 (100%)	75 (94%)	5 (6%)	16	43
50	CV	83/83 (100%)	75 (90%)	8 (10%)	8	28
50	DV	83/83 (100%)	77 (93%)	6 (7%)	13	39
51	CW	78/78 (100%)	72 (92%)	6 (8%)	12	36
51	DW	78/78 (100%)	74 (95%)	4 (5%)	21	50
52	CX	56/58 (97%)	53 (95%)	3 (5%)	20	48
52	DX	58/58 (100%)	55 (95%)	3 (5%)	21	49
53	CY	67/67 (100%)	61 (91%)	6 (9%)	9	31
53	DY	67/67 (100%)	62 (92%)	5 (8%)	12	38
54	CZ	54/54 (100%)	50 (93%)	4 (7%)	13	38
54	DZ	54/54 (100%)	50 (93%)	4 (7%)	13	38
55	DI	103/103 (100%)	96 (93%)	7 (7%)	14	40
All	All	9461/9478 (100%)	8740 (92%)	721 (8%)	12	37

All (721) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	44	GLU
2	AB	57	LEU
2	AB	93	ASN
2	AB	105	LYS
2	AB	106	THR
2	AB	125	THR
2	AB	129	LEU

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Mol	Chain	Res	Type
2	AB	130	THR
2	AB	135	LEU
2	AB	147	SER
2	AB	161	LEU
2	AB	183	VAL
2	AB	205	ASP
2	AB	207	ILE
3	AC	3	GLN
3	AC	21	THR
3	AC	33	LEU
3	AC	55	ILE
3	AC	75	ILE
3	AC	107	ARG
3	AC	121	THR
3	AC	128	VAL
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	48	LEU
4	AD	50	ASP
4	AD	132	ILE
4	AD	142	VAL
4	AD	143	VAL
4	AD	151	LYS
4	AD	194	ASP
5	AE	14	LYS
5	AE	26	LYS
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	88	VAL
5	AE	94	VAL
5	AE	100	SER
5	AE	106	ILE
5	AE	123	VAL

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Mol	Chain	Res	Type
5	AE	126	LYS
5	AE	131	THR
5	AE	134	ILE
5	AE	137	VAL
5	AE	142	ASP
5	AE	149	SER
5	AE	159	LYS
5	AE	160	SER
5	AE	164	ILE
6	AF	17	GLN
6	AF	36	ILE
6	AF	39	LEU
6	AF	62	MET
6	AF	68	GLN
6	AF	69	GLU
6	AF	71	ILE
6	AF	89	VAL
6	AF	93	LYS
7	AG	18	PHE
7	AG	22	LEU
7	AG	23	LEU
7	AG	30	LEU
7	AG	36	LYS
7	AG	58	GLU
7	AG	59	LEU
7	AG	63	GLU
7	AG	66	LEU
7	AG	70	ARG
7	AG	76	LYS
7	AG	83	SER
7	AG	95	ARG
7	AG	120	LEU
7	AG	131	LYS
7	AG	133	THR
7	AG	142	HIS
8	AH	3	MET
8	AH	31	LYS
8	AH	46	ILE
8	AH	47	GLU
8	AH	52	GLU
8	AH	54	ASP
8	AH	55	THR

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Mol	Chain	Res	Type
8	AH	60	GLU
8	AH	63	LEU
8	AH	83	LEU
8	AH	90	ASP
8	AH	96	MET
8	AH	101	ILE
8	AH	107	SER
8	AH	108	LYS
8	AH	117	ARG
9	AI	11	ARG
9	AI	36	GLU
9	AI	61	LEU
9	AI	63	LEU
9	AI	66	THR
10	AJ	6	ILE
10	AJ	62	ARG
10	AJ	63	ASP
10	AJ	69	THR
10	AJ	88	MET
10	AJ	89	ARG
10	AJ	90	LEU
11	AK	22	HIS
11	AK	55	SER
12	AL	3	THR
12	AL	24	LEU
12	AL	40	THR
12	AL	67	ILE
12	AL	82	ILE
12	AL	110	ARG
12	AL	121	ARG
13	AM	3	ARG
13	AM	7	ILE
13	AM	13	LYS
13	AM	27	LYS
13	AM	48	LEU
13	AM	58	ASP
14	AN	27	LEU
14	AN	31	ILE
15	AO	2	SER
15	AO	4	SER
15	AO	40	GLN
15	AO	70	LEU

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Mol	Chain	Res	Type
15	AO	88	ARG
15	AO	89	ARG
16	AP	18	GLN
16	AP	48	GLU
17	AQ	5	ILE
17	AQ	16	LYS
17	AQ	38	ILE
17	AQ	40	ARG
17	AQ	75	LEU
17	AQ	83	VAL
18	AR	47	THR
18	AR	66	SER
19	AS	5	LEU
19	AS	7	LYS
19	AS	11	ILE
19	AS	13	LEU
19	AS	27	ASP
19	AS	33	THR
19	AS	37	ARG
19	AS	60	VAL
19	AS	63	THR
19	AS	81	ARG
20	AT	5	LYS
20	AT	15	GLU
20	AT	27	MET
20	AT	44	LYS
20	AT	48	GLN
20	AT	85	LYS
21	AU	13	ASP
21	AU	16	LEU
21	AU	18	ARG
21	AU	31	GLU
21	AU	56	HIS
22	C1	40	ARG
22	C1	52	ARG
23	C2	8	LYS
23	C2	9	ILE
23	C2	46	HIS
23	C2	47	VAL
24	C3	1	MET
24	C3	24	THR
25	C4	51	SER

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Mol	Chain	Res	Type
25	C4	52	LYS
26	C5	26	ILE
27	C0	3	LYS
27	C0	4	THR
27	C0	5	ILE
27	C0	7	ILE
27	C0	19	LYS
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	57	LEU
2	BB	93	ASN
2	BB	105	LYS
2	BB	106	THR
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
3	BC	3	GLN
3	BC	21	THR
3	BC	33	LEU
3	BC	37	PHE
3	BC	38	LYS
3	BC	46	GLU
3	BC	55	ILE
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	193	TYR
3	BC	207	ILE
4	BD	17	THR

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Mol	Chain	Res	Type
4	BD	22	LYS
4	BD	26	ARG
4	BD	48	LEU
4	BD	50	ASP
4	BD	142	VAL
4	BD	143	VAL
4	BD	151	LYS
4	BD	173	VAL
4	BD	194	ASP
5	BE	14	LYS
5	BE	22	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
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	134	ILE
5	BE	137	VAL
5	BE	142	ASP
5	BE	149	SER
5	BE	151	GLU
5	BE	159	LYS
6	BF	7	VAL
6	BF	16	GLU
6	BF	17	GLN
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	89	VAL

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Mol	Chain	Res	Type
7	BG	4	ARG
7	BG	5	ARG
7	BG	10	ARG
7	BG	23	LEU
7	BG	30	LEU
7	BG	36	LYS
7	BG	50	LEU
7	BG	58	GLU
7	BG	59	LEU
7	BG	63	GLU
7	BG	66	LEU
7	BG	70	ARG
7	BG	72	THR
7	BG	76	LYS
7	BG	83	SER
7	BG	95	ARG
7	BG	120	LEU
7	BG	131	LYS
7	BG	133	THR
7	BG	141	VAL
7	BG	142	HIS
8	BH	3	MET
8	BH	46	ILE
8	BH	47	GLU
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	101	ILE
8	BH	107	SER
8	BH	108	LYS
8	BH	117	ARG
9	BI	11	ARG
9	BI	36	GLU
9	BI	61	LEU
9	BI	63	LEU
9	BI	66	THR
10	BJ	6	ILE

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Mol	Chain	Res	Type
10	BJ	59	LYS
10	BJ	62	ARG
10	BJ	63	ASP
10	BJ	69	THR
10	BJ	78	GLU
10	BJ	88	MET
10	BJ	89	ARG
10	BJ	90	LEU
11	BK	16	VAL
11	BK	18	ASP
11	BK	22	HIS
11	BK	31	ILE
11	BK	38	GLN
12	BL	3	THR
12	BL	24	LEU
12	BL	44	LYS
12	BL	49	LEU
12	BL	58	THR
12	BL	67	ILE
12	BL	90	LEU
12	BL	110	ARG
12	BL	121	ARG
13	BM	11	ASP
13	BM	16	VAL
13	BM	27	LYS
13	BM	48	LEU
14	BN	26	GLU
14	BN	27	LEU
15	BO	2	SER
15	BO	4	SER
15	BO	17	ARG
15	BO	40	GLN
15	BO	64	ARG
15	BO	66	LEU
15	BO	70	LEU
15	BO	87	LEU
16	BP	20	VAL
16	BP	36	VAL
16	BP	48	GLU
16	BP	76	LYS
17	BQ	17	MET
17	BQ	21	ILE

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Mol	Chain	Res	Type
17	BQ	26	GLU
17	BQ	38	ILE
17	BQ	40	ARG
17	BQ	51	ASN
17	BQ	67	LEU
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	37	ARG
19	BS	40	ILE
19	BS	60	VAL
19	BS	63	THR
20	BT	5	LYS
20	BT	12	ILE
20	BT	15	GLU
20	BT	48	GLN
20	BT	54	MET
20	BT	58	VAL
20	BT	64	LYS
20	BT	67	ILE
20	BT	69	LYS
21	BU	13	ASP
21	BU	16	LEU
21	BU	18	ARG
21	BU	31	GLU
21	BU	56	HIS
22	D1	26	THR
22	D1	52	ARG
22	D1	55	ILE
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
24	D3	24	THR
25	D4	52	LYS
26	D5	26	ILE

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Mol	Chain	Res	Type
27	D0	7	ILE
27	D0	10	THR
27	D0	19	LYS
27	D0	36	VAL
27	D0	39	GLU
29	CC	97	LYS
29	CC	110	LEU
29	CC	116	ILE
29	CC	117	GLN
29	CC	118	SER
29	CC	120	VAL
29	CC	156	ARG
29	CC	157	SER
29	CC	168	ASP
29	CC	192	LEU
29	CC	195	VAL
29	CC	204	VAL
29	CC	221	ARG
29	CC	236	GLU
30	CD	2	ILE
30	CD	18	ASP
30	CD	95	SER
30	CD	138	LEU
30	CD	150	GLN
30	CD	204	LYS
29	DC	43	ARG
29	DC	70	ASN
29	DC	97	LYS
29	DC	116	ILE
29	DC	117	GLN
29	DC	118	SER
29	DC	120	VAL
29	DC	192	LEU
29	DC	236	GLU
32	DD	2	ILE
32	DD	18	ASP
32	DD	95	SER
32	DD	138	LEU
32	DD	204	LYS
34	CE	7	ASP
34	CE	12	LEU
34	CE	25	GLU

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Mol	Chain	Res	Type
34	CE	40	ARG
34	CE	44	ARG
34	CE	72	SER
34	CE	80	SER
34	CE	83	VAL
34	CE	107	SER
34	CE	120	VAL
34	CE	122	GLU
34	CE	127	GLU
34	CE	149	ILE
34	CE	152	GLU
34	CE	176	ASP
34	CE	189	THR
34	CE	196	VAL
34	CE	199	MET
35	CF	31	VAL
35	CF	35	THR
35	CF	36	LEU
35	CF	49	LEU
35	CF	50	LEU
35	CF	57	LEU
35	CF	72	LYS
35	CF	80	ARG
35	CF	94	GLU
35	CF	117	LEU
35	CF	123	ASP
35	CF	134	GLU
35	CF	136	ILE
35	CF	141	ILE
35	CF	148	ARG
35	CF	149	VAL
35	CF	150	ARG
35	CF	152	LEU
35	CF	174	ASP
36	CG	18	LYS
36	CG	42	GLU
36	CG	72	LEU
36	CG	127	THR
36	CG	155	GLU
37	CH	1	MET
37	CH	7	ASP
37	CH	15	LEU

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Mol	Chain	Res	Type
37	CH	21	VAL
37	CH	44	ILE
37	CH	51	ARG
37	CH	53	GLU
37	CH	55	GLU
37	CH	62	LEU
37	CH	75	LEU
37	CH	76	GLU
37	CH	89	LYS
37	CH	112	LYS
37	CH	127	GLU
37	CH	145	ASN
38	CJ	13	VAL
38	CJ	28	LEU
38	CJ	53	LEU
38	CJ	55	ILE
38	CJ	101	ILE
38	CJ	113	LYS
39	CK	5	THR
39	CK	45	THR
39	CK	90	GLU
39	CK	101	ILE
39	CK	124	VAL
39	CK	142	ILE
40	CL	35	VAL
40	CL	49	ARG
40	CL	58	LEU
40	CL	70	ARG
40	CL	76	VAL
40	CL	98	ARG
40	CL	113	MET
40	CL	122	VAL
41	CM	33	ARG
41	CM	59	ARG
41	CM	92	LEU
41	CM	94	THR
41	CM	100	ILE
41	CM	103	ILE
41	CM	115	GLU
41	CM	120	VAL
42	CN	6	ARG
42	CN	14	LYS

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Mol	Chain	Res	Type
42	CN	20	LEU
42	CN	41	LEU
42	CN	42	THR
42	CN	59	ARG
42	CN	75	GLU
42	CN	100	LYS
43	CO	2	ARG
43	CO	14	SER
43	CO	51	LEU
43	CO	53	THR
43	CO	69	ARG
43	CO	71	ARG
43	CO	79	LEU
43	CO	95	THR
44	CP	20	GLU
44	CP	31	THR
44	CP	38	GLN
44	CP	45	SER
44	CP	47	VAL
44	CP	48	LEU
44	CP	78	VAL
44	CP	115	LEU
45	CQ	26	VAL
45	CQ	30	VAL
45	CQ	65	SER
45	CQ	96	LYS
45	CQ	102	GLU
45	CQ	114	LEU
46	CR	5	LYS
46	CR	9	ILE
46	CR	16	LYS
46	CR	51	ARG
46	CR	52	GLN
47	CS	12	HIS
47	CS	46	GLU
47	CS	48	LYS
47	CS	51	VAL
47	CS	74	ILE
48	CT	29	VAL
48	CT	86	MET
49	CU	2	ILE
49	CU	10	VAL

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Mol	Chain	Res	Type
49	CU	24	MET
49	CU	30	ILE
49	CU	69	ARG
49	CU	74	ILE
49	CU	93	LEU
50	CV	28	VAL
50	CV	34	VAL
50	CV	53	ASN
50	CV	61	LYS
50	CV	67	VAL
50	CV	72	ILE
50	CV	81	ASP
50	CV	98	SER
51	CW	1	MET
51	CW	7	GLU
51	CW	10	LYS
51	CW	18	ARG
51	CW	40	ILE
51	CW	61	LEU
52	CX	39	ARG
52	CX	78	LYS
52	CX	82	ILE
53	CY	25	THR
53	CY	35	SER
53	CY	44	LYS
53	CY	56	MET
53	CY	66	THR
53	CY	71	LEU
54	CZ	7	ARG
54	CZ	18	LEU
54	CZ	19	LEU
54	CZ	58	ASN
34	DE	12	LEU
34	DE	80	SER
34	DE	107	SER
34	DE	120	VAL
34	DE	127	GLU
34	DE	176	ASP
34	DE	189	THR
34	DE	196	VAL
34	DE	199	MET
35	DF	10	ASP

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Mol	Chain	Res	Type
35	DF	35	THR
35	DF	49	LEU
35	DF	50	LEU
35	DF	57	LEU
35	DF	72	LYS
35	DF	94	GLU
35	DF	115	ARG
35	DF	117	LEU
35	DF	120	LYS
35	DF	134	GLU
35	DF	136	ILE
35	DF	141	ILE
35	DF	148	ARG
35	DF	149	VAL
35	DF	150	ARG
35	DF	152	LEU
35	DF	174	ASP
36	DG	18	LYS
36	DG	42	GLU
36	DG	72	LEU
36	DG	127	THR
36	DG	155	GLU
37	DH	1	MET
37	DH	7	ASP
37	DH	15	LEU
37	DH	44	ILE
37	DH	53	GLU
37	DH	58	LEU
37	DH	60	GLU
37	DH	62	LEU
37	DH	75	LEU
37	DH	76	GLU
37	DH	83	LYS
37	DH	89	LYS
37	DH	112	LYS
37	DH	127	GLU
37	DH	145	ASN
38	DJ	11	LEU
38	DJ	13	VAL
38	DJ	28	LEU
38	DJ	53	LEU
38	DJ	55	ILE

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Mol	Chain	Res	Type
38	DJ	101	ILE
38	DJ	113	LYS
39	DK	45	THR
39	DK	101	ILE
39	DK	124	VAL
39	DK	142	ILE
40	DL	49	ARG
40	DL	58	LEU
40	DL	70	ARG
40	DL	109	SER
40	DL	110	GLU
40	DL	122	VAL
40	DL	123	LEU
41	DM	59	ARG
41	DM	91	ASP
41	DM	92	LEU
41	DM	94	THR
41	DM	107	PHE
41	DM	115	GLU
41	DM	120	VAL
42	DN	58	LYS
42	DN	75	GLU
42	DN	100	LYS
42	DN	115	GLU
43	DO	14	SER
43	DO	51	LEU
43	DO	53	THR
43	DO	69	ARG
43	DO	79	LEU
44	DP	20	GLU
44	DP	31	THR
44	DP	45	SER
44	DP	49	VAL
44	DP	78	VAL
44	DP	115	LEU
45	DQ	26	VAL
45	DQ	30	VAL
45	DQ	40	LEU
45	DQ	65	SER
45	DQ	96	LYS
45	DQ	102	GLU
45	DQ	111	LYS

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Mol	Chain	Res	Type
46	DR	5	LYS
46	DR	9	ILE
46	DR	11	ARG
46	DR	51	ARG
47	DS	38	VAL
47	DS	74	ILE
47	DS	87	GLN
48	DT	86	MET
49	DU	1	MET
49	DU	2	ILE
49	DU	10	VAL
49	DU	25	GLU
49	DU	74	ILE
50	DV	28	VAL
50	DV	34	VAL
50	DV	52	LEU
50	DV	61	LYS
50	DV	67	VAL
50	DV	72	ILE
51	DW	7	GLU
51	DW	40	ILE
51	DW	53	LYS
51	DW	61	LEU
52	DX	38	VAL
52	DX	39	ARG
52	DX	82	ILE
53	DY	11	ARG
53	DY	25	THR
53	DY	44	LYS
53	DY	48	THR
53	DY	66	THR
54	DZ	6	LEU
54	DZ	7	ARG
54	DZ	12	GLU
54	DZ	19	LEU
55	DI	16	SER
55	DI	53	ARG
55	DI	59	LEU
55	DI	60	LEU
55	DI	64	VAL
55	DI	117	LEU
55	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
2	AB	177	ASN
2	AB	178	ASN
3	AC	41	GLN
3	AC	100	GLN
3	AC	102	ASN
3	AC	123	GLN
4	AD	41	HIS
5	AE	70	ASN
5	AE	73	ASN
5	AE	77	ASN
5	AE	89	HIS
5	AE	122	ASN
5	AE	146	ASN
6	AF	17	GLN
6	AF	63	ASN
7	AG	130	ASN
8	AH	4	GLN
8	AH	38	ASN
9	AI	32	GLN
9	AI	126	GLN
10	AJ	56	HIS
11	AK	101	ASN
13	AM	12	HIS
14	AN	66	GLN
15	AO	28	GLN
15	AO	40	GLN
15	AO	50	HIS
15	AO	62	GLN
16	AP	63	GLN
19	AS	43	ASN
20	AT	20	HIS
20	AT	48	GLN
20	AT	61	GLN
22	C1	6	ASN
22	C1	42	HIS
24	C3	29	GLN
27	C0	9	GLN
27	C0	20	HIS

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Mol	Chain	Res	Type
27	C0	34	HIS
2	BB	39	HIS
2	BB	42	ASN
2	BB	93	ASN
2	BB	120	GLN
2	BB	178	ASN
3	BC	123	GLN
4	BD	41	HIS
4	BD	131	ASN
4	BD	140	ASN
5	BE	19	ASN
5	BE	89	HIS
5	BE	122	ASN
5	BE	146	ASN
6	BF	3	HIS
6	BF	14	GLN
6	BF	17	GLN
6	BF	46	GLN
7	BG	86	GLN
7	BG	130	ASN
7	BG	142	HIS
8	BH	4	GLN
8	BH	38	ASN
9	BI	32	GLN
9	BI	126	GLN
10	BJ	56	HIS
11	BK	101	ASN
15	BO	28	GLN
15	BO	40	GLN
15	BO	62	GLN
16	BP	40	ASN
16	BP	63	GLN
17	BQ	51	ASN
19	BS	43	ASN
20	BT	3	ASN
20	BT	48	GLN
20	BT	52	ASN
20	BT	78	ASN
20	BT	84	ASN
23	D2	45	GLN
25	D4	28	ASN
27	D0	49	ASN

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Mol	Chain	Res	Type
29	CC	142	HIS
29	CC	251	GLN
29	DC	142	HIS
29	DC	197	ASN
29	DC	251	GLN
32	DD	42	ASN
32	DD	173	GLN
34	CE	24	ASN
34	CE	136	GLN
34	CE	163	ASN
35	CF	23	ASN
35	CF	27	GLN
35	CF	52	ASN
36	CG	38	ASN
36	CG	104	ASN
36	CG	128	GLN
36	CG	139	GLN
37	CH	2	GLN
37	CH	20	ASN
39	CK	47	HIS
39	CK	138	GLN
44	CP	100	HIS
44	CP	104	GLN
44	CP	116	GLN
50	CV	46	GLN
50	CV	74	ASN
50	CV	99	ASN
52	CX	76	ASN
54	CZ	20	ASN
36	DG	104	ASN
36	DG	116	GLN
36	DG	128	GLN
37	DH	2	GLN
37	DH	18	GLN
37	DH	20	ASN
38	DJ	43	ASN
39	DK	136	GLN
42	DN	3	GLN
42	DN	97	GLN
43	DO	13	ASN
43	DO	107	ASN
44	DP	104	GLN

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Mol	Chain	Res	Type
44	DP	116	GLN
45	DQ	15	GLN
46	DR	52	GLN
50	DV	74	ASN
51	DW	12	GLN
53	DY	36	HIS
54	DZ	20	ASN
54	DZ	39	GLN
55	DI	4	ASN
55	DI	9	GLN
55	DI	88	HIS
55	DI	122	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1533/1534 (99%)	274 (17%)	38 (2%)
1	BA	1532/1534 (99%)	274 (17%)	44 (2%)
28	CB	117/120 (97%)	12 (10%)	0
28	DB	119/120 (99%)	12 (10%)	0
31	CA	2896/2904 (99%)	525 (18%)	94 (3%)
33	DA	2884/2903 (99%)	458 (15%)	72 (2%)
All	All	9081/9115 (99%)	1555 (17%)	248 (2%)

All (1555) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	8	A
1	AA	9	G
1	AA	22	G
1	AA	30	U
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	49	U

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Mol	Chain	Res	Type
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	69	G
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	92	U
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	128	G
1	AA	130	A
1	AA	131	A
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
1	AA	177	G
1	AA	197	A
1	AA	205	A
1	AA	210	C
1	AA	211	G
1	AA	212	G
1	AA	226	G

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Mol	Chain	Res	Type
1	AA	240	G
1	AA	245	U
1	AA	247	G
1	AA	251	G
1	AA	262	A
1	AA	266	G
1	AA	267	C
1	AA	281	G
1	AA	282	A
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	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	388	G
1	AA	398	U
1	AA	406	G
1	AA	411	A
1	AA	412	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	438	U
1	AA	439	U
1	AA	451	A
1	AA	457	G
1	AA	458	U
1	AA	466	A
1	AA	467	U
1	AA	468	A

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Mol	Chain	Res	Type
1	AA	474	G
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	505	G
1	AA	509	A
1	AA	511	C
1	AA	524	G
1	AA	527	G7M
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	596	A
1	AA	615	G
1	AA	633	G
1	AA	650	G
1	AA	653	U
1	AA	654	G
1	AA	661	G
1	AA	665	A
1	AA	675	A
1	AA	682	G
1	AA	687	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	764	C
1	AA	774	G
1	AA	777	A

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Mol	Chain	Res	Type
1	AA	793	U
1	AA	794	A
1	AA	809	G
1	AA	814	A
1	AA	815	A
1	AA	817	C
1	AA	818	G
1	AA	821	G
1	AA	828	U
1	AA	832	G
1	AA	836	G
1	AA	839	C
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	934	C
1	AA	935	A
1	AA	936	C
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	996	A
1	AA	1004	A
1	AA	1009	U
1	AA	1015	G
1	AA	1019	A
1	AA	1026	G
1	AA	1027	C
1	AA	1029	U
1	AA	1030	U
1	AA	1031	C

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Mol	Chain	Res	Type
1	AA	1032	G
1	AA	1033	G
1	AA	1036	A
1	AA	1037	C
1	AA	1043	G
1	AA	1046	A
1	AA	1053	G
1	AA	1054	C
1	AA	1065	U
1	AA	1066	C
1	AA	1086	U
1	AA	1087	G
1	AA	1094	G
1	AA	1095	U
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	1152	A
1	AA	1159	U
1	AA	1160	G
1	AA	1168	U
1	AA	1184	G
1	AA	1196	A
1	AA	1197	A
1	AA	1200	C
1	AA	1201	A
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
1	AA	1225	A

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Mol	Chain	Res	Type
1	AA	1226	C
1	AA	1227	A
1	AA	1236	A
1	AA	1238	A
1	AA	1239	A
1	AA	1256	A
1	AA	1257	A
1	AA	1260	G
1	AA	1280	A
1	AA	1281	C
1	AA	1286	U
1	AA	1287	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1312	G
1	AA	1317	C
1	AA	1318	A
1	AA	1319	A
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	1419	G
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	1487	G
1	AA	1492	A
1	AA	1493	A
1	AA	1497	G
1	AA	1499	A
1	AA	1503	A

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Mol	Chain	Res	Type
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	7	A
1	BA	8	A
1	BA	9	G
1	BA	22	G
1	BA	31	G
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	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	92	U
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	128	G
1	BA	130	A
1	BA	131	A
1	BA	141	G
1	BA	142	G
1	BA	143	A
1	BA	144	G
1	BA	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	251	G
1	BA	262	A
1	BA	266	G
1	BA	267	C
1	BA	281	G
1	BA	289	G
1	BA	306	A
1	BA	321	A
1	BA	328	C
1	BA	329	A
1	BA	330	C
1	BA	332	G
1	BA	346	G
1	BA	352	C
1	BA	354	G
1	BA	367	U
1	BA	372	C
1	BA	373	A

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Mol	Chain	Res	Type
1	BA	382	A
1	BA	384	G
1	BA	398	U
1	BA	406	G
1	BA	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	438	U
1	BA	439	U
1	BA	451	A
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	505	G
1	BA	509	A
1	BA	511	C
1	BA	524	G
1	BA	527	G7M
1	BA	531	U
1	BA	532	A
1	BA	533	A
1	BA	547	A
1	BA	559	A
1	BA	560	A
1	BA	561	U
1	BA	562	U
1	BA	564	C
1	BA	568	G
1	BA	572	A
1	BA	573	A
1	BA	576	C
1	BA	577	G

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Mol	Chain	Res	Type
1	BA	596	A
1	BA	615	G
1	BA	633	G
1	BA	650	G
1	BA	653	U
1	BA	654	G
1	BA	661	G
1	BA	665	A
1	BA	675	A
1	BA	682	G
1	BA	687	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	774	G
1	BA	777	A
1	BA	793	U
1	BA	794	A
1	BA	809	G
1	BA	814	A
1	BA	815	A
1	BA	817	C
1	BA	818	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	914	A
1	BA	926	G
1	BA	927	G
1	BA	934	C
1	BA	935	A

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Mol	Chain	Res	Type
1	BA	936	C
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
1	BA	993	G
1	BA	996	A
1	BA	1004	A
1	BA	1008	U
1	BA	1009	U
1	BA	1015	G
1	BA	1019	A
1	BA	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	1046	A
1	BA	1053	G
1	BA	1054	C
1	BA	1065	U
1	BA	1086	U
1	BA	1087	G
1	BA	1094	G
1	BA	1095	U
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

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Mol	Chain	Res	Type
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	1152	A
1	BA	1159	U
1	BA	1160	G
1	BA	1168	U
1	BA	1196	A
1	BA	1197	A
1	BA	1200	C
1	BA	1201	A
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	1286	U
1	BA	1287	A
1	BA	1300	G
1	BA	1302	C
1	BA	1305	G
1	BA	1312	G
1	BA	1317	C
1	BA	1318	A
1	BA	1319	A
1	BA	1320	C
1	BA	1323	G
1	BA	1346	A

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Mol	Chain	Res	Type
1	BA	1353	G
1	BA	1362	A
1	BA	1363	A
1	BA	1364	U
1	BA	1370	G
1	BA	1379	G
1	BA	1381	U
1	BA	1398	A
1	BA	1419	G
1	BA	1441	A
1	BA	1446	A
1	BA	1447	A
1	BA	1448	C
1	BA	1451	U
1	BA	1452	C
1	BA	1453	G
1	BA	1475	G
1	BA	1487	G
1	BA	1494	G
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

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Mol	Chain	Res	Type
31	CA	10	A
31	CA	34	U
31	CA	42	A
31	CA	46	G
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	86	G
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	177	G
31	CA	178	G
31	CA	181	A
31	CA	196	A
31	CA	197	A
31	CA	215	G
31	CA	216	A
31	CA	221	A
31	CA	222	A
31	CA	248	G
31	CA	250	G
31	CA	265	A
31	CA	266	G
31	CA	271	G
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	310	A
31	CA	311	A
31	CA	329	G
31	CA	330	A
31	CA	343	C
31	CA	345	A
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	387	U
31	CA	399	U
31	CA	403	U
31	CA	404	A
31	CA	405	U
31	CA	406	G
31	CA	411	G
31	CA	412	A
31	CA	420	C
31	CA	424	G
31	CA	451	U
31	CA	454	A
31	CA	455	C
31	CA	456	C
31	CA	457	A
31	CA	480	A
31	CA	481	G
31	CA	491	G
31	CA	496	G
31	CA	501	A
31	CA	503	A
31	CA	504	A
31	CA	505	A
31	CA	508	A
31	CA	517	C
31	CA	526	A
31	CA	528	A

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Mol	Chain	Res	Type
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
31	CA	551	G
31	CA	555	G
31	CA	556	A
31	CA	563	A
31	CA	572	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	622	G
31	CA	627	A
31	CA	634	C
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	696	G
31	CA	701	G
31	CA	702	U
31	CA	717	C
31	CA	730	A
31	CA	740	C
31	CA	746	PSU
31	CA	747	5MU

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Mol	Chain	Res	Type
31	CA	764	A
31	CA	765	C
31	CA	775	G
31	CA	776	G
31	CA	782	A
31	CA	783	A
31	CA	784	G
31	CA	785	G
31	CA	792	A
31	CA	798	G
31	CA	800	A
31	CA	802	A
31	CA	805	G
31	CA	812	C
31	CA	819	A
31	CA	827	U
31	CA	828	U
31	CA	845	A
31	CA	846	U
31	CA	847	U
31	CA	856	G
31	CA	858	G
31	CA	859	G
31	CA	866	A
31	CA	869	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	915	C
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	971	G
31	CA	973	A
31	CA	974	G

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Mol	Chain	Res	Type
31	CA	980	A
31	CA	981	A
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	1051	G
31	CA	1061	U
31	CA	1062	G
31	CA	1069	A
31	CA	1070	A
31	CA	1073	A
31	CA	1083	U
31	CA	1088	A
31	CA	1089	A
31	CA	1090	A
31	CA	1096	A
31	CA	1097	U
31	CA	1111	A
31	CA	1112	G
31	CA	1119	U
31	CA	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	1143	A
31	CA	1168	G

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Mol	Chain	Res	Type
31	CA	1169	A
31	CA	1171	G
31	CA	1175	A
31	CA	1176	U
31	CA	1177	G
31	CA	1179	G
31	CA	1180	U
31	CA	1182	G
31	CA	1186	G
31	CA	1195	G
31	CA	1212	G
31	CA	1227	G
31	CA	1236	G
31	CA	1238	G
31	CA	1247	A
31	CA	1248	G
31	CA	1253	A
31	CA	1256	G
31	CA	1262	A
31	CA	1266	G
31	CA	1271	G
31	CA	1272	A
31	CA	1273	U
31	CA	1300	G
31	CA	1301	A
31	CA	1306	C
31	CA	1312	U
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	1341	G
31	CA	1344	U
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

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Mol	Chain	Res	Type
31	CA	1395	A
31	CA	1403	A
31	CA	1416	G
31	CA	1417	C
31	CA	1419	A
31	CA	1420	A
31	CA	1428	C
31	CA	1434	A
31	CA	1437	C
31	CA	1438	U
31	CA	1452	G
31	CA	1453	A
31	CA	1458	U
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	1509	A
31	CA	1510	G
31	CA	1515	A
31	CA	1522	A
31	CA	1523	U
31	CA	1532	A
31	CA	1534	U
31	CA	1535	A
31	CA	1536	C
31	CA	1537	G
31	CA	1565	C
31	CA	1569	A
31	CA	1578	U
31	CA	1583	A
31	CA	1584	U
31	CA	1585	C
31	CA	1607	C
31	CA	1608	A
31	CA	1609	A
31	CA	1610	A
31	CA	1616	A
31	CA	1617	C

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Mol	Chain	Res	Type
31	CA	1647	U
31	CA	1648	U
31	CA	1649	G
31	CA	1660	G
31	CA	1674	G
31	CA	1675	C
31	CA	1694	C
31	CA	1695	G
31	CA	1703	G
31	CA	1715	G
31	CA	1729	U
31	CA	1730	C
31	CA	1732	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	1786	A
31	CA	1787	A
31	CA	1800	C
31	CA	1801	A
31	CA	1808	A
31	CA	1816	C
31	CA	1826	G
31	CA	1828	G
31	CA	1829	A
31	CA	1833	C
31	CA	1834	U
31	CA	1839	G
31	CA	1869	G
31	CA	1870	C
31	CA	1871	A
31	CA	1872	A
31	CA	1873	G
31	CA	1889	A
31	CA	1900	A
31	CA	1901	A
31	CA	1903	G
31	CA	1906	G

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Mol	Chain	Res	Type
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	2044	C
31	CA	2049	G
31	CA	2051	A
31	CA	2055	C
31	CA	2056	G
31	CA	2060	A
31	CA	2061	G
31	CA	2062	A
31	CA	2069	G7M
31	CA	2072	C
31	CA	2080	A
31	CA	2093	G
31	CA	2095	A
31	CA	2100	G
31	CA	2108	A
31	CA	2110	G
31	CA	2111	U
31	CA	2112	G
31	CA	2113	U
31	CA	2115	G
31	CA	2117	A

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Mol	Chain	Res	Type
31	CA	2118	U
31	CA	2119	A
31	CA	2120	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	2160	C
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	2195	U
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	2279	G
31	CA	2280	G
31	CA	2282	G

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Mol	Chain	Res	Type
31	CA	2283	C
31	CA	2286	G
31	CA	2287	A
31	CA	2288	A
31	CA	2305	U
31	CA	2311	A
31	CA	2322	A
31	CA	2326	C
31	CA	2327	A
31	CA	2331	G
31	CA	2333	A
31	CA	2335	A
31	CA	2343	U
31	CA	2345	G
31	CA	2347	C
31	CA	2350	C
31	CA	2354	C
31	CA	2357	G
31	CA	2361	G
31	CA	2383	G
31	CA	2385	C
31	CA	2388	A
31	CA	2393	U
31	CA	2402	U
31	CA	2403	C
31	CA	2406	A
31	CA	2410	G
31	CA	2423	U
31	CA	2424	C
31	CA	2425	A
31	CA	2426	A
31	CA	2429	G
31	CA	2430	A
31	CA	2435	A
31	CA	2436	G
31	CA	2441	U
31	CA	2448	A
31	CA	2465	C
31	CA	2476	A
31	CA	2484	G
31	CA	2491	U
31	CA	2494	G

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Mol	Chain	Res	Type
31	CA	2498	OMC
31	CA	2502	G
31	CA	2505	G
31	CA	2518	A
31	CA	2520	C
31	CA	2529	G
31	CA	2547	A
31	CA	2549	G
31	CA	2554	U
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	2599	G
31	CA	2603	G
31	CA	2606	C
31	CA	2609	U
31	CA	2613	U
31	CA	2629	U
31	CA	2630	G
31	CA	2634	A
31	CA	2645	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	2693	G
31	CA	2714	G
31	CA	2726	A
31	CA	2727	A
31	CA	2733	A
31	CA	2739	U
31	CA	2744	G
31	CA	2748	A
31	CA	2751	G
31	CA	2762	C
31	CA	2769	U

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Mol	Chain	Res	Type
31	CA	2776	A
31	CA	2777	G
31	CA	2778	A
31	CA	2779	U
31	CA	2780	G
31	CA	2791	G
31	CA	2794	C
31	CA	2799	A
31	CA	2820	A
31	CA	2825	G
31	CA	2835	A
31	CA	2836	U
31	CA	2849	U
31	CA	2850	A
31	CA	2861	U
31	CA	2867	G
31	CA	2877	G
31	CA	2883	A
31	CA	2886	A
31	CA	2891	U
31	CA	2903	U
28	DB	9	G
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
28	DB	120	U
33	DA	10	A
33	DA	12	U
33	DA	13	A
33	DA	34	U
33	DA	46	G
33	DA	51	G
33	DA	58	G
33	DA	63	A
33	DA	71	A

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Mol	Chain	Res	Type
33	DA	74	A
33	DA	75	G
33	DA	80	G
33	DA	84	A
33	DA	86	G
33	DA	101	A
33	DA	102	U
33	DA	118	A
33	DA	119	A
33	DA	120	U
33	DA	138	U
33	DA	139	U
33	DA	140	C
33	DA	141	G
33	DA	142	A
33	DA	196	A
33	DA	197	A
33	DA	199	A
33	DA	200	U
33	DA	215	G
33	DA	216	A
33	DA	221	A
33	DA	222	A
33	DA	248	G
33	DA	265	A
33	DA	266	G
33	DA	271	G
33	DA	272	A
33	DA	276	U
33	DA	277	G
33	DA	278	A
33	DA	279	A
33	DA	302	C
33	DA	308	G
33	DA	310	A
33	DA	311	A
33	DA	312	G
33	DA	329	G
33	DA	330	A
33	DA	343	C
33	DA	345	A
33	DA	346	A

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Mol	Chain	Res	Type
33	DA	352	A
33	DA	353	C
33	DA	362	A
33	DA	370	G
33	DA	372	G
33	DA	386	G
33	DA	387	U
33	DA	399	U
33	DA	403	U
33	DA	406	G
33	DA	411	G
33	DA	412	A
33	DA	420	C
33	DA	424	G
33	DA	451	U
33	DA	454	A
33	DA	455	C
33	DA	456	C
33	DA	459	U
33	DA	460	A
33	DA	480	A
33	DA	481	G
33	DA	491	G
33	DA	496	G
33	DA	503	A
33	DA	504	A
33	DA	505	A
33	DA	508	A
33	DA	518	G
33	DA	531	C
33	DA	532	A
33	DA	533	G
33	DA	543	G
33	DA	544	C
33	DA	546	U
33	DA	547	A
33	DA	548	G
33	DA	549	G
33	DA	550	C
33	DA	551	G
33	DA	563	A
33	DA	573	U

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Mol	Chain	Res	Type
33	DA	575	A
33	DA	586	A
33	DA	603	A
33	DA	613	A
33	DA	614	A
33	DA	615	U
33	DA	620	G
33	DA	621	A
33	DA	627	A
33	DA	634	C
33	DA	637	A
33	DA	645	C
33	DA	647	G
33	DA	653	U
33	DA	654	A
33	DA	655	A
33	DA	686	U
33	DA	687	C
33	DA	702	U
33	DA	717	C
33	DA	730	A
33	DA	747	5MU
33	DA	758	C
33	DA	764	A
33	DA	765	C
33	DA	775	G
33	DA	776	G
33	DA	782	A
33	DA	784	G
33	DA	785	G
33	DA	790	U
33	DA	792	A
33	DA	802	A
33	DA	805	G
33	DA	812	C
33	DA	827	U
33	DA	828	U
33	DA	858	G
33	DA	859	G
33	DA	866	A
33	DA	870	U
33	DA	878	A

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Mol	Chain	Res	Type
33	DA	883	G
33	DA	885	C
33	DA	896	A
33	DA	897	C
33	DA	910	A
33	DA	915	C
33	DA	931	U
33	DA	932	U
33	DA	946	C
33	DA	961	C
33	DA	962	G
33	DA	974	G
33	DA	983	A
33	DA	984	A
33	DA	985	C
33	DA	996	A
33	DA	1005	C
33	DA	1012	U
33	DA	1013	C
33	DA	1022	G
33	DA	1023	U
33	DA	1026	G
33	DA	1033	U
33	DA	1040	A
33	DA	1047	G
33	DA	1061	U
33	DA	1062	G
33	DA	1069	A
33	DA	1070	A
33	DA	1073	A
33	DA	1083	U
33	DA	1088	A
33	DA	1090	A
33	DA	1096	A
33	DA	1097	U
33	DA	1112	G
33	DA	1128	G
33	DA	1129	A
33	DA	1130	U
33	DA	1132	U
33	DA	1133	A
33	DA	1134	A

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Mol	Chain	Res	Type
33	DA	1135	C
33	DA	1136	G
33	DA	1142	A
33	DA	1168	G
33	DA	1172	C
33	DA	1174	U
33	DA	1176	U
33	DA	1177	G
33	DA	1180	U
33	DA	1182	G
33	DA	1210	G
33	DA	1227	G
33	DA	1238	G
33	DA	1253	A
33	DA	1256	G
33	DA	1271	G
33	DA	1272	A
33	DA	1273	U
33	DA	1284	A
33	DA	1300	G
33	DA	1301	A
33	DA	1306	C
33	DA	1321	A
33	DA	1329	U
33	DA	1341	G
33	DA	1352	U
33	DA	1365	A
33	DA	1376	C
33	DA	1379	U
33	DA	1380	G
33	DA	1383	A
33	DA	1386	C
33	DA	1403	A
33	DA	1416	G
33	DA	1417	C
33	DA	1420	A
33	DA	1427	A
33	DA	1428	C
33	DA	1434	A
33	DA	1452	G
33	DA	1453	A
33	DA	1458	U

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Mol	Chain	Res	Type
33	DA	1460	U
33	DA	1482	G
33	DA	1490	A
33	DA	1491	G
33	DA	1493	C
33	DA	1494	A
33	DA	1497	U
33	DA	1508	A
33	DA	1509	A
33	DA	1510	G
33	DA	1515	A
33	DA	1523	U
33	DA	1532	A
33	DA	1534	U
33	DA	1535	A
33	DA	1536	C
33	DA	1537	G
33	DA	1569	A
33	DA	1578	U
33	DA	1583	A
33	DA	1584	U
33	DA	1585	C
33	DA	1607	C
33	DA	1608	A
33	DA	1609	A
33	DA	1610	A
33	DA	1616	A
33	DA	1639	C
33	DA	1647	U
33	DA	1648	U
33	DA	1649	G
33	DA	1660	G
33	DA	1674	G
33	DA	1694	C
33	DA	1715	G
33	DA	1729	U
33	DA	1730	C
33	DA	1731	G
33	DA	1732	C
33	DA	1738	G
33	DA	1744	A
33	DA	1758	U

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Mol	Chain	Res	Type
33	DA	1764	C
33	DA	1773	A
33	DA	1782	U
33	DA	1800	C
33	DA	1801	A
33	DA	1808	A
33	DA	1816	C
33	DA	1826	G
33	DA	1869	G
33	DA	1870	C
33	DA	1871	A
33	DA	1872	A
33	DA	1873	G
33	DA	1900	A
33	DA	1906	G
33	DA	1907	G
33	DA	1913	A
33	DA	1914	C
33	DA	1929	G
33	DA	1930	G
33	DA	1931	U
33	DA	1937	A
33	DA	1938	A
33	DA	1939	5MU
33	DA	1955	U
33	DA	1965	C
33	DA	1967	C
33	DA	1970	A
33	DA	1972	G
33	DA	1991	U
33	DA	1993	U
33	DA	1997	C
33	DA	2018	G
33	DA	2023	C
33	DA	2028	U
33	DA	2030	6MZ
33	DA	2031	A
33	DA	2033	A
33	DA	2043	C
33	DA	2049	G
33	DA	2055	C
33	DA	2056	G

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Mol	Chain	Res	Type
33	DA	2060	A
33	DA	2061	G
33	DA	2062	A
33	DA	2069	G7M
33	DA	2080	A
33	DA	2093	G
33	DA	2097	A
33	DA	2098	U
33	DA	2100	G
33	DA	2105	U
33	DA	2111	U
33	DA	2112	G
33	DA	2113	U
33	DA	2116	G
33	DA	2117	A
33	DA	2118	U
33	DA	2119	A
33	DA	2120	G
33	DA	2123	G
33	DA	2125	G
33	DA	2126	A
33	DA	2128	G
33	DA	2131	U
33	DA	2132	U
33	DA	2133	G
33	DA	2134	A
33	DA	2135	A
33	DA	2145	C
33	DA	2146	C
33	DA	2148	G
33	DA	2157	G
33	DA	2158	A
33	DA	2159	G
33	DA	2160	C
33	DA	2161	C
33	DA	2162	G
33	DA	2163	A
33	DA	2164	C
33	DA	2165	C
33	DA	2167	U
33	DA	2168	G
33	DA	2169	A

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Mol	Chain	Res	Type
33	DA	2170	A
33	DA	2171	A
33	DA	2172	U
33	DA	2173	A
33	DA	2178	C
33	DA	2179	C
33	DA	2181	U
33	DA	2183	A
33	DA	2185	U
33	DA	2186	G
33	DA	2190	G
33	DA	2195	U
33	DA	2198	A
33	DA	2203	U
33	DA	2204	G
33	DA	2211	A
33	DA	2225	A
33	DA	2238	G
33	DA	2239	G
33	DA	2243	U
33	DA	2268	A
33	DA	2279	G
33	DA	2280	G
33	DA	2282	G
33	DA	2283	C
33	DA	2286	G
33	DA	2287	A
33	DA	2288	A
33	DA	2305	U
33	DA	2308	G
33	DA	2311	A
33	DA	2312	U
33	DA	2322	A
33	DA	2325	G
33	DA	2331	G
33	DA	2333	A
33	DA	2335	A
33	DA	2345	G
33	DA	2347	C
33	DA	2354	C
33	DA	2357	G
33	DA	2383	G

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Mol	Chain	Res	Type
33	DA	2385	C
33	DA	2393	U
33	DA	2402	U
33	DA	2403	C
33	DA	2406	A
33	DA	2407	A
33	DA	2410	G
33	DA	2423	U
33	DA	2424	C
33	DA	2425	A
33	DA	2435	A
33	DA	2441	U
33	DA	2445	2MG
33	DA	2448	A
33	DA	2476	A
33	DA	2484	G
33	DA	2491	U
33	DA	2494	G
33	DA	2502	G
33	DA	2505	G
33	DA	2518	A
33	DA	2529	G
33	DA	2547	A
33	DA	2566	A
33	DA	2567	G
33	DA	2573	C
33	DA	2585	U
33	DA	2586	U
33	DA	2603	G
33	DA	2609	U
33	DA	2613	U
33	DA	2623	G
33	DA	2629	U
33	DA	2630	G
33	DA	2634	A
33	DA	2661	G
33	DA	2663	G
33	DA	2682	A
33	DA	2689	U
33	DA	2690	U
33	DA	2691	C
33	DA	2714	G

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Mol	Chain	Res	Type
33	DA	2718	G
33	DA	2719	G
33	DA	2720	U
33	DA	2726	A
33	DA	2733	A
33	DA	2739	U
33	DA	2744	G
33	DA	2748	A
33	DA	2751	G
33	DA	2762	C
33	DA	2765	A
33	DA	2778	A
33	DA	2791	G
33	DA	2798	U
33	DA	2799	A
33	DA	2820	A
33	DA	2821	A
33	DA	2823	A
33	DA	2825	G
33	DA	2835	A
33	DA	2836	U
33	DA	2849	U
33	DA	2850	A
33	DA	2861	U
33	DA	2867	G
33	DA	2877	G
33	DA	2883	A
33	DA	2891	U
33	DA	2903	U

All (248) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	7	A
1	AA	30	U
1	AA	70	U
1	AA	88	U
1	AA	89	U
1	AA	181	A
1	AA	209	U
1	AA	281	G

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Mol	Chain	Res	Type
1	AA	305	G
1	AA	367	U
1	AA	413	G
1	AA	422	C
1	AA	438	U
1	AA	485	U
1	AA	653	U
1	AA	702	A
1	AA	733	G
1	AA	793	U
1	AA	841	C
1	AA	872	A
1	AA	884	U
1	AA	992	U
1	AA	1086	U
1	AA	1094	G
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1224	U
1	AA	1225	A
1	AA	1281	C
1	AA	1299	A
1	AA	1319	A
1	AA	1380	U
1	AA	1397	C
1	AA	1447	A
1	AA	1452	C
1	BA	5	U
1	BA	7	A
1	BA	30	U
1	BA	70	U
1	BA	86	G
1	BA	89	U
1	BA	181	A
1	BA	209	U
1	BA	246	A
1	BA	281	G
1	BA	305	G
1	BA	367	U
1	BA	411	A

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Mol	Chain	Res	Type
1	BA	422	C
1	BA	438	U
1	BA	485	U
1	BA	559	A
1	BA	561	U
1	BA	653	U
1	BA	702	A
1	BA	733	G
1	BA	793	U
1	BA	842	U
1	BA	872	A
1	BA	884	U
1	BA	992	U
1	BA	1008	U
1	BA	1086	U
1	BA	1094	G
1	BA	1137	C
1	BA	1139	G
1	BA	1140	C
1	BA	1141	C
1	BA	1224	U
1	BA	1225	A
1	BA	1281	C
1	BA	1299	A
1	BA	1319	A
1	BA	1362	A
1	BA	1363	A
1	BA	1380	U
1	BA	1447	A
1	BA	1452	C
1	BA	1493	A
31	CA	33	C
31	CA	62	U
31	CA	83	A
31	CA	138	U
31	CA	139	U
31	CA	141	G
31	CA	177	G
31	CA	196	A
31	CA	199	A
31	CA	228	C
31	CA	271	G

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Mol	Chain	Res	Type
31	CA	278	A
31	CA	310	A
31	CA	345	A
31	CA	361	G
31	CA	386	G
31	CA	387	U
31	CA	403	U
31	CA	404	A
31	CA	411	G
31	CA	455	C
31	CA	503	A
31	CA	506	G
31	CA	527	C
31	CA	555	G
31	CA	620	G
31	CA	684	G
31	CA	685	A
31	CA	764	A
31	CA	784	G
31	CA	846	U
31	CA	913	U
31	CA	961	C
31	CA	973	A
31	CA	980	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	1141	U
31	CA	1253	A
31	CA	1288	G
31	CA	1300	G
31	CA	1320	C
31	CA	1329	U
31	CA	1379	U
31	CA	1396	U

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Mol	Chain	Res	Type
31	CA	1452	G
31	CA	1490	A
31	CA	1497	U
31	CA	1509	A
31	CA	1535	A
31	CA	1536	C
31	CA	1607	C
31	CA	1609	A
31	CA	1647	U
31	CA	1730	C
31	CA	1786	A
31	CA	1800	C
31	CA	1818	U
31	CA	1870	C
31	CA	1871	A
31	CA	1900	A
31	CA	1966	A
31	CA	2035	G
31	CA	2043	C
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	2286	G
31	CA	2326	C
31	CA	2423	U
31	CA	2425	A
31	CA	2517	C
31	CA	2645	G
31	CA	2680	U
31	CA	2681	C
31	CA	2778	A
31	CA	2779	U
31	CA	2790	U
31	CA	2849	U
31	CA	2873	A
31	CA	2893	A
33	DA	62	U

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Mol	Chain	Res	Type
33	DA	101	A
33	DA	138	U
33	DA	141	G
33	DA	177	G
33	DA	196	A
33	DA	199	A
33	DA	228	C
33	DA	271	G
33	DA	278	A
33	DA	310	A
33	DA	345	A
33	DA	370	G
33	DA	387	U
33	DA	403	U
33	DA	455	C
33	DA	503	A
33	DA	532	A
33	DA	620	G
33	DA	764	A
33	DA	784	G
33	DA	961	C
33	DA	984	A
33	DA	1046	A
33	DA	1061	U
33	DA	1069	A
33	DA	1070	A
33	DA	1089	A
33	DA	1128	G
33	DA	1133	A
33	DA	1141	U
33	DA	1171	G
33	DA	1175	A
33	DA	1253	A
33	DA	1286	A
33	DA	1288	G
33	DA	1300	G
33	DA	1396	U
33	DA	1490	A
33	DA	1497	U
33	DA	1509	A
33	DA	1523	U
33	DA	1535	A

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Mol	Chain	Res	Type
33	DA	1536	C
33	DA	1565	C
33	DA	1607	C
33	DA	1609	A
33	DA	1647	U
33	DA	1730	C
33	DA	1800	C
33	DA	1870	C
33	DA	1871	A
33	DA	1939	5MU
33	DA	2097	A
33	DA	2119	A
33	DA	2127	G
33	DA	2146	C
33	DA	2157	G
33	DA	2158	A
33	DA	2164	C
33	DA	2282	G
33	DA	2286	G
33	DA	2311	A
33	DA	2406	A
33	DA	2423	U
33	DA	2585	U
33	DA	2778	A
33	DA	2779	U
33	DA	2790	U
33	DA	2798	U
33	DA	2849	U
33	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
1	G7M	AA	527	1	23,26,27	0.53	0	34,39,42	2.04	5 (14%)
33	2MG	DA	2445	33	23,26,27	0.49	0	33,38,41	0.36	0
42	4D4	CN	81	42	9,11,12	2.16	2 (22%)	7,13,15	2.38	2 (28%)
33	PSU	DA	2457	33	18,21,22	0.52	0	21,30,33	0.45	0
33	G7M	DA	2069	33	23,26,27	0.52	0	34,39,42	1.96	5 (14%)
31	PSU	CA	2580	31	18,21,22	0.47	0	21,30,33	0.56	0
33	PSU	DA	2605	33	18,21,22	0.40	0	21,30,33	0.59	0
1	5MC	AA	967	1	19,22,23	0.28	0	26,32,35	0.36	0
32	MEQ	DD	150[B]	32	8,9,10	1.14	1 (12%)	5,10,12	0.91	0
42	4D4	DN	81[A]	-	9,11,12	1.57	2 (22%)	7,13,15	2.66	2 (28%)
31	PSU	CA	2457	31	18,21,22	0.52	0	21,30,33	0.53	0
33	2MG	DA	1835	33	23,26,27	0.31	0	33,38,41	0.38	0
33	OMU	DA	2552	33	19,22,23	0.44	0	25,31,34	0.27	0
1	5MC	BA	967	1	19,22,23	0.30	0	26,32,35	0.36	0
31	2MA	CA	2503	31	22,25,26	0.75	0	32,37,40	1.84	6 (18%)
31	PSU	CA	2605	31	18,21,22	0.36	0	21,30,33	0.51	0
33	2MA	DA	2503	56,33	22,25,26	0.80	1 (4%)	32,37,40	1.96	6 (18%)
31	5MU	CA	747	31	19,22,23	0.21	0	27,32,35	0.32	0
1	5MC	AA	1407	1	19,22,23	0.32	0	26,32,35	0.46	0
33	5MU	DA	1939	33	19,22,23	0.62	0	27,32,35	0.43	0
1	UR3	AA	1498	1	19,22,23	0.49	0	26,32,35	0.43	0
31	2MG	CA	1835	31	23,26,27	0.34	0	33,38,41	0.38	0
31	5MU	CA	1939	31	19,22,23	0.38	0	27,32,35	0.30	0
33	OMC	DA	2498	56,33	19,22,23	0.50	0	25,31,34	0.44	0
12	D2T	BL	89	12	8,9,10	0.72	0	6,11,13	0.74	0
31	2MG	CA	2445	31	23,26,27	0.44	0	33,38,41	0.44	0
31	G7M	CA	2069	31	23,26,27	0.63	0	34,39,42	2.05	5 (14%)
33	OMG	DA	2251	33	23,26,27	0.31	0	32,38,41	0.36	0
42	4D4	DN	81[B]	-	9,11,12	1.76	1 (11%)	7,13,15	2.85	2 (28%)
31	5MC	CA	1962	31	19,22,23	0.23	0	26,32,35	0.38	0
1	2MG	AA	966	1	23,26,27	0.33	0	33,38,41	0.50	0
1	MA6	AA	1519	1	23,26,27	0.60	0	33,38,41	1.08	4 (12%)
1	2MG	AA	1207	1	23,26,27	0.25	0	33,38,41	0.41	0
31	6MZ	CA	2030	31	22,25,26	0.37	0	29,36,39	0.43	0
31	OMU	CA	2552	31	19,22,23	0.33	0	25,31,34	0.27	0
32	MEQ	DD	150[A]	32	8,9,10	0.43	0	5,10,12	0.66	0
1	2MG	AA	1516	1	23,26,27	0.31	0	33,38,41	0.43	0
1	5MC	BA	1407	1	19,22,23	0.38	0	26,32,35	0.45	0
33	PSU	DA	2504	33	18,21,22	0.55	0	21,30,33	0.33	0
1	4OC	BA	1402	1	20,23,24	0.35	0	25,32,35	0.54	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	PSU	DA	2580	33	18,21,22	0.57	0	21,30,33	0.57	0
33	PSU	DA	1917	33	18,21,22	0.44	0	21,30,33	0.44	0
1	PSU	BA	516	1	18,21,22	0.33	0	21,30,33	0.42	0
1	MA6	BA	1518	1	23,26,27	0.44	0	33,38,41	1.18	4 (12%)
31	1MG	CA	745	31	23,26,27	1.01	1 (4%)	33,39,42	0.63	0
31	PSU	CA	2504	31	18,21,22	0.38	0	21,30,33	0.38	0
1	UR3	BA	1498	1	19,22,23	0.37	0	26,32,35	0.39	0
33	5MC	DA	1962	33	19,22,23	0.42	0	26,32,35	0.44	0
31	3TD	CA	1915	31	19,22,23	0.47	0	23,32,35	0.74	1 (4%)
33	1MG	DA	745	33	23,26,27	1.20	1 (4%)	33,39,42	0.54	0
33	3TD	DA	1915	33	19,22,23	0.43	0	23,32,35	0.77	1 (4%)
33	H2U	DA	2449	33	18,21,22	0.78	0	19,30,33	0.44	0
1	2MG	BA	1207	1	23,26,27	0.29	0	33,38,41	0.42	0
1	MA6	BA	1519	1	23,26,27	0.53	0	33,38,41	1.07	4 (12%)
31	PSU	CA	1917	31	18,21,22	0.32	0	21,30,33	0.42	0
1	2MG	BA	1516	1	23,26,27	0.29	0	33,38,41	0.42	0
33	PSU	DA	1911	33	18,21,22	0.32	0	21,30,33	0.42	0
1	MA6	AA	1518	1	23,26,27	0.41	0	33,38,41	1.09	4 (12%)
33	6MZ	DA	2030	33	22,25,26	0.53	0	29,36,39	0.58	0
31	PSU	CA	746	31,56	18,21,22	0.69	1 (5%)	21,30,33	0.59	0
33	PSU	DA	746	56,33	18,21,22	0.98	2 (11%)	21,30,33	0.38	0
31	OMC	CA	2498	31,56	19,22,23	0.37	0	25,31,34	0.35	0
31	OMG	CA	2251	31	23,26,27	0.40	0	32,38,41	0.51	0
1	G7M	BA	527	1	23,26,27	0.67	0	34,39,42	2.06	5 (14%)
33	PSU	DA	955	33	18,21,22	0.49	0	21,30,33	0.44	0
31	PSU	CA	955	31	18,21,22	0.32	0	21,30,33	0.46	0
1	PSU	AA	516	56,1	18,21,22	0.31	0	21,30,33	0.42	0
12	D2T	AL	89	12	8,9,10	0.92	0	6,11,13	0.98	0
1	2MG	BA	966	1	23,26,27	0.31	0	33,38,41	0.40	0
31	PSU	CA	1911	31	18,21,22	0.32	0	21,30,33	0.43	0
33	6MZ	DA	1618	33	22,25,26	0.36	0	29,36,39	0.47	0
1	4OC	AA	1402	1	20,23,24	0.31	0	25,32,35	0.57	1 (4%)
33	5MU	DA	747	33	19,22,23	0.31	0	27,32,35	0.37	0
33	PSU	DA	2604	33	18,21,22	0.44	0	21,30,33	0.48	0
31	6MZ	CA	1618	31	22,25,26	0.48	0	29,36,39	0.81	1 (3%)

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
1	G7M	AA	527	1	-	2/7/25/26	0/3/3/3
33	2MG	DA	2445	33	-	2/9/27/28	0/3/3/3
42	4D4	CN	81	42	-	1/11/12/14	-
33	PSU	DA	2457	33	-	0/7/25/26	0/2/2/2
33	G7M	DA	2069	33	-	1/7/25/26	0/3/3/3
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
33	PSU	DA	2605	33	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
32	MEQ	DD	150[B]	32	-	4/8/9/11	-
42	4D4	DN	81[A]	-	-	1/11/12/14	-
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
33	2MG	DA	1835	33	-	1/9/27/28	0/3/3/3
33	OMU	DA	2552	33	-	0/9/27/28	0/2/2/2
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
31	2MA	CA	2503	31	-	1/7/25/26	0/3/3/3
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
33	2MA	DA	2503	56,33	-	1/7/25/26	0/3/3/3
31	5MU	CA	747	31	-	0/7/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
33	5MU	DA	1939	33	-	1/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
31	2MG	CA	1835	31	-	1/9/27/28	0/3/3/3
31	5MU	CA	1939	31	-	0/7/25/26	0/2/2/2
33	OMC	DA	2498	56,33	-	0/9/27/28	0/2/2/2
12	D2T	BL	89	12	-	6/7/12/14	-
31	2MG	CA	2445	31	-	1/9/27/28	0/3/3/3
31	G7M	CA	2069	31	-	1/7/25/26	0/3/3/3
33	OMG	DA	2251	33	-	1/9/27/28	0/3/3/3
42	4D4	DN	81[B]	-	-	3/11/12/14	-
31	5MC	CA	1962	31	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/9/27/28	0/3/3/3
1	MA6	AA	1519	1	-	2/11/29/30	0/3/3/3
1	2MG	AA	1207	1	-	0/9/27/28	0/3/3/3
31	6MZ	CA	2030	31	-	2/9/27/28	0/3/3/3
31	OMU	CA	2552	31	-	0/9/27/28	0/2/2/2
32	MEQ	DD	150[A]	32	-	4/8/9/11	-
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
33	PSU	DA	2504	33	-	0/7/25/26	0/2/2/2
1	4OC	BA	1402	1	-	0/9/29/30	0/2/2/2
33	PSU	DA	2580	33	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PSU	DA	1917	33	-	0/7/25/26	0/2/2/2
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
1	MA6	BA	1518	1	-	0/11/29/30	0/3/3/3
31	1MG	CA	745	31	-	0/7/25/26	0/3/3/3
31	PSU	CA	2504	31	-	1/7/25/26	0/2/2/2
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
33	5MC	DA	1962	33	-	0/7/25/26	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
33	1MG	DA	745	33	-	0/7/25/26	0/3/3/3
33	3TD	DA	1915	33	-	0/7/25/26	0/2/2/2
33	H2U	DA	2449	33	-	0/7/38/39	0/2/2/2
1	2MG	BA	1207	1	-	0/9/27/28	0/3/3/3
1	MA6	BA	1519	1	-	2/11/29/30	0/3/3/3
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
1	2MG	BA	1516	1	-	0/9/27/28	0/3/3/3
33	PSU	DA	1911	33	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/11/29/30	0/3/3/3
33	6MZ	DA	2030	33	-	0/9/27/28	0/3/3/3
31	PSU	CA	746	31,56	-	1/7/25/26	0/2/2/2
33	PSU	DA	746	56,33	-	1/7/25/26	0/2/2/2
31	OMC	CA	2498	31,56	-	2/9/27/28	0/2/2/2
31	OMG	CA	2251	31	-	1/9/27/28	0/3/3/3
1	G7M	BA	527	1	-	2/7/25/26	0/3/3/3
33	PSU	DA	955	33	-	0/7/25/26	0/2/2/2
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	56,1	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	3/7/12/14	-
1	2MG	BA	966	1	-	0/9/27/28	0/3/3/3
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
33	6MZ	DA	1618	33	-	0/9/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
33	5MU	DA	747	33	-	0/7/25/26	0/2/2/2
33	PSU	DA	2604	33	-	0/7/25/26	0/2/2/2
31	6MZ	CA	1618	31	-	1/9/27/28	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	CN	81	4D4	CZ-NE	5.77	1.44	1.33
33	DA	745	1MG	C2-N1	5.48	1.47	1.37
42	DN	81[B]	4D4	CZ-NE	4.76	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	745	1MG	C2-N1	4.44	1.45	1.37
42	DN	81[A]	4D4	CZ-NE	3.99	1.41	1.33
33	DA	746	PSU	O4'-C1'	-3.35	1.39	1.43
32	DD	150[B]	MEQ	CB-CA	3.04	1.58	1.53
42	CN	81	4D4	CZ-NH1	2.64	1.44	1.34
31	CA	746	PSU	O4'-C1'	-2.34	1.40	1.43
33	DA	2503	2MA	C6-N6	-2.14	1.28	1.34
33	DA	746	PSU	C2'-C1'	-2.10	1.50	1.53
42	DN	81[A]	4D4	CZ-NH1	2.01	1.41	1.34

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2069	G7M	C6-C5-N7	-8.72	121.24	132.17
33	DA	2503	2MA	N6-C6-N1	8.36	128.31	117.03
31	CA	2503	2MA	N6-C6-N1	7.92	127.71	117.03
33	DA	2069	G7M	C6-C5-N7	-7.86	122.32	132.17
1	AA	527	G7M	C6-C5-N7	-7.79	122.40	132.17
1	BA	527	G7M	C6-C5-N7	-7.63	122.60	132.17
42	DN	81[B]	4D4	NE-CZ-NH2	6.51	131.84	120.67
42	DN	81[A]	4D4	NE-CZ-NH2	5.77	130.58	120.67
1	BA	527	G7M	C6-C5-C4	-5.40	109.66	119.01
42	CN	81	4D4	NE-CZ-NH2	5.26	129.71	120.67
1	AA	527	G7M	C5-C4-N3	-5.23	118.26	128.15
31	CA	2069	G7M	C6-C5-C4	-5.22	109.97	119.01
33	DA	2069	G7M	C5-C4-N3	-5.12	118.47	128.15
1	BA	527	G7M	C5-C4-N3	-4.82	119.04	128.15
33	DA	2069	G7M	O4'-C1'-N9	4.41	118.36	108.36
33	DA	2503	2MA	C2-N1-C6	4.34	124.78	118.10
1	AA	527	G7M	C6-C5-C4	-4.26	111.63	119.01
31	CA	2069	G7M	C5-C4-N3	-4.21	120.20	128.15
31	CA	2503	2MA	C2-N1-C6	4.13	124.45	118.10
1	BA	527	G7M	O4'-C1'-N9	3.89	117.17	108.36
1	BA	1518	MA6	C4-C5-C6	-3.82	111.95	115.91
1	AA	527	G7M	C4-C5-N7	-3.52	101.91	107.67
33	DA	2069	G7M	C4-C5-N7	-3.48	101.97	107.67
1	AA	1518	MA6	C4-C5-C6	-3.45	112.34	115.91
42	DN	81[A]	4D4	NH1-CZ-NE	-3.42	111.48	119.27
31	CA	1618	6MZ	C9-N6-C6	3.35	125.96	122.85
1	BA	527	G7M	C4-C5-N7	-3.35	102.19	107.67
1	BA	1519	MA6	C4-C5-C6	-3.30	112.50	115.91
1	AA	1519	MA6	C4-C5-C6	-3.30	112.50	115.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	527	G7M	O4'-C1'-N9	3.25	115.72	108.36
31	CA	2069	G7M	C4-C5-N7	-3.16	102.50	107.67
42	DN	81[B]	4D4	NH1-CZ-NE	-3.09	112.24	119.27
1	BA	1518	MA6	N1-C6-N6	-2.99	113.22	116.86
33	DA	1915	3TD	C1'-C5-C4	2.94	122.07	117.61
31	CA	1915	3TD	C1'-C5-C4	2.81	121.88	117.61
31	CA	2069	G7M	O4'-C1'-N9	2.65	114.36	108.36
42	CN	81	4D4	NH1-CZ-NE	-2.63	113.29	119.27
33	DA	2503	2MA	C5-C6-N6	-2.61	116.82	123.29
33	DA	2503	2MA	C5-C6-N1	-2.59	114.88	118.90
1	BA	1518	MA6	C5-C6-N1	2.58	123.91	118.55
31	CA	2503	2MA	C5-C6-N1	-2.58	114.89	118.90
1	BA	1518	MA6	C6-C5-N7	2.50	137.43	133.43
33	DA	2503	2MA	N3-C2-N1	-2.48	121.39	125.77
1	AA	1518	MA6	N1-C6-N6	-2.46	113.86	116.86
1	AA	1518	MA6	C5-C6-N1	2.40	123.53	118.55
31	CA	2503	2MA	C5-C6-N6	-2.38	117.39	123.29
33	DA	2503	2MA	CM2-C2-N3	2.37	120.67	117.13
1	AA	1402	4OC	CM4-N4-C4	2.36	127.07	122.45
31	CA	2503	2MA	CM2-C2-N3	2.31	120.58	117.13
1	AA	1519	MA6	C5-C6-N1	2.26	123.23	118.55
1	AA	1518	MA6	C6-C5-N7	2.22	136.98	133.43
1	BA	1519	MA6	C5-C6-N1	2.21	123.14	118.55
31	CA	2503	2MA	N3-C2-N1	-2.21	121.87	125.77
1	BA	1402	4OC	CM4-N4-C4	2.17	126.70	122.45
1	AA	1519	MA6	N1-C6-N6	-2.16	114.23	116.86
1	BA	1519	MA6	N1-C6-N6	-2.13	114.26	116.86
1	BA	1519	MA6	C6-C5-N7	2.09	136.76	133.43
1	AA	1519	MA6	C6-C5-N7	2.08	136.76	133.43
33	DA	2069	G7M	C6-C5-C4	-2.05	115.46	119.01

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	AL	89	D2T	O-C-CA-CB
12	AL	89	D2T	CG-CB-SB-CB1
1	BA	527	G7M	O4'-C4'-C5'-O5'
1	BA	527	G7M	C3'-C4'-C5'-O5'
12	BL	89	D2T	O-C-CA-CB
12	BL	89	D2T	CA-CB-SB-CB1
12	BL	89	D2T	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
12	BL	89	D2T	CA-CB-CG-OD2
12	BL	89	D2T	SB-CB-CG-OD2
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
33	DA	2251	OMG	C1'-C2'-O2'-CM2
42	DN	81[B]	4D4	CA-CB-CG-CD
42	DN	81[B]	4D4	OB-CB-CG-CD
1	AA	527	G7M	O4'-C4'-C5'-O5'
1	AA	527	G7M	C3'-C4'-C5'-O5'
33	DA	2445	2MG	C3'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
1	BA	1519	MA6	O4'-C4'-C5'-O5'
33	DA	2445	2MG	O4'-C4'-C5'-O5'
32	DD	150[A]	MEQ	OE1-CD-CG-CB
32	DD	150[A]	MEQ	NE2-CD-CG-CB
32	DD	150[B]	MEQ	CA-CB-CG-CD
31	CA	746	PSU	O4'-C4'-C5'-O5'
31	CA	2030	6MZ	O4'-C4'-C5'-O5'
31	CA	1618	6MZ	C4'-C5'-O5'-P
1	AA	1519	MA6	C3'-C4'-C5'-O5'
1	BA	1519	MA6	C3'-C4'-C5'-O5'
31	CA	2445	2MG	C3'-C4'-C5'-O5'
12	AL	89	D2T	CA-CB-SB-CB1
31	CA	2251	OMG	C1'-C2'-O2'-CM2
33	DA	2069	G7M	C4'-C5'-O5'-P
33	DA	746	PSU	O4'-C1'-C5-C6
31	CA	2503	2MA	O4'-C4'-C5'-O5'
33	DA	1939	5MU	O4'-C4'-C5'-O5'
33	DA	2503	2MA	O4'-C4'-C5'-O5'
12	BL	89	D2T	CG-CB-SB-CB1
42	CN	81	4D4	O-C-CA-CB
42	DN	81[A]	4D4	O-C-CA-CB
42	DN	81[B]	4D4	O-C-CA-CB
31	CA	2030	6MZ	C3'-C4'-C5'-O5'
31	CA	2069	G7M	O4'-C4'-C5'-O5'
31	CA	1835	2MG	C3'-C4'-C5'-O5'
31	CA	2498	OMC	C4'-C5'-O5'-P
31	CA	2498	OMC	O4'-C4'-C5'-O5'
31	CA	2504	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
33	DA	1835	2MG	C3'-C4'-C5'-O5'

There are no ring outliers.

15 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	DD	150[B]	MEQ	1	0
31	CA	2503	2MA	1	0
33	DA	2503	2MA	1	0
31	CA	1835	2MG	1	0
12	BL	89	D2T	1	0
1	AA	1519	MA6	1	0
31	CA	2030	6MZ	1	0
31	CA	2552	OMU	1	0
32	DD	150[A]	MEQ	2	0
1	BA	1518	MA6	1	0
1	BA	1519	MA6	1	0
1	AA	1518	MA6	1	0
33	DA	2030	6MZ	1	0
31	CA	2251	OMG	1	0
12	AL	89	D2T	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 549 ligands modelled in this entry, 469 are monoatomic - leaving 80 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	MPD	DA	3207	-	7,7,7	0.67	0	9,10,10	0.43	0
64	SPD	DA	3185	-	9,9,9	0.12	0	8,8,8	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	EDO	DA	3227	-	3,3,3	0.53	0	2,2,2	0.36	0
57	PG4	BA	1642	-	12,12,12	0.17	0	11,11,11	0.16	0
58	MPD	DA	3204	-	7,7,7	0.54	0	9,10,10	0.53	0
63	PGE	DS	201	-	9,9,9	0.29	0	8,8,8	0.21	0
58	MPD	AA	1676	-	7,7,7	0.54	0	9,10,10	0.57	0
65	1PE	DA	3200	-	15,15,15	0.30	0	14,14,14	0.38	0
62	EDO	DA	3196	-	3,3,3	0.56	0	2,2,2	0.17	0
62	EDO	DA	3205	-	3,3,3	0.72	0	2,2,2	0.10	0
62	EDO	D1	101	-	3,3,3	0.58	0	2,2,2	0.10	0
65	1PE	DA	3183	-	15,15,15	0.18	0	14,14,14	0.15	0
57	PG4	DA	3213	-	12,12,12	0.14	0	11,11,11	0.16	0
59	PUT	AA	1673	-	5,5,5	0.09	0	4,4,4	0.09	0
66	ACY	DA	3194	-	3,3,3	2.36	1 (33%)	3,3,3	2.16	2 (66%)
59	PUT	DA	3202	-	5,5,5	0.09	0	4,4,4	0.09	0
58	MPD	DT	202	-	7,7,7	0.57	0	9,10,10	0.40	0
62	EDO	DA	3212	-	3,3,3	0.57	0	2,2,2	0.39	0
59	PUT	AA	1675	-	5,5,5	0.21	0	4,4,4	0.11	0
63	PGE	DA	3184	-	9,9,9	0.25	0	8,8,8	0.32	0
58	MPD	DN	201	-	7,7,7	0.81	0	9,10,10	0.49	0
58	MPD	DS	203	-	7,7,7	0.26	0	9,10,10	0.41	0
59	PUT	DA	3216	-	5,5,5	0.20	0	4,4,4	0.18	0
64	SPD	DA	3181	-	9,9,9	0.07	0	8,8,8	0.14	0
61	PEG	DP	201	-	6,6,6	0.12	0	5,5,5	0.04	0
59	PUT	DA	3186	-	5,5,5	0.30	0	4,4,4	0.20	0
62	EDO	DA	3206	-	3,3,3	0.58	0	2,2,2	0.28	0
61	PEG	AL	201	-	6,6,6	0.20	0	5,5,5	0.10	0
62	EDO	DA	3001	-	3,3,3	0.52	0	2,2,2	0.45	0
59	PUT	DA	3209	-	5,5,5	0.19	0	4,4,4	0.09	0
61	PEG	DA	3223	-	6,6,6	0.20	0	5,5,5	0.06	0
61	PEG	DA	3197	-	6,6,6	0.16	0	5,5,5	0.08	0
57	PG4	DS	202	-	12,12,12	0.29	0	11,11,11	0.23	0
58	MPD	DA	3201	-	7,7,7	0.54	0	9,10,10	0.51	0
59	PUT	DA	3226	-	5,5,5	0.10	0	4,4,4	0.08	0
61	PEG	DQ	201	-	6,6,6	0.11	0	5,5,5	0.07	0
63	PGE	DD	302	-	9,9,9	0.16	0	8,8,8	0.11	0
58	MPD	DE	301	-	7,7,7	0.70	0	9,10,10	0.49	0
59	PUT	DA	3220	-	5,5,5	0.14	0	4,4,4	0.07	0
59	PUT	AA	1674	-	5,5,5	0.14	0	4,4,4	0.06	0
58	MPD	DK	201	-	7,7,7	0.75	0	9,10,10	0.33	0
59	PUT	AA	1672	-	5,5,5	0.18	0	4,4,4	0.12	0
63	PGE	DT	201	-	9,9,9	0.14	0	8,8,8	0.12	0
61	PEG	DA	3198	-	6,6,6	0.21	0	5,5,5	0.15	0
68	TRS	DA	3217	-	7,7,7	0.27	0	9,9,9	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	PGE	DA	3211	-	9,9,9	0.10	0	8,8,8	0.08	0
63	PGE	D3	101	-	9,9,9	0.17	0	8,8,8	0.09	0
58	MPD	DA	3188	-	7,7,7	0.51	0	9,10,10	0.53	0
61	PEG	DA	3224	-	6,6,6	0.28	0	5,5,5	0.19	0
59	PUT	DA	3187	-	5,5,5	0.26	0	4,4,4	0.11	0
57	PG4	DA	3191	-	12,12,12	0.19	0	11,11,11	0.21	0
61	PEG	D3	102	-	6,6,6	0.25	0	5,5,5	0.17	0
59	PUT	DA	3210	-	5,5,5	0.19	0	4,4,4	0.08	0
57	PG4	AA	1670	-	12,12,12	0.25	0	11,11,11	0.22	0
63	PGE	DA	3222	-	9,9,9	0.15	0	8,8,8	0.27	0
58	MPD	DA	3190	-	7,7,7	0.51	0	9,10,10	0.64	0
66	ACY	DA	3189	-	3,3,3	0.60	0	3,3,3	0.98	0
58	MPD	DA	3228	-	7,7,7	0.54	0	9,10,10	0.34	0
66	ACY	DA	3199	-	3,3,3	0.66	0	3,3,3	0.97	0
62	EDO	D0	101	-	3,3,3	0.58	0	2,2,2	0.30	0
59	PUT	DA	3219	-	5,5,5	0.20	0	4,4,4	0.28	0
61	PEG	DL	201	-	6,6,6	0.17	0	5,5,5	0.08	0
58	MPD	AA	1671	-	7,7,7	0.60	0	9,10,10	0.44	0
59	PUT	DA	3218	-	5,5,5	0.16	0	4,4,4	0.13	0
61	PEG	D1	102	-	6,6,6	0.24	0	5,5,5	0.08	0
57	PG4	DQ	202	-	12,12,12	0.18	0	11,11,11	0.13	0
64	SPD	DA	3203	-	9,9,9	0.18	0	8,8,8	0.23	0
63	PGE	DU	101	-	9,9,9	0.25	0	8,8,8	0.18	0
62	EDO	DA	3192	-	3,3,3	0.50	0	2,2,2	0.34	0
62	EDO	DB	211	-	3,3,3	0.53	0	2,2,2	0.31	0
57	PG4	DR	203	-	12,12,12	0.20	0	11,11,11	0.22	0
63	PGE	DA	3214	-	9,9,9	0.16	0	8,8,8	0.14	0
62	EDO	DA	3195	-	3,3,3	0.57	0	2,2,2	0.32	0
67	GUN	DA	3208	-	12,12,12	0.37	0	15,17,17	0.28	0
59	PUT	DA	3193	-	5,5,5	0.33	0	4,4,4	0.38	0
62	EDO	DB	210	-	3,3,3	0.54	0	2,2,2	0.25	0
58	MPD	DE	302	-	7,7,7	0.62	0	9,10,10	0.52	0
59	PUT	DA	3182	-	5,5,5	0.13	0	4,4,4	0.13	0
64	SPD	DA	3221	-	9,9,9	0.10	0	8,8,8	0.33	0
61	PEG	DA	3215	-	6,6,6	0.15	0	5,5,5	0.04	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
58	MPD	DA	3207	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	SPD	DA	3185	-	-	1/7/7/7	-
62	EDO	DA	3227	-	-	0/1/1/1	-
57	PG4	BA	1642	-	-	1/10/10/10	-
58	MPD	DA	3204	-	-	2/5/5/5	-
63	PGE	DS	201	-	-	3/7/7/7	-
58	MPD	AA	1676	-	-	1/5/5/5	-
65	1PE	DA	3200	-	-	5/13/13/13	-
62	EDO	DA	3196	-	-	0/1/1/1	-
62	EDO	DA	3205	-	-	0/1/1/1	-
62	EDO	D1	101	-	-	0/1/1/1	-
65	1PE	DA	3183	-	-	5/13/13/13	-
57	PG4	DA	3213	-	-	4/10/10/10	-
59	PUT	AA	1673	-	-	0/3/3/3	-
59	PUT	DA	3202	-	-	1/3/3/3	-
58	MPD	DT	202	-	-	1/5/5/5	-
62	EDO	DA	3212	-	-	0/1/1/1	-
59	PUT	AA	1675	-	-	1/3/3/3	-
63	PGE	DA	3184	-	-	3/7/7/7	-
58	MPD	DN	201	-	-	3/5/5/5	-
58	MPD	DS	203	-	-	0/5/5/5	-
59	PUT	DA	3216	-	-	0/3/3/3	-
64	SPD	DA	3181	-	-	4/7/7/7	-
61	PEG	DP	201	-	-	2/4/4/4	-
59	PUT	DA	3186	-	-	0/3/3/3	-
62	EDO	DA	3206	-	-	0/1/1/1	-
61	PEG	AL	201	-	-	2/4/4/4	-
62	EDO	DA	3001	-	-	0/1/1/1	-
59	PUT	DA	3209	-	-	0/3/3/3	-
61	PEG	DA	3223	-	-	2/4/4/4	-
61	PEG	DA	3197	-	-	1/4/4/4	-
57	PG4	DS	202	-	-	2/10/10/10	-
58	MPD	DA	3201	-	-	4/5/5/5	-
59	PUT	DA	3226	-	-	0/3/3/3	-
61	PEG	DQ	201	-	-	1/4/4/4	-
63	PGE	DD	302	-	-	4/7/7/7	-
58	MPD	DE	301	-	-	1/5/5/5	-
59	PUT	DA	3220	-	-	1/3/3/3	-
59	PUT	AA	1674	-	-	1/3/3/3	-
58	MPD	DK	201	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PUT	AA	1672	-	-	0/3/3/3	-
63	PGE	DT	201	-	-	4/7/7/7	-
61	PEG	DA	3198	-	-	1/4/4/4	-
68	TRS	DA	3217	-	-	0/9/9/9	-
63	PGE	DA	3211	-	-	3/7/7/7	-
63	PGE	D3	101	-	-	2/7/7/7	-
58	MPD	DA	3188	-	-	2/5/5/5	-
61	PEG	DA	3224	-	-	0/4/4/4	-
59	PUT	DA	3187	-	-	0/3/3/3	-
57	PG4	DA	3191	-	-	5/10/10/10	-
61	PEG	D3	102	-	-	1/4/4/4	-
59	PUT	DA	3210	-	-	0/3/3/3	-
57	PG4	AA	1670	-	-	5/10/10/10	-
63	PGE	DA	3222	-	-	3/7/7/7	-
58	MPD	DA	3190	-	-	2/5/5/5	-
58	MPD	DA	3228	-	-	2/5/5/5	-
62	EDO	D0	101	-	-	1/1/1/1	-
59	PUT	DA	3219	-	-	1/3/3/3	-
61	PEG	DL	201	-	-	1/4/4/4	-
58	MPD	AA	1671	-	-	0/5/5/5	-
59	PUT	DA	3218	-	-	0/3/3/3	-
61	PEG	D1	102	-	-	2/4/4/4	-
57	PG4	DQ	202	-	-	3/10/10/10	-
64	SPD	DA	3203	-	-	1/7/7/7	-
63	PGE	DU	101	-	-	3/7/7/7	-
62	EDO	DA	3192	-	-	0/1/1/1	-
62	EDO	DB	211	-	-	0/1/1/1	-
57	PG4	DR	203	-	-	5/10/10/10	-
63	PGE	DA	3214	-	-	3/7/7/7	-
62	EDO	DA	3195	-	-	0/1/1/1	-
67	GUN	DA	3208	-	-	-	0/2/2/2
59	PUT	DA	3193	-	-	0/3/3/3	-
62	EDO	DB	210	-	-	0/1/1/1	-
58	MPD	DE	302	-	-	2/5/5/5	-
59	PUT	DA	3182	-	-	0/3/3/3	-
64	SPD	DA	3221	-	-	2/7/7/7	-
61	PEG	DA	3215	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	DA	3194	ACY	O-C	3.75	1.38	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	DA	3194	ACY	OXT-C-CH3	2.93	127.32	115.05
66	DA	3194	ACY	O-C-CH3	-2.18	113.59	122.53

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AA	1676	MPD	C2-C3-C4-O4
58	DA	3201	MPD	C2-C3-C4-O4
58	DA	3201	MPD	C2-C3-C4-C5
58	DE	302	MPD	C2-C3-C4-O4
64	DA	3181	SPD	C3-C4-C5-N6
57	DR	203	PG4	O2-C3-C4-O3
65	DA	3200	1PE	OH5-C14-C24-OH4
57	DR	203	PG4	O3-C5-C6-O4
65	DA	3200	1PE	OH4-C13-C23-OH3
57	DS	202	PG4	O1-C1-C2-O2
63	DS	201	PGE	O2-C3-C4-O3
63	DA	3211	PGE	O2-C3-C4-O3
57	DQ	202	PG4	O1-C1-C2-O2
63	DA	3211	PGE	O1-C1-C2-O2
63	DU	101	PGE	O3-C5-C6-O4
64	DA	3181	SPD	C2-C3-C4-C5
65	DA	3183	1PE	OH2-C12-C22-OH3
59	DA	3219	PUT	C1-C2-C3-C4
63	DA	3184	PGE	O3-C5-C6-O4
65	DA	3200	1PE	OH2-C12-C22-OH3
62	D0	101	EDO	O1-C1-C2-O2
64	DA	3185	SPD	C2-C3-C4-C5
59	DA	3202	PUT	C1-C2-C3-C4
59	DA	3220	PUT	C1-C2-C3-C4
64	DA	3221	SPD	C4-C5-N6-C7
57	DR	203	PG4	C4-C3-O2-C2
61	DQ	201	PEG	C1-C2-O2-C3
63	DA	3214	PGE	C3-C4-O3-C5
61	DA	3215	PEG	C1-C2-O2-C3
61	DA	3223	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
63	DT	201	PGE	C3-C4-O3-C5
57	DA	3213	PG4	C3-C4-O3-C5
63	DA	3184	PGE	C4-C3-O2-C2
61	DL	201	PEG	C4-C3-O2-C2
57	DR	203	PG4	C6-C5-O3-C4
61	AL	201	PEG	C1-C2-O2-C3
63	DA	3211	PGE	C4-C3-O2-C2
63	DU	101	PGE	C6-C5-O3-C4
57	DA	3213	PG4	C8-C7-O4-C6
57	DS	202	PG4	C4-C3-O2-C2
57	DA	3191	PG4	C4-C3-O2-C2
61	D1	102	PEG	C4-C3-O2-C2
65	DA	3183	1PE	C24-C14-OH5-C25
63	DA	3222	PGE	C1-C2-O2-C3
61	DA	3198	PEG	C4-C3-O2-C2
63	DA	3214	PGE	C6-C5-O3-C4
65	DA	3200	1PE	C12-C22-OH3-C23
63	DA	3184	PGE	C3-C4-O3-C5
63	D3	101	PGE	C4-C3-O2-C2
63	DS	201	PGE	C6-C5-O3-C4
58	DK	201	MPD	O2-C2-C3-C4
58	DT	202	MPD	O2-C2-C3-C4
61	DA	3223	PEG	C4-C3-O2-C2
65	DA	3183	1PE	C16-C26-OH6-C15
61	DA	3215	PEG	C4-C3-O2-C2
58	DA	3190	MPD	C2-C3-C4-O4
63	DA	3214	PGE	C4-C3-O2-C2
58	DA	3204	MPD	C1-C2-C3-C4
58	DA	3228	MPD	C1-C2-C3-C4
61	DP	201	PEG	C1-C2-O2-C3
65	DA	3183	1PE	OH6-C15-C25-OH5
63	DA	3222	PGE	C4-C3-O2-C2
59	AA	1675	PUT	C1-C2-C3-C4
63	DS	201	PGE	C1-C2-O2-C3
57	DA	3191	PG4	C6-C5-O3-C4
58	DA	3188	MPD	C2-C3-C4-C5
58	DA	3190	MPD	C2-C3-C4-C5
58	DE	301	MPD	C2-C3-C4-C5
57	BA	1642	PG4	C8-C7-O4-C6
57	AA	1670	PG4	O4-C7-C8-O5
63	DT	201	PGE	C4-C3-O2-C2
63	DA	3222	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
57	AA	1670	PG4	C5-C6-O4-C7
63	DT	201	PGE	O3-C5-C6-O4
63	DT	201	PGE	C1-C2-O2-C3
57	DA	3191	PG4	O3-C5-C6-O4
61	D3	102	PEG	C4-C3-O2-C2
61	AL	201	PEG	C4-C3-O2-C2
63	DD	302	PGE	O2-C3-C4-O3
63	DD	302	PGE	C4-C3-O2-C2
64	DA	3181	SPD	C8-C7-N6-C5
61	DP	201	PEG	C4-C3-O2-C2
63	D3	101	PGE	C1-C2-O2-C3
64	DA	3221	SPD	C8-C7-N6-C5
65	DA	3183	1PE	C12-C22-OH3-C23
63	DD	302	PGE	C1-C2-O2-C3
65	DA	3200	1PE	C15-C25-OH5-C14
57	DA	3213	PG4	O4-C7-C8-O5
57	DQ	202	PG4	C1-C2-O2-C3
63	DU	101	PGE	O1-C1-C2-O2
57	AA	1670	PG4	C3-C4-O3-C5
57	DQ	202	PG4	C5-C6-O4-C7
57	AA	1670	PG4	C4-C3-O2-C2
63	DD	302	PGE	C3-C4-O3-C5
64	DA	3203	SPD	C8-C7-N6-C5
61	D1	102	PEG	C1-C2-O2-C3
57	DA	3213	PG4	O1-C1-C2-O2
61	DA	3197	PEG	C1-C2-O2-C3
57	AA	1670	PG4	O1-C1-C2-O2
57	DR	203	PG4	C3-C4-O3-C5
58	DA	3188	MPD	C2-C3-C4-O4
58	DN	201	MPD	C2-C3-C4-O4
58	DA	3201	MPD	C1-C2-C3-C4
58	DA	3201	MPD	CM-C2-C3-C4
58	DA	3204	MPD	CM-C2-C3-C4
58	DA	3228	MPD	CM-C2-C3-C4
58	DE	302	MPD	C1-C2-C3-C4
58	DN	201	MPD	C1-C2-C3-C4
58	DN	201	MPD	CM-C2-C3-C4
64	DA	3181	SPD	C7-C8-C9-N10
57	DA	3191	PG4	O2-C3-C4-O3
57	DA	3191	PG4	O4-C7-C8-O5
59	AA	1674	PUT	C1-C2-C3-C4

There are no ring outliers.

16 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	BA	1642	PG4	1	0
63	DS	201	PGE	2	0
65	DA	3183	1PE	1	0
62	DA	3206	EDO	1	0
57	DS	202	PG4	1	0
58	DE	301	MPD	1	0
68	DA	3217	TRS	1	0
57	DA	3191	PG4	1	0
59	DA	3210	PUT	1	0
57	AA	1670	PG4	1	0
63	DA	3222	PGE	2	0
58	DA	3190	MPD	1	0
58	AA	1671	MPD	1	0
61	D1	102	PEG	2	0
57	DR	203	PG4	3	0
59	DA	3193	PUT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1523/1534 (99%)	-0.26	11 (0%) 84 68	40, 90, 219, 296	0
1	BA	1522/1534 (99%)	0.39	82 (5%) 31 17	46, 131, 271, 279	0
2	AB	224/224 (100%)	0.42	7 (3%) 51 31	65, 116, 194, 247	0
2	BB	224/224 (100%)	0.56	10 (4%) 38 21	91, 129, 190, 236	0
3	AC	206/206 (100%)	-0.04	1 (0%) 87 73	67, 95, 126, 146	0
3	BC	206/206 (100%)	0.48	5 (2%) 59 38	86, 134, 172, 196	0
4	AD	205/205 (100%)	0.17	0 100 100	63, 99, 125, 146	0
4	BD	205/205 (100%)	-0.19	0 100 100	42, 72, 104, 134	0
5	AE	155/155 (100%)	-0.00	1 (0%) 85 70	48, 82, 118, 155	0
5	BE	150/155 (96%)	0.16	0 100 100	60, 83, 132, 206	0
6	AF	106/106 (100%)	0.12	0 100 100	68, 94, 118, 143	0
6	BF	100/106 (94%)	0.34	2 (2%) 65 44	79, 114, 141, 155	0
7	AG	151/151 (100%)	0.41	8 (5%) 32 17	81, 116, 143, 156	0
7	BG	151/151 (100%)	1.01	22 (14%) 6 3	125, 189, 206, 220	0
8	AH	129/129 (100%)	0.02	2 (1%) 70 49	54, 84, 111, 121	0
8	BH	129/129 (100%)	0.45	4 (3%) 51 31	76, 108, 142, 160	0
9	AI	127/127 (100%)	0.51	5 (3%) 43 24	76, 114, 149, 158	0
9	BI	127/127 (100%)	0.96	20 (15%) 5 2	125, 158, 188, 202	0
10	AJ	99/99 (100%)	0.63	2 (2%) 65 44	70, 106, 135, 146	0
10	BJ	98/99 (98%)	1.15	14 (14%) 6 3	121, 165, 189, 199	0
11	AK	117/117 (100%)	0.35	1 (0%) 81 63	54, 106, 141, 153	0
11	BK	117/117 (100%)	0.39	4 (3%) 48 28	80, 117, 144, 170	0
12	AL	122/123 (99%)	-0.00	1 (0%) 82 64	49, 69, 99, 124	0
12	BL	122/123 (99%)	0.50	4 (3%) 49 29	62, 90, 116, 145	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.61	3 (2%) 57 36	89, 118, 154, 171	0
13	BM	114/114 (100%)	0.92	9 (7%) 18 10	195, 227, 238, 248	0
14	AN	100/100 (100%)	0.66	3 (3%) 52 32	71, 104, 179, 192	0
14	BN	100/100 (100%)	1.13	16 (16%) 5 2	114, 173, 217, 228	0
15	AO	88/88 (100%)	0.03	0 100 100	58, 81, 108, 136	0
15	BO	88/88 (100%)	0.38	0 100 100	70, 111, 132, 159	0
16	AP	82/82 (100%)	0.27	2 (2%) 59 38	62, 82, 127, 146	0
16	BP	82/82 (100%)	1.31	13 (15%) 5 2	95, 114, 151, 162	0
17	AQ	80/80 (100%)	0.24	2 (2%) 58 37	54, 79, 116, 139	0
17	BQ	80/80 (100%)	0.84	5 (6%) 26 14	82, 125, 147, 160	0
18	AR	55/55 (100%)	0.04	0 100 100	53, 87, 117, 153	0
18	BR	55/55 (100%)	0.32	2 (3%) 46 26	60, 88, 124, 154	0
19	AS	79/79 (100%)	0.60	4 (5%) 33 18	90, 114, 145, 152	0
19	BS	79/79 (100%)	1.05	13 (16%) 4 2	200, 222, 234, 239	0
20	AT	86/86 (100%)	0.42	1 (1%) 76 58	64, 83, 113, 136	0
20	BT	85/86 (98%)	1.36	16 (18%) 3 2	108, 138, 167, 180	0
21	AU	56/56 (100%)	0.87	9 (16%) 4 2	93, 124, 166, 180	0
21	BU	56/56 (100%)	0.53	2 (3%) 46 26	81, 107, 154, 167	0
22	C1	56/56 (100%)	1.84	24 (42%) 0 0	124, 162, 181, 184	0
22	D1	56/56 (100%)	-0.59	0 100 100	14, 39, 71, 99	0
23	C2	50/51 (98%)	1.15	9 (18%) 3 2	139, 161, 173, 186	0
23	D2	51/51 (100%)	-0.23	0 100 100	54, 67, 101, 110	0
24	C3	46/46 (100%)	2.36	25 (54%) 0 0	119, 143, 157, 165	0
24	D3	46/46 (100%)	-0.36	1 (2%) 62 41	29, 40, 64, 112	0
25	C4	64/64 (100%)	2.23	33 (51%) 0 0	116, 138, 155, 161	0
25	D4	64/64 (100%)	-0.46	0 100 100	26, 41, 53, 73	0
26	C5	38/38 (100%)	1.68	14 (36%) 1 1	108, 126, 139, 143	0
26	D5	38/38 (100%)	-0.36	0 100 100	33, 45, 69, 87	0
27	C0	58/58 (100%)	1.47	16 (27%) 1 1	115, 135, 151, 156	0
27	D0	58/58 (100%)	-0.42	2 (3%) 48 28	17, 32, 59, 94	2 (3%)
28	CB	118/120 (98%)	0.66	0 100 100	135, 190, 241, 251	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	120/120 (100%)	-0.84	0 100 100	28, 57, 87, 143	0
29	CC	271/271 (100%)	0.91	42 (15%) 5 2	80, 113, 143, 167	0
29	DC	271/271 (100%)	-0.35	2 (0%) 84 68	23, 53, 84, 113	0
30	CD	209/209 (100%)	1.42	59 (28%) 1 1	102, 136, 165, 177	0
31	CA	2876/2904 (99%)	1.17	465 (16%) 4 2	69, 185, 272, 290	0
32	DD	208/209 (99%)	-0.63	0 100 100	15, 40, 73, 98	0
33	DA	2873/2903 (98%)	-0.82	44 (1%) 72 52	13, 46, 203, 298	11 (0%)
34	CE	201/201 (100%)	1.62	71 (35%) 1 1	121, 176, 206, 224	0
34	DE	201/201 (100%)	-0.39	0 100 100	17, 57, 103, 139	0
35	CF	177/177 (100%)	0.88	10 (5%) 30 16	194, 215, 226, 232	0
35	DF	177/177 (100%)	-0.02	0 100 100	52, 80, 120, 145	0
36	CG	176/176 (100%)	0.91	13 (7%) 20 11	146, 178, 208, 222	0
36	DG	176/176 (100%)	-0.19	1 (0%) 85 70	33, 70, 99, 136	0
37	CH	149/149 (100%)	0.44	4 (2%) 56 35	89, 149, 170, 178	0
37	DH	149/149 (100%)	0.38	1 (0%) 84 68	73, 154, 190, 203	0
38	CJ	134/134 (100%)	1.27	25 (18%) 3 2	236, 254, 265, 273	0
38	DJ	134/134 (100%)	1.31	25 (18%) 3 2	193, 222, 235, 242	0
39	CK	142/142 (100%)	1.54	47 (33%) 1 1	106, 132, 169, 195	0
39	DK	142/142 (100%)	-0.57	0 100 100	18, 35, 66, 88	0
40	CL	122/123 (99%)	1.01	10 (8%) 17 9	96, 118, 151, 168	0
40	DL	123/123 (100%)	-0.55	0 100 100	26, 44, 70, 112	0
41	CM	144/144 (100%)	1.80	57 (39%) 1 0	117, 169, 227, 247	0
41	DM	144/144 (100%)	-0.39	0 100 100	14, 54, 87, 128	0
42	CN	135/136 (99%)	1.14	20 (14%) 5 3	92, 125, 151, 178	0
42	DN	135/136 (99%)	-0.62	0 100 100	20, 41, 73, 89	1 (0%)
43	CO	120/125 (96%)	1.89	43 (35%) 1 1	110, 141, 163, 197	0
43	DO	125/125 (100%)	-0.64	0 100 100	18, 36, 84, 137	0
44	CP	116/117 (99%)	1.11	19 (16%) 4 2	140, 171, 187, 195	0
44	DP	117/117 (100%)	-0.34	0 100 100	34, 55, 88, 95	0
45	CQ	114/114 (100%)	1.17	19 (16%) 4 2	113, 131, 157, 180	0
45	DQ	114/114 (100%)	-0.46	0 100 100	29, 51, 80, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
46	CR	117/117 (100%)	1.96	51 (43%) 0 0	108, 137, 166, 175	0
46	DR	117/117 (100%)	-0.67	0 100 100	14, 30, 50, 80	0
47	CS	103/103 (100%)	1.72	32 (31%) 1 1	124, 149, 173, 187	0
47	DS	103/103 (100%)	-0.64	0 100 100	19, 43, 76, 103	0
48	CT	110/110 (100%)	1.91	45 (40%) 0 0	123, 155, 177, 188	0
48	DT	110/110 (100%)	-0.62	0 100 100	19, 33, 66, 126	0
49	CU	93/93 (100%)	1.63	29 (31%) 1 1	136, 168, 193, 201	0
49	DU	93/93 (100%)	-0.07	0 100 100	26, 55, 126, 141	0
50	CV	102/102 (100%)	2.08	41 (40%) 0 0	147, 176, 207, 219	0
50	DV	102/102 (100%)	-0.30	0 100 100	41, 62, 104, 139	0
51	CW	94/94 (100%)	0.80	6 (6%) 25 14	128, 153, 165, 173	0
51	DW	94/94 (100%)	-0.43	2 (2%) 63 42	29, 54, 86, 99	0
52	CX	75/76 (98%)	1.29	13 (17%) 4 2	109, 140, 152, 186	0
52	DX	76/76 (100%)	-0.43	0 100 100	16, 40, 74, 114	1 (1%)
53	CY	77/77 (100%)	1.35	20 (25%) 1 1	108, 123, 156, 170	0
53	DY	77/77 (100%)	-0.28	0 100 100	32, 55, 88, 98	0
54	CZ	62/62 (100%)	1.85	22 (35%) 1 1	161, 179, 190, 196	0
54	DZ	62/62 (100%)	-0.07	0 100 100	44, 74, 108, 140	0
55	DI	135/135 (100%)	0.77	12 (8%) 15 8	78, 153, 204, 224	1 (0%)
All	All	20634/20744 (99%)	0.34	1680 (8%) 18 10	13, 111, 241, 298	16 (0%)

All (1680) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
41	CM	27	LEU	6.8
48	CT	47	VAL	6.7
46	CR	8	VAL	6.6
43	CO	46	ARG	6.5
43	CO	25	ALA	6.5
41	CM	71	ALA	6.1
24	D3	46	LYS	6.0
33	DA	2886[A]	A	6.0
54	CZ	18	LEU	6.0
46	CR	37	GLN	5.8
47	CS	81	LYS	5.8

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Mol	Chain	Res	Type	RSRZ
50	CV	67	VAL	5.7
41	CM	19	LEU	5.6
54	CZ	22	LEU	5.6
41	CM	35	HIS	5.4
48	CT	45	VAL	5.4
47	CS	96	VAL	5.3
12	AL	124	ALA	5.3
40	CL	28	SER	5.3
46	CR	11	ARG	5.3
22	C1	7	LYS	5.2
43	CO	28	LEU	5.2
25	C4	15	LYS	5.2
47	CS	80	ARG	5.2
41	CM	15	ALA	5.2
34	CE	73	ILE	5.2
24	C3	24	THR	5.2
8	AH	2	SER	5.1
35	CF	156	ILE	5.1
25	C4	57	LEU	5.0
39	CK	47	HIS	5.0
50	CV	5	ILE	5.0
1	BA	1362	A	5.0
50	CV	39	ILE	5.0
30	CD	8	LYS	5.0
20	BT	68	HIS	4.9
20	BT	69	LYS	4.9
50	CV	36	VAL	4.9
30	CD	128	ARG	4.9
50	CV	3	ALA	4.9
31	CA	411	G	4.9
50	CV	35	ILE	4.9
41	CM	72	ALA	4.9
48	CT	46	LEU	4.9
22	C1	2	ALA	4.8
24	C3	42	LEU	4.8
48	CT	105	VAL	4.8
46	CR	35	ALA	4.8
47	CS	82	HIS	4.8
23	C2	24	THR	4.8
31	CA	125	A	4.8
42	CN	56	ALA	4.8
38	CJ	54	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
38	DJ	53	LEU	4.7
45	CQ	95	ALA	4.7
50	CV	2	ALA	4.7
43	CO	105	GLY	4.7
36	CG	172	LYS	4.7
24	C3	19	ARG	4.7
20	BT	4	ILE	4.7
31	CA	448	U	4.7
30	CD	126	ASN	4.7
39	CK	119	PHE	4.7
50	CV	64	ALA	4.6
22	C1	6	ASN	4.6
18	BR	20	GLU	4.6
46	CR	9	ILE	4.6
2	BB	135	LEU	4.6
29	CC	228	VAL	4.6
14	AN	21	PHE	4.6
38	DJ	79	LEU	4.6
29	CC	227	PRO	4.5
1	BA	222	C	4.5
25	C4	37	ALA	4.5
36	CG	166	ASP	4.5
44	CP	2	ASP	4.5
25	C4	46	PRO	4.5
9	BI	128	SER	4.4
54	CZ	15	ASN	4.4
43	CO	113	ILE	4.4
38	CJ	24	VAL	4.4
41	CM	81	ASP	4.4
54	CZ	6	LEU	4.4
1	BA	208	U	4.4
46	CR	4	VAL	4.4
46	CR	32	TYR	4.4
31	CA	331	C	4.4
25	C4	60	ALA	4.4
30	CD	168	GLU	4.4
41	CM	28	GLY	4.4
41	CM	114	GLY	4.4
48	CT	99	ARG	4.4
48	CT	40	ASN	4.4
29	CC	234	GLY	4.3
31	CA	1248	G	4.3

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Mol	Chain	Res	Type	RSRZ
30	CD	131	ASP	4.3
17	BQ	8	LEU	4.3
31	CA	1205	A	4.3
30	CD	130	GLN	4.3
7	AG	5	ARG	4.3
41	CM	14	LYS	4.2
43	CO	29	VAL	4.3
39	CK	81	ILE	4.2
31	CA	387	U	4.2
31	CA	504	A	4.2
43	CO	26	GLY	4.2
16	BP	42	ILE	4.2
47	CS	75	VAL	4.2
38	DJ	80	LEU	4.2
7	BG	62	PHE	4.2
17	BQ	70	THR	4.2
46	CR	29	SER	4.1
31	CA	2820	A	4.1
10	BJ	74	VAL	4.1
22	C1	3	VAL	4.1
22	C1	15	MET	4.1
49	CU	43	ILE	4.1
34	CE	50	ALA	4.1
34	CE	93	SER	4.1
39	CK	120	ARG	4.1
47	CS	77	PHE	4.1
48	CT	48	LYS	4.1
46	CR	2	ALA	4.1
34	CE	33	VAL	4.1
31	CA	1326	U	4.1
46	CR	38	ALA	4.1
46	CR	44	GLN	4.1
30	CD	26	VAL	4.1
25	C4	25	LYS	4.1
24	C3	13	ASN	4.0
39	CK	73	VAL	4.0
48	CT	42	LYS	4.0
31	CA	1323	C	4.0
47	CS	78	ARG	4.0
27	C0	18	PRO	4.0
38	DJ	54	PRO	4.0
31	CA	355	U	4.0

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Mol	Chain	Res	Type	RSRZ
24	C3	23	ALA	4.0
39	CK	46	PRO	4.0
30	CD	142	VAL	4.0
44	CP	107	ALA	4.0
46	CR	18	LEU	4.0
43	CO	47	VAL	4.0
50	CV	13	VAL	3.9
1	BA	121	U	3.9
24	C3	26	ASN	3.9
1	AA	121	U	3.9
1	AA	1492	A	3.9
31	CA	326	G	3.9
36	CG	103	ILE	3.9
25	C4	36	LYS	3.9
50	CV	33	LYS	3.9
2	BB	130	THR	3.9
47	CS	76	LYS	3.9
14	BN	45	VAL	3.8
21	AU	36	GLU	3.8
47	CS	73	LYS	3.8
22	C1	20	ASP	3.8
31	CA	1324	G	3.8
43	CO	18	GLN	3.8
50	CV	80	ALA	3.8
30	CD	25	THR	3.8
41	CM	18	ARG	3.8
27	C0	56	LYS	3.8
31	CA	2677	G	3.8
41	CM	20	GLY	3.8
30	CD	167	ASN	3.8
34	CE	182	ALA	3.8
50	CV	83	VAL	3.8
25	C4	39	LYS	3.8
31	CA	354	A	3.8
31	CA	680	C	3.8
31	CA	388	G	3.8
46	CR	52	GLN	3.8
2	BB	132	LYS	3.8
50	CV	26	LYS	3.8
41	CM	1	MET	3.8
53	CY	28	ARG	3.8
38	CJ	79	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
54	CZ	14	LEU	3.8
24	C3	43	THR	3.8
20	BT	13	GLN	3.7
39	CK	86	GLN	3.7
43	CO	40	LYS	3.7
50	CV	65	ILE	3.7
52	CX	78	LYS	3.7
31	CA	394	C	3.7
31	CA	2000	C	3.7
31	CA	1250	G	3.7
10	BJ	26	VAL	3.7
38	DJ	78	VAL	3.7
41	CM	21	ARG	3.7
41	CM	92	LEU	3.7
31	CA	914	G	3.7
1	BA	207	C	3.7
24	C3	25	LYS	3.7
29	CC	242	LYS	3.7
48	CT	49	LYS	3.7
48	CT	98	LYS	3.7
1	BA	211	G	3.6
1	BA	220	G	3.6
31	CA	682	G	3.6
55	DI	83	ALA	3.6
34	CE	69	ARG	3.6
38	DJ	117	MET	3.6
31	CA	631	A	3.6
31	CA	2406	A	3.6
39	CK	115	GLY	3.6
34	CE	135	ALA	3.6
41	CM	100	ILE	3.6
31	CA	2817	U	3.6
46	CR	5	LYS	3.6
1	AA	1441	A	3.6
51	CW	84	PRO	3.6
49	CU	67	VAL	3.6
52	CX	23	VAL	3.6
41	CM	58	TYR	3.6
48	CT	38	TYR	3.6
55	DI	38	MET	3.6
23	C2	36	LEU	3.6
24	C3	4	THR	3.6

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Mol	Chain	Res	Type	RSRZ
24	C3	31	LEU	3.6
34	CE	147	LEU	3.6
38	CJ	53	LEU	3.6
9	BI	117	GLY	3.6
30	CD	111	GLY	3.6
39	CK	48	VAL	3.6
1	BA	212	G	3.6
1	BA	380	G	3.6
31	CA	75	G	3.6
30	CD	129	THR	3.6
9	BI	16	ALA	3.6
38	CJ	13	VAL	3.6
20	BT	5	LYS	3.6
39	CK	118	MET	3.6
48	CT	36	LEU	3.6
45	CQ	110	ILE	3.6
46	CR	17	ILE	3.6
50	CV	31	SER	3.6
1	BA	108	G	3.5
10	BJ	77	VAL	3.5
49	CU	47	VAL	3.5
54	CZ	50	VAL	3.5
25	C4	47	LYS	3.5
43	CO	79	LEU	3.5
34	CE	70	SER	3.5
34	CE	72	SER	3.5
34	CE	131	THR	3.5
22	C1	5	GLN	3.5
42	CN	8	LYS	3.5
48	CT	44	ALA	3.5
25	C4	29	LEU	3.5
31	CA	68	G	3.5
53	CY	56	MET	3.5
11	BK	110	ILE	3.5
26	C5	18	LYS	3.5
48	CT	7	HIS	3.5
22	C1	24	ALA	3.5
44	CP	87	ILE	3.5
46	CR	6	ARG	3.5
47	CS	84	ARG	3.5
31	CA	126	A	3.5
31	CA	795	C	3.5

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Mol	Chain	Res	Type	RSRZ
29	CC	255	LYS	3.5
51	CW	22	ALA	3.5
30	CD	143	PRO	3.5
38	CJ	74	PRO	3.5
48	CT	97	LEU	3.5
34	CE	31	VAL	3.5
43	CO	7	GLY	3.5
24	C3	10	LEU	3.5
30	CD	31	ALA	3.5
10	BJ	39	PRO	3.5
31	CA	1639	C	3.5
2	BB	131	LYS	3.4
16	BP	27	ALA	3.4
38	CJ	28	LEU	3.4
24	C3	1	MET	3.4
25	C4	32	ILE	3.4
1	BA	223	A	3.4
31	CA	1598	A	3.4
39	CK	71	ASP	3.4
39	CK	72	LYS	3.4
31	CA	2383	G	3.4
50	CV	14	LEU	3.4
50	CV	29	LEU	3.4
30	CD	132	ALA	3.4
34	CE	37	ALA	3.4
25	C4	43	HIS	3.4
31	CA	412	A	3.4
54	CZ	11	VAL	3.4
25	C4	33	LEU	3.4
42	CN	20	LEU	3.4
46	CR	28	ARG	3.4
31	CA	1252	G	3.4
33	DA	2141	G	3.4
25	C4	61	CYS	3.4
38	CJ	11	LEU	3.4
50	CV	25	VAL	3.4
43	CO	8	ARG	3.4
22	C1	23	THR	3.4
41	CM	30	THR	3.4
9	AI	129	LYS	3.4
22	C1	12	LYS	3.4
31	CA	390	U	3.4

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Mol	Chain	Res	Type	RSRZ
31	CA	1779	U	3.4
9	BI	124	ARG	3.4
19	BS	15	LEU	3.4
34	CE	49	ARG	3.4
44	CP	103	VAL	3.4
31	CA	389	G	3.4
31	CA	410	G	3.4
29	CC	92	ALA	3.4
18	BR	21	ILE	3.4
49	CU	15	HIS	3.4
49	CU	60	THR	3.4
29	CC	46	ASN	3.3
31	CA	2690	U	3.3
25	C4	28	ASN	3.3
31	CA	681	G	3.3
31	CA	1236	G	3.3
31	CA	2726	A	3.3
33	DA	1847	A	3.3
48	CT	83	LYS	3.3
48	CT	43	ALA	3.3
1	AA	1017	U	3.3
34	CE	157	LEU	3.3
41	CM	57	LEU	3.3
43	CO	44	LEU	3.3
30	CD	9	VAL	3.3
41	CM	70	LYS	3.3
31	CA	289	G	3.3
31	CA	291	G	3.3
31	CA	1346	G	3.3
42	CN	126	ILE	3.3
46	CR	33	ARG	3.3
1	BA	330	C	3.3
31	CA	2045	C	3.3
50	CV	85	PHE	3.3
26	C5	22	VAL	3.3
24	C3	20	ALA	3.3
29	CC	54	ILE	3.3
7	AG	8	GLY	3.3
24	C3	17	GLY	3.3
30	CD	139	SER	3.3
38	CJ	80	LEU	3.3
25	C4	58	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
39	CK	105	VAL	3.3
41	CM	29	LYS	3.3
31	CA	563	A	3.3
31	CA	810	U	3.3
31	CA	1396	U	3.3
9	BI	112	GLU	3.3
31	CA	1646	C	3.3
46	CR	23	GLY	3.3
13	BM	96	PRO	3.2
20	BT	64	LYS	3.2
53	CY	25	THR	3.2
19	BS	49	ILE	3.2
34	CE	78	TRP	3.2
46	CR	99	ALA	3.2
50	CV	58	ILE	3.2
34	CE	64	GLY	3.2
29	CC	218	PRO	3.2
41	CM	17	LYS	3.2
47	CS	20	VAL	3.2
43	CO	36	THR	3.2
27	C0	32	ILE	3.2
48	CT	82	MET	3.2
29	CC	254	GLY	3.2
31	CA	409	G	3.2
38	DJ	13	VAL	3.2
43	CO	21	PHE	3.2
24	C3	35	ARG	3.2
27	D0	2[A]	ALA	3.2
30	CD	158	GLY	3.2
39	CK	83	GLY	3.2
34	CE	164	LEU	3.2
8	BH	2	SER	3.2
31	CA	1325	U	3.2
31	CA	2506	U	3.2
34	CE	75	SER	3.2
34	CE	94	GLN	3.2
39	CK	49	ASP	3.2
31	CA	2059	A	3.2
31	CA	512	G	3.2
31	CA	225	C	3.2
31	CA	257	C	3.2
25	C4	44	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
54	CZ	21	LEU	3.2
41	CM	107	PHE	3.2
34	CE	62	GLN	3.2
34	CE	77	ILE	3.2
38	DJ	128	SER	3.2
9	BI	121	ALA	3.2
21	BU	57	ALA	3.2
14	BN	12	LYS	3.1
19	BS	12	ASP	3.1
48	CT	6	LYS	3.1
23	C2	42	VAL	3.1
31	CA	968	C	3.1
31	CA	1625	C	3.1
31	CA	2755	C	3.1
47	CS	86	GLN	3.1
14	BN	99	ALA	3.1
34	CE	34	ALA	3.1
46	CR	22	LYS	3.1
55	DI	93	ALA	3.1
41	CM	53	GLY	3.1
49	CU	11	LEU	3.1
31	CA	2629	U	3.1
31	CA	2743	U	3.1
29	CC	220	VAL	3.1
47	CS	51	VAL	3.1
53	CY	29	PHE	3.1
46	CR	25	TYR	3.1
31	CA	1247	A	3.1
31	CA	1322	A	3.1
14	BN	60	GLN	3.1
23	C2	22	THR	3.1
31	CA	1135	C	3.1
6	BF	100	SER	3.1
1	BA	201	G	3.1
31	CA	953	G	3.1
31	CA	1288	G	3.1
31	CA	1380	G	3.1
43	CO	43	GLU	3.1
46	CR	36	PHE	3.1
54	CZ	46	VAL	3.1
53	CY	22	LEU	3.1
31	CA	586	A	3.1

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Mol	Chain	Res	Type	RSRZ
31	CA	1808	A	3.1
1	BA	221	C	3.1
27	C0	11	ARG	3.1
34	CE	168	ASP	3.1
38	DJ	24	VAL	3.1
47	CS	79	ARG	3.1
39	CK	111	LYS	3.1
1	BA	134	G	3.1
33	DA	2133	G	3.1
39	CK	84	ILE	3.1
22	C1	21	ALA	3.1
46	CR	59	GLN	3.1
22	C1	25	VAL	3.1
34	CE	52	VAL	3.1
47	CS	72	VAL	3.1
23	C2	38	LYS	3.1
31	CA	472	A	3.1
46	CR	41	LYS	3.1
43	CO	24	MET	3.1
31	CA	393	C	3.0
31	CA	587	C	3.0
20	BT	66	LEU	3.0
30	CD	192	ALA	3.0
34	CE	3	LEU	3.0
41	CM	61	LEU	3.0
50	CV	75	ALA	3.0
48	CT	31	GLN	3.0
7	BG	5	ARG	3.0
31	CA	1136	G	3.0
46	CR	7	GLY	3.0
36	CG	171	THR	3.0
1	AA	632	U	3.0
31	CA	2689	U	3.0
9	BI	72	ILE	3.0
41	CM	23	ILE	3.0
1	BA	196	A	3.0
31	CA	515	A	3.0
31	CA	2725	A	3.0
43	CO	22	ARG	3.0
50	CV	27	ASN	3.0
54	CZ	25	GLN	3.0
31	CA	22	C	3.0

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Mol	Chain	Res	Type	RSRZ
2	AB	132	LYS	3.0
25	C4	35	LYS	3.0
39	CK	50	THR	3.0
39	CK	85	LYS	3.0
39	CK	100	VAL	3.0
50	CV	70	VAL	3.0
31	CA	1778	U	3.0
31	CA	1381	G	3.0
31	CA	2890	G	3.0
31	CA	2892	G	3.0
33	DA	2885[A]	G	3.0
41	CM	3	LEU	3.0
16	BP	31	ARG	3.0
41	CM	31	GLY	3.0
1	BA	135	C	3.0
31	CA	1330	C	3.0
41	CM	51	GLU	3.0
46	CR	47	TYR	3.0
31	CA	2585	U	3.0
13	BM	99	GLY	3.0
20	BT	65	GLY	3.0
31	CA	30	G	3.0
31	CA	2360	G	3.0
34	CE	178	VAL	3.0
25	C4	14	PHE	3.0
10	BJ	76	ILE	3.0
43	CO	97	ILE	3.0
31	CA	1133	A	3.0
31	CA	1302	A	3.0
31	CA	1552	A	3.0
9	BI	122	ARG	3.0
21	AU	57	ALA	3.0
21	AU	46	LYS	3.0
31	CA	531	C	3.0
31	CA	678	C	3.0
34	CE	96	VAL	3.0
1	AA	1039	G	2.9
31	CA	859	G	2.9
20	BT	33	LYS	2.9
30	CD	123	LYS	2.9
30	CD	157	LYS	2.9
34	CE	36	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
38	CJ	14	ALA	2.9
45	CQ	111	LYS	2.9
31	CA	654	A	2.9
31	CA	781	A	2.9
26	C5	3	VAL	2.9
52	CX	54	GLY	2.9
38	DJ	12	GLN	2.9
31	CA	672	C	2.9
31	CA	1289	C	2.9
31	CA	1606	C	2.9
3	BC	162	ILE	2.9
24	C3	21	ARG	2.9
31	CA	12	U	2.9
43	CO	10	LEU	2.9
14	BN	7	LYS	2.9
22	C1	8	PRO	2.9
49	CU	36	LYS	2.9
7	BG	39	ALA	2.9
7	BG	37	SER	2.9
31	CA	26	G	2.9
31	CA	2780	G	2.9
5	AE	97	GLN	2.9
14	BN	54	ASP	2.9
43	CO	1	MET	2.9
48	CT	96	ILE	2.9
31	CA	1600	C	2.9
33	DA	1092	C	2.9
37	CH	23	ALA	2.9
33	DA	2166	U	2.9
34	CE	187	VAL	2.9
13	AM	99	GLY	2.9
27	C0	48	ILE	2.9
46	CR	50	ARG	2.9
40	CL	66	LYS	2.9
16	BP	3	THR	2.9
31	CA	27	G	2.9
31	CA	1651	G	2.9
38	CJ	76	ALA	2.9
39	CK	8	PRO	2.9
31	CA	508	A	2.9
31	CA	528	A	2.9
46	CR	39	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
31	CA	1278	C	2.9
31	CA	1291	C	2.9
31	CA	1607	C	2.9
31	CA	2507	C	2.9
31	CA	1249	U	2.9
39	CK	116	ARG	2.9
16	BP	67	ILE	2.9
38	CJ	128	SER	2.9
9	BI	129	LYS	2.9
44	CP	48	LEU	2.9
46	CR	109	LEU	2.9
46	CR	20	GLN	2.9
27	C0	50	ALA	2.9
30	CD	54	ALA	2.9
34	CE	104	ALA	2.9
34	CE	177	PRO	2.9
13	BM	22	ILE	2.9
31	CA	583	G	2.9
31	CA	669	G	2.9
31	CA	1093	G	2.9
31	CA	1216	G	2.9
31	CA	1277	G	2.9
31	CA	1331	G	2.9
31	CA	2363	G	2.9
38	DJ	129	ILE	2.9
48	CT	74	ILE	2.9
1	BA	106	C	2.8
31	CA	946	C	2.8
38	DJ	76	ALA	2.8
38	CJ	73	THR	2.8
43	CO	48	VAL	2.8
50	CV	34	VAL	2.8
37	CH	27	ARG	2.8
48	CT	11	ARG	2.8
9	BI	127	PHE	2.8
45	CQ	23	GLY	2.8
50	CV	44	LYS	2.8
47	CS	83	TYR	2.8
49	CU	70	HIS	2.8
31	CA	1214	A	2.8
43	CO	104	ALA	2.8
1	BA	202	G	2.8

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Mol	Chain	Res	Type	RSRZ
31	CA	2891	U	2.8
43	CO	109	PRO	2.8
29	CC	236	GLU	2.8
31	CA	517	C	2.8
31	CA	1251	C	2.8
41	CM	78	ARG	2.8
51	DW	69	GLU	2.8
21	AU	54	LYS	2.8
25	C4	23	LYS	2.8
44	CP	4	LYS	2.8
16	BP	4	ILE	2.8
34	CE	85	PHE	2.8
41	CM	79	LEU	2.8
49	CU	30	ILE	2.8
29	CC	15	HIS	2.8
19	BS	35	SER	2.8
29	CC	259	SER	2.8
41	CM	75	ALA	2.8
41	CM	80	SER	2.8
26	C5	19	ARG	2.8
52	CX	55	ARG	2.8
7	BG	27	VAL	2.8
10	BJ	44	THR	2.8
47	CS	70	GLU	2.8
52	CX	44	LYS	2.8
1	BA	325	A	2.8
7	BG	103	TRP	2.8
1	BA	173	U	2.8
1	BA	219	U	2.8
1	BA	1364	U	2.8
29	CC	90	ASN	2.8
31	CA	1468	U	2.8
39	CK	79	GLY	2.8
40	CL	26	GLY	2.8
53	CY	23	ASN	2.8
31	CA	585	G	2.8
31	CA	2066	C	2.8
31	CA	2621	G	2.8
31	CA	2767	C	2.8
12	BL	2	ALA	2.8
21	AU	26	ALA	2.8
49	CU	41	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
7	BG	69	VAL	2.8
46	CR	31	VAL	2.8
54	CZ	54	LYS	2.8
42	CN	95	LEU	2.8
55	DI	126	LEU	2.8
25	C4	49	MET	2.8
26	C5	23	ILE	2.8
39	CK	93	ILE	2.8
50	CV	32	GLY	2.8
1	BA	632	U	2.8
31	CA	332	A	2.8
31	CA	392	U	2.8
31	CA	1287	A	2.8
31	CA	2346	A	2.8
31	CA	2713	U	2.8
1	BA	63	C	2.8
13	BM	106	ALA	2.8
23	C2	52	ALA	2.8
14	BN	19	LYS	2.8
31	CA	128	C	2.8
31	CA	786	C	2.8
31	CA	46	G	2.8
31	CA	559	G	2.8
30	CD	95	SER	2.8
44	CP	5	SER	2.8
42	CN	129	THR	2.8
47	CS	23	GLU	2.8
20	BT	67	ILE	2.8
41	CM	55	MET	2.7
16	BP	23	ASP	2.7
30	CD	198	GLY	2.7
48	CT	84	ARG	2.7
14	BN	47	LYS	2.7
20	BT	9	LYS	2.7
34	CE	39	ALA	2.7
52	CX	75	LYS	2.7
53	CY	54	LYS	2.7
30	CD	122	VAL	2.7
31	CA	67	U	2.7
31	CA	330	A	2.7
31	CA	1213	A	2.7
34	CE	32	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
35	CF	84	PRO	2.7
46	CR	40	ILE	2.7
41	CM	16	GLY	2.7
49	CU	71	GLY	2.7
1	BA	200	G	2.7
31	CA	15	G	2.7
31	CA	356	G	2.7
31	CA	801	G	2.7
33	DA	2110	G	2.7
25	C4	40	ARG	2.7
14	BN	3	LYS	2.7
39	CK	75	TYR	2.7
50	CV	40	ASN	2.7
7	BG	65	ALA	2.7
30	CD	148	GLN	2.7
46	CR	34	VAL	2.7
31	CA	288	U	2.7
33	DA	846[A]	U	2.7
33	DA	2167	U	2.7
1	AA	1016	A	2.7
29	CC	12	GLY	2.7
30	CD	166	GLY	2.7
31	CA	391	A	2.7
31	CA	514	A	2.7
31	CA	1650	A	2.7
48	CT	37	THR	2.7
50	CV	78	GLY	2.7
29	CC	52	ARG	2.7
31	CA	76	C	2.7
31	CA	264	C	2.7
31	CA	564	C	2.7
31	CA	1208	C	2.7
47	CS	36	ALA	2.7
48	CT	5	ALA	2.7
53	CY	17	ASN	2.7
54	CZ	43	LEU	2.7
7	BG	106	GLU	2.7
24	C3	28	ARG	2.7
50	CV	57	GLY	2.7
30	CD	151	THR	2.7
30	CD	154	LYS	2.7
38	DJ	118	THR	2.7

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Mol	Chain	Res	Type	RSRZ
41	CM	74	THR	2.7
43	CO	15	SER	2.7
48	CT	81	SER	2.7
31	CA	2441	U	2.7
1	BA	66	A	2.7
1	BA	199	A	2.7
31	CA	677	A	2.7
34	CE	161	ALA	2.7
39	CK	117	ALA	2.7
46	CR	21	ALA	2.7
55	DI	111	ALA	2.7
39	CK	80	HIS	2.7
49	CU	61	LEU	2.7
31	CA	1092	C	2.7
33	DA	1732	C	2.7
25	C4	22	PHE	2.7
41	CM	33	ARG	2.7
49	CU	76	ARG	2.7
38	CJ	10	LYS	2.7
1	BA	107	G	2.7
1	BA	326	G	2.7
31	CA	17	G	2.7
31	CA	386	G	2.7
31	CA	446	G	2.7
33	DA	1091	G	2.7
9	AI	128	SER	2.7
43	CO	68	ALA	2.7
53	CY	24	ALA	2.7
31	CA	566	U	2.7
38	DJ	106	LEU	2.7
53	CY	30	LEU	2.7
31	CA	675	A	2.6
31	CA	1328	A	2.6
31	CA	1641	A	2.6
34	CE	181	ILE	2.6
35	CF	34	ILE	2.6
41	CM	56	PRO	2.6
47	CS	49	ILE	2.6
41	CM	102	GLY	2.6
53	CY	55	GLY	2.6
31	CA	11	C	2.6
31	CA	445	C	2.6

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Mol	Chain	Res	Type	RSRZ
31	CA	584	C	2.6
31	CA	2827	C	2.6
7	AG	6	VAL	2.6
13	BM	89	LEU	2.6
16	BP	52	LEU	2.6
45	CQ	92	VAL	2.6
49	CU	46	ALA	2.6
31	CA	663	G	2.6
31	CA	1389	G	2.6
31	CA	1555	G	2.6
26	C5	9	LYS	2.6
27	D0	3[A]	LYS	2.6
31	CA	29	U	2.6
31	CA	65	U	2.6
31	CA	72	U	2.6
33	DA	2797	U	2.6
34	CE	183	PHE	2.6
47	CS	71	LYS	2.6
1	AA	1019	A	2.6
3	BC	170	GLU	2.6
31	CA	1253	A	2.6
7	BG	43	VAL	2.6
34	CE	134	LEU	2.6
34	CE	186	VAL	2.6
38	DJ	77	ALA	2.6
43	CO	98	LEU	2.6
54	CZ	32	ALA	2.6
31	CA	1349	C	2.6
33	DA	2153	C	2.6
33	DA	2175	C	2.6
25	C4	26	HIS	2.6
49	CU	68	LYS	2.6
31	CA	767	U	2.6
54	CZ	24	GLU	2.6
31	CA	1068	G	2.6
31	CA	1239	G	2.6
31	CA	1642	G	2.6
31	CA	2414	G	2.6
33	DA	2120	G	2.6
30	CD	138	LEU	2.6
50	CV	41	LEU	2.6
54	CZ	19	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
27	C0	13	ALA	2.6
22	C1	17	ARG	2.6
31	CA	676	A	2.6
31	CA	1237	A	2.6
31	CA	1327	A	2.6
31	CA	2058	A	2.6
31	CA	2530	A	2.6
31	CA	2602	A	2.6
34	CE	74	LYS	2.6
34	CE	119	ILE	2.6
8	BH	3	MET	2.6
30	CD	156	PHE	2.6
31	CA	1350	C	2.6
31	CA	2452	C	2.6
41	CM	54	GLN	2.6
44	CP	93	ASP	2.6
48	CT	51	LEU	2.6
20	BT	63	ALA	2.6
43	CO	70	THR	2.6
45	CQ	108	ALA	2.6
54	CZ	53	VAL	2.6
1	BA	4	U	2.6
17	AQ	53	CYS	2.6
1	AA	1018	G	2.6
1	BA	203	G	2.6
31	CA	7	G	2.6
31	CA	51	G	2.6
31	CA	327	G	2.6
31	CA	1259	G	2.6
39	CK	74	TYR	2.6
48	CT	102	HIS	2.6
31	CA	63	A	2.6
31	CA	320	A	2.6
31	CA	1597	A	2.6
31	CA	2873	A	2.6
41	CM	11	GLY	2.6
31	CA	129	C	2.6
31	CA	335	C	2.6
31	CA	455	C	2.6
7	BG	35	LYS	2.6
39	CK	106	LYS	2.6
41	CM	69	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
54	CZ	29	ARG	2.6
3	BC	26	THR	2.6
34	CE	53	THR	2.6
29	CC	64	ILE	2.5
48	CT	86	MET	2.5
41	CM	64	PHE	2.5
31	CA	1379	U	2.5
29	DC	38	SER	2.5
30	CD	144	GLY	2.5
30	CD	187	LEU	2.5
39	CK	25	LEU	2.5
48	CT	19	LEU	2.5
48	CT	23	LEU	2.5
1	BA	198	G	2.5
29	CC	48	ARG	2.5
31	CA	971	G	2.5
31	CA	1215	G	2.5
31	CA	1235	G	2.5
31	CA	1300	G	2.5
31	CA	2010	G	2.5
33	DA	2152	G	2.5
33	DA	2168	G	2.5
39	CK	9	GLU	2.5
45	CQ	102	GLU	2.5
46	CR	16	LYS	2.5
20	BT	47	ALA	2.5
30	CD	65	ALA	2.5
3	BC	94	ILE	2.5
27	C0	10	THR	2.5
41	CM	101	ILE	2.5
41	CM	105	ILE	2.5
48	CT	4	ILE	2.5
31	CA	57	C	2.5
31	CA	209	C	2.5
31	CA	444	C	2.5
1	BA	1240	U	2.5
19	BS	13	LEU	2.5
46	CR	87	SER	2.5
31	CA	224	U	2.5
31	CA	1217	U	2.5
31	CA	2068	U	2.5
49	CU	72	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
54	CZ	28	LEU	2.5
25	C4	3	LYS	2.5
53	CY	26	LYS	2.5
16	BP	2	VAL	2.5
38	CJ	78	VAL	2.5
16	BP	29	ASN	2.5
34	CE	175	ILE	2.5
48	CT	103	ILE	2.5
49	CU	74	ILE	2.5
48	CT	100	THR	2.5
1	BA	1363	A	2.5
31	CA	21	A	2.5
31	CA	1321	A	2.5
1	BA	213	G	2.5
53	CY	12	PRO	2.5
19	AS	5	LEU	2.5
42	CN	2	LEU	2.5
46	CR	60	LEU	2.5
31	CA	806	C	2.5
36	CG	169	VAL	2.5
37	CH	108	VAL	2.5
50	CV	59	VAL	2.5
47	CS	103	ALA	2.5
50	CV	71	ALA	2.5
31	CA	292	U	2.5
31	CA	1240	U	2.5
30	CD	146	ILE	2.5
2	AB	27	MET	2.5
34	CE	60	TRP	2.5
46	CR	106	PHE	2.5
26	C5	31	PRO	2.5
7	AG	109	ARG	2.5
22	C1	39	LEU	2.5
27	C0	17	LEU	2.5
29	CC	14	ARG	2.5
30	CD	116	LYS	2.5
44	CP	26	LEU	2.5
1	BA	1437	A	2.5
31	CA	256	A	2.5
31	CA	265	A	2.5
31	CA	2814	A	2.5
31	CA	2882	A	2.5

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Mol	Chain	Res	Type	RSRZ
36	CG	102	VAL	2.5
41	CM	38	GLN	2.5
1	BA	100	G	2.5
1	BA	799	G	2.5
25	C4	27	ALA	2.5
31	CA	333	G	2.5
31	CA	530	G	2.5
31	CA	1202	G	2.5
31	CA	1218	G	2.5
31	CA	1228	G	2.5
31	CA	2004	G	2.5
31	CA	2630	G	2.5
33	DA	1093	G	2.5
43	CO	111	ALA	2.5
44	CP	6	ALA	2.5
31	CA	343	C	2.5
31	CA	961	C	2.5
31	CA	1335	C	2.5
31	CA	2691	C	2.5
54	CZ	30	MET	2.5
10	BJ	75	ASP	2.5
55	DI	96	PHE	2.5
1	BA	224	U	2.5
1	BA	1286	U	2.5
31	CA	234	U	2.5
31	CA	2245	U	2.5
31	CA	2818	U	2.5
26	C5	34	LYS	2.5
34	CE	63	LYS	2.5
2	AB	135	LEU	2.5
7	BG	71	PRO	2.5
13	BM	48	LEU	2.5
34	CE	118	LEU	2.5
49	CU	32	LEU	2.5
40	CL	27	GLY	2.5
30	CD	207	VAL	2.5
36	CG	168	VAL	2.5
49	CU	34	VAL	2.5
22	C1	4	GLN	2.5
46	CR	56	GLN	2.5
2	BB	134	ALA	2.4
38	CJ	109	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	BB	136	MET	2.4
31	CA	53	A	2.4
31	CA	1262	A	2.4
31	CA	1938	A	2.4
35	CF	32	GLU	2.4
39	CK	4	PHE	2.4
8	BH	90	ASP	2.4
25	C4	41	LYS	2.4
29	CC	229	ASP	2.4
34	CE	67	ARG	2.4
41	CM	60	ARG	2.4
48	CT	8	ARG	2.4
1	BA	104	G	2.4
1	BA	136	C	2.4
1	BA	214	C	2.4
29	CC	33	LEU	2.4
29	CC	202	LEU	2.4
31	CA	16	C	2.4
31	CA	212	G	2.4
31	CA	297	G	2.4
31	CA	325	G	2.4
31	CA	2838	G	2.4
39	CK	114	LEU	2.4
43	CO	95	THR	2.4
52	CX	21	LEU	2.4
34	CE	59	PRO	2.4
47	CS	52	PRO	2.4
13	AM	86	TYR	2.4
31	CA	25	U	2.4
31	CA	1647	U	2.4
33	DA	139	U	2.4
34	CE	193	VAL	2.4
41	CM	34	GLY	2.4
46	CR	100	VAL	2.4
50	CV	12	ILE	2.4
2	BB	147	SER	2.4
45	CQ	43	PHE	2.4
2	BB	139	ARG	2.4
47	CS	48	LYS	2.4
1	BA	65	A	2.4
1	BA	101	A	2.4
10	AJ	75	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
16	AP	69	ASP	2.4
31	CA	794	A	2.4
33	DA	2142	A	2.4
48	CT	104	THR	2.4
38	DJ	23	PRO	2.4
19	BS	58	VAL	2.4
27	C0	15	GLY	2.4
30	CD	10	GLY	2.4
31	CA	66	C	2.4
31	CA	1345	C	2.4
31	CA	2260	C	2.4
38	CJ	55	ILE	2.4
38	CJ	59	ILE	2.4
46	CR	42	ALA	2.4
1	BA	1032	G	2.4
31	CA	329	G	2.4
31	CA	431	U	2.4
31	CA	588	U	2.4
31	CA	790	U	2.4
31	CA	811	U	2.4
31	CA	974	G	2.4
31	CA	1139	G	2.4
31	CA	1311	G	2.4
31	CA	1337	G	2.4
48	CT	85	ILE	2.4
40	CL	1	MET	2.4
34	CE	57	LYS	2.4
34	CE	132	LYS	2.4
50	CV	47	LYS	2.4
30	CD	127	PHE	2.4
38	DJ	67	PHE	2.4
45	CQ	68	GLU	2.4
29	CC	38	SER	2.4
45	CQ	8	LEU	2.4
9	BI	125	PRO	2.4
10	BJ	41	PRO	2.4
49	CU	62	VAL	2.4
29	CC	235	GLY	2.4
34	CE	92	HIS	2.4
41	CM	26	GLY	2.4
1	BA	1441	A	2.4
7	AG	7	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
31	CA	866	A	2.4
31	CA	1156	A	2.4
31	CA	1274	A	2.4
31	CA	1307	A	2.4
47	CS	97	LYS	2.4
1	BA	1325	C	2.4
10	BJ	102	LEU	2.4
31	CA	69	C	2.4
31	CA	106	C	2.4
31	CA	565	C	2.4
31	CA	1200	C	2.4
31	CA	1348	C	2.4
31	CA	2861	U	2.4
48	CT	101	SER	2.4
55	DI	24	SER	2.4
1	BA	94	G	2.4
31	CA	539	G	2.4
31	CA	664	G	2.4
31	CA	916	G	2.4
31	CA	1334	G	2.4
25	C4	38	THR	2.4
30	CD	203	VAL	2.4
10	BJ	8	ILE	2.4
34	CE	149	ILE	2.4
39	CK	6	ALA	2.4
39	CK	103	ILE	2.4
46	CR	45	TYR	2.4
50	CV	72	ILE	2.4
23	C2	10	LYS	2.4
20	AT	28	MET	2.4
34	CE	88	ARG	2.4
38	CJ	38	PHE	2.4
31	CA	979	A	2.4
31	CA	2037	A	2.4
33	DA	1090	A	2.4
55	DI	40	GLU	2.4
29	CC	248	TRP	2.4
38	CJ	9	VAL	2.4
39	CK	110	PRO	2.4
44	CP	27	VAL	2.4
1	BA	175	C	2.3
1	BA	381	C	2.3

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Mol	Chain	Res	Type	RSRZ
23	C2	23	THR	2.3
31	CA	210	C	2.3
31	CA	595	C	2.3
29	CC	233	GLY	2.3
41	CM	45	GLY	2.3
14	BN	29	ALA	2.3
17	BQ	21	ILE	2.3
35	CF	119	ALA	2.3
40	CL	29	HIS	2.3
43	CO	23	ASN	2.3
46	CR	27	ALA	2.3
50	CV	24	LYS	2.3
36	CG	157	TYR	2.3
37	DH	97	ARG	2.3
31	CA	189	G	2.3
31	CA	215	G	2.3
31	CA	1653	G	2.3
31	CA	2027	G	2.3
31	CA	2067	G	2.3
30	CD	188	LEU	2.3
42	CN	130	PHE	2.3
52	CX	45	PHE	2.3
9	AI	116	VAL	2.3
34	CE	146	VAL	2.3
42	CN	36	VAL	2.3
42	CN	135	VAL	2.3
1	BA	60	A	2.3
22	C1	11	SER	2.3
31	CA	222	A	2.3
31	CA	443	A	2.3
31	CA	505	A	2.3
31	CA	1654	A	2.3
31	CA	2211	A	2.3
31	CA	2813	A	2.3
29	CC	9	THR	2.3
41	CM	36	LYS	2.3
42	CN	14	LYS	2.3
34	CE	61	ARG	2.3
42	CN	24	THR	2.3
52	CX	37	ILE	2.3
52	CX	41	ARG	2.3
11	BK	21	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
46	CR	14	HIS	2.3
52	CX	47	ALA	2.3
52	CX	53	CYS	2.3
31	CA	1624	U	2.3
39	CK	44	TYR	2.3
1	BA	379	C	2.3
1	BA	470	C	2.3
29	CC	34	LEU	2.3
29	CC	93	LEU	2.3
31	CA	823	C	2.3
31	CA	2573	C	2.3
1	BA	454	G	2.3
19	BS	60	VAL	2.3
31	CA	60	G	2.3
31	CA	474	G	2.3
31	CA	1382	G	2.3
31	CA	2029	G	2.3
31	CA	2812	G	2.3
33	DA	2140	G	2.3
19	BS	76	PRO	2.3
46	CR	30	ARG	2.3
48	CT	95	ARG	2.3
19	AS	8	GLY	2.3
34	CE	55	SER	2.3
38	DJ	35	ILE	2.3
43	CO	34	ILE	2.3
19	BS	33	THR	2.3
24	C3	22	MET	2.3
26	C5	10	LEU	2.3
1	BA	1534	A	2.3
31	CA	513	A	2.3
31	CA	793	A	2.3
31	CA	2872	A	2.3
7	BG	15	ASP	2.3
31	CA	1599	U	2.3
33	DA	546	U	2.3
31	CA	353	C	2.3
33	DA	885	C	2.3
48	CT	29	VAL	2.3
50	CV	28	VAL	2.3
26	C5	38	GLY	2.3
34	CE	81	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
44	CP	35	ILE	2.3
51	CW	6	ALA	2.3
2	AB	130	THR	2.3
8	AH	3	MET	2.3
14	AN	50	THR	2.3
47	CS	19	THR	2.3
19	BS	14	HIS	2.3
53	CY	52	SER	2.3
1	BA	69	G	2.3
31	CA	338	G	2.3
31	CA	350	G	2.3
31	CA	776	G	2.3
31	CA	1227	G	2.3
31	CA	1660	G	2.3
33	DA	1087	G	2.3
33	DA	2138	G	2.3
35	CF	128	TYR	2.3
51	CW	87	GLN	2.3
1	BA	109	A	2.3
1	BA	1016	A	2.3
17	BQ	63	GLU	2.3
31	CA	10	A	2.3
38	CJ	58	VAL	2.3
48	CT	52	GLU	2.3
31	CA	235	U	2.3
31	CA	686	U	2.3
31	CA	741	U	2.3
31	CA	803	U	2.3
31	CA	1255	U	2.3
31	CA	1390	U	2.3
33	DA	1094	U	2.3
33	DA	2111	U	2.3
24	C3	7	PRO	2.3
9	BI	108	ALA	2.3
39	CK	87	ALA	2.3
1	BA	985	C	2.3
31	CA	433	C	2.3
31	CA	1574	C	2.3
31	CA	2047	C	2.3
31	CA	2874	C	2.3
13	BM	21	SER	2.3
9	BI	120	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
14	BN	97	LYS	2.3
30	CD	7	LYS	2.3
36	CG	6	LYS	2.3
41	CM	104	GLN	2.3
49	CU	66	LYS	2.3
7	BG	33	ASP	2.3
45	CQ	61	VAL	2.3
45	CQ	9	GLU	2.2
31	CA	117	G	2.2
31	CA	537	G	2.2
31	CA	577	G	2.2
31	CA	777	G	2.2
31	CA	805	G	2.2
31	CA	1091	G	2.2
31	CA	2808	G	2.2
31	CA	2895	G	2.2
13	BM	77	ILE	2.2
29	CC	104	ILE	2.2
39	CK	101	ILE	2.2
26	C5	29	ALA	2.2
46	CR	26	GLY	2.2
55	DI	112	ALA	2.2
1	BA	1285	A	2.2
22	C1	22	LEU	2.2
31	CA	479	A	2.2
31	CA	615	U	2.2
31	CA	804	A	2.2
31	CA	941	A	2.2
31	CA	945	A	2.2
31	CA	1780	A	2.2
31	CA	1956	U	2.2
33	DA	1058	U	2.2
33	DA	1083	U	2.2
33	DA	2169	A	2.2
35	CF	103	LEU	2.2
42	CN	124	LEU	2.2
24	C3	16	HIS	2.2
55	DI	131	THR	2.2
6	BF	93	LYS	2.2
9	BI	68	LYS	2.2
45	CQ	94	LYS	2.2
30	CD	141	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	336	C	2.2
31	CA	660	C	2.2
31	CA	673	C	2.2
31	CA	679	C	2.2
31	CA	1233	C	2.2
42	CN	10	ARG	2.2
49	CU	57	VAL	2.2
2	AB	169	GLU	2.2
16	BP	53	ASP	2.2
22	C1	43	ILE	2.2
44	CP	8	ILE	2.2
47	CS	27	ILE	2.2
19	BS	71	LEU	2.2
22	C1	28	LEU	2.2
26	C5	1	MET	2.2
26	C5	21	GLY	2.2
39	CK	109	LEU	2.2
41	CM	82	LEU	2.2
47	CS	8	GLY	2.2
26	C5	32	LYS	2.2
30	CD	112	THR	2.2
31	CA	185	G	2.2
31	CA	536	G	2.2
31	CA	561	G	2.2
31	CA	809	G	2.2
31	CA	1388	G	2.2
31	CA	1514	G	2.2
31	CA	2040	G	2.2
31	CA	2731	G	2.2
33	DA	1074	G	2.2
42	CN	118	LYS	2.2
49	CU	44	LYS	2.2
1	BA	1307	U	2.2
30	CD	77	ARG	2.2
31	CA	846	U	2.2
31	CA	2172	U	2.2
31	CA	2213	U	2.2
48	CT	92	ARG	2.2
53	CY	3	ARG	2.2
31	CA	447	A	2.2
31	CA	626	A	2.2
31	CA	2019	A	2.2

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Mol	Chain	Res	Type	RSRZ
33	DA	613	A	2.2
33	DA	2887[A]	A	2.2
24	C3	9	VAL	2.2
27	C0	7	ILE	2.2
31	CA	31	C	2.2
31	CA	1404	C	2.2
31	CA	1605	C	2.2
31	CA	2575	C	2.2
12	BL	24	LEU	2.2
34	CE	171	ASP	2.2
52	CX	56	ASP	2.2
29	CC	8	PRO	2.2
34	CE	71	GLY	2.2
38	DJ	14	ALA	2.2
19	BS	17	LYS	2.2
43	CO	78	LYS	2.2
49	CU	33	LYS	2.2
50	CV	21	LYS	2.2
29	CC	30	PHE	2.2
19	AS	3	ARG	2.2
25	C4	42	ARG	2.2
7	BG	72	THR	2.2
30	CD	140	HIS	2.2
34	CE	65	THR	2.2
34	CE	165	HIS	2.2
38	CJ	70	VAL	2.2
39	CK	56	VAL	2.2
44	CP	28	VAL	2.2
31	CA	546	U	2.2
31	CA	2609	U	2.2
33	DA	2118	U	2.2
3	BC	10	ILE	2.2
22	C1	55	ILE	2.2
29	CC	49	ILE	2.2
30	CD	27	ILE	2.2
30	CD	96	ILE	2.2
1	BA	532	A	2.2
31	CA	205	G	2.2
7	BG	13	LEU	2.2
31	CA	219	A	2.2
31	CA	478	A	2.2
31	CA	495	G	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	501	A	2.2
31	CA	608	A	2.2
31	CA	939	G	2.2
31	CA	1131	G	2.2
31	CA	1137	G	2.2
31	CA	1353	A	2.2
31	CA	1525	A	2.2
31	CA	1632	A	2.2
31	CA	2267	A	2.2
31	CA	2828	G	2.2
33	DA	1057	A	2.2
34	CE	138	LEU	2.2
34	CE	143	LEU	2.2
39	CK	43	GLU	2.2
7	BG	61	ALA	2.2
10	BJ	79	PRO	2.2
29	CC	231	PRO	2.2
38	DJ	52	GLY	2.2
41	CM	52	GLY	2.2
9	BI	13	LYS	2.2
21	AU	49	LYS	2.2
30	CD	200	ASP	2.2
41	CM	84	LYS	2.2
1	BA	194	C	2.2
1	BA	328	C	2.2
31	CA	32	C	2.2
31	CA	323	C	2.2
31	CA	812	C	2.2
31	CA	1774	C	2.2
22	C1	42	HIS	2.2
25	C4	24	HIS	2.2
43	CO	116	VAL	2.2
3	AC	207	ILE	2.2
30	CD	137	SER	2.2
30	CD	199	SER	2.2
40	CL	99	ILE	2.2
7	BG	66	LEU	2.2
14	BN	98	LYS	2.2
16	BP	26	ASN	2.2
30	CD	194	PRO	2.2
39	CK	39	LYS	2.2
43	CO	39	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
29	CC	203	ARG	2.2
21	AU	37	PHE	2.2
31	CA	1254	A	2.2
31	CA	1469	A	2.2
1	BA	384	G	2.2
31	CA	23	G	2.2
31	CA	696	G	2.2
31	CA	1206	G	2.2
31	CA	1464	G	2.2
31	CA	1649	G	2.2
31	CA	1770	G	2.2
31	CA	2894	G	2.2
33	DA	2112	G	2.2
43	CO	3	HIS	2.2
47	CS	12	HIS	2.2
19	AS	39	THR	2.1
40	CL	35	VAL	2.1
42	CN	132	THR	2.1
54	CZ	16	THR	2.1
8	BH	128	TYR	2.1
1	BA	1218	C	2.1
10	AJ	6	ILE	2.1
31	CA	337	C	2.1
31	CA	1658	C	2.1
38	CJ	49	ILE	2.1
14	BN	16	LEU	2.1
2	AB	136	MET	2.1
21	BU	15	ALA	2.1
24	C3	15	SER	2.1
42	CN	100	LYS	2.1
43	CO	14	SER	2.1
14	BN	70	PRO	2.1
27	C0	16	ARG	2.1
29	CC	217	ARG	2.1
30	CD	6	GLY	2.1
34	CE	42	GLY	2.1
36	CG	170	ARG	2.1
29	CC	226	ASN	2.1
38	DJ	38	PHE	2.1
1	AA	723	U	2.1
51	CW	45	ASP	2.1
22	C1	19	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
40	CL	122	VAL	2.1
7	BG	38	THR	2.1
22	C1	9	THR	2.1
1	BA	1287	A	2.1
31	CA	14	A	2.1
31	CA	1393	A	2.1
43	CO	38	LEU	2.1
45	CQ	114	LEU	2.1
54	CZ	42	LEU	2.1
1	AA	1015	G	2.1
1	BA	1432	G	2.1
20	BT	25	ARG	2.1
29	CC	221	ARG	2.1
31	CA	473	G	2.1
31	CA	1197	G	2.1
31	CA	1238	G	2.1
31	CA	1303	G	2.1
31	CA	1332	G	2.1
31	CA	2239	G	2.1
30	CD	196	ALA	2.1
44	CP	7	ARG	2.1
44	CP	14	ALA	2.1
46	CR	13	ARG	2.1
49	CU	83	ALA	2.1
10	BJ	66	GLU	2.1
17	AQ	10	GLY	2.1
29	CC	47	GLY	2.1
39	CK	113	PRO	2.1
42	CN	99	GLY	2.1
47	CS	50	GLY	2.1
31	CA	237	C	2.1
31	CA	456	C	2.1
50	CV	48	PRO	2.1
13	AM	105	ASN	2.1
35	CF	23	ASN	2.1
14	BN	101	TRP	2.1
39	CK	124	VAL	2.1
49	CU	10	VAL	2.1
1	BA	209	U	2.1
10	BJ	46	LYS	2.1
29	CC	18	LYS	2.1
31	CA	50	U	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	641	U	2.1
31	CA	828	U	2.1
34	CE	166	LYS	2.1
43	CO	112	TYR	2.1
48	CT	73	LYS	2.1
11	AK	66	ALA	2.1
14	AN	22	ALA	2.1
25	C4	65	ALA	2.1
45	CQ	91	ALA	2.1
55	DI	25	ALA	2.1
27	C0	28	GLY	2.1
31	CA	911	A	2.1
31	CA	1439	A	2.1
31	CA	1690	A	2.1
39	CK	98	GLU	2.1
45	CQ	22	PRO	2.1
55	DI	106	PHE	2.1
53	CY	16	ASN	2.1
1	BA	79	G	2.1
31	CA	180	G	2.1
31	CA	376	G	2.1
31	CA	488	G	2.1
31	CA	729	G	2.1
31	CA	1212	G	2.1
31	CA	1245	G	2.1
31	CA	1776	G	2.1
31	CA	1984	G	2.1
31	CA	2574	G	2.1
31	CA	2576	G	2.1
31	CA	2655	G	2.1
33	DA	1059	G	2.1
41	CM	46	VAL	2.1
53	CY	51	VAL	2.1
31	CA	1314	C	2.1
31	CA	1704	C	2.1
31	CA	2443	C	2.1
11	BK	14	LYS	2.1
11	BK	22	HIS	2.1
47	CS	55	ASP	2.1
51	DW	34	LYS	2.1
19	BS	16	LEU	2.1
44	CP	30	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
54	CZ	47	ARG	2.1
9	BI	44	ALA	2.1
31	CA	1199	U	2.1
42	CN	97	GLN	2.1
24	C3	27	GLY	2.1
7	AG	26	PHE	2.1
38	CJ	23	PRO	2.1
50	CV	37	GLU	2.1
53	CY	31	PRO	2.1
9	BI	104	VAL	2.1
34	CE	167	VAL	2.1
49	CU	63	VAL	2.1
1	BA	174	A	2.1
12	BL	44	LYS	2.1
20	BT	8	LYS	2.1
30	CD	160	LYS	2.1
31	CA	216	A	2.1
31	CA	218	A	2.1
31	CA	352	A	2.1
31	CA	590	A	2.1
31	CA	614	A	2.1
31	CA	1745	A	2.1
33	DA	1095	A	2.1
33	DA	2108	A	2.1
49	CU	64	LYS	2.1
7	BG	7	ILE	2.1
9	BI	119	ARG	2.1
20	BT	32	ILE	2.1
24	C3	12	ARG	2.1
24	C3	14	ARG	2.1
27	C0	25	LEU	2.1
39	CK	122	LEU	2.1
51	CW	89	ILE	2.1
53	CY	18	ARG	2.1
42	CN	70	ASP	2.1
34	CE	84	THR	2.1
1	BA	210	C	2.1
1	BA	352	C	2.1
1	BA	1317	C	2.1
31	CA	238	C	2.1
31	CA	440	C	2.1
31	CA	509	C	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	557	C	2.1
31	CA	623	C	2.1
31	CA	1556	C	2.1
31	CA	1764	C	2.1
31	CA	2422	C	2.1
1	BA	378	G	2.1
1	BA	976	G	2.1
31	CA	1573	G	2.1
31	CA	1661	G	2.1
31	CA	1980	G	2.1
31	CA	2608	G	2.1
31	CA	2686	G	2.1
31	CA	2732	G	2.1
36	CG	150	ALA	2.1
40	CL	16	ALA	2.1
35	CF	100	PHE	2.1
38	DJ	20	PRO	2.1
41	CM	106	GLU	2.1
1	BA	229	U	2.0
30	CD	170	VAL	2.0
31	CA	328	U	2.0
31	CA	441	U	2.0
31	CA	1982	U	2.0
36	CG	162	VAL	2.0
38	DJ	98	VAL	2.0
43	CO	60	VAL	2.0
43	CO	76	VAL	2.0
48	CT	41	LYS	2.0
53	CY	35	SER	2.0
7	BG	23	LEU	2.0
30	CD	58	ASN	2.0
30	CD	186	LEU	2.0
37	CH	11	ASN	2.0
44	CP	106	LEU	2.0
36	DG	111	HIS	2.0
1	BA	172	A	2.0
9	BI	9	THR	2.0
16	BP	22	ALA	2.0
23	C2	21	TYR	2.0
27	C0	22	ALA	2.0
31	CA	1241	A	2.0
31	CA	1336	A	2.0

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Mol	Chain	Res	Type	RSRZ
31	CA	2587	A	2.0
31	CA	2893	A	2.0
33	DA	1067	A	2.0
33	DA	2170	A	2.0
43	CO	53	THR	2.0
46	CR	24	TYR	2.0
10	BJ	64	GLN	2.0
16	AP	10	GLY	2.0
27	C0	9	GLN	2.0
29	DC	251	GLN	2.0
34	CE	90	GLN	2.0
30	CD	55	LYS	2.0
7	BG	73	VAL	2.0
21	AU	53	VAL	2.0
31	CA	211	C	2.0
31	CA	486	C	2.0
31	CA	1290	C	2.0
31	CA	1748	C	2.0
31	CA	2579	C	2.0
31	CA	2610	C	2.0
36	CG	138	LYS	2.0
38	DJ	10	LYS	2.0
46	CR	93	LYS	2.0
2	AB	161	LEU	2.0
21	AU	35	ARG	2.0
31	CA	1	G	2.0
31	CA	35	G	2.0
31	CA	186	G	2.0
31	CA	830	G	2.0
31	CA	1210	G	2.0
31	CA	1310	G	2.0
31	CA	1374	G	2.0
31	CA	1633	G	2.0
31	CA	1857	G	2.0
31	CA	1983	G	2.0
31	CA	2319	G	2.0
33	DA	2116	G	2.0
38	DJ	88	SER	2.0
45	CQ	64	ILE	2.0
12	BL	5	ASN	2.0
49	CU	1	MET	2.0
2	BB	34	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
25	C4	17	THR	2.0
46	CR	10	ALA	2.0
50	CV	77	THR	2.0
7	AG	112	GLY	2.0
9	AI	20	PHE	2.0
45	CQ	105	GLY	2.0
9	BI	100	LYS	2.0
13	BM	27	LYS	2.0
1	BA	949	A	2.0
2	BB	133	GLU	2.0
7	AG	58	GLU	2.0
14	BN	34	VAL	2.0
17	BQ	59	VAL	2.0
25	C4	7	VAL	2.0
29	CC	19	VAL	2.0
31	CA	432	A	2.0
31	CA	449	A	2.0
31	CA	480	A	2.0
31	CA	1572	A	2.0
31	CA	2439	A	2.0
47	CS	64	VAL	2.0
34	CE	200	LEU	2.0
45	CQ	100	LEU	2.0
9	AI	21	ILE	2.0
35	CF	106	ILE	2.0
38	CJ	122	ILE	2.0
44	CP	40	ILE	2.0
1	BA	1462	C	2.0
31	CA	20	C	2.0
31	CA	485	C	2.0
31	CA	2073	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
31	PSU	CA	1917	20/21	0.62	0.12	120,122,127,127	0
31	6MZ	CA	1618	23/24	0.72	0.17	165,167,172,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	PSU	CA	1911	20/21	0.74	0.08	128,136,137,138	0
1	2MG	BA	966	24/25	0.75	0.14	140,144,153,153	0
31	3TD	CA	1915	21/22	0.78	0.08	139,145,147,148	0
31	PSU	CA	955	20/21	0.78	0.14	108,113,117,117	0
31	2MA	CA	2503	23/24	0.79	0.17	101,104,114,114	0
1	2MG	BA	1207	24/25	0.81	0.11	154,155,158,161	0
31	PSU	CA	2580	20/21	0.81	0.15	105,112,116,117	0
31	PSU	CA	2504	20/21	0.82	0.16	91,98,101,102	0
31	6MZ	CA	2030	23/24	0.82	0.15	117,125,129,130	0
1	5MC	BA	967	21/22	0.83	0.12	135,141,145,145	0
31	PSU	CA	2457	20/21	0.84	0.14	109,112,117,118	0
31	PSU	CA	746	20/21	0.85	0.16	127,129,130,130	0
42	4D4	CN	81	12/13	0.85	0.12	99,103,115,116	0
12	D2T	BL	89	10/11	0.88	0.14	79,85,97,98	0
31	2MG	CA	2445	24/25	0.89	0.15	79,94,103,104	0
31	OMU	CA	2552	21/22	0.89	0.15	100,103,113,115	0
1	PSU	BA	516	20/21	0.89	0.11	78,85,90,91	0
31	G7M	CA	2069	24/25	0.89	0.16	105,111,117,118	0
31	1MG	CA	745	24/25	0.90	0.17	117,123,124,126	0
1	5MC	BA	1407	21/22	0.90	0.11	93,96,104,107	0
31	OMG	CA	2251	24/25	0.90	0.14	95,101,105,106	0
31	5MU	CA	747	21/22	0.90	0.11	129,137,142,144	0
31	PSU	CA	2605	20/21	0.90	0.12	81,87,95,96	0
33	PSU	DA	1917	20/21	0.90	0.08	83,86,95,95	0
12	D2T	AL	89	10/11	0.90	0.13	59,63,78,81	0
31	2MG	CA	1835	24/25	0.91	0.11	76,80,82,83	0
31	5MU	CA	1939	21/22	0.91	0.12	79,86,88,89	0
1	2MG	BA	1516	24/25	0.92	0.10	82,87,93,93	0
33	3TD	DA	1915	21/22	0.92	0.09	110,116,120,122	0
1	2MG	AA	966	24/25	0.92	0.09	83,86,88,88	0
1	2MG	AA	1207	24/25	0.92	0.08	90,100,107,107	0
31	5MC	CA	1962	21/22	0.93	0.10	76,79,80,85	0
1	MA6	BA	1518	24/25	0.93	0.11	71,77,85,86	0
1	5MC	AA	967	21/22	0.93	0.10	84,88,89,89	0
31	OMC	CA	2498	21/22	0.93	0.11	98,104,108,109	0
1	UR3	BA	1498	21/22	0.94	0.09	83,84,89,89	0
1	PSU	AA	516	20/21	0.94	0.08	77,81,84,85	0
33	PSU	DA	1911	20/21	0.94	0.07	86,90,91,92	0
1	MA6	BA	1519	24/25	0.95	0.10	78,82,85,85	0
1	UR3	AA	1498	21/22	0.95	0.09	54,58,62,64	0
1	G7M	BA	527	24/25	0.95	0.09	69,73,78,78	0
33	PSU	DA	2604	20/21	0.95	0.08	31,43,54,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	G7M	AA	527	24/25	0.95	0.09	57,62,67,70	0
1	4OC	BA	1402	22/23	0.96	0.07	72,74,77,78	0
1	MA6	AA	1519	24/25	0.97	0.08	46,51,55,59	0
1	5MC	AA	1407	21/22	0.97	0.06	54,55,57,58	0
1	4OC	AA	1402	22/23	0.97	0.07	60,63,64,65	0
33	5MU	DA	1939	21/22	0.97	0.09	38,40,48,50	0
1	MA6	AA	1518	24/25	0.97	0.07	45,48,54,54	0
33	2MG	DA	1835	24/25	0.97	0.08	44,48,54,61	0
42	4D4	DN	81[A]	12/13	0.97	0.08	29,36,47,49	9
42	4D4	DN	81[B]	12/13	0.97	0.08	13,22,30,31	9
33	2MA	DA	2503	23/24	0.98	0.07	16,28,36,40	0
33	PSU	DA	2504	20/21	0.98	0.06	29,34,37,41	0
33	5MU	DA	747	21/22	0.98	0.06	26,28,35,37	0
33	PSU	DA	2605	20/21	0.98	0.05	33,40,41,41	0
1	2MG	AA	1516	24/25	0.98	0.06	51,53,55,57	0
33	5MC	DA	1962	21/22	0.98	0.06	40,46,48,48	0
33	G7M	DA	2069	24/25	0.98	0.07	34,37,43,45	0
33	OMG	DA	2251	24/25	0.99	0.04	28,30,40,44	0
33	2MG	DA	2445	24/25	0.99	0.05	16,25,30,31	0
33	H2U	DA	2449	20/21	0.99	0.06	12,22,32,33	0
33	PSU	DA	2457	20/21	0.99	0.04	24,25,30,32	0
33	OMC	DA	2498	21/22	0.99	0.05	15,20,26,33	0
33	1MG	DA	745	24/25	0.99	0.05	26,32,36,38	0
33	PSU	DA	746	20/21	0.99	0.04	16,22,31,32	0
33	OMU	DA	2552	21/22	0.99	0.06	25,30,35,42	0
33	PSU	DA	2580	20/21	0.99	0.05	18,26,29,31	0
32	MEQ	DD	150[A]	10/11	0.99	0.09	9,14,29,29	10
33	PSU	DA	955	20/21	0.99	0.05	17,22,24,25	0
33	6MZ	DA	1618	23/24	0.99	0.04	17,28,32,32	0
33	6MZ	DA	2030	23/24	0.99	0.04	16,20,26,27	0
32	MEQ	DD	150[B]	10/11	0.99	0.09	26,31,38,40	10

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3110	1/1	0.06	0.41	168,168,168,168	0
56	MG	CA	3124	1/1	0.11	0.25	165,165,165,165	0
56	MG	CA	3146	1/1	0.11	0.25	220,220,220,220	0
56	MG	CA	3007	1/1	0.31	0.13	256,256,256,256	0
56	MG	CA	3038	1/1	0.37	0.10	250,250,250,250	0
56	MG	CA	3115	1/1	0.38	0.44	85,85,85,85	0
56	MG	CA	3123	1/1	0.44	0.26	200,200,200,200	0
56	MG	CA	3003	1/1	0.52	0.31	280,280,280,280	0
56	MG	CA	3132	1/1	0.53	0.19	116,116,116,116	0
56	MG	AA	1628	1/1	0.57	0.22	177,177,177,177	0
56	MG	AA	1606	1/1	0.57	0.46	106,106,106,106	0
56	MG	CA	3002	1/1	0.58	0.20	273,273,273,273	0
56	MG	DA	3166	1/1	0.59	0.27	141,141,141,141	0
56	MG	CA	3092	1/1	0.61	0.14	210,210,210,210	0
56	MG	BA	1624	1/1	0.61	0.27	274,274,274,274	0
56	MG	CA	3139	1/1	0.62	0.28	100,100,100,100	0
56	MG	CA	3075	1/1	0.63	0.24	241,241,241,241	0
56	MG	BA	1604	1/1	0.64	0.15	218,218,218,218	0
56	MG	CA	3104	1/1	0.64	0.13	234,234,234,234	0
56	MG	CA	3111	1/1	0.65	0.24	121,121,121,121	0
56	MG	CA	3077	1/1	0.65	0.09	240,240,240,240	0
56	MG	CA	3061	1/1	0.66	0.15	264,264,264,264	0
56	MG	CA	3034	1/1	0.66	0.19	239,239,239,239	0
56	MG	AA	1619	1/1	0.67	0.21	98,98,98,98	0
56	MG	CA	3032	1/1	0.67	0.15	257,257,257,257	0
56	MG	CA	3005	1/1	0.67	0.18	250,250,250,250	0
56	MG	CA	3154	1/1	0.68	0.23	132,132,132,132	0
56	MG	CA	3067	1/1	0.68	0.17	283,283,283,283	0
56	MG	BA	1625	1/1	0.69	0.15	269,269,269,269	0
56	MG	CA	3060	1/1	0.70	0.13	259,259,259,259	0
56	MG	CA	3152	1/1	0.71	0.15	167,167,167,167	0
56	MG	CA	3014	1/1	0.71	0.16	256,256,256,256	0
56	MG	CA	3026	1/1	0.71	0.12	201,201,201,201	0
56	MG	CA	3083	1/1	0.73	0.17	263,263,263,263	0
56	MG	CA	3021	1/1	0.74	0.38	272,272,272,272	0
56	MG	CA	3028	1/1	0.74	0.12	263,263,263,263	0
56	MG	CA	3155	1/1	0.76	0.19	196,196,196,196	0
56	MG	CA	3135	1/1	0.76	0.30	96,96,96,96	0
56	MG	CA	3156	1/1	0.77	0.11	252,252,252,252	0
61	PEG	DP	201	7/7	0.77	0.24	136,137,140,141	0
56	MG	CA	3047	1/1	0.78	0.35	230,230,230,230	0
56	MG	CA	3009	1/1	0.78	0.13	271,271,271,271	0
56	MG	CA	3008	1/1	0.78	0.17	251,251,251,251	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	1606	1/1	0.79	0.18	249,249,249,249	0
56	MG	CA	3140	1/1	0.79	0.16	112,112,112,112	0
58	MPD	DK	201	8/8	0.79	0.20	138,140,140,141	0
56	MG	CA	3122	1/1	0.79	0.19	81,81,81,81	0
56	MG	CA	3141	1/1	0.80	0.24	72,72,72,72	0
58	MPD	DE	301	8/8	0.80	0.22	151,152,153,153	0
56	MG	CA	3151	1/1	0.81	0.28	81,81,81,81	0
56	MG	CA	3129	1/1	0.81	0.19	109,109,109,109	0
56	MG	AA	1605	1/1	0.81	0.36	98,98,98,98	0
56	MG	CA	3133	1/1	0.81	0.15	112,112,112,112	0
56	MG	BA	1640	1/1	0.81	0.21	131,131,131,131	0
56	MG	DA	3159	1/1	0.81	0.33	60,60,60,60	0
56	MG	AA	1609	1/1	0.81	0.19	72,72,72,72	0
56	MG	CA	3071	1/1	0.81	0.10	230,230,230,230	0
56	MG	AA	1661	1/1	0.81	0.11	166,166,166,166	0
59	PUT	AA	1673	6/6	0.81	0.12	91,92,94,95	0
56	MG	CA	3126	1/1	0.81	0.08	74,74,74,74	0
56	MG	CA	3073	1/1	0.82	0.20	212,212,212,212	0
56	MG	CA	3023	1/1	0.82	0.24	206,206,206,206	0
56	MG	DA	3157	1/1	0.82	0.12	67,67,67,67	0
56	MG	CA	3039	1/1	0.82	0.17	203,203,203,203	0
56	MG	BA	1639	1/1	0.82	0.11	70,70,70,70	0
56	MG	CA	3019	1/1	0.82	0.12	71,71,71,71	0
56	MG	BA	1603	1/1	0.82	0.10	254,254,254,254	0
56	MG	CA	3022	1/1	0.82	0.21	235,235,235,235	0
59	PUT	AA	1675	6/6	0.82	0.27	111,112,113,113	0
56	MG	CA	3037	1/1	0.82	0.19	206,206,206,206	0
56	MG	DA	3169	1/1	0.83	0.11	86,86,86,86	0
56	MG	DA	3171	1/1	0.83	0.31	106,106,106,106	0
56	MG	AA	1624	1/1	0.83	0.23	85,85,85,85	0
56	MG	CA	3072	1/1	0.83	0.11	273,273,273,273	0
56	MG	CA	3064	1/1	0.83	0.16	283,283,283,283	0
59	PUT	AA	1674	6/6	0.83	0.29	108,109,110,110	0
56	MG	CA	3010	1/1	0.83	0.13	250,250,250,250	0
56	MG	CA	3131	1/1	0.83	0.16	75,75,75,75	0
56	MG	AA	1623	1/1	0.84	0.11	60,60,60,60	0
56	MG	BA	1607	1/1	0.84	0.13	203,203,203,203	0
56	MG	CA	3006	1/1	0.84	0.10	240,240,240,240	0
56	MG	BA	1636	1/1	0.84	0.28	91,91,91,91	0
62	EDO	DA	3001	4/4	0.84	0.23	95,95,95,96	0
56	MG	CA	3112	1/1	0.85	0.23	85,85,85,85	0
56	MG	DA	3170	1/1	0.85	0.31	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3036	1/1	0.85	0.21	194,194,194,194	0
58	MPD	DA	3188	8/8	0.85	0.20	91,94,96,98	0
56	MG	CA	3120	1/1	0.85	0.15	135,135,135,135	0
56	MG	CA	3091	1/1	0.85	0.10	137,137,137,137	0
56	MG	AA	1660	1/1	0.85	0.15	278,278,278,278	0
56	MG	CA	3076	1/1	0.85	0.12	214,214,214,214	0
56	MG	CA	3065	1/1	0.85	0.12	151,151,151,151	0
59	PUT	DA	3218	6/6	0.85	0.24	122,122,123,123	0
61	PEG	DA	3197	7/7	0.85	0.22	91,99,102,102	0
56	MG	DA	3160	1/1	0.85	0.15	87,87,87,87	0
61	PEG	DQ	201	7/7	0.85	0.15	118,119,121,121	0
56	MG	CA	3082	1/1	0.85	0.16	152,152,152,152	0
58	MPD	DA	3201	8/8	0.86	0.26	125,126,127,128	0
56	MG	CA	3121	1/1	0.86	0.17	63,63,63,63	0
56	MG	AA	1615	1/1	0.86	0.56	110,110,110,110	0
56	MG	AA	1608	1/1	0.86	0.20	83,83,83,83	0
56	MG	CA	3105	1/1	0.86	0.19	254,254,254,254	0
56	MG	BA	1629	1/1	0.86	0.16	195,195,195,195	0
56	MG	CA	3004	1/1	0.86	0.14	203,203,203,203	0
59	PUT	DA	3219	6/6	0.86	0.18	55,57,61,62	0
56	MG	AA	1622	1/1	0.86	0.17	70,70,70,70	0
56	MG	AA	1602	1/1	0.86	0.13	80,80,80,80	0
56	MG	DA	3178	1/1	0.86	0.11	105,105,105,105	0
56	MG	CA	3051	1/1	0.86	0.15	183,183,183,183	0
56	MG	CA	3094	1/1	0.87	0.15	139,139,139,139	0
58	MPD	DN	201	8/8	0.87	0.18	90,95,96,96	0
56	MG	AA	1603	1/1	0.87	0.19	91,91,91,91	0
56	MG	CA	3068	1/1	0.87	0.21	266,266,266,266	0
56	MG	CA	3134	1/1	0.87	0.13	134,134,134,134	0
56	MG	CA	3125	1/1	0.87	0.11	85,85,85,85	0
56	MG	CA	3109	1/1	0.87	0.18	80,80,80,80	0
57	PG4	DQ	202	13/13	0.87	0.14	65,68,81,81	0
56	MG	DA	3129	1/1	0.87	0.09	46,46,46,46	0
56	MG	CA	3127	1/1	0.87	0.17	71,71,71,71	0
56	MG	BA	1617	1/1	0.87	0.10	160,160,160,160	0
59	PUT	AA	1672	6/6	0.88	0.27	88,89,89,90	0
57	PG4	BA	1642	13/13	0.88	0.14	94,97,106,107	0
57	PG4	DA	3213	13/13	0.88	0.18	101,107,112,112	0
56	MG	DA	3122	1/1	0.88	0.31	86,86,86,86	0
59	PUT	DA	3182	6/6	0.88	0.23	77,78,80,80	0
56	MG	AA	1664	1/1	0.88	0.08	147,147,147,147	0
56	MG	DA	3137	1/1	0.88	0.51	29,29,29,29	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MPD	DA	3204	8/8	0.88	0.18	93,94,97,97	0
56	MG	DA	3146	1/1	0.88	0.16	117,117,117,117	0
56	MG	CA	3054	1/1	0.88	0.12	180,180,180,180	0
56	MG	CA	3063	1/1	0.88	0.21	181,181,181,181	0
63	PGE	DS	201	10/10	0.88	0.12	68,74,77,77	0
66	ACY	DA	3194	4/4	0.88	0.18	52,56,56,58	0
56	MG	CA	3084	1/1	0.89	0.12	196,196,196,196	0
56	MG	CA	3107	1/1	0.89	0.26	67,67,67,67	0
56	MG	CA	3057	1/1	0.89	0.07	143,143,143,143	0
56	MG	DA	3176	1/1	0.89	0.11	59,59,59,59	0
61	PEG	AL	201	7/7	0.89	0.11	78,79,84,85	0
61	PEG	D3	102	7/7	0.89	0.26	105,109,110,111	0
58	MPD	DE	302	8/8	0.89	0.26	116,118,121,121	0
56	MG	CA	3137	1/1	0.89	0.06	137,137,137,137	0
57	PG4	AA	1670	13/13	0.89	0.12	77,84,91,92	0
56	MG	BA	1623	1/1	0.89	0.16	193,193,193,193	0
62	EDO	DA	3212	4/4	0.89	0.14	72,73,74,75	0
56	MG	CA	3074	1/1	0.89	0.11	142,142,142,142	0
63	PGE	DT	201	10/10	0.89	0.21	137,138,140,140	0
56	MG	BA	1619	1/1	0.89	0.19	198,198,198,198	0
56	MG	DA	3136	1/1	0.90	0.12	91,91,91,91	0
56	MG	CA	3087	1/1	0.90	0.11	196,196,196,196	0
59	PUT	DA	3193	6/6	0.90	0.30	88,90,92,92	0
59	PUT	DA	3210	6/6	0.90	0.32	108,110,112,113	0
56	MG	CA	3090	1/1	0.90	0.25	222,222,222,222	0
56	MG	DA	3155	1/1	0.90	0.09	47,47,47,47	0
56	MG	DA	3156	1/1	0.90	0.10	45,45,45,45	0
56	MG	CA	3145	1/1	0.90	0.13	50,50,50,50	0
56	MG	AA	1626	1/1	0.90	0.08	77,77,77,77	0
56	MG	CA	3001	1/1	0.90	0.17	294,294,294,294	0
56	MG	CA	3093	1/1	0.90	0.07	140,140,140,140	0
56	MG	AA	1612	1/1	0.90	0.14	59,59,59,59	0
56	MG	CA	3012	1/1	0.90	0.12	130,130,130,130	0
56	MG	AA	1635	1/1	0.90	0.23	209,209,209,209	0
56	MG	CA	3055	1/1	0.90	0.05	145,145,145,145	0
56	MG	CA	3085	1/1	0.90	0.09	67,67,67,67	0
68	TRS	DA	3217	8/8	0.90	0.15	149,150,153,155	0
56	MG	DA	3174	1/1	0.91	0.16	99,99,99,99	0
56	MG	CA	3142	1/1	0.91	0.13	73,73,73,73	0
56	MG	DA	3131	1/1	0.91	0.12	43,43,43,43	0
56	MG	DA	3180	1/1	0.91	0.14	72,72,72,72	0
56	MG	CA	3099	1/1	0.91	0.15	189,189,189,189	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	PUT	DA	3216	6/6	0.91	0.19	71,72,72,72	0
56	MG	CA	3102	1/1	0.91	0.11	92,92,92,92	0
57	PG4	DA	3191	13/13	0.91	0.18	76,87,103,103	0
56	MG	CA	3029	1/1	0.91	0.16	181,181,181,181	0
56	MG	DA	3151	1/1	0.91	0.25	82,82,82,82	0
56	MG	BA	1612	1/1	0.91	0.21	200,200,200,200	0
61	PEG	DA	3198	7/7	0.91	0.29	118,120,124,124	0
56	MG	CA	3153	1/1	0.91	0.10	49,49,49,49	0
56	MG	CA	3106	1/1	0.91	0.10	81,81,81,81	0
62	EDO	DB	210	4/4	0.91	0.18	87,88,89,90	0
56	MG	CA	3119	1/1	0.91	0.08	68,68,68,68	0
62	EDO	DA	3206	4/4	0.91	0.25	104,104,105,105	0
56	MG	AA	1647	1/1	0.91	0.14	217,217,217,217	0
56	MG	DA	3061	1/1	0.91	0.07	209,209,209,209	0
56	MG	DA	3118	1/1	0.91	0.09	62,62,62,62	0
56	MG	CA	3108	1/1	0.91	0.17	74,74,74,74	0
56	MG	DA	3125	1/1	0.91	0.19	48,48,48,48	0
56	MG	CA	3138	1/1	0.92	0.12	67,67,67,67	0
56	MG	CA	3059	1/1	0.92	0.09	120,120,120,120	0
56	MG	CA	3116	1/1	0.92	0.25	62,62,62,62	0
56	MG	DB	207	1/1	0.92	0.16	74,74,74,74	0
57	PG4	DR	203	13/13	0.92	0.28	151,153,155,155	0
57	PG4	DS	202	13/13	0.92	0.12	73,75,77,77	0
56	MG	DA	3006	1/1	0.92	0.08	118,118,118,118	0
56	MG	CA	3048	1/1	0.92	0.10	112,112,112,112	0
56	MG	AA	1630	1/1	0.92	0.08	124,124,124,124	0
58	MPD	DA	3228	8/8	0.92	0.23	92,96,99,99	0
56	MG	DA	3167	1/1	0.92	0.08	23,23,23,23	0
56	MG	CA	3062	1/1	0.92	0.09	191,191,191,191	0
56	MG	DA	3124	1/1	0.92	0.18	59,59,59,59	0
56	MG	AA	1654	1/1	0.92	0.13	200,200,200,200	0
56	MG	CA	3148	1/1	0.92	0.30	27,27,27,27	1
56	MG	CA	3149	1/1	0.92	0.28	52,52,52,52	0
56	MG	AA	1617	1/1	0.92	0.18	63,63,63,63	0
56	MG	BA	1609	1/1	0.92	0.11	203,203,203,203	0
67	GUN	DA	3208	11/11	0.92	0.19	111,112,113,113	0
56	MG	CA	3088	1/1	0.92	0.10	75,75,75,75	0
58	MPD	AA	1676	8/8	0.93	0.21	96,98,102,102	0
56	MG	DA	3130	1/1	0.93	0.21	76,76,76,76	0
56	MG	CA	3130	1/1	0.93	0.11	75,75,75,75	0
56	MG	BA	1616	1/1	0.93	0.08	169,169,169,169	0
56	MG	AA	1614	1/1	0.93	0.24	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3142	1/1	0.93	0.13	58,58,58,58	0
56	MG	DB	208	1/1	0.93	0.22	60,60,60,60	0
61	PEG	DA	3224	7/7	0.93	0.18	75,76,78,79	0
61	PEG	DL	201	7/7	0.93	0.09	78,80,83,84	0
56	MG	CA	3086	1/1	0.93	0.07	67,67,67,67	0
56	MG	BA	1627	1/1	0.93	0.12	109,109,109,109	0
56	MG	DA	3110	1/1	0.93	0.19	273,273,273,273	0
56	MG	CA	3044	1/1	0.93	0.15	102,102,102,102	0
56	MG	CA	3113	1/1	0.93	0.16	50,50,50,50	0
56	MG	AA	1601	1/1	0.93	0.20	48,48,48,48	0
62	EDO	DA	3227	4/4	0.93	0.27	123,124,125,126	0
63	PGE	D3	101	10/10	0.93	0.16	93,97,100,100	0
56	MG	BA	1634	1/1	0.93	0.09	133,133,133,133	0
56	MG	AA	1677	1/1	0.93	0.11	121,121,121,121	0
64	SPD	DA	3203	10/10	0.93	0.21	93,98,105,106	0
65	1PE	DA	3183	16/16	0.93	0.13	46,56,86,87	0
59	PUT	DA	3202	6/6	0.93	0.21	95,96,96,96	0
66	ACY	DA	3199	4/4	0.93	0.19	83,84,85,85	0
59	PUT	DA	3209	6/6	0.93	0.15	80,83,87,88	0
58	MPD	AA	1671	8/8	0.93	0.15	110,112,114,115	0
56	MG	CA	3033	1/1	0.94	0.19	154,154,154,154	0
56	MG	DA	3165	1/1	0.94	0.28	118,118,118,118	0
58	MPD	DA	3190	8/8	0.94	0.17	99,100,101,101	0
56	MG	BA	1633	1/1	0.94	0.11	248,248,248,248	0
56	MG	CA	3035	1/1	0.94	0.17	102,102,102,102	0
61	PEG	DA	3215	7/7	0.94	0.25	126,128,134,135	0
56	MG	DA	3168	1/1	0.94	0.21	47,47,47,47	0
56	MG	CA	3128	1/1	0.94	0.08	65,65,65,65	0
56	MG	CA	3018	1/1	0.94	0.08	131,131,131,131	0
56	MG	AA	1642	1/1	0.94	0.12	173,173,173,173	0
62	EDO	D1	101	4/4	0.94	0.08	53,53,53,54	0
56	MG	AA	1616	1/1	0.94	0.29	55,55,55,55	0
58	MPD	DT	202	8/8	0.94	0.23	117,118,119,119	0
56	MG	CA	3096	1/1	0.94	0.11	105,105,105,105	0
56	MG	CA	3098	1/1	0.94	0.07	101,101,101,101	0
56	MG	BA	1637	1/1	0.94	0.13	63,63,63,63	0
56	MG	BA	1638	1/1	0.94	0.23	64,64,64,64	0
63	PGE	DD	302	10/10	0.94	0.24	75,77,78,79	0
56	MG	DA	3143	1/1	0.94	0.13	111,111,111,111	0
59	PUT	DA	3187	6/6	0.94	0.09	36,42,42,42	0
56	MG	CA	3136	1/1	0.94	0.14	66,66,66,66	0
64	SPD	DA	3221	10/10	0.94	0.15	47,58,65,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DB	206	1/1	0.94	0.05	61,61,61,61	0
65	1PE	DA	3200	16/16	0.94	0.18	62,67,77,77	0
56	MG	AA	1665	1/1	0.94	0.10	153,153,153,153	0
56	MG	AA	1621	1/1	0.94	0.20	59,59,59,59	0
56	MG	AA	1656	1/1	0.94	0.09	132,132,132,132	0
56	MG	AA	1610	1/1	0.94	0.10	76,76,76,76	0
56	MG	CA	3013	1/1	0.95	0.07	91,91,91,91	0
56	MG	DA	3097	1/1	0.95	0.15	187,187,187,187	0
56	MG	BA	1608	1/1	0.95	0.07	122,122,122,122	0
56	MG	DA	3173	1/1	0.95	0.13	73,73,73,73	0
56	MG	DA	3112	1/1	0.95	0.09	94,94,94,94	0
56	MG	AA	1669	1/1	0.95	0.09	91,91,91,91	0
56	MG	DA	3177	1/1	0.95	0.18	118,118,118,118	0
56	MG	CA	3078	1/1	0.95	0.08	128,128,128,128	0
60	ZN	C5	101	1/1	0.95	0.07	149,149,149,149	0
56	MG	CA	3101	1/1	0.95	0.07	164,164,164,164	0
61	PEG	D1	102	7/7	0.95	0.12	61,65,68,69	0
56	MG	DR	202	1/1	0.95	0.08	29,29,29,29	0
56	MG	CA	3079	1/1	0.95	0.10	156,156,156,156	0
56	MG	DA	3126	1/1	0.95	0.22	55,55,55,55	0
56	MG	AA	1657	1/1	0.95	0.07	152,152,152,152	0
61	PEG	DA	3223	7/7	0.95	0.16	82,82,84,85	0
56	MG	CA	3147	1/1	0.95	0.32	50,50,50,50	1
56	MG	BA	1614	1/1	0.95	0.11	127,127,127,127	0
56	MG	BA	1601	1/1	0.95	0.08	140,140,140,140	0
56	MG	CA	3150	1/1	0.95	0.05	50,50,50,50	0
56	MG	DA	3141	1/1	0.95	0.25	46,46,46,46	0
56	MG	AA	1613	1/1	0.95	0.11	52,52,52,52	0
56	MG	AA	1650	1/1	0.95	0.09	149,149,149,149	0
62	EDO	DA	3196	4/4	0.95	0.28	86,88,89,89	0
62	EDO	DA	3205	4/4	0.95	0.17	79,82,83,83	0
56	MG	DA	3145	1/1	0.95	0.17	58,58,58,58	0
56	MG	BA	1622	1/1	0.95	0.07	150,150,150,150	0
56	MG	AA	1618	1/1	0.95	0.18	57,57,57,57	0
56	MG	CA	3089	1/1	0.95	0.12	69,69,69,69	0
56	MG	CA	3053	1/1	0.95	0.06	84,84,84,84	0
63	PGE	DA	3184	10/10	0.95	0.11	39,51,60,63	0
63	PGE	DA	3211	10/10	0.95	0.14	81,82,90,93	0
63	PGE	DA	3214	10/10	0.95	0.12	81,82,84,85	0
63	PGE	DA	3222	10/10	0.95	0.17	79,90,99,99	0
56	MG	DB	205	1/1	0.95	0.12	64,64,64,64	0
56	MG	AA	1644	1/1	0.95	0.08	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
63	PGE	DU	101	10/10	0.95	0.11	79,83,88,88	0
64	SPD	DA	3181	10/10	0.95	0.11	66,69,73,73	0
56	MG	BA	1641	1/1	0.95	0.09	72,72,72,72	0
56	MG	DA	3163	1/1	0.95	0.33	70,70,70,70	0
56	MG	DA	3164	1/1	0.95	0.17	78,78,78,78	0
56	MG	CA	3056	1/1	0.95	0.22	48,48,48,48	0
56	MG	DB	209	1/1	0.95	0.21	105,105,105,105	0
56	MG	DD	301	1/1	0.95	0.12	53,53,53,53	0
56	MG	CA	3117	1/1	0.95	0.16	64,64,64,64	0
59	PUT	DA	3186	6/6	0.95	0.12	44,49,50,51	0
56	MG	AA	1627	1/1	0.96	0.07	55,55,55,55	0
56	MG	CA	3046	1/1	0.96	0.11	123,123,123,123	0
56	MG	CA	3030	1/1	0.96	0.04	76,76,76,76	0
56	MG	CA	3031	1/1	0.96	0.04	102,102,102,102	0
56	MG	DA	3138	1/1	0.96	0.11	43,43,43,43	0
62	EDO	DB	211	4/4	0.96	0.14	96,96,96,96	0
56	MG	DA	3140	1/1	0.96	0.09	54,54,54,54	0
62	EDO	DA	3192	4/4	0.96	0.17	92,92,93,94	0
62	EDO	DA	3195	4/4	0.96	0.14	71,73,74,75	0
56	MG	BA	1630	1/1	0.96	0.07	165,165,165,165	0
56	MG	BA	1632	1/1	0.96	0.08	72,72,72,72	0
56	MG	DA	3004	1/1	0.96	0.09	107,107,107,107	0
56	MG	DA	3179	1/1	0.96	0.27	56,56,56,56	0
56	MG	DA	3144	1/1	0.96	0.09	65,65,65,65	0
56	MG	DR	201	1/1	0.96	0.17	228,228,228,228	0
56	MG	AA	1607	1/1	0.96	0.15	52,52,52,52	0
56	MG	AA	1638	1/1	0.96	0.06	105,105,105,105	0
56	MG	CB	201	1/1	0.96	0.06	169,169,169,169	0
56	MG	DA	3152	1/1	0.96	0.40	59,59,59,59	0
56	MG	DA	3153	1/1	0.96	0.13	47,47,47,47	0
56	MG	CB	203	1/1	0.96	0.05	106,106,106,106	0
56	MG	BA	1635	1/1	0.96	0.06	96,96,96,96	0
59	PUT	DA	3220	6/6	0.96	0.23	77,80,81,81	0
56	MG	BA	1628	1/1	0.96	0.05	80,80,80,80	0
56	MG	CA	3040	1/1	0.96	0.06	134,134,134,134	0
56	MG	DA	3123	1/1	0.96	0.20	66,66,66,66	0
56	MG	CA	3042	1/1	0.96	0.07	93,93,93,93	0
56	MG	CA	3097	1/1	0.96	0.10	123,123,123,123	0
56	MG	CA	3080	1/1	0.96	0.18	160,160,160,160	0
56	MG	DA	3128	1/1	0.96	0.20	52,52,52,52	0
58	MPD	DA	3207	8/8	0.96	0.15	64,70,73,78	0
56	MG	CA	3081	1/1	0.96	0.07	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	1613	1/1	0.97	0.07	86,86,86,86	0
56	MG	AA	1636	1/1	0.97	0.07	89,89,89,89	0
56	MG	AA	1658	1/1	0.97	0.05	58,58,58,58	0
56	MG	AA	1611	1/1	0.97	0.09	50,50,50,50	0
62	EDO	D0	101	4/4	0.97	0.13	67,67,68,69	0
56	MG	DA	3132	1/1	0.97	0.07	57,57,57,57	0
56	MG	DA	3133	1/1	0.97	0.10	55,55,55,55	0
56	MG	CA	3058	1/1	0.97	0.10	203,203,203,203	0
56	MG	CA	3114	1/1	0.97	0.05	40,40,40,40	0
56	MG	CA	3024	1/1	0.97	0.07	153,153,153,153	0
56	MG	CA	3025	1/1	0.97	0.11	109,109,109,109	0
56	MG	CA	3011	1/1	0.97	0.05	68,68,68,68	0
56	MG	CA	3118	1/1	0.97	0.10	52,52,52,52	0
56	MG	CA	3027	1/1	0.97	0.06	118,118,118,118	0
56	MG	BA	1618	1/1	0.97	0.09	91,91,91,91	0
56	MG	CA	3100	1/1	0.97	0.09	104,104,104,104	0
56	MG	CA	3144	1/1	0.97	0.04	54,54,54,54	0
56	MG	DA	3148	1/1	0.97	0.12	34,34,34,34	0
56	MG	DA	3150	1/1	0.97	0.10	41,41,41,41	0
56	MG	AA	1634	1/1	0.97	0.06	141,141,141,141	0
56	MG	BA	1602	1/1	0.97	0.04	79,79,79,79	0
56	MG	CA	3103	1/1	0.97	0.04	93,93,93,93	0
59	PUT	DA	3226	6/6	0.97	0.15	74,74,75,75	0
60	ZN	AB	301	1/1	0.97	0.04	125,125,125,125	0
56	MG	DA	3120	1/1	0.97	0.09	64,64,64,64	0
56	MG	DA	3121	1/1	0.97	0.25	51,51,51,51	0
56	MG	CA	3066	1/1	0.97	0.07	133,133,133,133	0
56	MG	CA	3016	1/1	0.97	0.07	107,107,107,107	0
56	MG	CA	3017	1/1	0.97	0.08	87,87,87,87	0
66	ACY	DA	3189	4/4	0.97	0.11	65,66,66,67	0
56	MG	DA	3161	1/1	0.97	0.14	48,48,48,48	0
56	MG	DA	3162	1/1	0.97	0.16	50,50,50,50	0
56	MG	CA	3070	1/1	0.97	0.04	94,94,94,94	0
56	MG	AA	1604	1/1	0.97	0.24	57,57,57,57	0
56	MG	DA	3135	1/1	0.98	0.07	25,25,25,25	0
56	MG	DA	3036	1/1	0.98	0.09	16,16,16,16	0
58	MPD	DS	203	8/8	0.98	0.09	59,60,62,64	0
56	MG	AA	1640	1/1	0.98	0.04	80,80,80,80	0
56	MG	DA	3070	1/1	0.98	0.08	58,58,58,58	0
56	MG	DA	3071	1/1	0.98	0.07	102,102,102,102	0
56	MG	DA	3081	1/1	0.98	0.04	80,80,80,80	0
56	MG	DA	3175	1/1	0.98	0.09	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CB	202	1/1	0.98	0.08	123,123,123,123	0
56	MG	DA	3098	1/1	0.98	0.05	19,19,19,19	0
56	MG	AA	1659	1/1	0.98	0.04	94,94,94,94	0
56	MG	CA	3052	1/1	0.98	0.05	80,80,80,80	0
56	MG	DA	3116	1/1	0.98	0.11	33,33,33,33	0
56	MG	DA	3147	1/1	0.98	0.17	46,46,46,46	0
56	MG	AA	1629	1/1	0.98	0.05	100,100,100,100	0
56	MG	DA	3119	1/1	0.98	0.12	56,56,56,56	0
56	MG	AA	1643	1/1	0.98	0.03	65,65,65,65	0
56	MG	BA	1626	1/1	0.98	0.08	138,138,138,138	0
56	MG	AA	1655	1/1	0.98	0.05	101,101,101,101	0
56	MG	DA	3154	1/1	0.98	0.09	62,62,62,62	0
56	MG	CA	3143	1/1	0.98	0.05	54,54,54,54	0
56	MG	AA	1620	1/1	0.98	0.05	79,79,79,79	0
56	MG	AA	1667	1/1	0.98	0.05	33,33,33,33	0
64	SPD	DA	3185	10/10	0.98	0.11	52,53,57,58	0
56	MG	CA	3043	1/1	0.98	0.04	72,72,72,72	0
56	MG	DA	3127	1/1	0.98	0.24	24,24,24,24	0
56	MG	AA	1645	1/1	0.98	0.09	54,54,54,54	0
56	MG	DA	3003	1/1	0.98	0.05	93,93,93,93	0
56	MG	CA	3045	1/1	0.98	0.08	78,78,78,78	0
56	MG	BA	1631	1/1	0.98	0.04	42,42,42,42	0
56	MG	DA	3010	1/1	0.98	0.06	145,145,145,145	0
56	MG	DA	3029	1/1	0.98	0.05	68,68,68,68	0
56	MG	DA	3134	1/1	0.98	0.05	120,120,120,120	0
56	MG	CA	3015	1/1	0.99	0.13	59,59,59,59	0
56	MG	DA	3078	1/1	0.99	0.04	127,127,127,127	0
56	MG	DA	3079	1/1	0.99	0.02	44,44,44,44	0
56	MG	DA	3158	1/1	0.99	0.09	61,61,61,61	0
56	MG	CA	3049	1/1	0.99	0.05	53,53,53,53	0
56	MG	DA	3083	1/1	0.99	0.02	23,23,23,23	0
56	MG	DA	3084	1/1	0.99	0.04	56,56,56,56	0
56	MG	DA	3088	1/1	0.99	0.03	13,13,13,13	0
56	MG	DA	3093	1/1	0.99	0.06	17,17,17,17	0
56	MG	DA	3094	1/1	0.99	0.03	54,54,54,54	0
56	MG	CA	3069	1/1	0.99	0.03	81,81,81,81	0
56	MG	CA	3050	1/1	0.99	0.04	58,58,58,58	0
56	MG	DA	3107	1/1	0.99	0.02	26,26,26,26	0
56	MG	AA	1649	1/1	0.99	0.03	62,62,62,62	0
56	MG	AA	1641	1/1	0.99	0.03	44,44,44,44	0
56	MG	AA	1651	1/1	0.99	0.03	61,61,61,61	0
56	MG	DB	201	1/1	0.99	0.03	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	DA	3172	1/1	0.99	0.05	48,48,48,48	0
56	MG	DB	204	1/1	0.99	0.03	56,56,56,56	0
56	MG	AA	1663	1/1	0.99	0.05	65,65,65,65	0
56	MG	CA	3095	1/1	0.99	0.04	80,80,80,80	0
56	MG	CA	3020	1/1	0.99	0.03	73,73,73,73	0
56	MG	BA	1620	1/1	0.99	0.04	90,90,90,90	0
56	MG	BA	1605	1/1	0.99	0.05	58,58,58,58	0
56	MG	AA	1631	1/1	0.99	0.05	42,42,42,42	0
56	MG	DA	3002	1/1	0.99	0.05	77,77,77,77	0
56	MG	DA	3230	1/1	0.99	0.03	60,60,60,60	0
56	MG	DA	3231	1/1	0.99	0.05	43,43,43,43	0
56	MG	AA	1632	1/1	0.99	0.04	88,88,88,88	0
56	MG	CA	3041	1/1	0.99	0.06	47,47,47,47	0
56	MG	DA	3005	1/1	0.99	0.04	78,78,78,78	0
56	MG	AA	1666	1/1	0.99	0.05	56,56,56,56	0
56	MG	AA	1633	1/1	0.99	0.03	76,76,76,76	0
56	MG	DA	3013	1/1	0.99	0.05	92,92,92,92	0
56	MG	DA	3014	1/1	0.99	0.05	56,56,56,56	0
56	MG	DA	3017	1/1	0.99	0.03	53,53,53,53	0
56	MG	DA	3026	1/1	0.99	0.03	39,39,39,39	0
56	MG	DA	3027	1/1	0.99	0.05	136,136,136,136	0
56	MG	BA	1610	1/1	0.99	0.03	97,97,97,97	0
56	MG	AA	1668	1/1	0.99	0.07	62,62,62,62	0
56	MG	DA	3139	1/1	0.99	0.10	73,73,73,73	0
56	MG	DA	3042	1/1	0.99	0.06	24,24,24,24	0
56	MG	DA	3043	1/1	0.99	0.05	84,84,84,84	0
56	MG	DA	3044	1/1	0.99	0.04	73,73,73,73	0
56	MG	DA	3045	1/1	0.99	0.03	25,25,25,25	0
56	MG	DA	3046	1/1	0.99	0.05	46,46,46,46	0
56	MG	DA	3050	1/1	0.99	0.03	44,44,44,44	0
56	MG	DA	3051	1/1	0.99	0.04	52,52,52,52	0
56	MG	DA	3053	1/1	0.99	0.03	68,68,68,68	0
56	MG	AA	1639	1/1	0.99	0.03	82,82,82,82	0
56	MG	DA	3149	1/1	0.99	0.02	38,38,38,38	0
56	MG	DA	3062	1/1	0.99	0.04	110,110,110,110	0
56	MG	DA	3063	1/1	0.99	0.06	83,83,83,83	0
56	MG	DA	3067	1/1	0.99	0.05	43,43,43,43	0
56	MG	DA	3069	1/1	0.99	0.06	65,65,65,65	0
56	MG	AA	1625	1/1	0.99	0.05	61,61,61,61	0
56	MG	DA	3225	1/1	1.00	0.03	14,14,14,14	0
56	MG	DA	3229	1/1	1.00	0.02	45,45,45,45	0
56	MG	DA	3095	1/1	1.00	0.03	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3096	1/1	1.00	0.02	36,36,36,36	0
56	MG	AA	1662	1/1	1.00	0.03	66,66,66,66	0
56	MG	BA	1611	1/1	1.00	0.02	31,31,31,31	0
56	MG	DA	3099	1/1	1.00	0.01	9,9,9,9	0
56	MG	DA	3100	1/1	1.00	0.06	53,53,53,53	0
56	MG	DA	3101	1/1	1.00	0.02	26,26,26,26	0
56	MG	DA	3102	1/1	1.00	0.03	38,38,38,38	0
56	MG	DA	3103	1/1	1.00	0.03	22,22,22,22	0
56	MG	DA	3104	1/1	1.00	0.04	20,20,20,20	0
56	MG	DA	3105	1/1	1.00	0.03	11,11,11,11	0
56	MG	DA	3106	1/1	1.00	0.03	32,32,32,32	0
56	MG	DA	3028	1/1	1.00	0.06	21,21,21,21	0
56	MG	DA	3108	1/1	1.00	0.01	36,36,36,36	0
56	MG	DA	3109	1/1	1.00	0.02	13,13,13,13	0
56	MG	DD	303	1/1	1.00	0.04	37,37,37,37	0
56	MG	DA	3111	1/1	1.00	0.02	21,21,21,21	0
56	MG	DA	3030	1/1	1.00	0.03	26,26,26,26	0
56	MG	DA	3113	1/1	1.00	0.03	30,30,30,30	0
56	MG	DA	3114	1/1	1.00	0.01	7,7,7,7	0
56	MG	DA	3115	1/1	1.00	0.01	32,32,32,32	0
56	MG	DA	3031	1/1	1.00	0.04	16,16,16,16	0
56	MG	DA	3117	1/1	1.00	0.02	43,43,43,43	0
56	MG	DA	3032	1/1	1.00	0.02	21,21,21,21	0
56	MG	DA	3033	1/1	1.00	0.01	10,10,10,10	0
56	MG	DA	3034	1/1	1.00	0.05	28,28,28,28	0
56	MG	DA	3035	1/1	1.00	0.04	15,15,15,15	0
56	MG	AA	1652	1/1	1.00	0.11	18,18,18,18	0
56	MG	DA	3037	1/1	1.00	0.03	26,26,26,26	0
56	MG	DA	3038	1/1	1.00	0.01	29,29,29,29	0
56	MG	DA	3039	1/1	1.00	0.02	43,43,43,43	0
56	MG	DA	3040	1/1	1.00	0.12	10,10,10,10	0
56	MG	DA	3041	1/1	1.00	0.01	25,25,25,25	0
56	MG	BA	1621	1/1	1.00	0.09	13,13,13,13	0
56	MG	DB	202	1/1	1.00	0.05	60,60,60,60	0
56	MG	DB	203	1/1	1.00	0.02	27,27,27,27	0
56	MG	AA	1653	1/1	1.00	0.03	32,32,32,32	0
56	MG	DA	3007	1/1	1.00	0.02	19,19,19,19	0
56	MG	DA	3047	1/1	1.00	0.03	47,47,47,47	0
56	MG	DA	3048	1/1	1.00	0.04	67,67,67,67	0
56	MG	DA	3049	1/1	1.00	0.02	10,10,10,10	0
56	MG	DA	3008	1/1	1.00	0.01	15,15,15,15	0
56	MG	DA	3009	1/1	1.00	0.03	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	ZN	D5	101	1/1	1.00	0.02	55,55,55,55	0
56	MG	DA	3052	1/1	1.00	0.01	53,53,53,53	0
56	MG	AA	1646	1/1	1.00	0.02	50,50,50,50	0
56	MG	DA	3054	1/1	1.00	0.04	27,27,27,27	0
56	MG	DA	3055	1/1	1.00	0.02	19,19,19,19	0
56	MG	DA	3056	1/1	1.00	0.01	7,7,7,7	0
56	MG	DA	3057	1/1	1.00	0.02	33,33,33,33	0
56	MG	DA	3058	1/1	1.00	0.02	22,22,22,22	0
56	MG	DA	3059	1/1	1.00	0.03	25,25,25,25	0
56	MG	DA	3060	1/1	1.00	0.02	32,32,32,32	0
56	MG	DA	3011	1/1	1.00	0.01	9,9,9,9	0
56	MG	DA	3012	1/1	1.00	0.01	18,18,18,18	0
56	MG	BA	1615	1/1	1.00	0.02	44,44,44,44	0
56	MG	DA	3064	1/1	1.00	0.01	24,24,24,24	0
56	MG	DA	3065	1/1	1.00	0.02	24,24,24,24	0
56	MG	DA	3066	1/1	1.00	0.04	49,49,49,49	0
56	MG	AA	1637	1/1	1.00	0.03	47,47,47,47	0
56	MG	DA	3068	1/1	1.00	0.05	52,52,52,52	0
56	MG	DA	3015	1/1	1.00	0.02	28,28,28,28	0
56	MG	DA	3016	1/1	1.00	0.02	32,32,32,32	0
56	MG	AA	1648	1/1	1.00	0.03	55,55,55,55	0
56	MG	DA	3072	1/1	1.00	0.02	26,26,26,26	0
56	MG	DA	3073	1/1	1.00	0.03	37,37,37,37	0
56	MG	DA	3074	1/1	1.00	0.01	26,26,26,26	0
56	MG	DA	3075	1/1	1.00	0.04	26,26,26,26	0
56	MG	DA	3076	1/1	1.00	0.03	34,34,34,34	0
56	MG	DA	3077	1/1	1.00	0.02	34,34,34,34	0
56	MG	DA	3018	1/1	1.00	0.15	10,10,10,10	0
56	MG	DA	3019	1/1	1.00	0.02	54,54,54,54	0
56	MG	DA	3080	1/1	1.00	0.03	28,28,28,28	0
56	MG	DA	3020	1/1	1.00	0.03	23,23,23,23	0
56	MG	DA	3082	1/1	1.00	0.04	64,64,64,64	0
56	MG	DA	3021	1/1	1.00	0.01	9,9,9,9	0
56	MG	DA	3022	1/1	1.00	0.02	21,21,21,21	0
56	MG	DA	3085	1/1	1.00	0.01	27,27,27,27	0
56	MG	DA	3086	1/1	1.00	0.03	17,17,17,17	0
56	MG	DA	3087	1/1	1.00	0.02	58,58,58,58	0
56	MG	DA	3023	1/1	1.00	0.02	29,29,29,29	0
56	MG	DA	3089	1/1	1.00	0.03	16,16,16,16	0
56	MG	DA	3090	1/1	1.00	0.01	11,11,11,11	0
56	MG	DA	3091	1/1	1.00	0.03	24,24,24,24	0
56	MG	DA	3092	1/1	1.00	0.02	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3024	1/1	1.00	0.01	45,45,45,45	0
56	MG	DA	3025	1/1	1.00	0.06	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.