Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2026 – 11:40 PM EDT

PDB ID	:	5J91 / pdb_00005j91
Title	:	Structure of the Wild-type 70S E coli ribosome bound to Tigecycline
Authors	:	Cocozaki, A.; Ferguson, A.
Deposited on	:	2016-04-08
Resolution	:	2.96 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 (i) 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 (i)) were used in the production of this report:

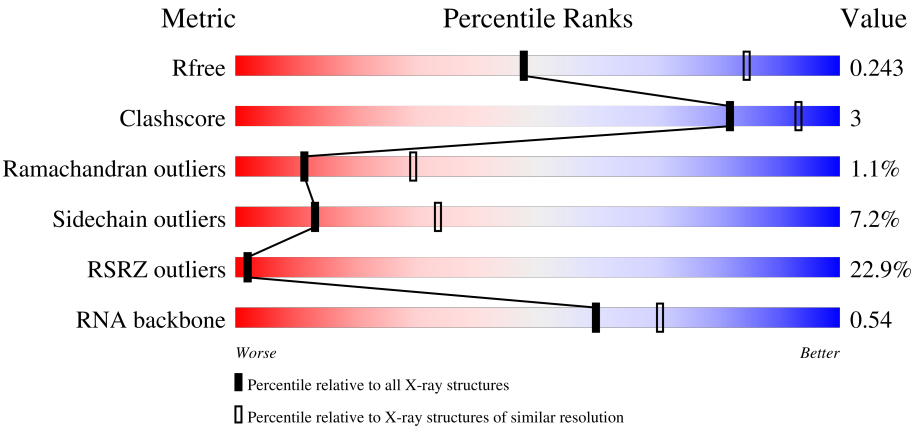
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.96 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)
RNA backbone	3983	1046 (3.16-2.76)

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 <=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	9% 77% 20% .
1	BA	1534	20% 77% 21% .
2	AB	224	19% 85% 12% .
2	BB	224	20% 83% 14% .

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Mol	Chain	Length	Quality of chain
3	AC	206	11% 85% 14%
3	BC	206	28% 81% 18%
4	AD	205	10% 85% 12%
4	BD	205	5% 83% 15%
5	AE	155	14% 77% 18%
5	BE	155	16% 61% 32%
6	AF	106	9% 77% 22%
6	BF	106	6% 61% 31% 6%
7	AG	151	23% 85% 13%
7	BG	151	46% 84% 16%
8	AH	129	12% 79% 20%
8	BH	129	17% 81% 19%
9	AI	127	29% 90% 8%
9	BI	127	46% 90% 8%
10	AJ	99	33% 73% 25%
10	BJ	99	46% 72% 20% 6%
11	AK	117	16% 78% 21%
11	BK	117	21% 71% 26%
12	AL	123	10% 80% 17%
12	BL	123	27% 80% 16%
13	AM	114	39% 75% 19% 5%
13	BM	114	36% 75% 21%
14	AN	100	45% 84% 16%
14	BN	100	55% 84% 16%
15	AO	88	11% 91% 9%

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Mol	Chain	Length	Quality of chain
15	BO	88	14% 90% 10%
16	AP	82	7% 90% 10%
16	BP	82	65% 79% 18%
17	AQ	80	5% 76% 24%
17	BQ	80	36% 74% 22%
18	AR	55	13% 82% 15%
18	BR	55	11% 85% 15%
19	AS	79	37% 80% 15% 5%
19	BS	79	38% 82% 14%
20	AT	86	13% 91% 8%
20	BT	86	56% 72% 17% 8%
21	AU	56	12% 84% 16%
21	BU	56	14% 86% 14%
22	C1	56	66% 66% 29% 5%
22	D1	56	2% 71% 29%
23	C2	51	45% 73% 25%
23	D2	51	18% 78% 18%
24	C3	46	89% 67% 30%
24	D3	46	7% 85% 15%
25	C4	64	86% 80% 17%
25	D4	64	3% 81% 19%
26	C5	38	58% 74% 24%
26	D5	38	5% 92% 8%
27	C0	58	53% 83% 12% 5%
27	D0	58	9% 90% 9%

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Mol	Chain	Length	Quality of chain
28	CB	120	14% 86% 12%
28	DB	120	89% 10%
29	CC	272	44% 82% 14%
29	DC	272	6% 88% 10%
30	CD	209	59% 86% 13%
31	CA	2904	41% 75% 22%
32	DD	209	% 86% 11%
33	CE	201	56% 86% 12%
33	DE	201	% 89% 11%
34	CF	178	21% 78% 19%
34	DF	178	3% 78% 20%
35	CG	176	25% 87% 13%
35	DG	176	5% 88% 12%
36	CH	149	17% 74% 23%
36	DH	149	22% 77% 22%
37	CJ	134	40% 87% 11%
37	DJ	134	47% 85% 13%
38	CK	142	52% 89% 8%
38	DK	142	% 92% 8%
39	CL	123	35% 84% 13%
39	DL	123	% 87% 11%
40	CM	144	68% 76% 22%
40	DM	144	9% 81% 17%
41	CN	136	38% 85% 13%
41	DN	136	88% 11%

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Mol	Chain	Length	Quality of chain
42	CO	125	59% 84% 10%
42	DO	125	% 91% 8%
43	CP	117	22% 82% 15%
43	DP	117	2% 86% 11%
44	CQ	114	36% 86% 13%
44	DQ	114	% 87% 13%
45	CR	117	61% 84% 16%
45	DR	117	% 89% 10%
46	CS	103	53% 83% 14%
46	DS	103	2% 90% 8%
47	CT	110	74% 79% 17%
47	DT	110	2% 85% 14%
48	CU	93	67% 75% 22%
48	DU	93	5% 87% 13%
49	CV	103	66% 78% 18%
49	DV	103	5% 86% 10%
50	CW	94	18% 88% 12%
50	DW	94	2% 90% 10%
51	CX	76	42% 91% 8%
51	DX	76	3% 87% 12%
52	CY	77	58% 79% 21%
52	DY	77	3% 84% 16%
53	CZ	62	56% 89% 10%
53	DZ	62	5% 92% 8%
54	DI	135	36% 67% 30%

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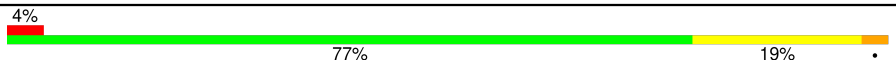
Mol	Chain	Length	Quality of chain
55	DA	2904	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	1601	-	-	-	X
56	MG	AA	1603	-	-	-	X
56	MG	AA	1605	-	-	-	X
56	MG	AA	1606	-	-	-	X
56	MG	AA	1608	-	-	-	X
56	MG	AA	1616	-	-	-	X
56	MG	BA	1640	-	-	-	X
56	MG	CA	3056	-	-	-	X
56	MG	CA	3107	-	-	-	X
56	MG	CA	3108	-	-	-	X
56	MG	CA	3110	-	-	-	X
56	MG	CA	3113	-	-	-	X
56	MG	CA	3116	-	-	-	X
56	MG	CA	3117	-	-	-	X
56	MG	CA	3130	-	-	-	X
56	MG	CA	3133	-	-	-	X
56	MG	CA	3139	-	-	-	X
56	MG	CA	3141	-	-	-	X
56	MG	CA	3147	-	-	-	X
56	MG	CA	3148	-	-	-	X
56	MG	DA	3124	-	-	-	X
56	MG	DA	3128	-	-	-	X
56	MG	DA	3139	-	-	-	X
56	MG	DA	3143	-	-	-	X
56	MG	DA	3153	-	-	-	X
59	PUT	AA	1672	-	-	-	X

2 Entry composition (i)

There are 70 unique types of molecules in this entry. The entry contains 295202 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
			2082	1288	423	364	7			
29	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CO	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DO	125	Total	C	N	O	S	0	0	0
			993	613	202	173	5			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	71	Total 71	Mg 71	0	0
56	BA	43	Total 43	Mg 43	0	0
56	CB	3	Total 3	Mg 3	0	0
56	CA	156	Total 156	Mg 156	0	0
56	DD	2	Total 2	Mg 2	0	0
56	DM	1	Total 1	Mg 1	0	0
56	DR	2	Total 2	Mg 2	0	0
56	DB	9	Total 9	Mg 9	0	0

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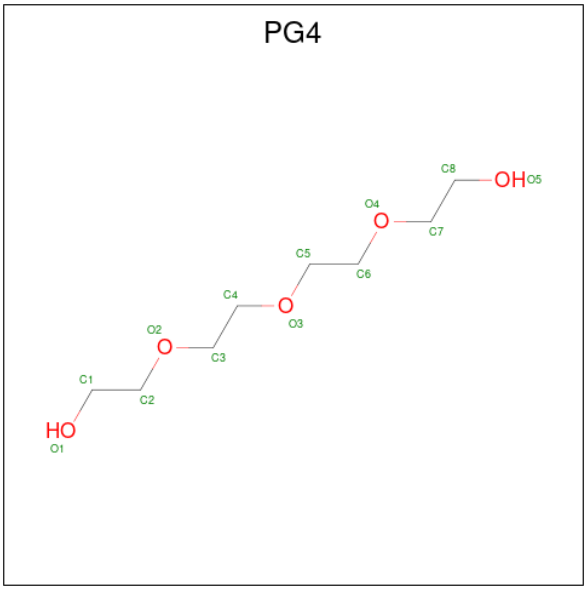
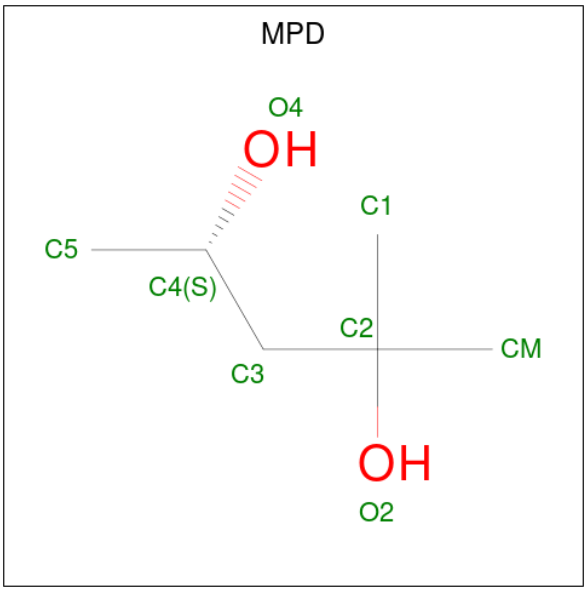
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DA	182	Total Mg 182 182	0	0

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



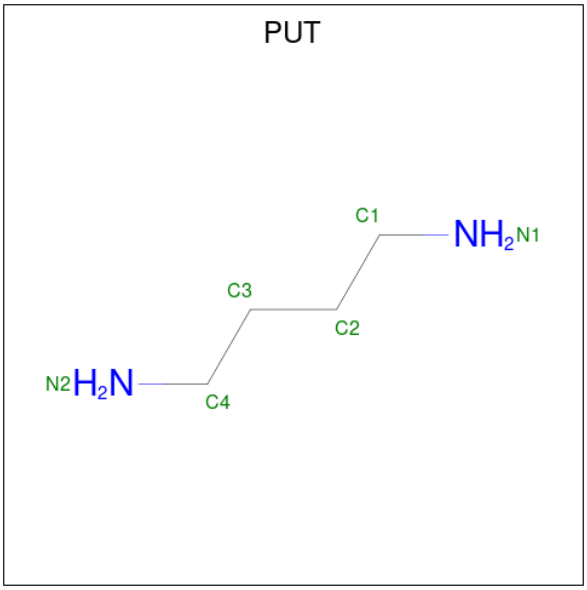
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	1	Total C O 13 8 5	0	0
57	BA	1	Total C O 13 8 5	0	0
57	DQ	1	Total C O 13 8 5	0	0
57	DR	1	Total C O 13 8 5	0	0
57	DS	1	Total C O 13 8 5	0	0
57	DA	1	Total C O 13 8 5	0	0
57	DA	1	Total C O 13 8 5	0	0

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



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

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



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

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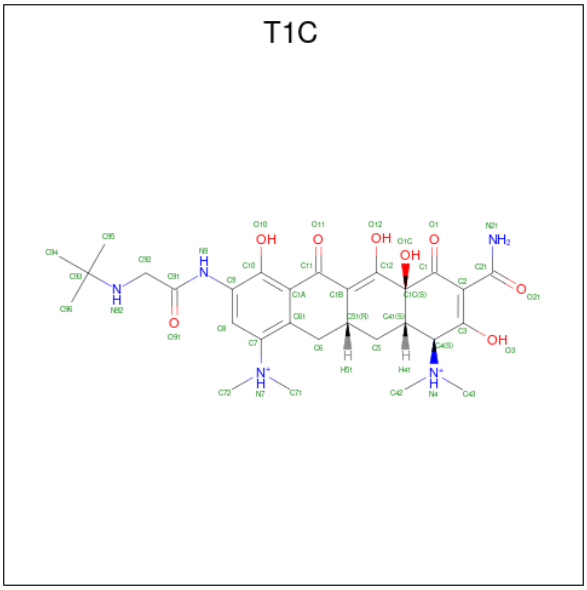
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0
59	DA	1	Total C N 6 4 2	0	0

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

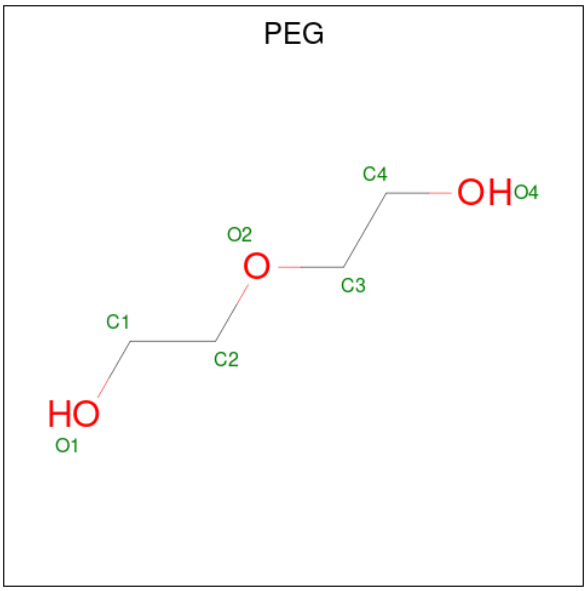


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AA	1	Total C N O 42 29 5 8	0	0
60	BA	1	Total C N O 42 29 5 8	0	0

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

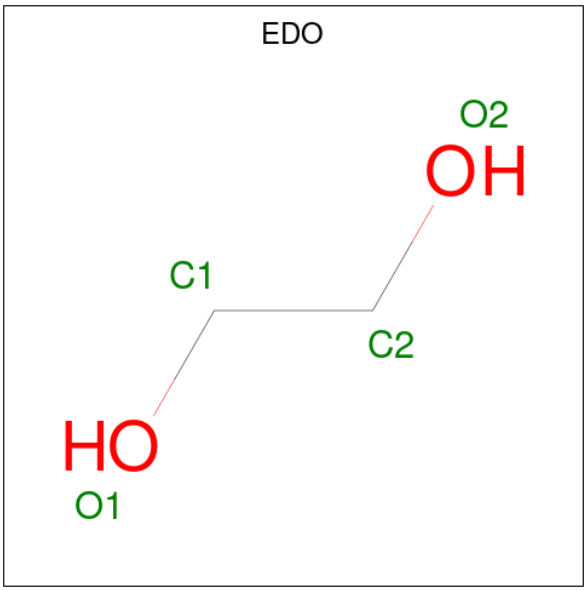
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AB	1	Total Zn 1 1	0	0
61	C5	1	Total Zn 1 1	0	0
61	D5	1	Total Zn 1 1	0	0

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



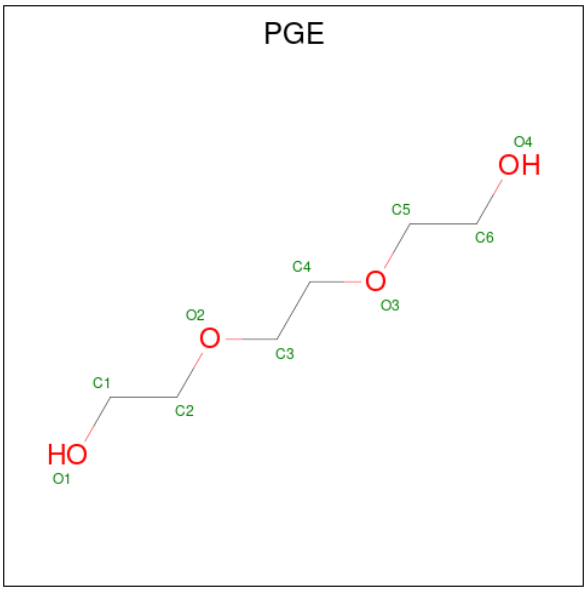
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
62	AL	1	7	4	3	0	0
62	D1	1	7	4	3	0	0
62	D3	1	7	4	3	0	0
62	DL	1	7	4	3	0	0
62	DP	1	7	4	3	0	0
62	DQ	1	7	4	3	0	0
62	DA	1	7	4	3	0	0
62	DA	1	7	4	3	0	0
62	DA	1	7	4	3	0	0
62	DA	1	7	4	3	0	0
62	DA	1	7	4	3	0	0

- Molecule 63 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



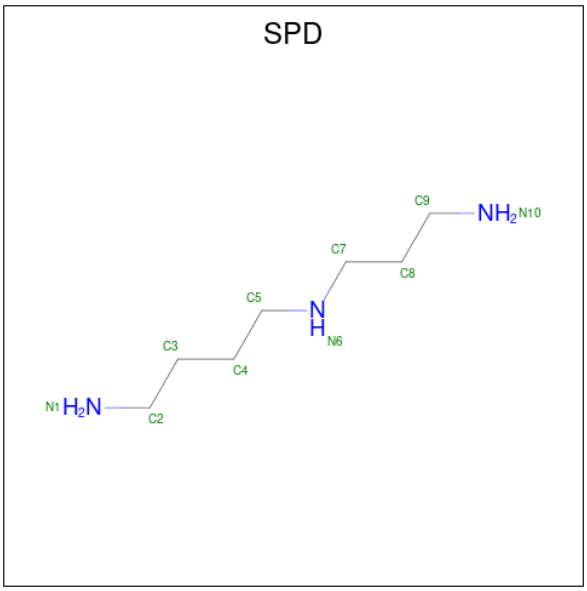
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			4	2	2		
63	DB	1	Total	C	O	0	0
			4	2	2		
63	DB	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4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

- Molecule 64 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



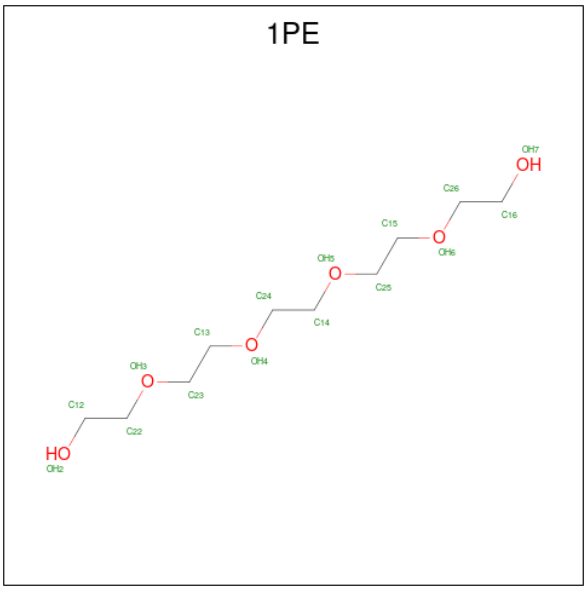
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	D1	1	Total C O 10 6 4	0	0
64	D3	1	Total C O 10 6 4	0	0
64	DD	1	Total C O 10 6 4	0	0
64	DS	1	Total C O 10 6 4	0	0
64	DU	1	Total C O 10 6 4	0	0
64	DA	1	Total C O 10 6 4	0	0
64	DA	1	Total C O 10 6 4	0	0
64	DA	1	Total C O 10 6 4	0	0
64	DA	1	Total C O 10 6 4	0	0

- Molecule 65 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



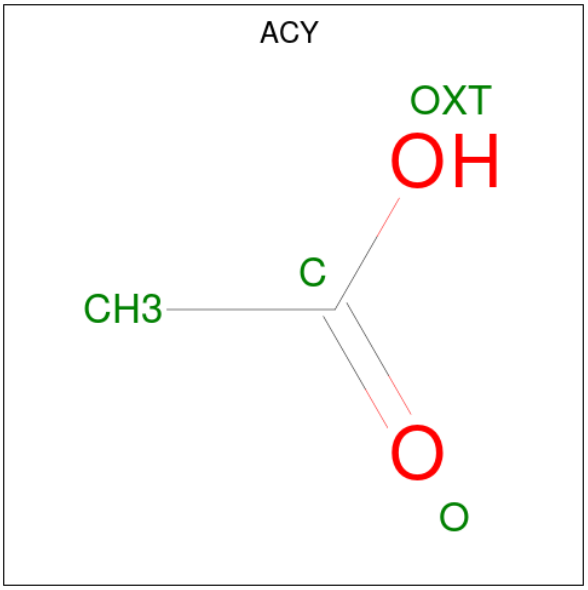
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
65	DA	1	Total C N 10 7 3	0	0
65	DA	1	Total C N 10 7 3	0	0
65	DA	1	Total C N 10 7 3	0	0
65	DA	1	Total C N 10 7 3	0	0

- Molecule 66 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



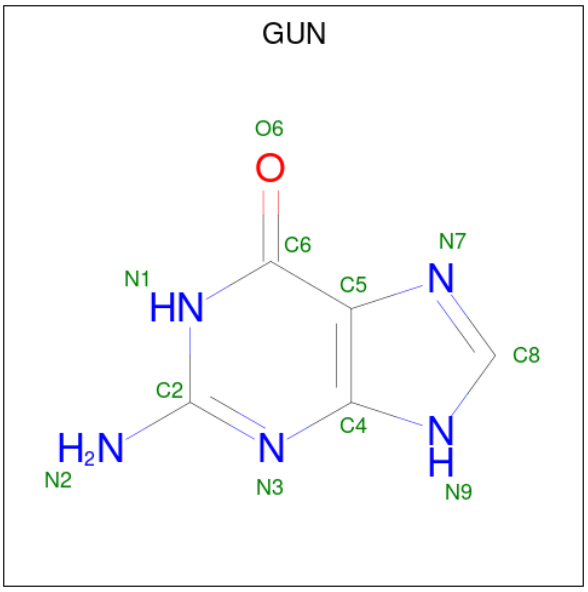
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
66	DA	1	Total C O 16 10 6	0	0
66	DA	1	Total C O 16 10 6	0	0

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



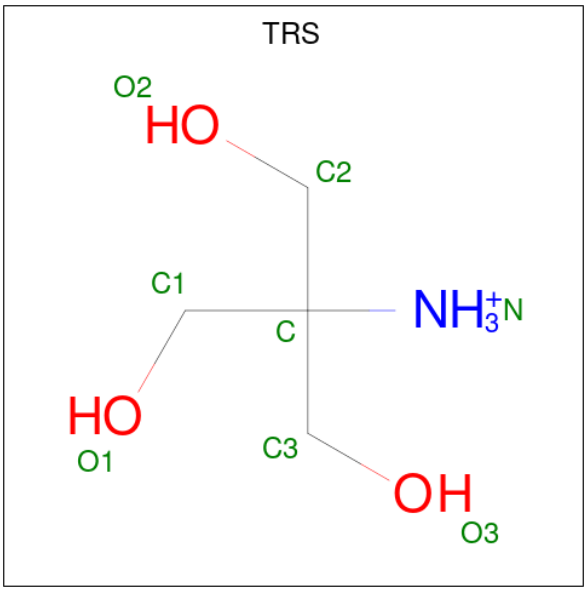
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
67	DA	1	Total C O 4 2 2	0	0
67	DA	1	Total C O 4 2 2	0	0
67	DA	1	Total C O 4 2 2	0	0

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



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

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



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

- Molecule 70 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
70	AA	507	Total O 507 507	0	0
70	AC	4	Total O 4 4	0	0
70	AD	2	Total O 2 2	0	0
70	AE	4	Total O 4 4	0	0
70	AF	1	Total O 1 1	0	0
70	AG	1	Total O 1 1	0	0
70	AH	1	Total O 1 1	0	0
70	AJ	2	Total O 2 2	0	0
70	AK	5	Total O 5 5	0	0
70	AL	8	Total O 8 8	0	0
70	AM	4	Total O 4 4	0	0
70	AN	5	Total O 5 5	0	0
70	AO	2	Total O 2 2	0	0
70	AP	2	Total O 2 2	0	0
70	AR	1	Total O 1 1	0	0
70	AS	1	Total O 1 1	0	0
70	AT	2	Total O 2 2	0	0
70	AU	3	Total O 3 3	0	0
70	C3	3	Total O 3 3	0	0
70	C4	1	Total O 1 1	0	0
70	BA	287	Total O 287 287	0	0
70	BD	13	Total O 13 13	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
70	BE	1	Total O 1 1	0	0
70	BF	1	Total O 1 1	0	0
70	BK	1	Total O 1 1	0	0
70	BL	3	Total O 3 3	0	0
70	BN	2	Total O 2 2	0	0
70	BO	1	Total O 1 1	0	0
70	BP	3	Total O 3 3	0	0
70	BR	1	Total O 1 1	0	0
70	BT	4	Total O 4 4	0	0
70	BU	2	Total O 2 2	0	0
70	D1	42	Total O 42 42	0	0
70	D2	7	Total O 7 7	0	0
70	D3	25	Total O 25 25	0	0
70	D4	32	Total O 32 32	0	0
70	D5	13	Total O 13 13	0	0
70	D0	25	Total O 25 25	0	0
70	CB	13	Total O 13 13	0	0
70	CC	10	Total O 10 10	0	0
70	CD	5	Total O 5 5	0	0
70	CA	694	Total O 694 694	0	0
70	DC	102	Total O 102 102	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
70	DD	105	Total O 105 105	0	0
70	CE	6	Total O 6 6	0	0
70	CL	1	Total O 1 1	0	0
70	CM	3	Total O 3 3	0	0
70	CO	1	Total O 1 1	0	0
70	CU	3	Total O 3 3	0	0
70	CV	1	Total O 1 1	0	0
70	CW	1	Total O 1 1	0	0
70	CY	1	Total O 1 1	0	0
70	DE	63	Total O 63 63	0	0
70	DF	14	Total O 14 14	0	0
70	DG	6	Total O 6 6	0	0
70	DH	2	Total O 2 2	0	0
70	DK	58	Total O 58 58	0	0
70	DL	51	Total O 51 51	0	0
70	DM	60	Total O 60 60	0	0
70	DN	71	Total O 71 71	0	0
70	DO	44	Total O 44 44	0	0
70	DP	35	Total O 35 35	0	0
70	DQ	27	Total O 27 27	0	0
70	DR	64	Total O 64 64	0	0

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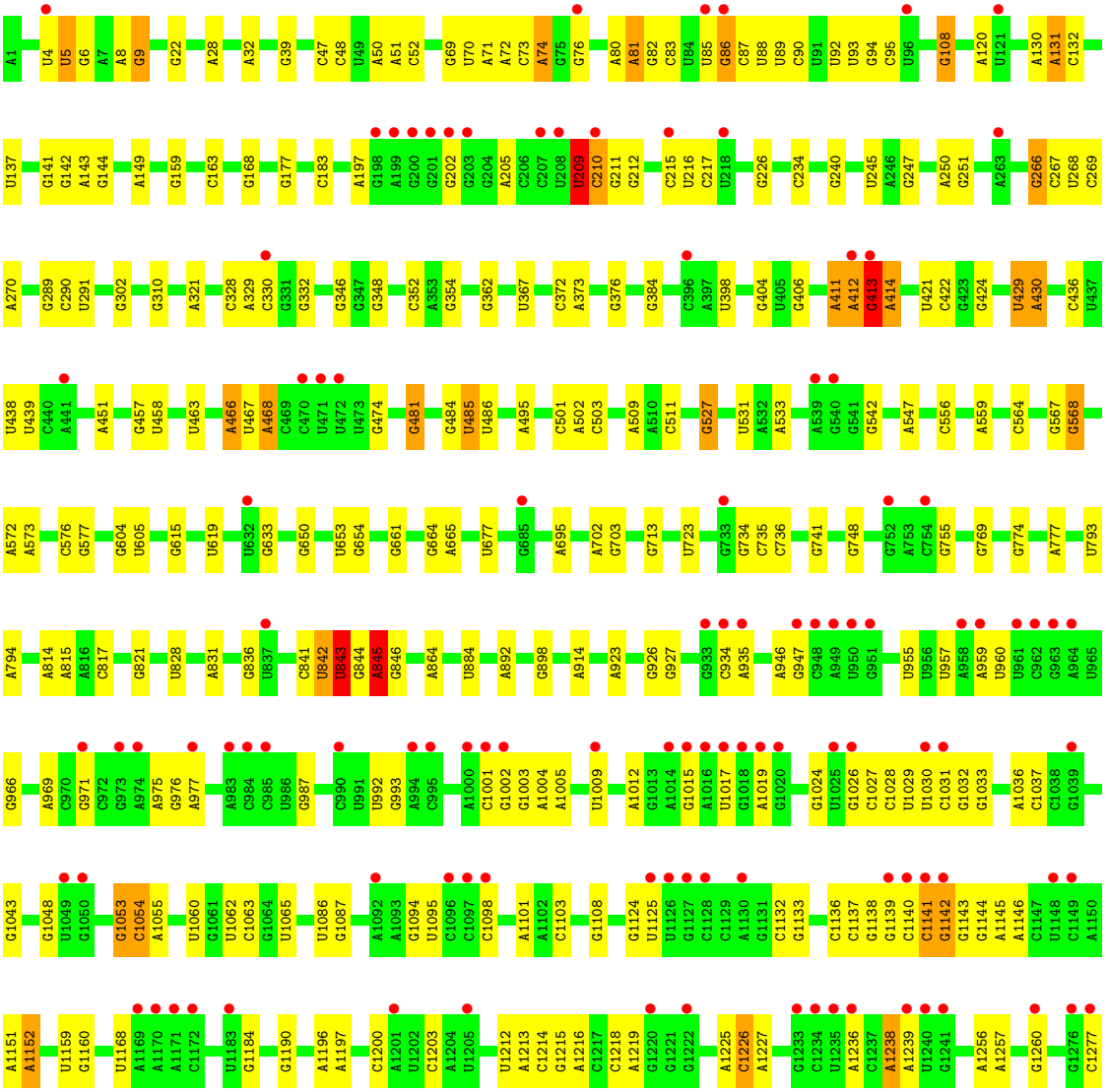
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
70	DS	51	Total O 51 51	0	0
70	DT	70	Total O 70 70	0	0
70	DU	17	Total O 17 17	0	0
70	DV	19	Total O 19 19	0	0
70	DW	31	Total O 31 31	0	0
70	DX	30	Total O 30 30	0	0
70	DY	9	Total O 9 9	0	0
70	DZ	7	Total O 7 7	0	0
70	DB	213	Total O 213 213	0	0
70	DA	4836	Total O 4836 4836	0	0

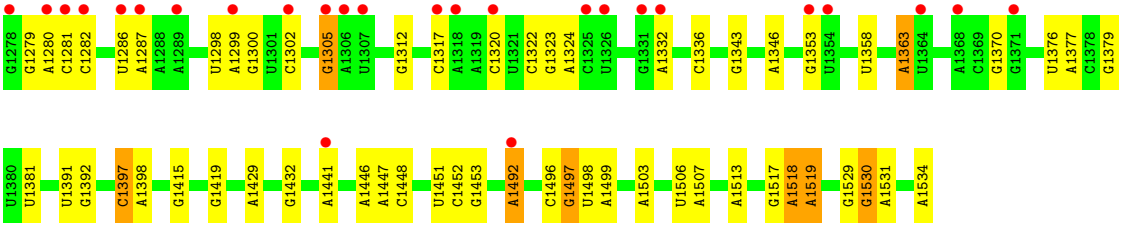
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

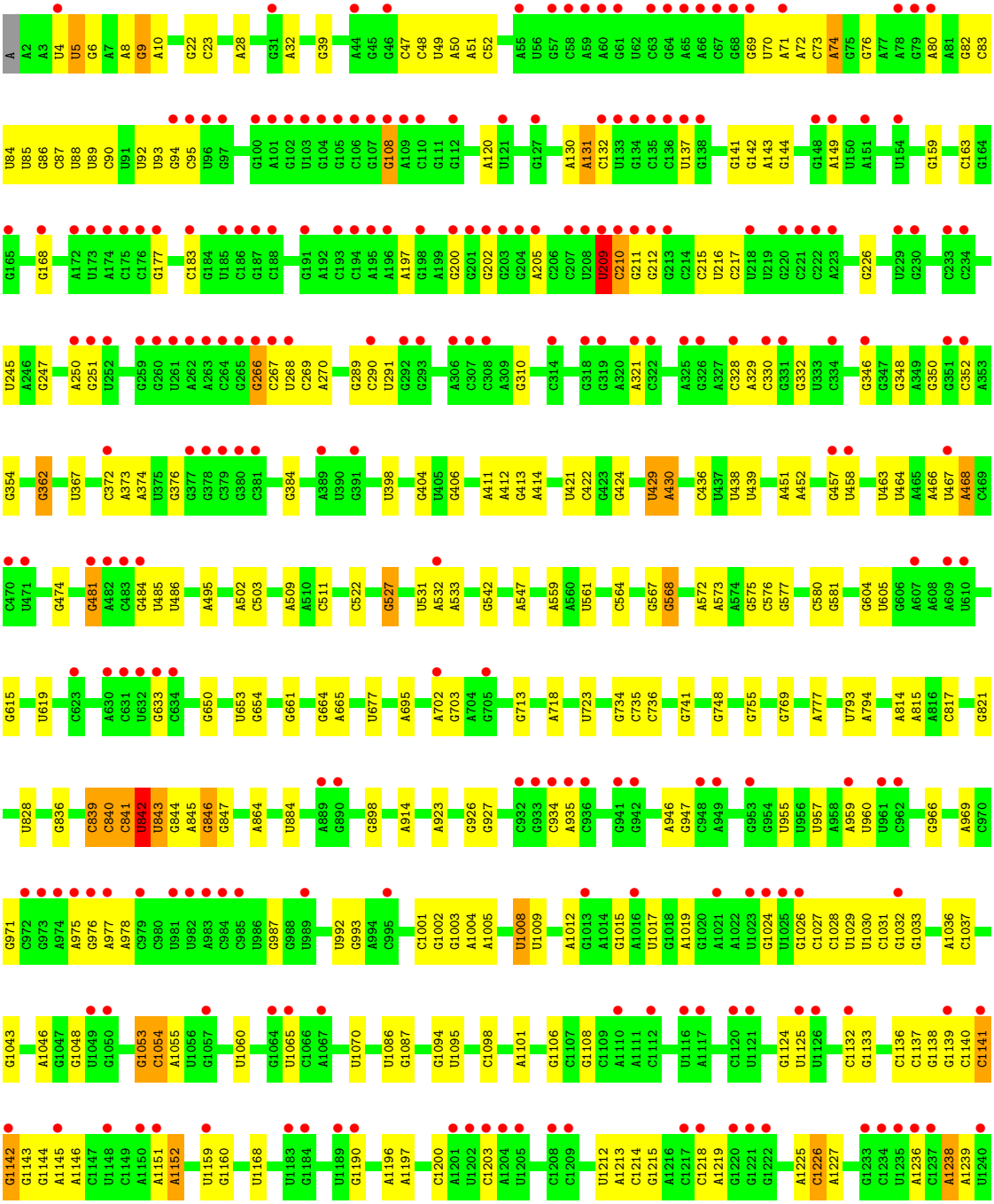
Chain AA:

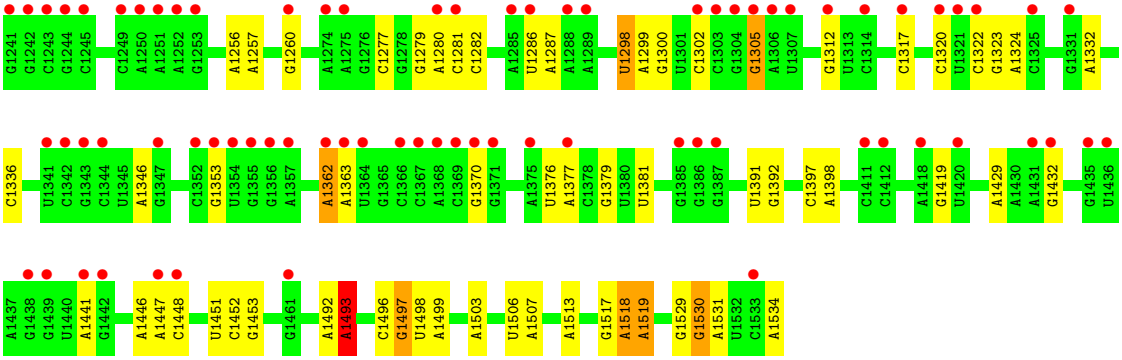




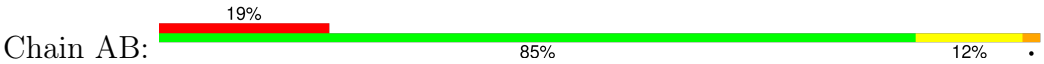
• Molecule 1: 16S rRNA

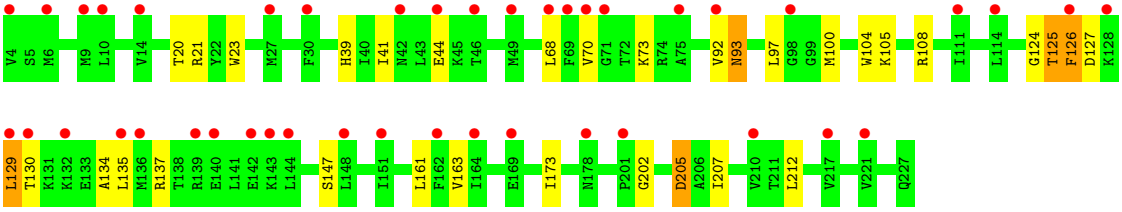
Chain BA:



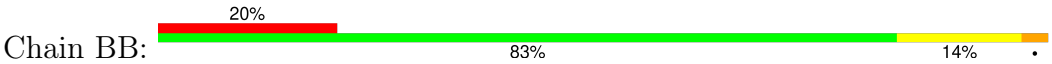


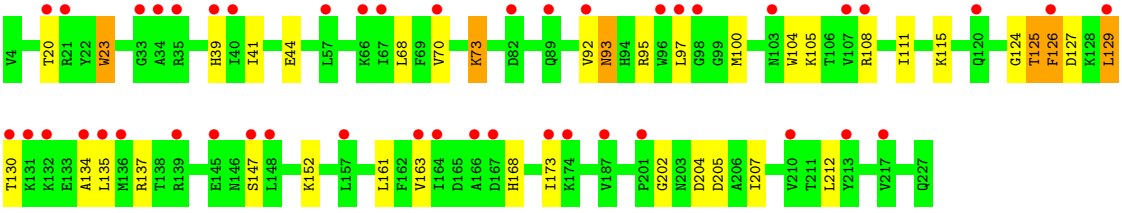
• Molecule 2: 30S ribosomal protein S2



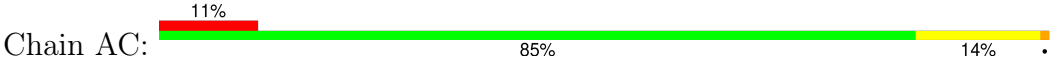


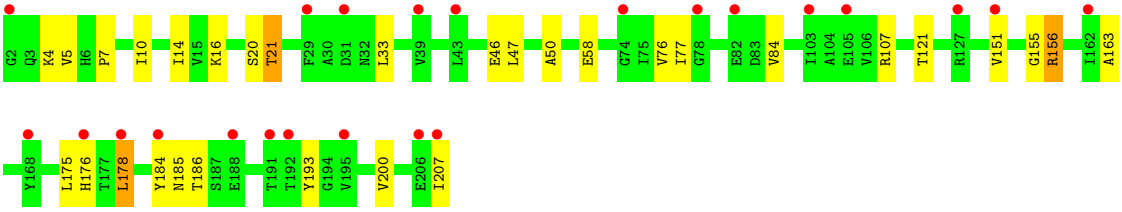
• Molecule 2: 30S ribosomal protein S2



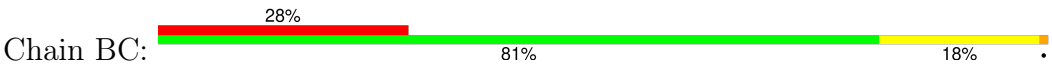


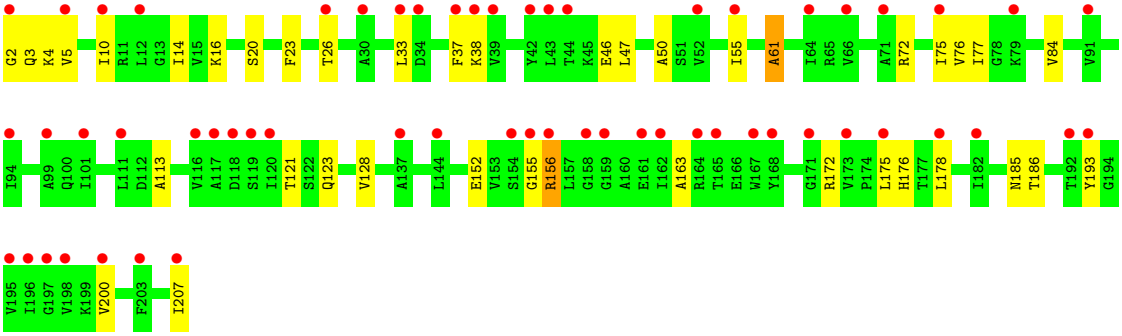
• Molecule 3: 30S ribosomal protein S3



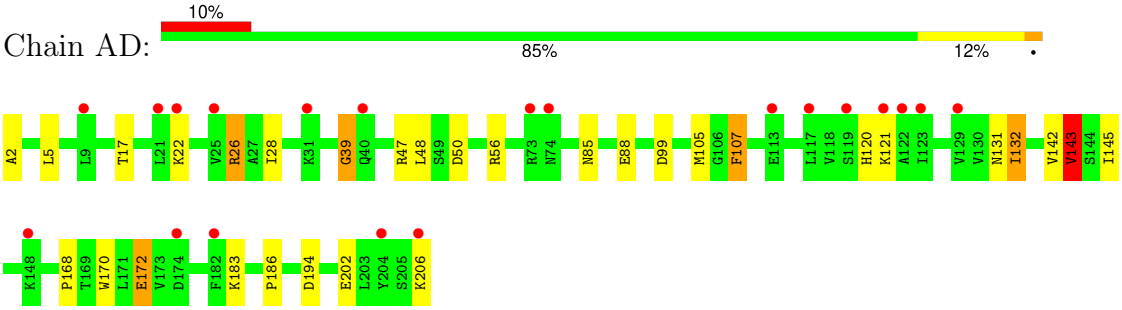


• Molecule 3: 30S ribosomal protein S3

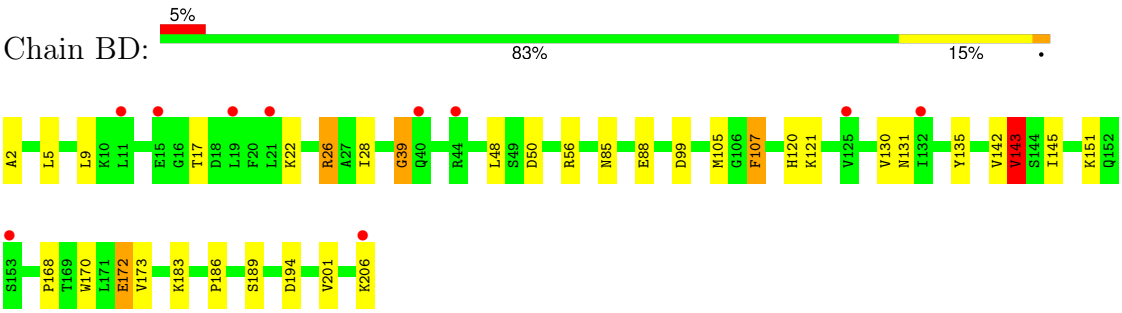




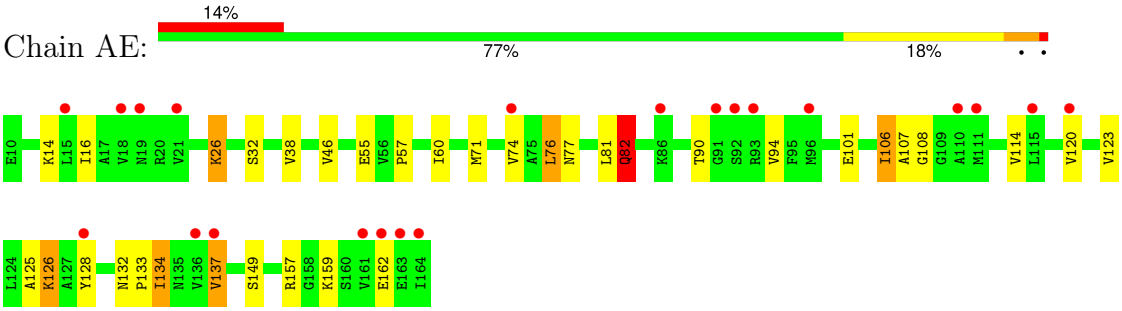
• Molecule 4: 30S ribosomal protein S4



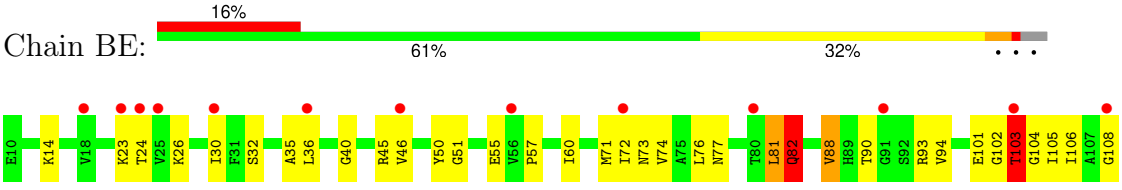
• Molecule 4: 30S ribosomal protein S4

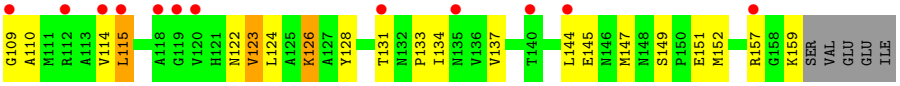


• Molecule 5: 30S ribosomal protein S5



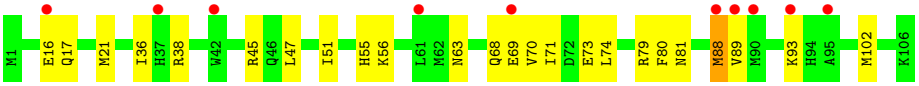
• Molecule 5: 30S ribosomal protein S5





• Molecule 6: 30S ribosomal protein S6

Chain AF:



• Molecule 6: 30S ribosomal protein S6

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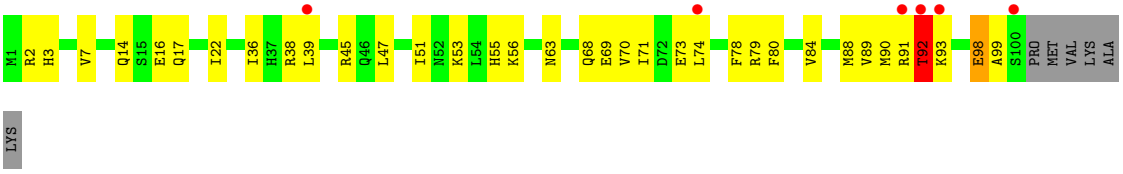
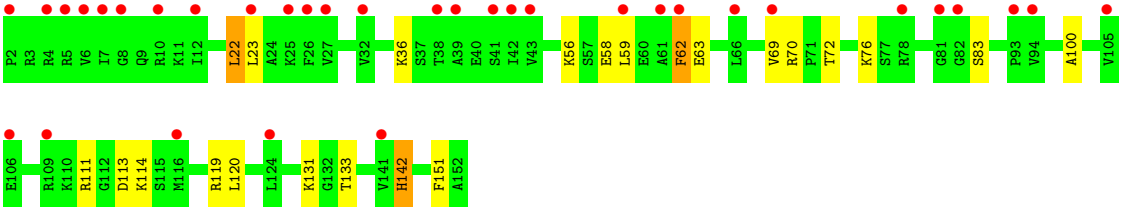


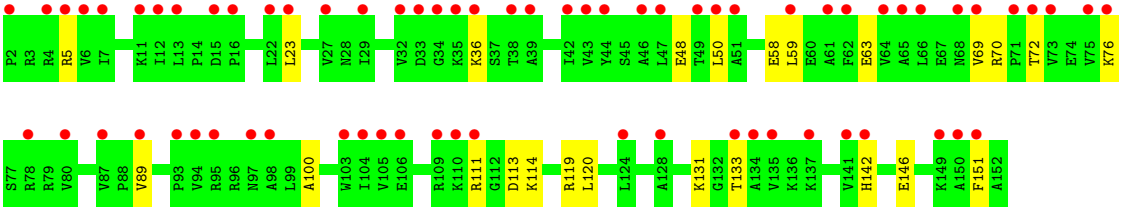
• Molecule 7: 30S ribosomal protein S7

Chain AG:



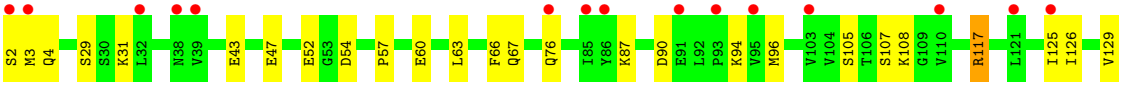
• Molecule 7: 30S ribosomal protein S7

Chain BG:



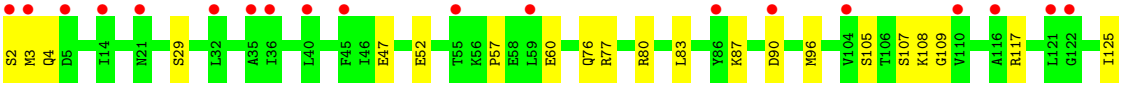
• Molecule 8: 30S ribosomal protein S8

Chain AH:



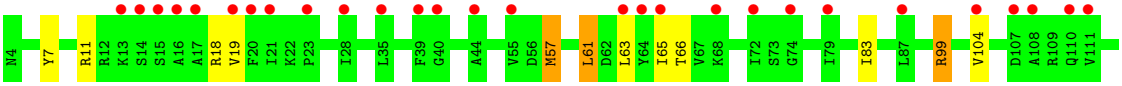
• Molecule 8: 30S ribosomal protein S8

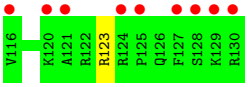
Chain BH:



• Molecule 9: 30S ribosomal protein S9

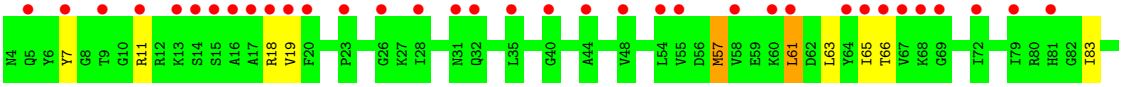
Chain AI:

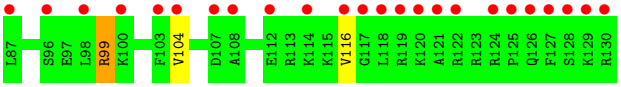




• Molecule 9: 30S ribosomal protein S9

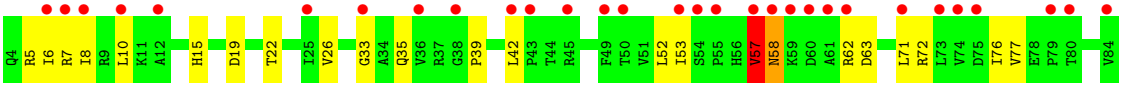
Chain BI:

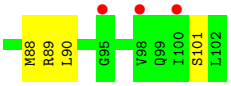




• Molecule 10: 30S ribosomal protein S10

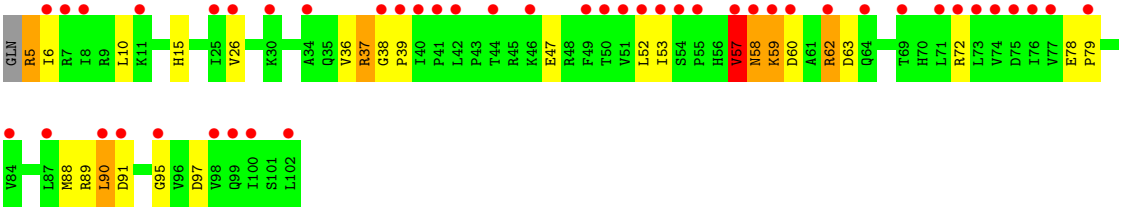
Chain AJ:



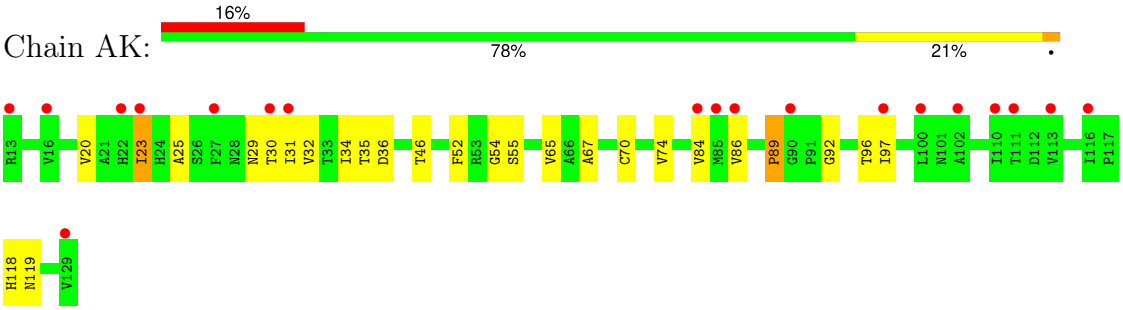


• Molecule 10: 30S ribosomal protein S10

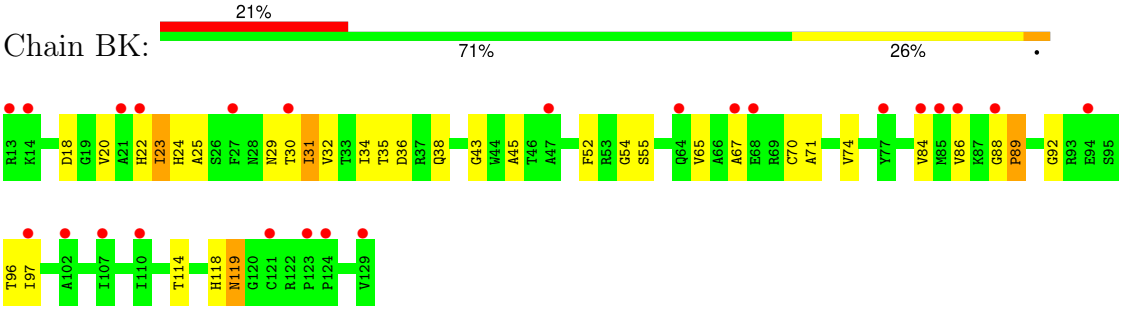
Chain BJ:



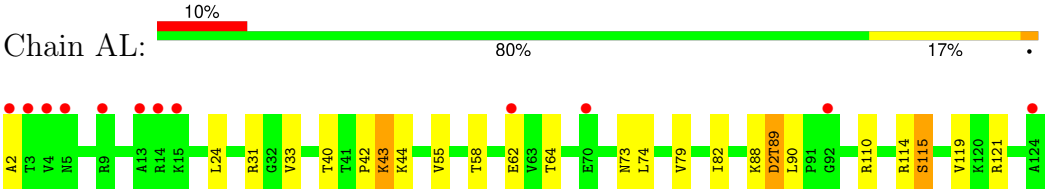
• Molecule 11: 30S ribosomal protein S11



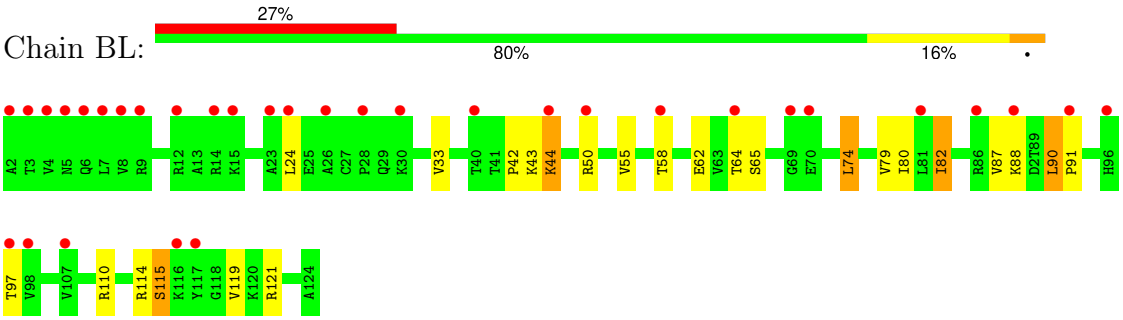
• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12

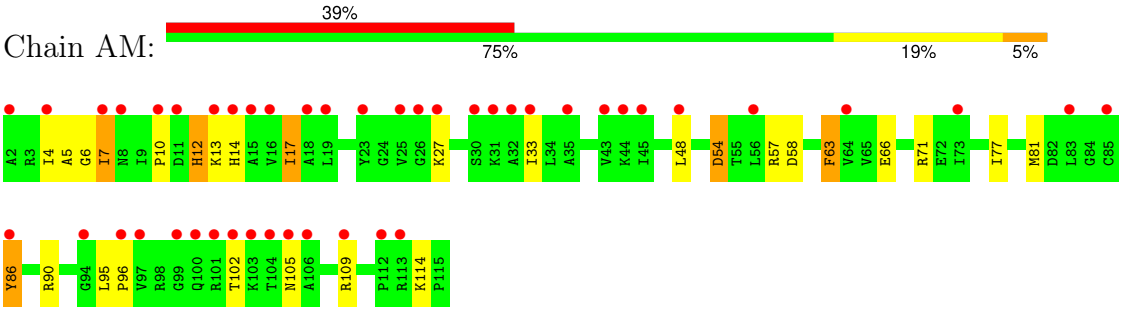


• Molecule 12: 30S ribosomal protein S12



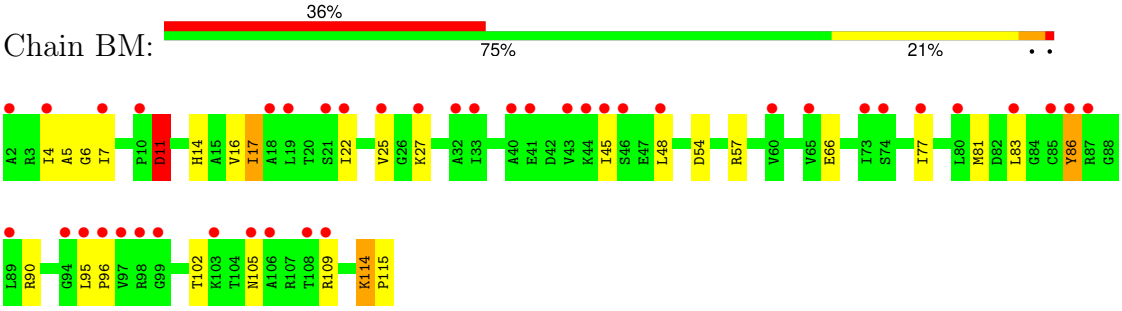
• Molecule 13: 30S ribosomal protein S13

Chain AM:



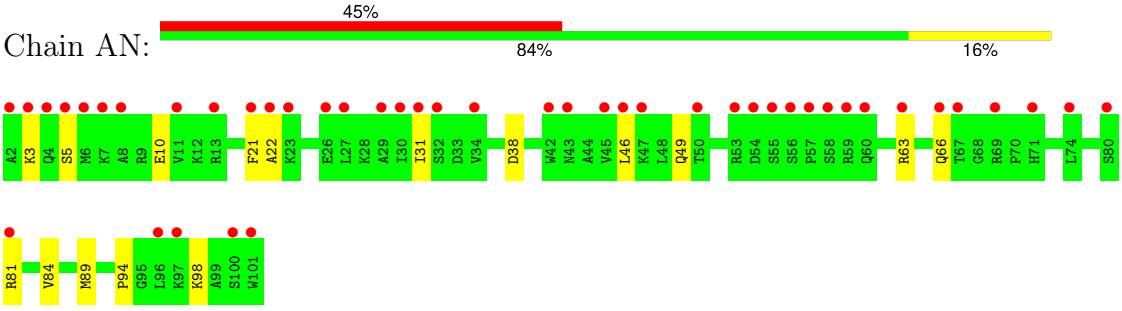
• Molecule 13: 30S ribosomal protein S13

Chain BM:



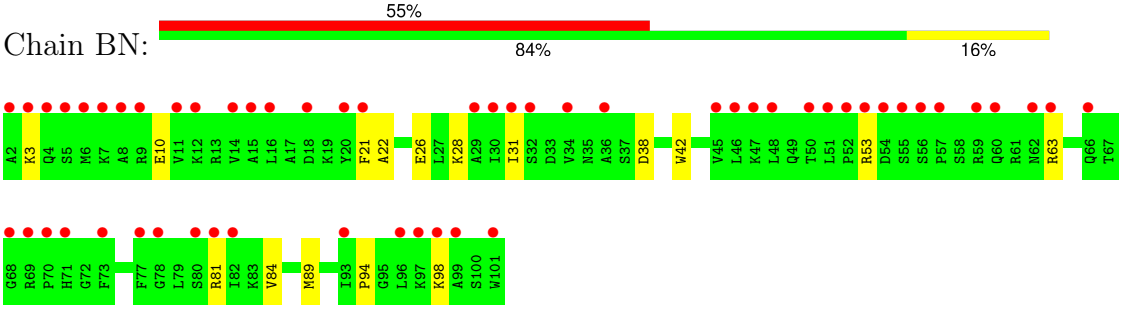
• Molecule 14: 30S ribosomal protein S14

Chain AN:



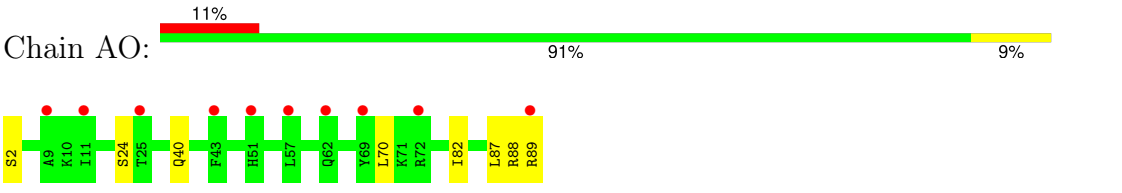
• Molecule 14: 30S ribosomal protein S14

Chain BN:



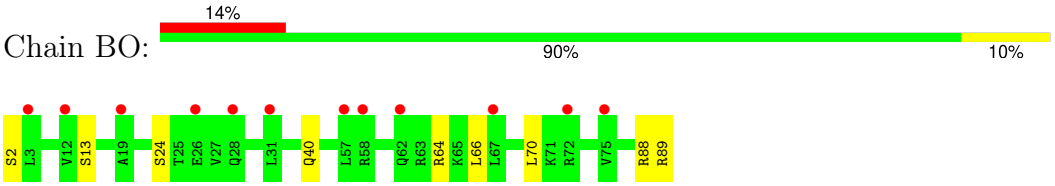
• Molecule 15: 30S ribosomal protein S15

Chain AO:



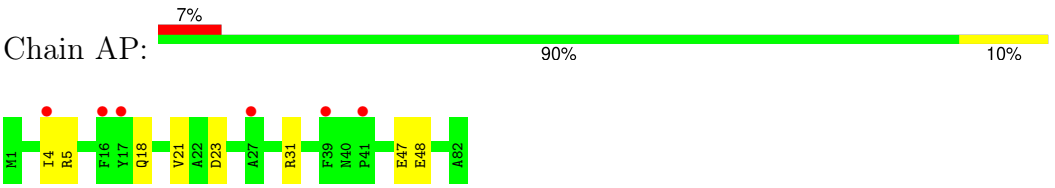
• Molecule 15: 30S ribosomal protein S15

Chain BO:



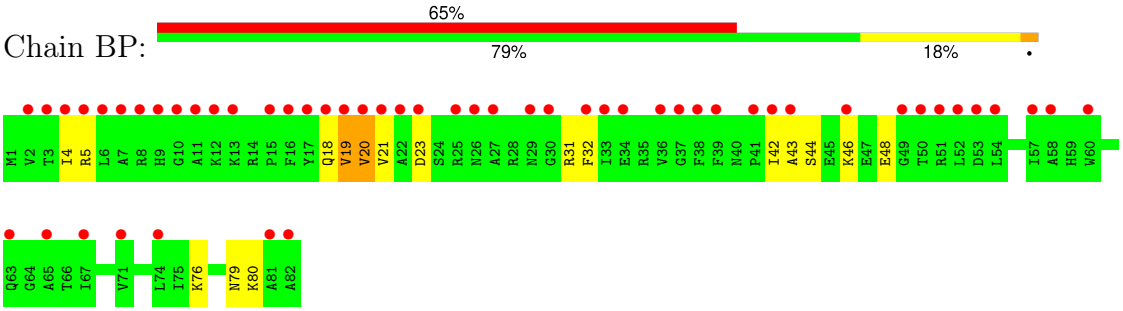
• Molecule 16: 30S ribosomal protein S16

Chain AP:



• Molecule 16: 30S ribosomal protein S16

Chain BP:



• Molecule 17: 30S ribosomal protein S17

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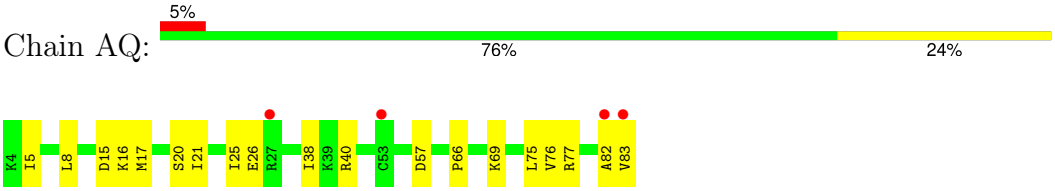
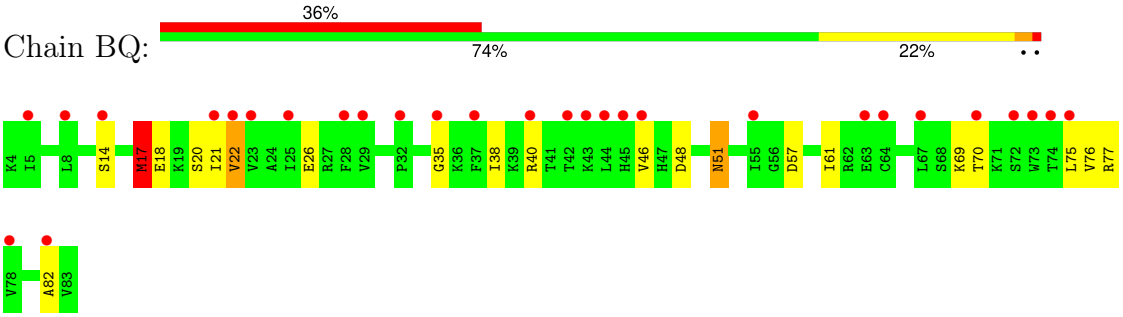


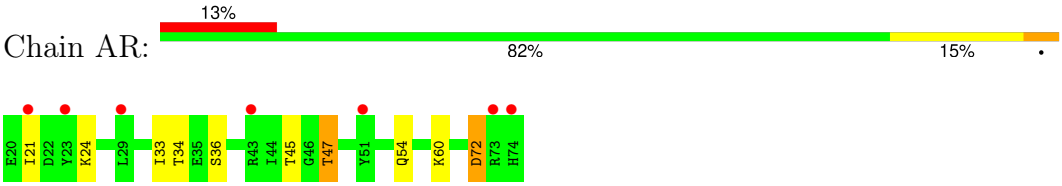
• Molecule 17: 30S ribosomal protein S17

Chain BQ:



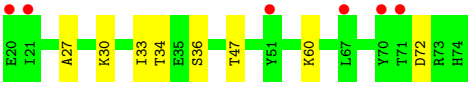
• Molecule 18: 30S ribosomal protein S18

Chain AR:



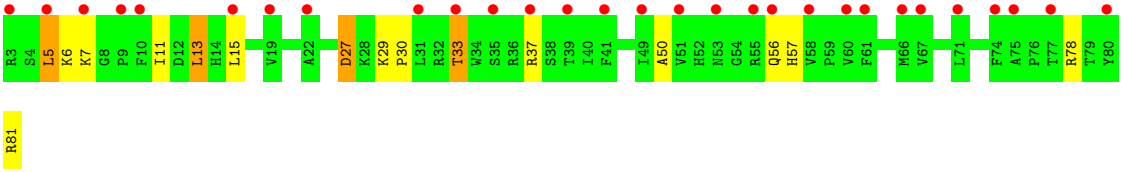
• Molecule 18: 30S ribosomal protein S18

Chain BR:



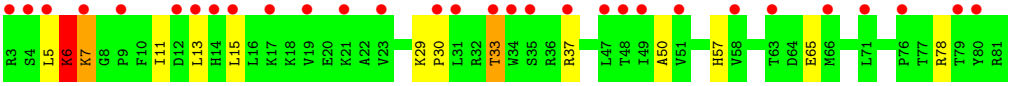
• Molecule 19: 30S ribosomal protein S19

Chain AS:



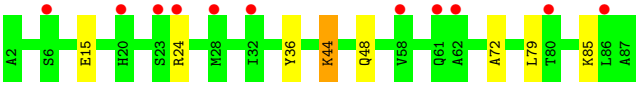
• Molecule 19: 30S ribosomal protein S19

Chain BS:



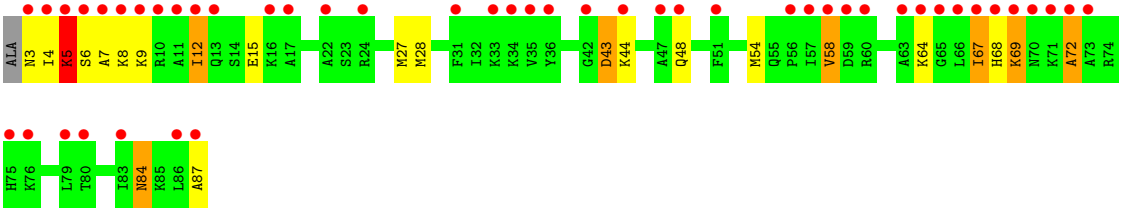
• Molecule 20: 30S ribosomal protein S20

Chain AT:



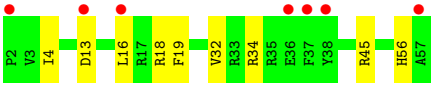
• Molecule 20: 30S ribosomal protein S20

Chain BT:



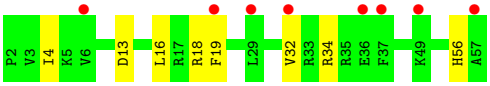
• Molecule 21: 30S ribosomal protein S21

Chain AU:



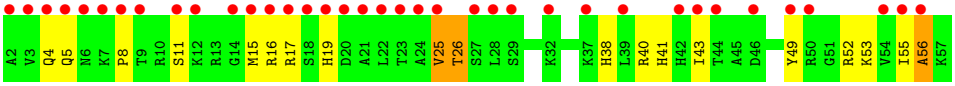
• Molecule 21: 30S ribosomal protein S21

Chain BU:



• Molecule 22: 50S ribosomal protein L32

Chain C1:



• Molecule 22: 50S ribosomal protein L32

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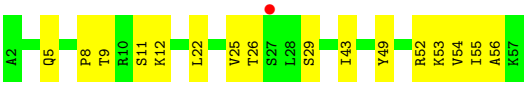
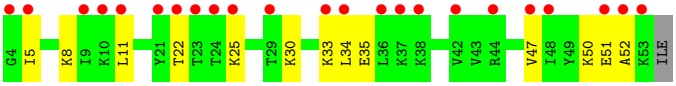


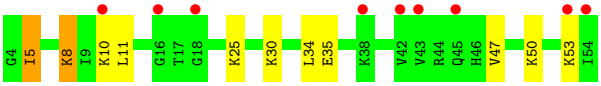
• Molecule 23: 50S ribosomal protein L33

Chain C2:



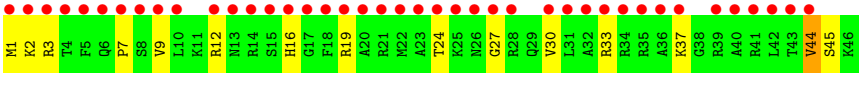
• Molecule 23: 50S ribosomal protein L33

Chain D2:



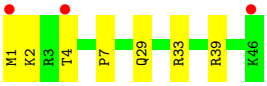
• Molecule 24: 50S ribosomal protein L34

Chain C3:



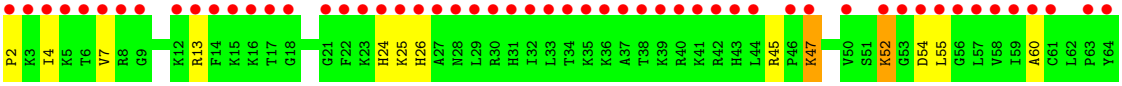
• Molecule 24: 50S ribosomal protein L34

Chain D3:



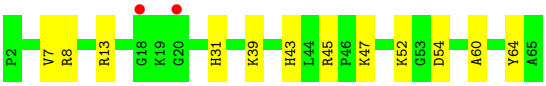
• Molecule 25: 50S ribosomal protein L35

Chain C4:



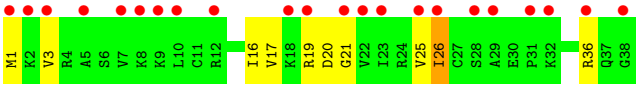
• Molecule 25: 50S ribosomal protein L35

Chain D4:



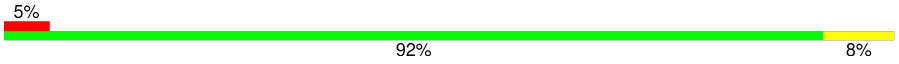
• Molecule 26: 50S ribosomal protein L36

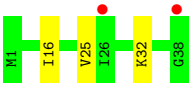
Chain C5:



• Molecule 26: 50S ribosomal protein L36

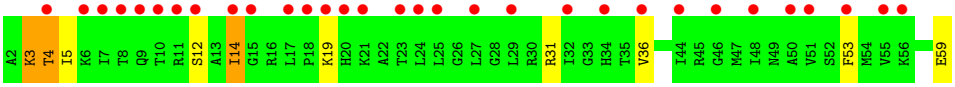
Chain D5:





• Molecule 27: 50S ribosomal protein L30

Chain C0:

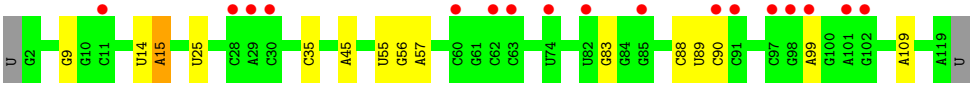


• Molecule 27: 50S ribosomal protein L30

Chain D0:

• Molecule 28: 5S rRNA

Chain CB:

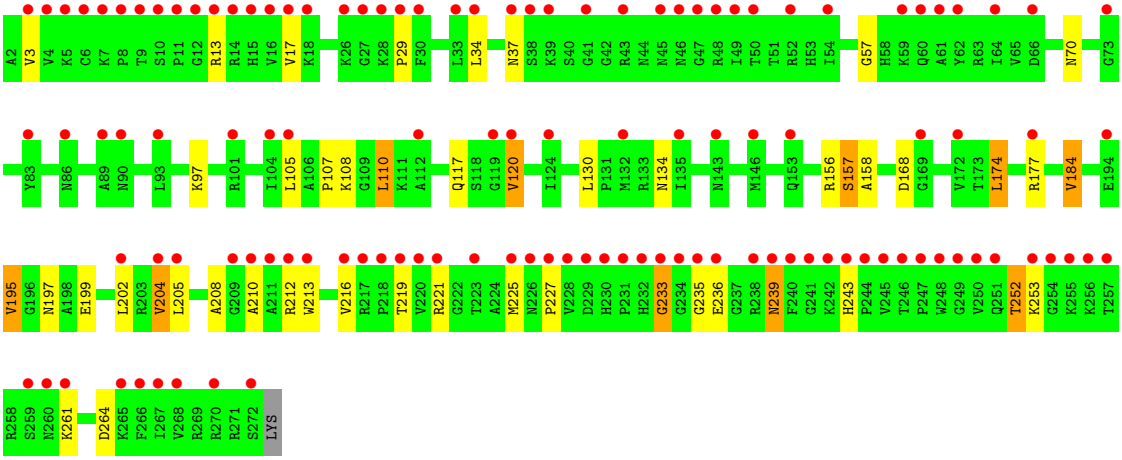


• Molecule 28: 5S rRNA

Chain DB:

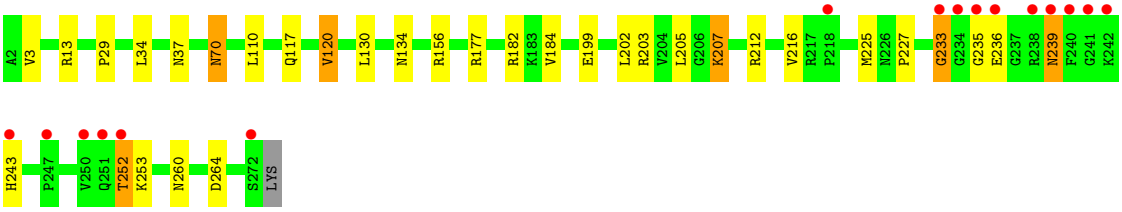
• Molecule 29: 50S ribosomal protein L2

Chain CC:



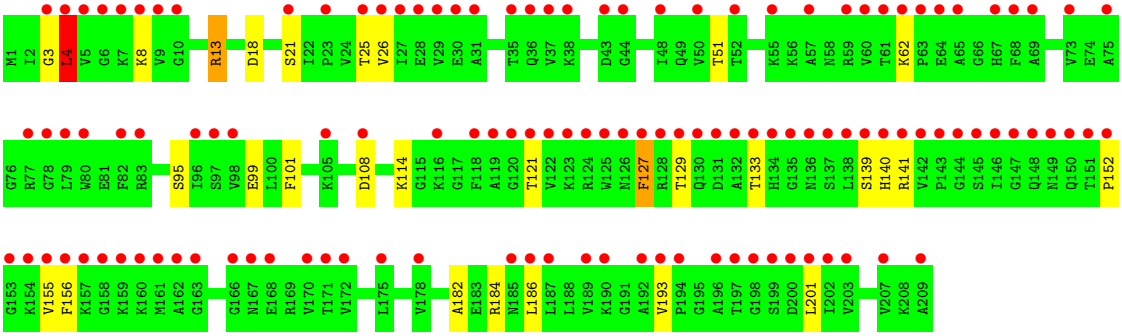
• Molecule 29: 50S ribosomal protein L2

Chain DC:



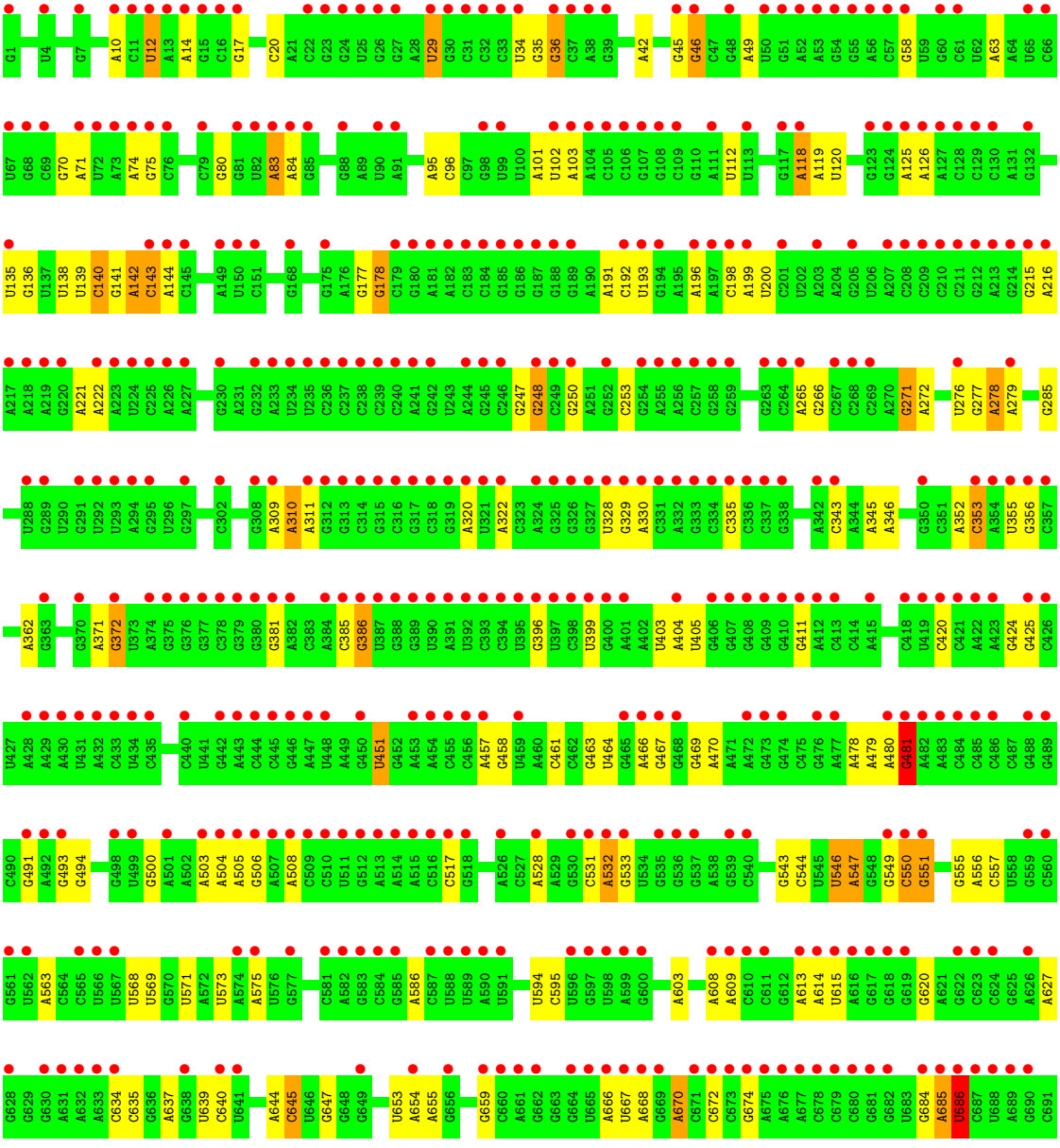
• Molecule 30: 50S ribosomal protein L3

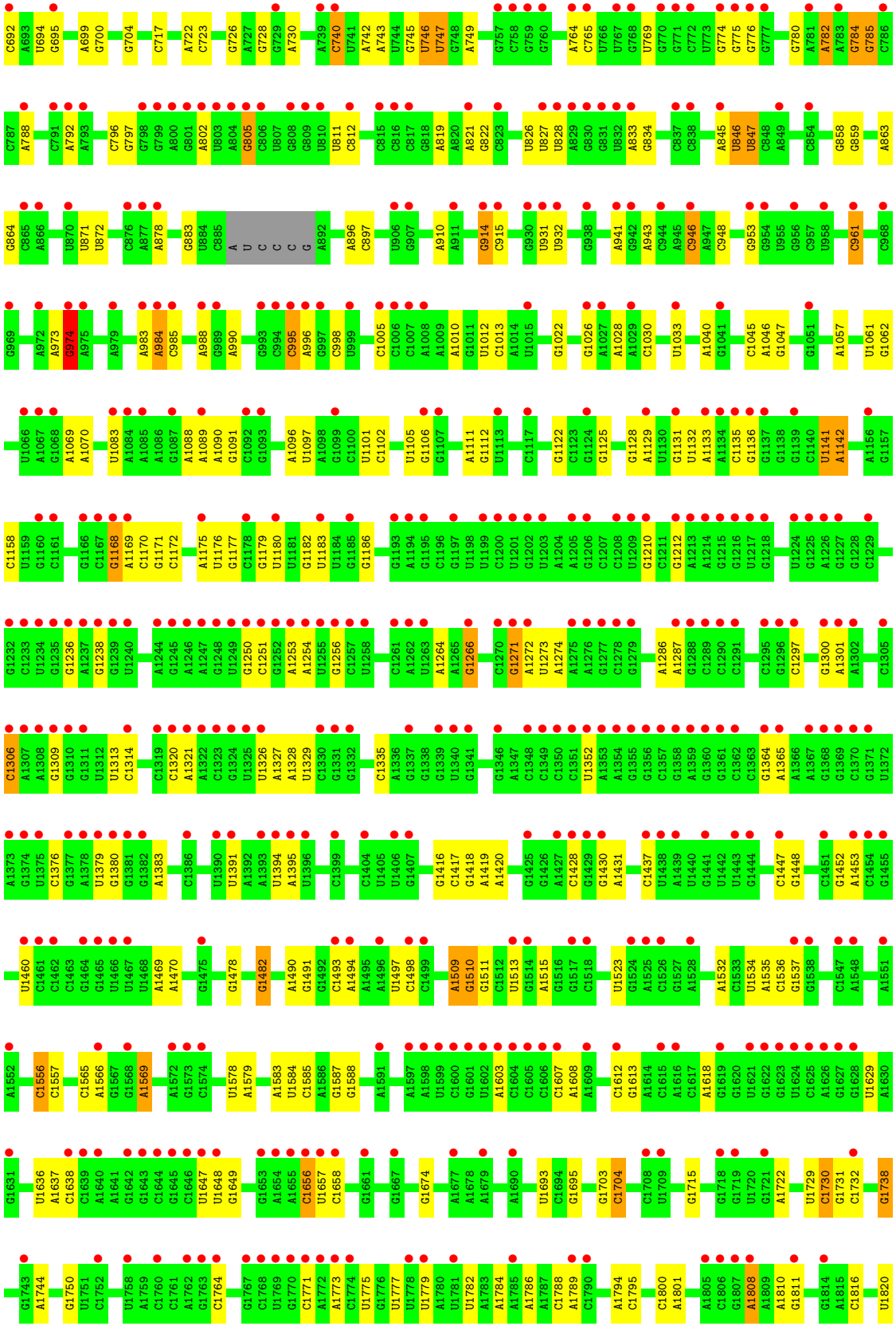
Chain CD:



• Molecule 31: 23S rRNA

Chain CA:

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C787 A788 C791 A792 A793 C796 G797 G798 G799 A800 G801 A802 U803 A804 G805 C806 U807 G808 G809 U810 U811 C812 C815 C816 C817 G818 A819 A820 A821 G822 C823 U826 U827 U828 A829 G830 G831 U832 A833 G834 C837 C838 A845 U846 U847 C848 A849 C854 G858 G859 A863
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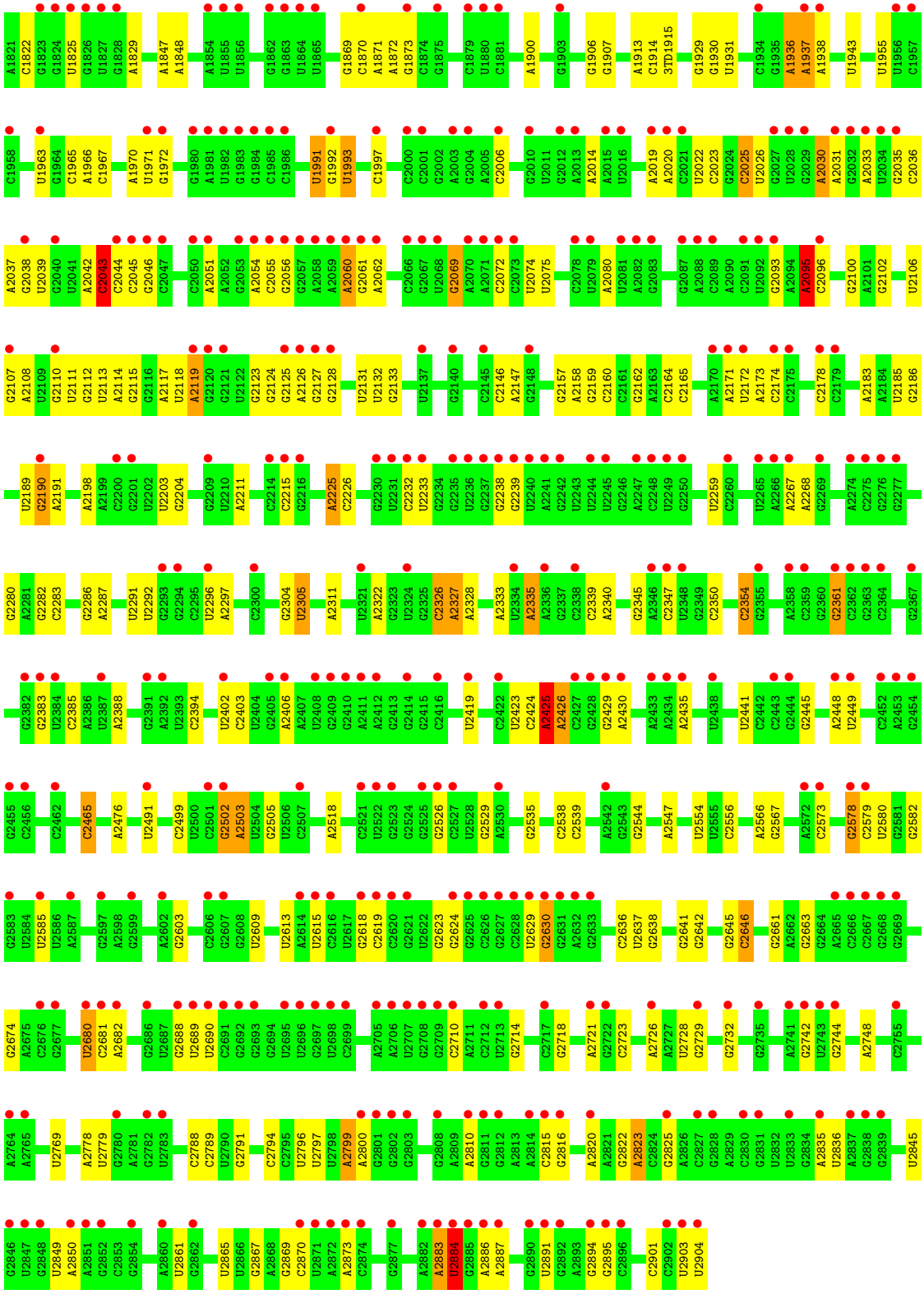
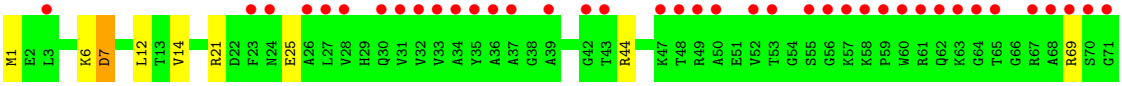


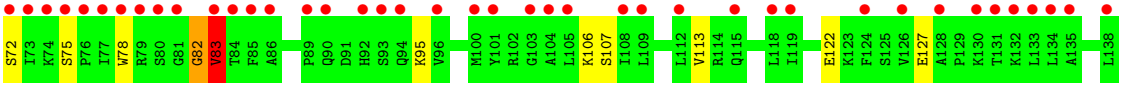
• Molecule 32: 50S ribosomal protein L3

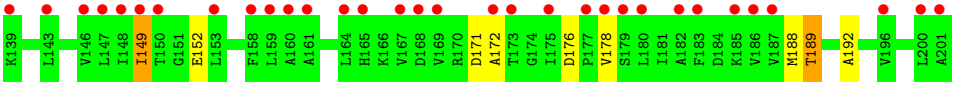
Chain DD:

• Molecule 33: 50S ribosomal protein L4

Chain CE:

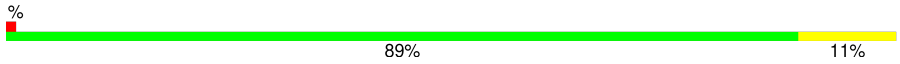


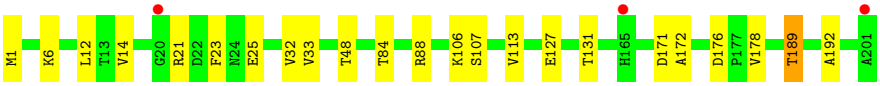




• Molecule 33: 50S ribosomal protein L4

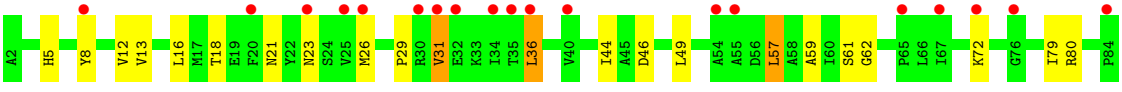
Chain DE:

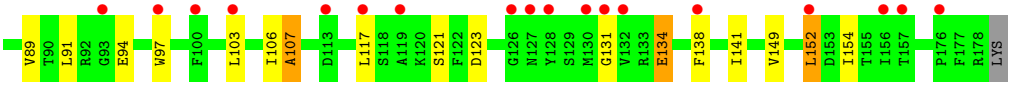




• Molecule 34: 50S ribosomal protein L5

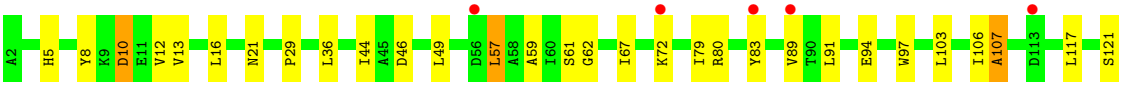
Chain CF:

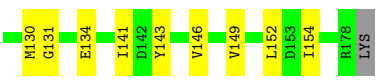




• Molecule 34: 50S ribosomal protein L5

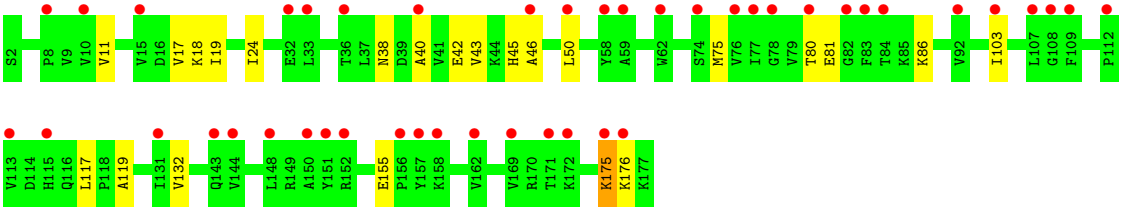
Chain DF:



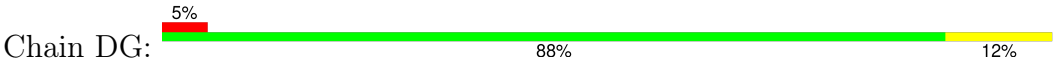


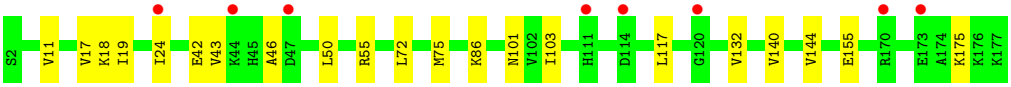
• Molecule 35: 50S ribosomal protein L6

Chain CG:

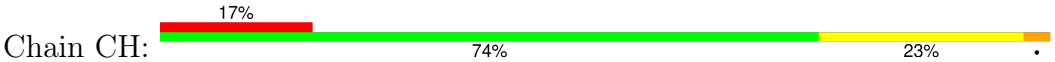


• Molecule 35: 50S ribosomal protein L6

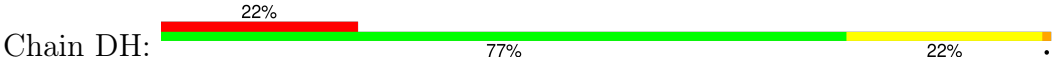


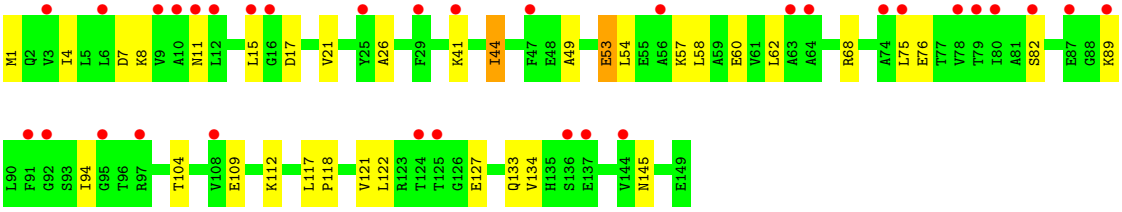


• Molecule 36: 50S ribosomal protein L9

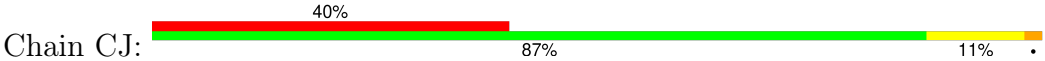


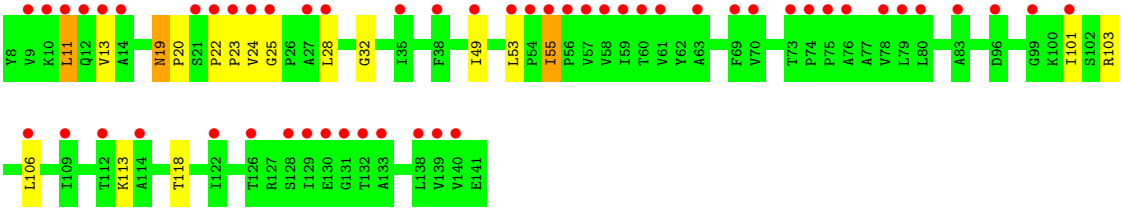
• Molecule 36: 50S ribosomal protein L9



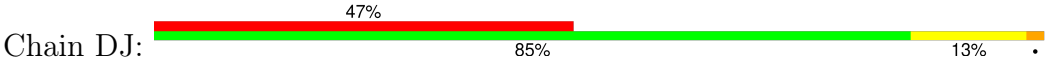


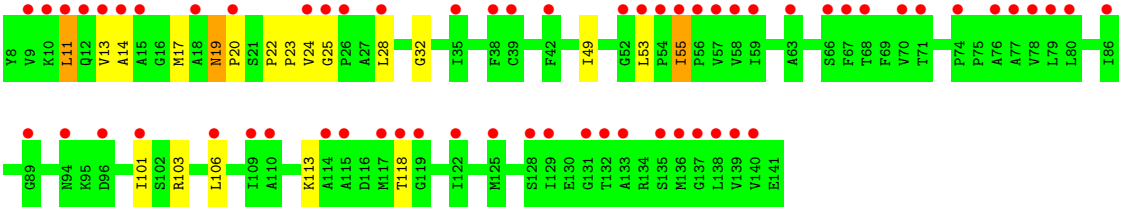
• Molecule 37: 50S ribosomal protein L11



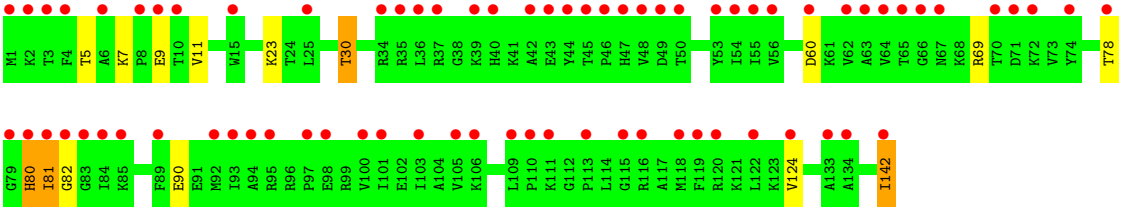


• Molecule 37: 50S ribosomal protein L11

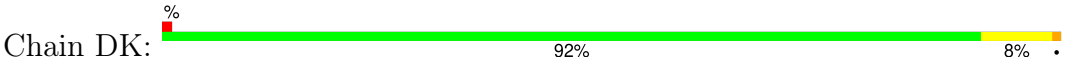




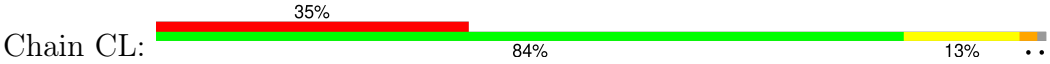
• Molecule 38: 50S ribosomal protein L13

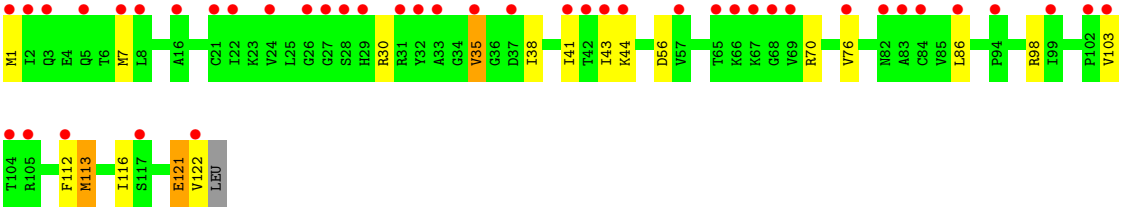


• Molecule 38: 50S ribosomal protein L13

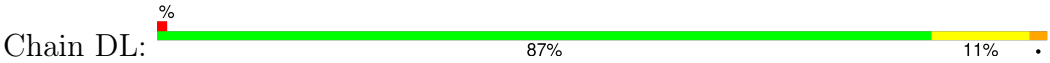


• Molecule 39: 50S ribosomal protein L14

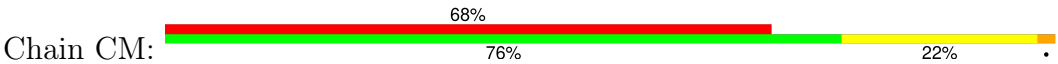


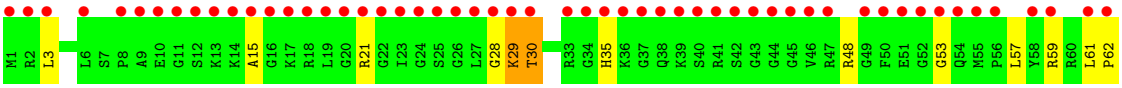


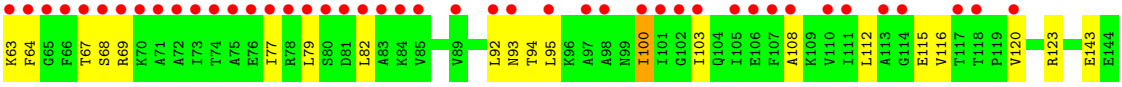
• Molecule 39: 50S ribosomal protein L14



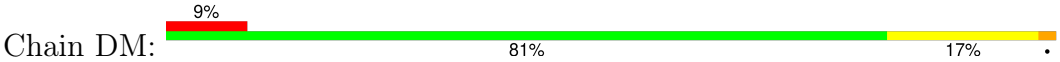
• Molecule 40: 50S ribosomal protein L15

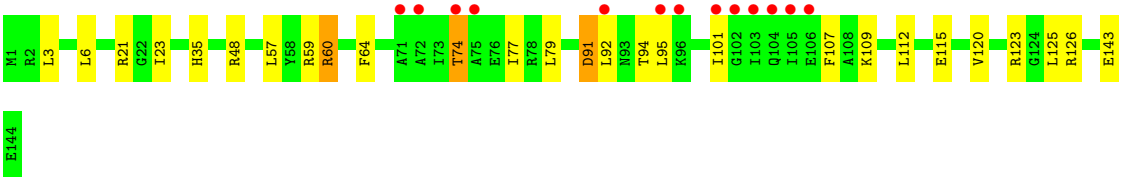




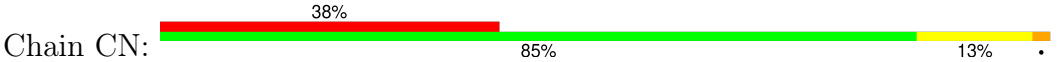


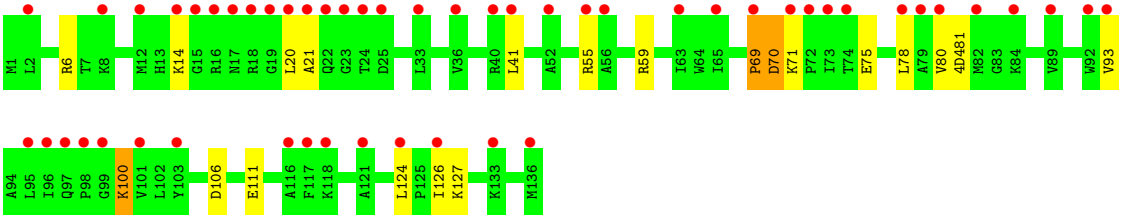
• Molecule 40: 50S ribosomal protein L15



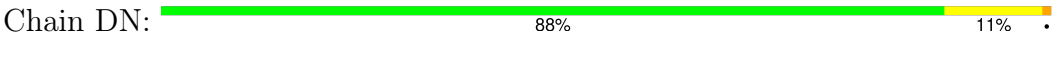


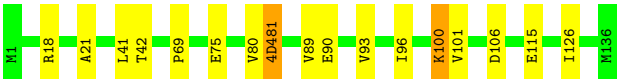
• Molecule 41: 50S ribosomal protein L16



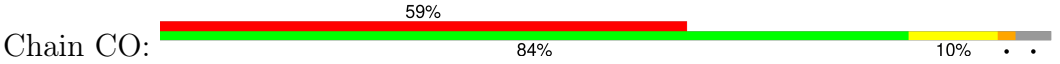


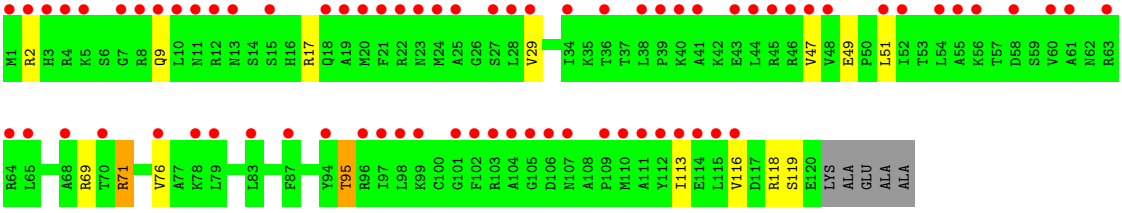
• Molecule 41: 50S ribosomal protein L16



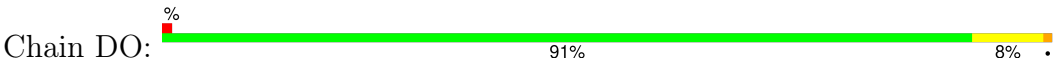


• Molecule 42: 50S ribosomal protein L17



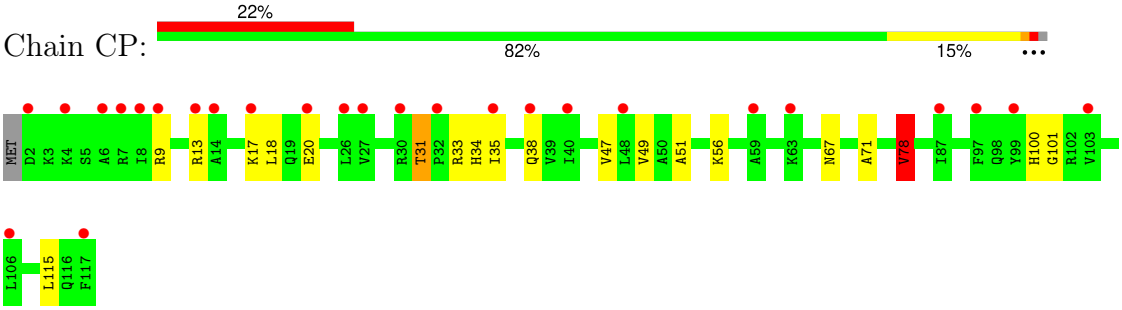


• Molecule 42: 50S ribosomal protein L17



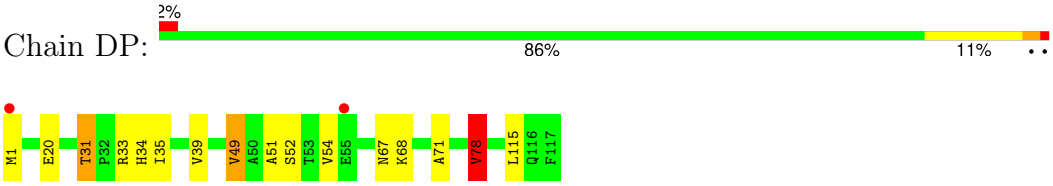
• Molecule 43: 50S ribosomal protein L18

Chain CP:



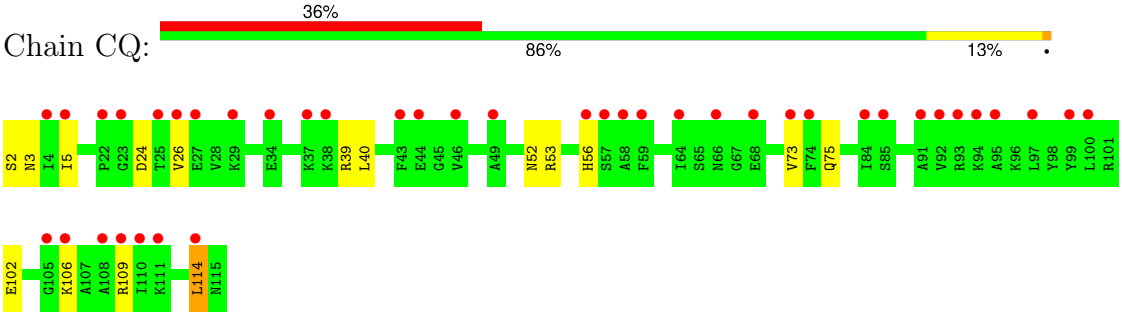
• Molecule 43: 50S ribosomal protein L18

Chain DP:



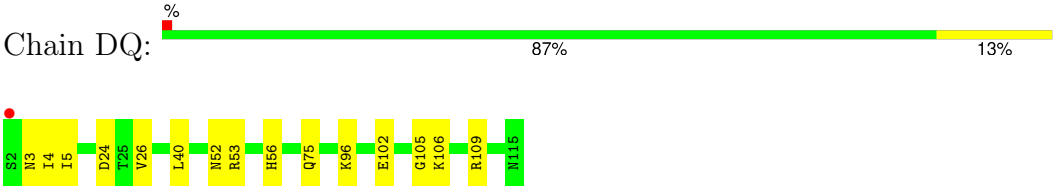
• Molecule 44: 50S ribosomal protein L19

Chain CQ:



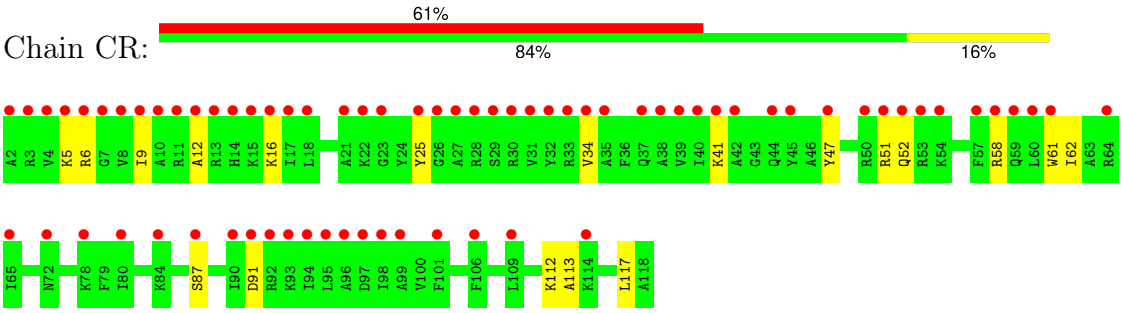
• Molecule 44: 50S ribosomal protein L19

Chain DQ:



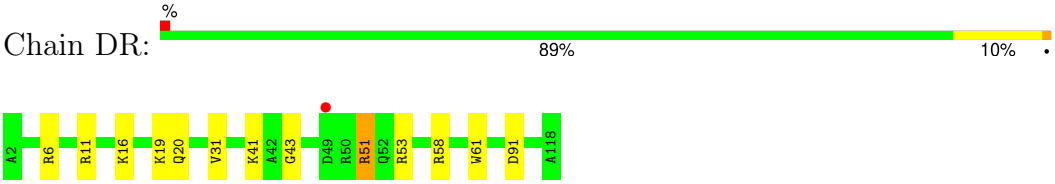
• Molecule 45: 50S ribosomal protein L20

Chain CR:



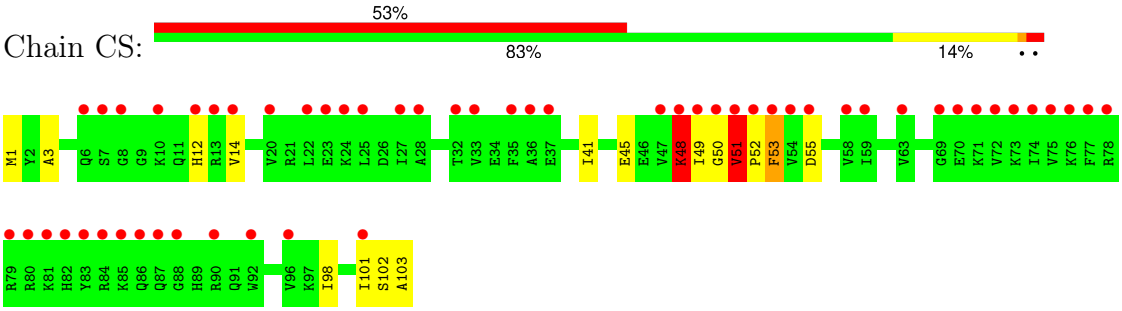
• Molecule 45: 50S ribosomal protein L20

Chain DR:



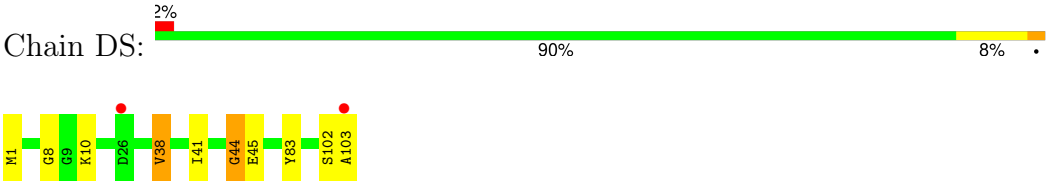
• Molecule 46: 50S ribosomal protein L21

Chain CS:



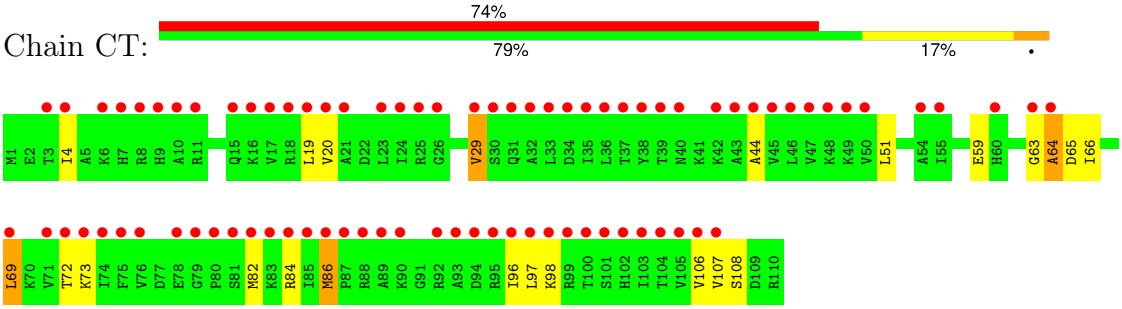
• Molecule 46: 50S ribosomal protein L21

Chain DS:



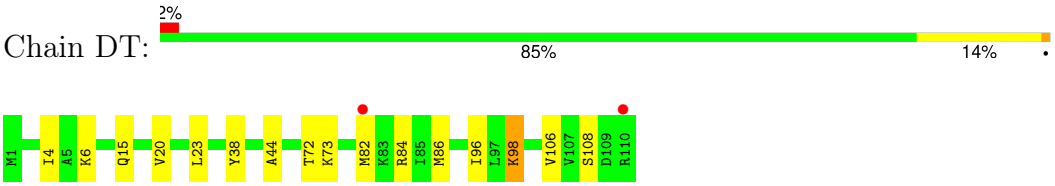
• Molecule 47: 50S ribosomal protein L22

Chain CT:



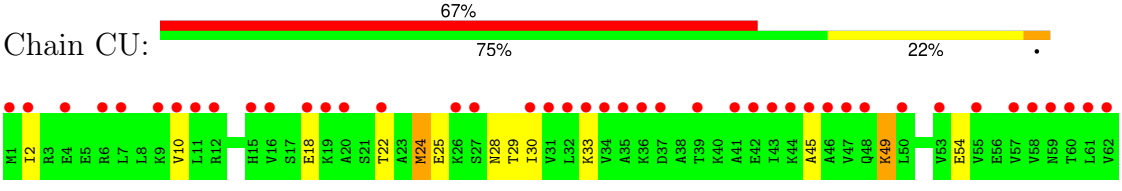
• Molecule 47: 50S ribosomal protein L22

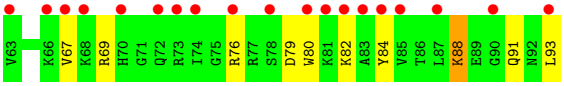
Chain DT:



• Molecule 48: 50S ribosomal protein L23

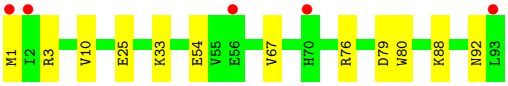
Chain CU:





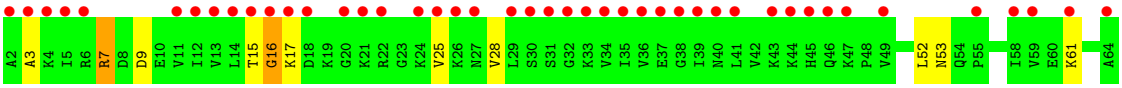
• Molecule 48: 50S ribosomal protein L23

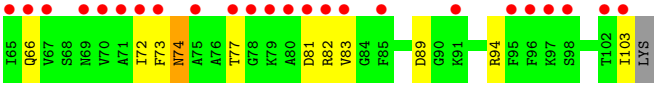
Chain DU:



• Molecule 49: 50S ribosomal protein L24

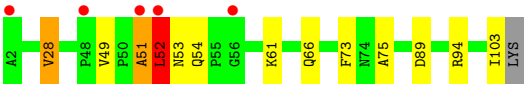
Chain CV:





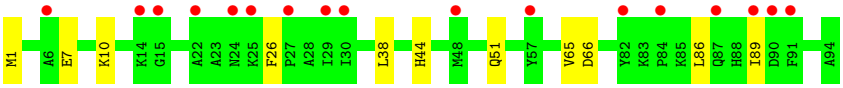
• Molecule 49: 50S ribosomal protein L24

Chain DV:



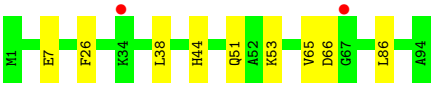
• Molecule 50: 50S ribosomal protein L25

Chain CW:



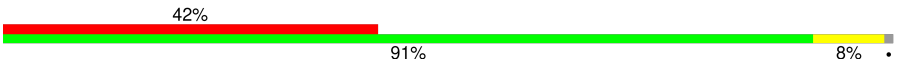
• Molecule 50: 50S ribosomal protein L25

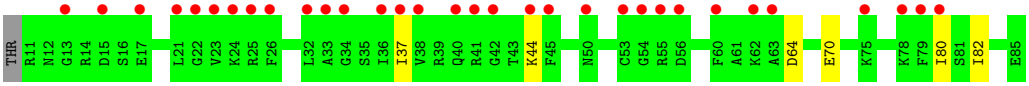
Chain DW:



• Molecule 51: 50S ribosomal protein L27

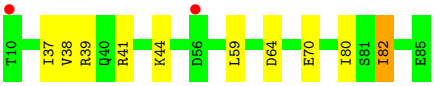
Chain CX:





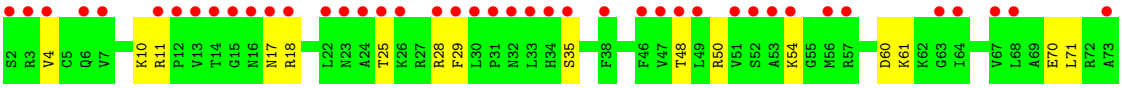
• Molecule 51: 50S ribosomal protein L27

Chain DX:



• Molecule 52: 50S ribosomal protein L28

Chain CY:

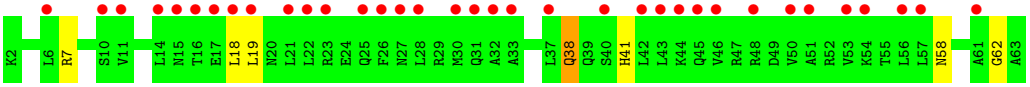


• Molecule 52: 50S ribosomal protein L28

Chain DY:

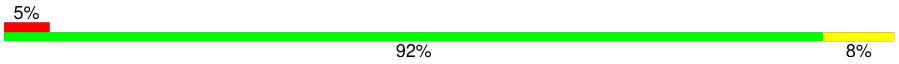
• Molecule 53: 50S ribosomal protein L29

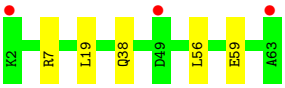
Chain CZ:



• Molecule 53: 50S ribosomal protein L29

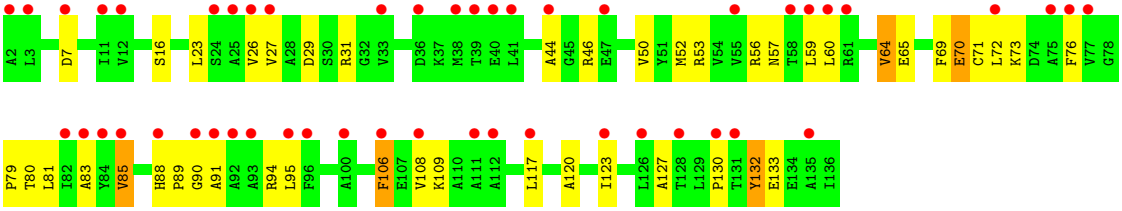
Chain DZ:





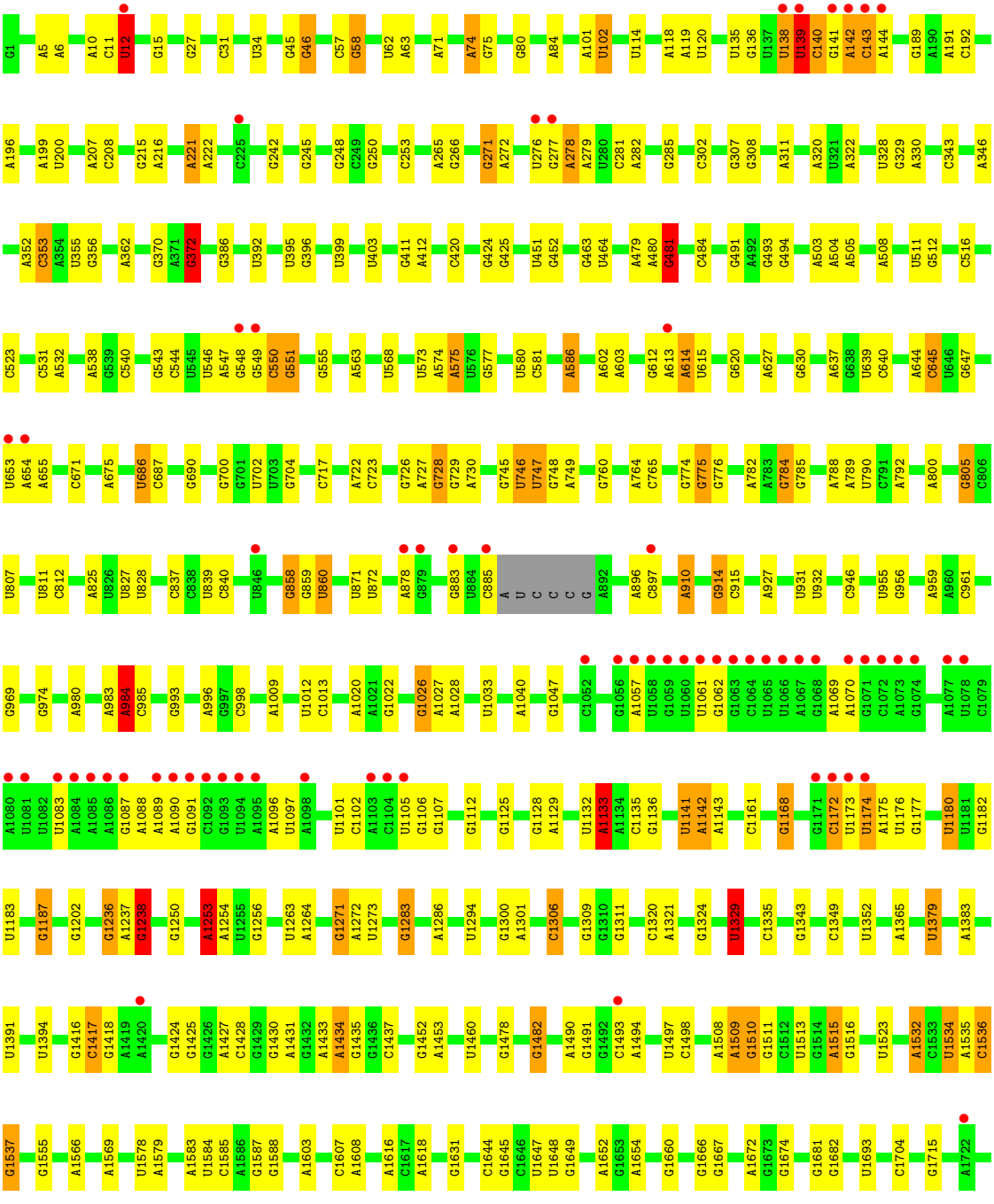
• Molecule 54: 50S ribosomal protein L10

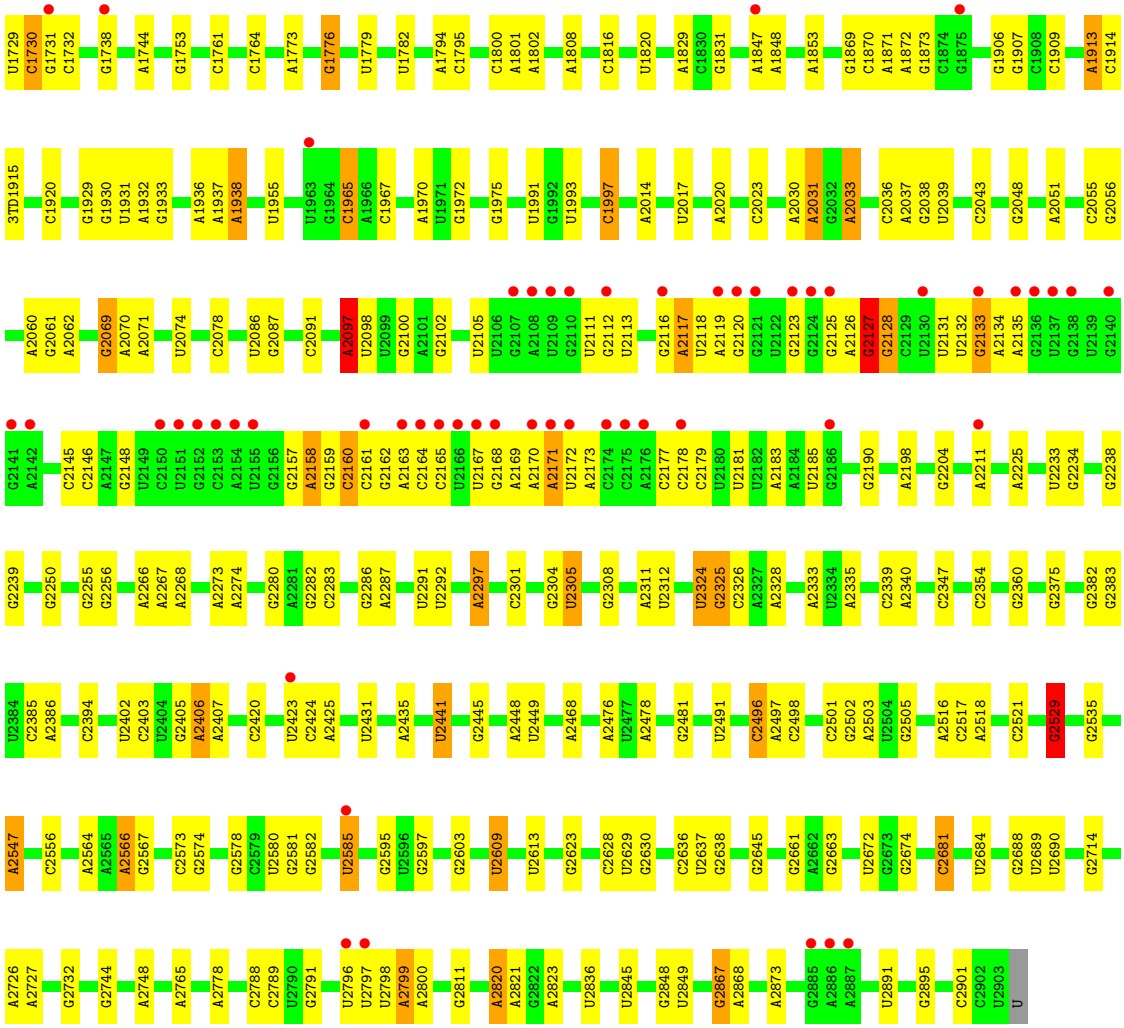
Chain DI:



• Molecule 55: 23S rRNA

Chain DA:




U1729 C1730 G1731 C1732 G1738 A1744 G1753 C1761 C1764 A1773 G1776 U1779 U1782 A1794 C1795 C1800 A1801 A1802 A1808 C1816 U1820 A1829 C1830 G1831 A1847 A1848 A1853 G1869 C1870 A1871 A1872 G1873 C1874 G1875 G1906 G1907 C1908 C1909 A1913 C1914
3TD1915 C1920 G1929 G1930 U1931 A1932 G1933 A1936 A1937 A1938 U1955 U1963 G1964 C1965 A1966 C1967 A1970 U1971 G1972 G1975 U1991 G1992 U1993 C1997 A2014 U2017 A2020 C2023 A2030 A2031 G2032 A2033 C2036 A2037 G2038 U2039 C2043 G2048 A2051 C2055 G2056
A2060 G2061 A2062 G2069 A2070 A2071 U2074 C2078 U2086 G2087 C2091 A2097 U2098 U2099 G2100 A2101 G2102 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2128 C2129 U2130 U2131 U2132 G2133 A2134 A2135 G2136 U2137 G2138 U2139 G2140
G2141 A2142 C2145 C2146 A2147 G2148 U2149 C2150 U2151 G2152 C2153 A2154 U2155 G2156 G2157 A2158 G2159 C2160 C2161 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 U2181 U2182 A2183 A2184 U2185 G2186 G2190 A2198 G2204 A2211 A2225 U2233 G2234 G2238
G2239 G2250 G2255 G2256 A2266 A2267 A2268 A2273 A2274 G2280 A2281 G2282 C2283 G2286 A2287 U2291 U2292 A2297 C2301 G2304 U2305 G2308 A2311 U2312 U2324 G2325 C2326 A2327 A2328 A2333 U2334 A2335 C2339 A2340 C2347 C2354 G2360 G2375 G2382 G2383
U2384 C2385 A2386 C2394 U2402 C2403 U2404 G2405 A2406 A2407 C2420 U2423 C2424 A2425 U2431 A2435 U2441 G2445 A2448 U2449 A2468 A2476 U2477 A2478 G2481 U2491 C2496 A2497 C2498 C2501 G2502 A2503 U2504 G2505 A2516 C2517 A2518 C2521 G2529 G2535
A2547 C2556 A2564 A2565 A2566 G2567 C2573 G2574 G2578 C2579 U2580 G2581 G2582 U2585 G2595 U2596 G2597 G2603 U2609 U2613 G2623 C2628 U2629 G2630 C2636 U2637 G2638 G2645 G2661 A2662 G2663 U2672 G2673 G2674 C2681 U2684 G2688 U2689 U2690 G2714
A2726 A2727 G2732 G2744 A2748 A2765 A2778 C2788 C2789 U2790 G2791 U2796 U2797 U2798 A2799 A2800 G2811 A2820 A2821 G2822 A2823 U2836 U2845 G2848 U2849 G2867 A2868 A2873 G2885 A2886 A2887 U2891 G2895 C2901 C2902 U2903 U

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	212.18Å 434.82Å 624.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.51 – 2.96 48.51 – 2.96	Depositor EDS
% Data completeness (in resolution range)	88.6 (48.51-2.96) 88.6 (48.51-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	21.17 (at 2.96Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, R_{free}	0.208 , 0.221 0.227 , 0.243	Depositor DCC
R_{free} test set	4163 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å^2)	57.6	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 106.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	295202	wwPDB-VP
Average B, all atoms (Å^2)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, D2T, 2MG, 4OC, T1C, 1MG, 5MC, UR3, SPD, PG4, MG, OMC, EDO, PGE, MEQ, 4D4, 2MA, TRS, PUT, MPD, MA6, G7M, ACY, H2U, GUN, PSU, OMG, 1PE, 5MU, OMU, 6MZ, 3TD, ZN

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	0.72	14/36593 (0.0%)	0.68	1/57081 (0.0%)
1	BA	0.72	11/36568 (0.0%)	0.68	2/57042 (0.0%)
2	AB	0.88	0/1784	1.41	4/2403 (0.2%)
2	BB	0.87	0/1784	1.41	4/2403 (0.2%)
3	AC	0.87	0/1652	1.34	2/2225 (0.1%)
3	BC	0.86	0/1652	1.34	6/2225 (0.3%)
4	AD	0.78	0/1665	1.43	11/2227 (0.5%)
4	BD	0.76	0/1665	1.45	10/2227 (0.4%)
5	AE	0.87	0/1157	1.43	3/1557 (0.2%)
5	BE	0.90	0/1118	1.45	3/1504 (0.2%)
6	AF	0.85	1/881 (0.1%)	1.36	6/1189 (0.5%)
6	BF	0.86	0/835	1.50	13/1128 (1.2%)
7	AG	0.83	0/1196	1.40	3/1602 (0.2%)
7	BG	0.84	0/1196	1.39	1/1602 (0.1%)
8	AH	0.82	0/989	1.35	0/1326
8	BH	0.84	0/989	1.34	1/1326 (0.1%)
9	AI	0.82	0/1034	1.34	2/1375 (0.1%)
9	BI	0.82	0/1034	1.33	2/1375 (0.1%)
10	AJ	0.82	1/806 (0.1%)	1.30	4/1089 (0.4%)
10	BJ	0.91	1/797 (0.1%)	1.35	6/1077 (0.6%)
11	AK	0.83	0/893	1.25	4/1205 (0.3%)
11	BK	0.83	0/893	1.29	5/1205 (0.4%)
12	AL	0.77	0/960	1.25	4/1286 (0.3%)
12	BL	0.82	0/960	1.26	3/1286 (0.2%)
13	AM	0.94	1/893 (0.1%)	1.54	9/1193 (0.8%)
13	BM	0.92	0/893	1.54	8/1193 (0.7%)
14	AN	0.83	0/817	1.37	2/1088 (0.2%)
14	BN	0.80	0/817	1.35	2/1088 (0.2%)
15	AO	0.83	0/722	1.48	1/964 (0.1%)
15	BO	0.84	0/722	1.52	0/964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	AP	0.86	0/659	1.32	3/884 (0.3%)
16	BP	0.89	0/659	1.41	7/884 (0.8%)
17	AQ	0.86	0/658	1.24	1/881 (0.1%)
17	BQ	0.91	0/658	1.37	4/881 (0.5%)
18	AR	0.93	0/463	1.46	3/621 (0.5%)
18	BR	0.88	0/463	1.41	2/621 (0.3%)
19	AS	0.86	0/653	1.23	1/877 (0.1%)
19	BS	0.85	0/653	1.23	0/877
20	AT	0.85	0/676	1.61	2/895 (0.2%)
20	BT	0.93	0/671	1.65	5/888 (0.6%)
21	AU	0.79	0/472	1.42	2/627 (0.3%)
21	BU	0.77	0/472	1.46	0/627
22	C1	0.87	0/450	1.35	4/599 (0.7%)
22	D1	0.99	0/450	1.41	2/599 (0.3%)
23	C2	0.83	0/416	1.26	0/554
23	D2	0.86	0/421	1.28	1/561 (0.2%)
24	C3	0.77	0/380	1.44	0/498
24	D3	0.89	0/380	1.51	2/498 (0.4%)
25	C4	0.81	0/513	1.33	1/676 (0.1%)
25	D4	0.90	0/513	1.38	1/676 (0.1%)
26	C5	0.80	0/303	1.19	2/397 (0.5%)
26	D5	0.92	0/303	1.18	0/397
27	C0	0.96	0/453	1.45	2/605 (0.3%)
27	D0	1.01	1/467 (0.2%)	1.45	3/623 (0.5%)
28	CB	0.69	0/2828	0.68	1/4410 (0.0%)
28	DB	0.79	3/2872 (0.1%)	0.72	0/4478
29	CC	0.80	0/2121	1.30	15/2852 (0.5%)
29	DC	0.85	0/2121	1.28	11/2852 (0.4%)
30	CD	0.76	0/1586	1.20	5/2134 (0.2%)
31	CA	0.74	54/69165 (0.1%)	0.69	7/107896 (0.0%)
32	DD	0.88	0/1576	1.22	5/2119 (0.2%)
33	CE	0.82	0/1571	1.40	8/2113 (0.4%)
33	DE	0.88	0/1571	1.39	8/2113 (0.4%)
34	CF	0.79	0/1434	1.38	10/1926 (0.5%)
34	DF	0.82	0/1434	1.39	11/1926 (0.6%)
35	CG	0.79	0/1343	1.29	4/1816 (0.2%)
35	DG	0.80	0/1343	1.27	3/1816 (0.2%)
36	CH	0.89	0/1121	1.34	3/1515 (0.2%)
36	DH	0.89	0/1121	1.35	4/1515 (0.3%)
37	CJ	0.93	0/993	1.35	3/1341 (0.2%)
37	DJ	0.93	0/993	1.34	3/1341 (0.2%)
38	CK	0.76	0/1152	1.35	3/1551 (0.2%)
38	DK	0.92	0/1152	1.38	3/1551 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	CL	0.84	0/947	1.24	4/1268 (0.3%)
39	DL	0.93	0/955	1.23	0/1279
40	CM	0.81	0/1062	1.37	10/1413 (0.7%)
40	DM	0.82	0/1062	1.37	7/1413 (0.5%)
41	CN	0.78	0/1081	1.32	5/1443 (0.3%)
41	DN	0.91	0/1092	1.33	4/1457 (0.3%)
42	CO	0.81	0/973	1.38	2/1301 (0.2%)
42	DO	0.95	0/1006	1.49	3/1345 (0.2%)
43	CP	0.77	0/902	1.47	4/1209 (0.3%)
43	DP	0.81	0/910	1.45	2/1219 (0.2%)
44	CQ	0.72	0/929	1.20	5/1242 (0.4%)
44	DQ	0.80	0/929	1.22	4/1242 (0.3%)
45	CR	0.83	0/960	1.52	5/1278 (0.4%)
45	DR	0.99	0/960	1.57	7/1278 (0.5%)
46	CS	0.81	0/829	1.20	5/1107 (0.5%)
46	DS	0.89	0/829	1.24	1/1107 (0.1%)
47	CT	0.77	0/864	1.39	2/1156 (0.2%)
47	DT	0.91	0/864	1.37	4/1156 (0.3%)
48	CU	0.80	0/745	1.31	1/994 (0.1%)
48	DU	0.83	0/745	1.32	3/994 (0.3%)
49	CV	0.81	0/787	1.36	11/1051 (1.0%)
49	DV	0.84	0/787	1.33	7/1051 (0.7%)
50	CW	0.74	0/766	1.21	0/1025
50	DW	0.86	0/766	1.26	0/1025
51	CX	0.69	0/576	1.16	2/762 (0.3%)
51	DX	0.84	1/598 (0.2%)	1.21	2/790 (0.3%)
52	CY	0.72	0/635	1.38	3/848 (0.4%)
52	DY	0.77	0/635	1.35	2/848 (0.2%)
53	CZ	0.75	0/502	1.49	0/667
53	DZ	0.76	0/502	1.51	0/667
54	DI	0.94	0/1037	1.48	6/1402 (0.4%)
55	DA	0.86	52/69364 (0.1%)	0.78	9/108207 (0.0%)
All	All	0.79	140/309267 (0.0%)	0.93	397/462210 (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	3
1	BA	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	AE	0	1
10	BJ	0	1
31	CA	0	12
55	DA	0	87
All	All	0	108

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2095	A	O5'-C5'	-9.33	1.28	1.42
55	DA	2585	U	C1'-N1	7.89	1.59	1.47
55	DA	12	U	C1'-N1	7.78	1.60	1.48
55	DA	2097	A	O5'-C5'	-7.58	1.31	1.42
31	CA	769	U	C1'-N1	7.42	1.59	1.48
31	CA	12	U	C1'-N1	7.26	1.59	1.48
31	CA	546	U	C1'-N1	6.96	1.58	1.48
55	DA	484	C	C1'-N1	6.96	1.58	1.48
13	AM	114	LYS	CA-C	6.88	1.58	1.52
1	BA	5	U	C1'-N1	6.73	1.58	1.48
1	BA	28	A	O5'-C5'	-6.67	1.32	1.42
55	DA	671	C	C1'-N1	6.54	1.58	1.48
55	DA	1306	C	C1'-N1	6.49	1.58	1.48
55	DA	998	C	C1'-N1	6.43	1.58	1.48
55	DA	2547	A	O5'-C5'	-6.38	1.32	1.42
1	BA	1493	A	C3'-O3'	6.37	1.51	1.42
31	CA	2069	G7M	O3'-P	6.30	1.62	1.56
28	DB	90	C	O5'-C5'	-6.26	1.33	1.42
1	AA	28	A	O5'-C5'	-6.25	1.33	1.42
31	CA	451	U	C1'-N1	6.21	1.56	1.47
1	BA	1008	U	O5'-C5'	-6.13	1.33	1.42
55	DA	1965	C	C1'-N1	6.12	1.57	1.48
31	CA	253	C	C1'-N1	6.08	1.57	1.48
55	DA	1294	U	O5'-C5'	-6.07	1.33	1.42
1	AA	5	U	C1'-N1	6.06	1.57	1.48
55	DA	2297	A	O5'-C5'	-6.06	1.33	1.42
31	CA	1306	C	C1'-N1	6.00	1.57	1.48
31	CA	2619	C	C1'-N1	5.98	1.57	1.48
31	CA	2579	C	C1'-N1	5.96	1.57	1.48
31	CA	1788	C	C1'-N1	5.94	1.57	1.48
55	DA	140	C	C1'-N1	5.86	1.56	1.47
1	BA	290	C	C1'-N1	5.85	1.57	1.48
55	DA	1534	U	C1'-N1	5.85	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2425	A	C3'-O3'	5.84	1.51	1.43
31	CA	1314	C	C1'-N1	5.83	1.57	1.48
55	DA	1133	A	O5'-C5'	-5.78	1.34	1.42
31	CA	995	C	O5'-C5'	-5.78	1.34	1.42
55	DA	139	U	C1'-N1	5.77	1.56	1.47
31	CA	1658	C	C1'-N1	5.74	1.57	1.48
55	DA	1920	C	C1'-N1	5.74	1.57	1.48
31	CA	2006	C	C1'-N1	5.69	1.56	1.48
55	DA	1660	G	O5'-C5'	-5.68	1.33	1.42
1	AA	1203	C	C1'-N1	5.59	1.56	1.48
31	CA	946	C	C1'-N1	5.59	1.56	1.48
31	CA	2233	U	C1'-N1	5.59	1.56	1.48
55	DA	12	U	O5'-C5'	5.58	1.50	1.42
1	AA	485	U	C1'-N1	5.57	1.55	1.47
10	AJ	57	VAL	CA-C	5.56	1.59	1.52
31	CA	1825	U	C1'-N1	5.54	1.56	1.48
31	CA	461	C	C1'-N1	5.54	1.56	1.48
1	BA	209	U	C1'-N1	5.51	1.55	1.47
55	DA	2036	C	C1'-N1	5.51	1.56	1.48
31	CA	961	C	C1'-N1	5.50	1.55	1.47
55	DA	653	U	C1'-N1	5.50	1.56	1.48
31	CA	557	C	C1'-N1	5.50	1.56	1.48
31	CA	1629	U	C1'-N1	5.49	1.56	1.48
31	CA	2723	C	C1'-N1	5.48	1.56	1.48
31	CA	1730	C	C1'-N1	5.47	1.55	1.47
31	CA	653	U	C1'-N1	5.46	1.56	1.48
55	DA	1730	C	C1'-N1	5.45	1.55	1.47
10	BJ	57	VAL	CA-C	5.45	1.59	1.52
1	AA	1498	UR3	O3'-P	5.44	1.61	1.56
31	CA	198	C	C1'-N1	5.44	1.56	1.48
31	CA	1771	C	C1'-N1	5.42	1.56	1.48
31	CA	2646	C	C1'-N1	5.42	1.56	1.48
55	DA	1584	U	C1'-N1	5.41	1.56	1.48
1	BA	291	U	C1'-N1	5.41	1.56	1.48
55	DA	2127	G	C3'-O3'	5.40	1.50	1.42
55	DA	2521	C	C1'-N1	5.40	1.56	1.48
55	DA	2901	C	C1'-N1	5.39	1.56	1.48
55	DA	1253	A	O5'-C5'	-5.38	1.34	1.42
55	DA	581	C	C1'-N1	5.37	1.56	1.48
31	CA	1971	U	C1'-N1	5.36	1.56	1.48
6	AF	88	MET	SD-CE	-5.36	1.66	1.79
55	DA	574	A	O5'-C5'	-5.36	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	845	A	O5'-C5'	5.34	1.50	1.42
55	DA	353	C	C1'-N1	5.34	1.56	1.48
31	CA	2465	C	C1'-N1	5.33	1.56	1.48
55	DA	1704	C	C1'-N1	5.32	1.56	1.48
1	AA	290	C	C1'-N1	5.31	1.56	1.48
55	DA	2069	G7M	O3'-P	5.31	1.61	1.56
31	CA	672	C	C1'-N1	5.31	1.56	1.48
51	DX	82	ILE	CG1-CD1	-5.29	1.31	1.51
31	CA	2044	C	C1'-N1	5.28	1.56	1.48
31	CA	2354	C	C1'-N1	5.28	1.56	1.48
31	CA	2901	C	C1'-N1	5.27	1.56	1.48
31	CA	1704	C	C1'-N1	5.27	1.56	1.48
27	D0	47	MET	SD-CE	-5.26	1.66	1.79
55	DA	2301	C	C1'-N1	5.26	1.56	1.48
55	DA	114	U	C1'-N1	5.24	1.56	1.48
31	CA	692	C	C1'-N1	5.24	1.56	1.48
55	DA	1776	G	O5'-C5'	-5.23	1.34	1.42
1	AA	843	U	C1'-N1	5.23	1.56	1.48
55	DA	2354	C	O5'-C5'	-5.22	1.34	1.42
31	CA	20	C	C1'-N1	5.21	1.56	1.48
55	DA	1644	C	C1'-N1	5.21	1.56	1.48
31	CA	2215	C	C1'-N1	5.20	1.56	1.48
55	DA	1335	C	C1'-N1	5.20	1.56	1.48
55	DA	1965	C	O5'-C5'	-5.20	1.34	1.42
1	AA	955	U	C1'-N1	5.19	1.56	1.48
55	DA	511	U	C1'-N1	5.19	1.56	1.48
55	DA	2496	C	O5'-C5'	-5.19	1.34	1.42
1	BA	1298	U	C1'-N1	5.18	1.55	1.47
31	CA	2043	C	C1'-N1	5.18	1.56	1.48
31	CA	1656	C	C1'-N1	5.17	1.56	1.48
55	DA	1909	C	C1'-N1	5.17	1.56	1.48
31	CA	2232	C	C1'-N1	5.17	1.56	1.48
55	DA	392	U	C1'-N1	5.17	1.56	1.48
31	CA	2225	A	C3'-O3'	5.16	1.50	1.43
1	AA	209	U	C1'-N1	5.15	1.56	1.48
31	CA	1657	U	C1'-N1	5.15	1.56	1.48
55	DA	1965	C	C3'-O3'	-5.15	1.34	1.42
1	AA	1397	C	C1'-N1	5.14	1.55	1.47
31	CA	29	U	C1'-N1	5.14	1.56	1.48
31	CA	1584	U	C1'-N1	5.14	1.56	1.48
28	DB	91	C	C1'-N1	5.14	1.56	1.48
55	DA	860	U	C1'-N1	5.13	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	516	C	C1'-N1	5.12	1.56	1.48
1	BA	1203	C	C1'-N1	5.12	1.56	1.48
55	DA	1437	C	O5'-C5'	-5.12	1.34	1.42
31	CA	2025	C	C1'-N1	5.10	1.56	1.48
31	CA	2680	U	C3'-O3'	5.09	1.49	1.42
1	BA	955	U	C1'-N1	5.09	1.56	1.48
31	CA	1556	C	C1'-N1	5.08	1.56	1.48
55	DA	1174	U	C1'-N1	5.08	1.56	1.48
1	BA	839	C	C1'-N1	5.08	1.56	1.48
1	AA	501	C	C1'-N1	5.07	1.56	1.48
31	CA	140	C	C1'-N1	5.06	1.55	1.47
55	DA	1329	U	C1'-N1	5.05	1.55	1.47
55	DA	702	U	C1'-N1	5.04	1.56	1.48
1	AA	291	U	C1'-N1	5.04	1.56	1.48
55	DA	2672	U	C1'-N1	5.03	1.55	1.48
31	CA	2823	A	C3'-O3'	5.03	1.49	1.42
55	DA	2867	G	C3'-O3'	5.02	1.50	1.43
28	DB	19	C	C1'-N1	5.02	1.55	1.48
1	AA	1103	C	C1'-N1	5.02	1.55	1.48
31	CA	353	C	C1'-N1	5.01	1.55	1.48
31	CA	1335	C	C1'-N1	5.01	1.55	1.48
31	CA	2884	U	C1'-N1	5.00	1.55	1.48
55	DA	372	G	C3'-O3'	5.00	1.50	1.43

All (397) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	CN	69	PRO	CA-C-N	9.76	140.18	121.54
41	CN	69	PRO	C-N-CA	9.76	140.18	121.54
54	DI	132	TYR	CA-C-N	9.74	139.24	121.70
54	DI	132	TYR	C-N-CA	9.74	139.24	121.70
34	DF	10	ASP	CA-CB-CG	9.13	121.73	112.60
17	BQ	51	ASN	CA-CB-CG	8.73	121.33	112.60
23	D2	5	ILE	N-CA-C	-8.36	104.23	112.17
6	BF	90	MET	CA-C-N	8.32	133.05	120.82
6	BF	90	MET	C-N-CA	8.32	133.05	120.82
54	DI	106	PHE	CA-CB-CG	8.04	121.84	113.80
41	DN	106	ASP	CA-CB-CG	7.67	120.27	112.60
40	DM	91	ASP	CA-CB-CG	7.63	120.23	112.60
6	BF	17	GLN	CA-C-N	7.54	127.67	120.43
6	BF	17	GLN	C-N-CA	7.54	127.67	120.43
6	AF	17	GLN	CA-C-N	7.53	127.66	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	AF	17	GLN	C-N-CA	7.53	127.66	120.43
41	CN	106	ASP	CA-CB-CG	7.50	120.11	112.60
27	D0	10	THR	N-CA-CB	-7.28	101.22	110.90
20	BT	6	SER	N-CA-C	-7.17	104.56	113.38
1	BA	842	U	C2'-C3'-O3'	7.09	120.13	109.50
31	CA	2425	A	C4'-C3'-O3'	7.05	119.98	109.40
45	DR	91	ASP	CA-CB-CG	7.05	119.65	112.60
10	AJ	76	ILE	CA-C-N	7.02	129.40	120.56
10	AJ	76	ILE	C-N-CA	7.02	129.40	120.56
40	CM	68	SER	CA-C-N	6.87	134.66	121.54
40	CM	68	SER	C-N-CA	6.87	134.66	121.54
29	CC	239	ASN	CA-CB-CG	6.86	119.46	112.60
38	DK	60	ASP	CA-CB-CG	6.82	119.42	112.60
38	CK	60	ASP	CA-CB-CG	6.80	119.40	112.60
2	AB	126	PHE	CA-CB-CG	6.73	120.53	113.80
2	BB	126	PHE	CA-CB-CG	6.72	120.52	113.80
38	CK	80	HIS	CA-C-N	6.66	133.96	121.97
38	CK	80	HIS	C-N-CA	6.66	133.96	121.97
5	AE	55	GLU	CA-C-N	6.66	126.82	120.43
5	AE	55	GLU	C-N-CA	6.66	126.82	120.43
34	CF	134	GLU	CB-CG-CD	6.64	123.88	112.60
20	BT	43	ASP	CA-CB-CG	6.63	119.23	112.60
6	BF	79	ARG	CA-C-N	6.63	129.16	120.28
6	BF	79	ARG	C-N-CA	6.63	129.16	120.28
29	DC	239	ASN	CA-CB-CG	6.62	119.22	112.60
35	CG	175	LYS	CA-C-N	6.57	134.08	121.54
35	CG	175	LYS	C-N-CA	6.57	134.08	121.54
16	BP	42	ILE	CA-C-N	6.54	129.37	120.54
16	BP	42	ILE	C-N-CA	6.54	129.37	120.54
34	CF	46	ASP	CA-CB-CG	6.52	119.12	112.60
15	AO	88	ARG	N-CA-C	-6.48	100.02	110.32
43	CP	78	VAL	N-CA-CB	6.47	118.12	110.55
6	BF	91	ARG	N-CA-C	6.47	118.65	110.24
29	DC	260	ASN	CA-C-N	6.45	129.57	120.28
29	DC	260	ASN	C-N-CA	6.45	129.57	120.28
43	DP	78	VAL	N-CA-CB	6.45	118.09	110.55
39	CL	121	GLU	CA-C-N	6.43	133.28	121.70
39	CL	121	GLU	C-N-CA	6.43	133.28	121.70
1	AA	413	G	C1'-O4'-C4'	-6.41	103.29	109.70
55	DA	271	G	C2'-C3'-O3'	6.40	119.10	109.50
13	AM	96	PRO	CA-C-N	6.37	129.47	120.42
13	AM	96	PRO	C-N-CA	6.37	129.47	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	BE	55	GLU	CA-C-N	6.37	126.55	120.43
5	BE	55	GLU	C-N-CA	6.37	126.55	120.43
41	DN	69	PRO	CB-CA-C	-6.34	102.37	112.27
52	CY	17	ASN	N-CA-C	-6.32	98.92	108.96
6	BF	55	HIS	N-CA-C	-6.31	98.61	108.90
3	BC	178	LEU	CA-C-N	6.31	129.36	120.28
3	BC	178	LEU	C-N-CA	6.31	129.36	120.28
29	DC	207	LYS	CA-C-N	6.30	128.63	120.44
29	DC	207	LYS	C-N-CA	6.30	128.63	120.44
36	CH	8	LYS	CA-C-N	6.29	133.29	121.97
36	CH	8	LYS	C-N-CA	6.29	133.29	121.97
32	DD	139	SER	N-CA-C	6.27	117.97	110.44
13	BM	96	PRO	CA-C-N	6.27	129.33	120.42
13	BM	96	PRO	C-N-CA	6.27	129.33	120.42
40	DM	23	ILE	CA-C-N	6.27	127.06	120.03
40	DM	23	ILE	C-N-CA	6.27	127.06	120.03
51	CX	44	LYS	N-CA-C	-6.27	104.53	111.36
33	DE	171	ASP	CA-CB-CG	6.26	118.86	112.60
52	DY	17	ASN	N-CA-C	-6.26	99.01	108.96
49	DV	53	ASN	CA-C-N	6.25	129.05	120.67
49	DV	53	ASN	C-N-CA	6.25	129.05	120.67
5	AE	106	ILE	CB-CA-C	6.23	118.81	111.59
6	BF	92	THR	CA-C-N	6.22	131.22	122.08
6	BF	92	THR	C-N-CA	6.22	131.22	122.08
32	DD	176	ASP	CA-CB-CG	6.22	118.82	112.60
4	BD	143	VAL	N-CA-CB	6.21	118.44	110.99
29	DC	70	ASN	CA-CB-CG	6.21	118.81	112.60
4	AD	143	VAL	N-CA-CB	6.19	118.42	110.99
30	CD	4	LEU	CD1-CG-CD2	6.19	124.41	110.80
10	BJ	58	ASN	CA-C-N	6.18	128.56	120.28
10	BJ	58	ASN	C-N-CA	6.18	128.56	120.28
49	CV	9	ASP	CA-CB-CG	6.16	118.76	112.60
34	CF	21	ASN	CA-CB-CG	6.13	118.73	112.60
13	BM	11	ASP	CA-C-N	6.12	130.82	122.19
13	BM	11	ASP	C-N-CA	6.12	130.82	122.19
44	DQ	3	ASN	CA-C-N	6.12	128.39	120.56
44	DQ	3	ASN	C-N-CA	6.12	128.39	120.56
43	DP	67	ASN	CA-CB-CG	6.10	118.70	112.60
29	DC	264	ASP	CA-CB-CG	6.08	118.68	112.60
20	BT	84	ASN	CA-CB-CG	6.08	118.68	112.60
36	DH	8	LYS	CA-C-N	6.08	131.10	123.14
36	DH	8	LYS	C-N-CA	6.08	131.10	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	BJ	37	ARG	CA-C-N	6.07	131.40	121.87
10	BJ	37	ARG	C-N-CA	6.07	131.40	121.87
33	CE	83	VAL	CA-C-N	6.07	128.33	120.44
33	CE	83	VAL	C-N-CA	6.07	128.33	120.44
13	AM	54	ASP	CA-CB-CG	6.07	118.67	112.60
34	CF	13	VAL	CA-C-N	6.06	128.73	120.54
34	CF	13	VAL	C-N-CA	6.06	128.73	120.54
34	CF	23	ASN	CA-CB-CG	6.06	118.66	112.60
16	BP	19	VAL	N-CA-CB	6.05	117.73	110.95
7	AG	151	PHE	CA-CB-CG	6.05	119.85	113.80
34	DF	13	VAL	CA-C-N	6.05	128.71	120.54
34	DF	13	VAL	C-N-CA	6.05	128.71	120.54
12	AL	73	ASN	CA-CB-CG	6.05	118.65	112.60
55	DA	1379	U	C2'-C3'-O3'	-6.04	104.64	113.70
3	AC	178	LEU	CA-C-N	6.04	128.97	120.28
3	AC	178	LEU	C-N-CA	6.04	128.97	120.28
10	AJ	58	ASN	CA-C-N	6.03	128.35	120.28
10	AJ	58	ASN	C-N-CA	6.03	128.35	120.28
33	CE	7	ASP	CA-CB-CG	6.01	118.61	112.60
35	DG	101	ASN	CA-CB-CG	6.01	118.61	112.60
42	DO	29	VAL	CA-C-N	6.01	128.59	120.65
42	DO	29	VAL	C-N-CA	6.01	128.59	120.65
34	CF	107	ALA	CA-C-N	6.01	124.03	120.24
34	CF	107	ALA	C-N-CA	6.01	124.03	120.24
45	CR	91	ASP	CA-CB-CG	6.01	118.61	112.60
29	DC	252	THR	N-CA-C	-6.01	102.06	110.35
40	CM	68	SER	N-CA-C	6.00	118.34	111.02
34	DF	107	ALA	CA-C-N	5.99	124.02	120.24
34	DF	107	ALA	C-N-CA	5.99	124.02	120.24
4	AD	107	PHE	CA-C-N	5.99	125.72	121.65
4	AD	107	PHE	C-N-CA	5.99	125.72	121.65
12	AL	64	THR	CB-CA-C	5.99	119.62	109.75
12	BL	64	THR	CB-CA-C	5.97	119.60	109.75
35	DG	75	MET	CA-C-N	5.97	128.09	120.56
35	DG	75	MET	C-N-CA	5.97	128.09	120.56
3	BC	61	ALA	CA-C-N	5.97	130.64	122.34
3	BC	61	ALA	C-N-CA	5.97	130.64	122.34
35	CG	75	MET	CA-C-N	5.97	128.08	120.56
35	CG	75	MET	C-N-CA	5.97	128.08	120.56
55	DA	784	G	P-O3'-C3'	5.96	129.13	120.20
6	AF	80	PHE	CA-CB-CG	5.96	119.75	113.80
18	AR	34	THR	CA-C-N	5.94	128.24	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	AR	34	THR	C-N-CA	5.94	128.24	120.28
49	CV	3	ALA	CA-C-N	5.94	132.88	121.54
49	CV	3	ALA	C-N-CA	5.94	132.88	121.54
46	CS	50	GLY	CA-C-N	5.93	131.36	122.17
46	CS	50	GLY	C-N-CA	5.93	131.36	122.17
6	AF	55	HIS	N-CA-C	-5.93	99.24	108.90
16	AP	47	GLU	CA-C-N	5.92	132.84	121.54
16	AP	47	GLU	C-N-CA	5.92	132.84	121.54
41	DN	101	VAL	N-CA-C	-5.92	99.79	108.54
13	AM	86	TYR	CA-C-N	5.91	128.20	120.28
13	AM	86	TYR	C-N-CA	5.91	128.20	120.28
29	DC	156	ARG	CB-CG-CD	-5.91	97.71	111.30
49	DV	53	ASN	N-CA-C	-5.88	105.68	112.86
22	D1	11	SER	CA-C-N	5.87	128.07	120.44
22	D1	11	SER	C-N-CA	5.87	128.07	120.44
40	DM	59	ARG	CA-C-N	5.86	128.13	120.28
40	DM	59	ARG	C-N-CA	5.86	128.13	120.28
44	CQ	3	ASN	CA-C-N	5.86	128.06	120.56
44	CQ	3	ASN	C-N-CA	5.86	128.06	120.56
31	CA	974	G	N9-C1'-C2'	5.84	122.76	114.00
14	AN	84	VAL	N-CA-C	-5.83	105.05	110.53
14	BN	84	VAL	N-CA-C	-5.80	105.08	110.53
43	CP	17	LYS	CA-C-N	5.80	128.05	120.28
43	CP	17	LYS	C-N-CA	5.80	128.05	120.28
13	BM	86	TYR	CA-C-N	5.79	128.04	120.28
13	BM	86	TYR	C-N-CA	5.79	128.04	120.28
11	BK	118	HIS	CA-C-N	5.77	132.56	121.54
11	BK	118	HIS	C-N-CA	5.77	132.56	121.54
37	CJ	22	PRO	N-CA-C	5.77	117.74	110.70
25	D4	7	VAL	N-CA-C	-5.76	99.19	107.37
18	BR	34	THR	CA-C-N	5.75	127.99	120.28
18	BR	34	THR	C-N-CA	5.75	127.99	120.28
54	DI	46	ARG	CA-C-N	5.75	127.99	120.28
54	DI	46	ARG	C-N-CA	5.75	127.99	120.28
4	BD	107	PHE	CA-C-N	5.75	125.56	121.65
4	BD	107	PHE	C-N-CA	5.75	125.56	121.65
40	CM	59	ARG	CA-C-N	5.75	127.98	120.28
40	CM	59	ARG	C-N-CA	5.75	127.98	120.28
46	DS	38	VAL	N-CA-CB	5.75	117.89	110.99
43	CP	67	ASN	CA-CB-CG	5.74	118.34	112.60
37	DJ	22	PRO	N-CA-C	5.73	117.69	110.70
51	DX	44	LYS	N-CA-C	-5.73	105.12	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	CC	157	SER	CA-C-N	5.70	132.43	121.54
29	CC	157	SER	C-N-CA	5.70	132.43	121.54
34	DF	46	ASP	CA-CB-CG	5.68	118.28	112.60
4	BD	99	ASP	CA-CB-CG	5.68	118.28	112.60
4	AD	99	ASP	CA-CB-CG	5.68	118.28	112.60
6	BF	98	GLU	CA-C-N	5.68	132.38	121.54
6	BF	98	GLU	C-N-CA	5.68	132.38	121.54
6	BF	80	PHE	CA-CB-CG	5.67	119.47	113.80
29	CC	252	THR	N-CA-C	-5.66	102.54	110.35
44	CQ	75	GLN	CA-C-N	5.65	128.12	120.38
44	CQ	75	GLN	C-N-CA	5.65	128.12	120.38
11	BK	71	ALA	N-CA-C	-5.65	105.20	111.36
29	CC	208	ALA	CA-C-N	5.65	126.25	119.98
29	CC	208	ALA	C-N-CA	5.65	126.25	119.98
29	DC	243	HIS	N-CA-C	-5.65	101.39	109.24
31	CA	2095	A	C5'-C4'-C3'	-5.64	107.55	116.00
2	BB	124	GLY	CA-C-N	5.62	132.28	121.54
2	BB	124	GLY	C-N-CA	5.62	132.28	121.54
29	CC	264	ASP	CA-C-N	5.62	128.08	120.38
29	CC	264	ASP	C-N-CA	5.62	128.08	120.38
2	AB	124	GLY	CA-C-N	5.62	132.26	121.54
2	AB	124	GLY	C-N-CA	5.62	132.26	121.54
4	AD	131	ASN	CA-CB-CG	5.61	118.21	112.60
49	DV	51	ALA	CA-C-N	5.61	132.26	121.54
49	DV	51	ALA	C-N-CA	5.61	132.26	121.54
30	CD	139	SER	N-CA-C	5.60	117.16	110.44
46	CS	51	VAL	N-CA-C	-5.58	102.70	109.01
47	DT	98	LYS	CA-C-N	5.58	128.79	120.87
47	DT	98	LYS	C-N-CA	5.58	128.79	120.87
49	CV	53	ASN	CA-C-N	5.57	127.06	120.09
49	CV	53	ASN	C-N-CA	5.57	127.06	120.09
48	CU	79	ASP	CA-CB-CG	5.57	118.17	112.60
33	DE	172	ALA	CA-C-N	5.55	128.17	120.29
33	DE	172	ALA	C-N-CA	5.55	128.17	120.29
54	DI	7	ASP	CA-CB-CG	5.54	118.14	112.60
33	CE	82	GLY	CA-C-N	5.54	131.93	121.97
33	CE	82	GLY	C-N-CA	5.54	131.93	121.97
41	CN	70	ASP	CA-CB-CG	5.51	118.11	112.60
33	DE	171	ASP	N-CA-C	-5.51	102.36	110.52
33	CE	171	ASP	CA-CB-CG	5.51	118.11	112.60
18	AR	72	ASP	CA-CB-CG	5.50	118.10	112.60
31	CA	2326	C	C4'-C3'-O3'	5.50	117.65	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	DJ	118	THR	CA-C-N	5.50	125.32	120.10
37	DJ	118	THR	C-N-CA	5.50	125.32	120.10
11	BK	36	ASP	CA-CB-CG	5.48	118.08	112.60
41	DN	90	GLU	CB-CG-CD	5.47	121.91	112.60
42	DO	2	ARG	N-CA-CB	-5.47	102.18	111.27
6	AF	79	ARG	CA-C-N	5.47	127.61	120.28
6	AF	79	ARG	C-N-CA	5.47	127.61	120.28
32	DD	127	PHE	CA-CB-CG	5.47	119.27	113.80
44	DQ	75	GLN	N-CA-C	-5.46	99.62	108.41
51	DX	64	ASP	CA-CB-CG	5.46	118.06	112.60
4	AD	39	GLY	CA-C-N	5.44	128.32	120.38
4	AD	39	GLY	C-N-CA	5.44	128.32	120.38
42	CO	29	VAL	CA-C-N	5.43	127.82	120.65
42	CO	29	VAL	C-N-CA	5.43	127.82	120.65
16	BP	43	ALA	N-CA-C	5.43	117.63	111.11
17	BQ	57	ASP	CA-CB-CG	5.43	118.03	112.60
37	CJ	118	THR	CA-C-N	5.43	125.26	120.10
37	CJ	118	THR	C-N-CA	5.43	125.26	120.10
7	BG	151	PHE	CA-CB-CG	5.42	119.22	113.80
26	C5	19	ARG	CA-C-N	5.42	131.89	121.54
26	C5	19	ARG	C-N-CA	5.42	131.89	121.54
13	BM	14	HIS	CA-C-N	5.42	127.85	120.54
13	BM	14	HIS	C-N-CA	5.42	127.85	120.54
17	BQ	48	ASP	CA-CB-CG	5.41	118.01	112.60
48	DU	92	ASN	CA-C-N	5.41	131.44	121.70
48	DU	92	ASN	C-N-CA	5.41	131.44	121.70
11	AK	36	ASP	CA-CB-CG	5.40	118.00	112.60
49	CV	83	VAL	CA-C-N	5.40	126.22	121.58
49	CV	83	VAL	C-N-CA	5.40	126.22	121.58
17	BQ	22	VAL	N-CA-CB	5.39	117.52	111.21
45	CR	12	ALA	CA-C-N	5.39	127.50	120.28
45	CR	12	ALA	C-N-CA	5.39	127.50	120.28
12	AL	42	PRO	CA-C-N	5.39	131.19	121.06
12	AL	42	PRO	C-N-CA	5.39	131.19	121.06
29	CC	37	ASN	CA-CB-CG	5.39	117.99	112.60
40	DM	60	ARG	CG-CD-NE	5.38	123.84	112.00
13	AM	14	HIS	CA-C-N	5.37	127.79	120.54
13	AM	14	HIS	C-N-CA	5.37	127.79	120.54
28	CB	15	A	O4'-C1'-N9	5.37	116.25	108.20
41	CN	111	GLU	CB-CG-CD	5.36	121.71	112.60
25	C4	7	VAL	N-CA-C	-5.36	99.76	107.37
29	CC	156	ARG	CB-CG-CD	-5.36	98.98	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	DV	49	VAL	CA-C-O	-5.36	117.24	120.88
29	CC	243	HIS	N-CA-C	-5.35	101.80	109.24
34	DF	21	ASN	CA-CB-CG	5.35	117.95	112.60
22	C1	11	SER	CA-C-N	5.35	127.45	120.28
22	C1	11	SER	C-N-CA	5.35	127.45	120.28
55	DA	2820	A	C4'-C3'-O3'	-5.35	104.98	113.00
55	DA	2820	A	P-O3'-C3'	5.34	128.21	120.20
13	AM	12	HIS	CA-C-N	5.34	132.09	122.64
13	AM	12	HIS	C-N-CA	5.34	132.09	122.64
7	AG	62	PHE	CA-C-N	5.32	127.41	120.28
7	AG	62	PHE	C-N-CA	5.32	127.41	120.28
9	BI	99	ARG	CA-C-N	5.32	127.67	120.38
9	BI	99	ARG	C-N-CA	5.32	127.67	120.38
36	DH	26	ALA	CA-C-N	5.31	127.34	120.44
36	DH	26	ALA	C-N-CA	5.31	127.34	120.44
1	BA	1362	A	C1'-O4'-C4'	-5.30	104.40	109.70
29	CC	195	VAL	N-CA-CB	5.30	116.30	110.53
31	CA	686	U	O5'-C5'-C4'	-5.29	103.76	111.70
29	CC	70	ASN	CA-CB-CG	5.29	117.89	112.60
39	CL	1	MET	CA-C-N	5.29	129.60	122.93
39	CL	1	MET	C-N-CA	5.29	129.60	122.93
19	AS	27	ASP	CA-CB-CG	5.28	117.88	112.60
40	CM	35	HIS	N-CA-C	5.27	117.00	108.41
47	CT	64	ALA	CA-C-N	5.27	131.60	121.54
47	CT	64	ALA	C-N-CA	5.27	131.60	121.54
55	DA	2280	G	C4'-C3'-C2'	-5.27	97.33	102.60
16	BP	23	ASP	CA-CB-CG	5.26	117.86	112.60
47	DT	15	GLN	CA-C-N	5.26	127.33	120.28
47	DT	15	GLN	C-N-CA	5.26	127.33	120.28
29	DC	37	ASN	CA-CB-CG	5.25	117.85	112.60
34	DF	67	ILE	N-CA-CB	5.25	116.83	110.95
4	AD	168	PRO	CA-C-N	5.24	127.83	120.28
4	AD	168	PRO	C-N-CA	5.24	127.83	120.28
34	DF	59	ALA	CA-C-N	5.24	127.17	120.56
34	DF	59	ALA	C-N-CA	5.24	127.17	120.56
11	AK	118	HIS	CA-C-N	5.24	131.55	121.54
11	AK	118	HIS	C-N-CA	5.24	131.55	121.54
3	BC	26	THR	CA-C-N	5.24	127.57	120.65
3	BC	26	THR	C-N-CA	5.24	127.57	120.65
31	CA	271	G	C2'-C3'-O3'	5.24	117.36	109.50
40	DM	35	HIS	N-CA-C	5.23	117.05	108.52
52	CY	70	GLU	CA-C-N	5.23	127.29	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	CY	70	GLU	C-N-CA	5.23	127.29	120.28
22	C1	55	ILE	CA-C-N	5.23	131.53	121.54
22	C1	55	ILE	C-N-CA	5.23	131.53	121.54
5	BE	82	GLN	CB-CG-CD	5.23	121.48	112.60
16	AP	23	ASP	CA-CB-CG	5.22	117.82	112.60
11	AK	29	ASN	CA-CB-CG	5.21	117.81	112.60
27	C0	3	LYS	CA-C-N	5.21	131.49	121.54
27	C0	3	LYS	C-N-CA	5.21	131.49	121.54
4	BD	39	GLY	CA-C-N	5.20	127.97	120.38
4	BD	39	GLY	C-N-CA	5.20	127.97	120.38
32	DD	108	ASP	CA-CB-CG	5.20	117.80	112.60
27	D0	51	VAL	CA-C-N	5.19	127.96	120.38
27	D0	51	VAL	C-N-CA	5.19	127.96	120.38
45	CR	47	TYR	CA-C-N	5.19	127.24	120.28
45	CR	47	TYR	C-N-CA	5.19	127.24	120.28
9	AI	99	ARG	CA-C-N	5.18	127.48	120.38
9	AI	99	ARG	C-N-CA	5.18	127.48	120.38
45	DR	53	ARG	CA-C-N	5.18	127.74	120.28
45	DR	53	ARG	C-N-CA	5.18	127.74	120.28
32	DD	186	LEU	N-CA-C	5.18	118.00	109.72
40	CM	15	ALA	N-CA-C	5.17	117.31	111.11
55	DA	807	U	C4'-C3'-C2'	-5.17	97.43	102.60
14	BN	21	PHE	CA-CB-CG	5.16	118.96	113.80
51	CX	64	ASP	CA-CB-CG	5.16	117.76	112.60
17	AQ	57	ASP	CA-CB-CG	5.16	117.76	112.60
33	DE	113	VAL	CA-C-N	5.16	127.19	120.28
33	DE	113	VAL	C-N-CA	5.16	127.19	120.28
33	DE	131	THR	CA-C-N	5.15	127.18	120.28
33	DE	131	THR	C-N-CA	5.15	127.18	120.28
12	BL	42	PRO	CA-C-N	5.15	128.39	120.82
12	BL	42	PRO	C-N-CA	5.15	128.39	120.82
2	AB	205	ASP	CA-CB-CG	5.14	117.74	112.60
40	CM	30	THR	N-CA-CB	5.13	119.16	110.49
55	DA	1238	G	C4'-C3'-C2'	-5.13	97.47	102.60
4	BD	168	PRO	CA-C-N	5.12	127.66	120.28
4	BD	168	PRO	C-N-CA	5.12	127.66	120.28
11	BK	29	ASN	CA-CB-CG	5.12	117.72	112.60
34	CF	59	ALA	CA-C-N	5.12	127.01	120.56
34	CF	59	ALA	C-N-CA	5.12	127.01	120.56
38	DK	33	ALA	CA-C-N	5.11	127.08	120.44
38	DK	33	ALA	C-N-CA	5.11	127.08	120.44
31	CA	2225	A	C2'-C3'-O3'	5.10	117.16	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	BT	72	ALA	CA-C-N	5.09	127.11	120.28
20	BT	72	ALA	C-N-CA	5.09	127.11	120.28
45	DR	43	GLY	CA-C-N	5.09	127.06	120.44
45	DR	43	GLY	C-N-CA	5.09	127.06	120.44
4	BD	9	LEU	CA-C-N	5.09	127.10	120.28
4	BD	9	LEU	C-N-CA	5.09	127.10	120.28
8	BH	109	GLY	N-CA-C	5.09	119.30	112.17
30	CD	186	LEU	N-CA-C	5.09	117.86	109.72
46	CS	53	PHE	CA-C-N	5.08	127.97	120.91
46	CS	53	PHE	C-N-CA	5.08	127.97	120.91
52	DY	60	ASP	CA-CB-CG	5.08	117.68	112.60
55	DA	1997	C	C4'-C3'-C2'	-5.08	97.52	102.60
48	DU	79	ASP	CA-CB-CG	5.07	117.67	112.60
30	CD	108	ASP	CA-CB-CG	5.07	117.67	112.60
36	CH	37	VAL	CB-CA-C	5.07	114.30	109.33
49	CV	73	PHE	CA-C-N	5.07	127.07	120.28
49	CV	73	PHE	C-N-CA	5.07	127.07	120.28
33	CE	113	VAL	CA-C-N	5.06	127.06	120.28
33	CE	113	VAL	C-N-CA	5.06	127.06	120.28
20	AT	72	ALA	CA-C-N	5.06	127.06	120.28
20	AT	72	ALA	C-N-CA	5.06	127.06	120.28
34	DF	146	VAL	N-CA-CB	5.06	116.44	110.82
30	CD	127	PHE	CA-CB-CG	5.05	118.86	113.80
16	BP	79	ASN	CA-C-N	5.05	131.18	121.54
16	BP	79	ASN	C-N-CA	5.05	131.18	121.54
29	CC	261	LYS	CA-C-N	5.05	127.46	120.29
29	CC	261	LYS	C-N-CA	5.05	127.46	120.29
44	CQ	24	ASP	CA-CB-CG	5.05	117.65	112.60
49	CV	74	ASN	CA-C-N	5.05	131.18	121.54
49	CV	74	ASN	C-N-CA	5.05	131.18	121.54
14	AN	21	PHE	CA-CB-CG	5.04	118.84	113.80
4	AD	47	ARG	CA-C-N	5.04	127.93	120.82
4	AD	47	ARG	C-N-CA	5.04	127.93	120.82
10	BJ	90	LEU	CA-C-N	5.04	131.18	121.54
10	BJ	90	LEU	C-N-CA	5.04	131.18	121.54
45	DR	16	LYS	CA-C-N	5.04	127.01	120.56
45	DR	16	LYS	C-N-CA	5.04	127.01	120.56
49	DV	28	VAL	N-CA-CB	5.04	117.81	111.46
2	BB	204	ASP	CA-CB-CG	5.03	117.63	112.60
24	D3	39	ARG	CA-C-N	5.03	126.97	120.44
24	D3	39	ARG	C-N-CA	5.03	126.97	120.44
21	AU	45	ARG	CA-C-N	5.02	127.42	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AU	45	ARG	C-N-CA	5.02	127.42	120.29
40	CM	67	THR	CA-C-N	5.02	127.77	120.79
40	CM	67	THR	C-N-CA	5.02	127.77	120.79
44	DQ	24	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (108) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1432	G	Sidechain
1	AA	362	G	Sidechain
1	AA	898	G	Sidechain
5	AE	82	GLN	Sidechain
1	BA	1432	G	Sidechain
1	BA	362	G	Sidechain
1	BA	575	G	Sidechain
1	BA	898	G	Sidechain
10	BJ	37	ARG	Mainchain
31	CA	1693	U	Sidechain
31	CA	1777	U	Sidechain
31	CA	1936	A	Sidechain
31	CA	1937	A	Sidechain
31	CA	2267	A	Sidechain
31	CA	2638	G	Sidechain
31	CA	2732	G	Sidechain
31	CA	463	G	Sidechain
31	CA	481	G	Sidechain
31	CA	704	G	Sidechain
31	CA	726	G	Sidechain
31	CA	805	G	Sidechain
55	DA	1009	A	Sidechain
55	DA	1142	A	Sidechain
55	DA	1236	G	Sidechain
55	DA	1253	A	Sidechain
55	DA	1283	G	Sidechain
55	DA	1311	G	Sidechain
55	DA	1324	G	Sidechain
55	DA	1343	G	Sidechain
55	DA	1425	G	Sidechain
55	DA	15	G	Sidechain
55	DA	1631	G	Sidechain
55	DA	1645	G	Sidechain

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Mol	Chain	Res	Type	Group
55	DA	1666	G	Sidechain
55	DA	1667	G	Sidechain
55	DA	1672	A	Sidechain
55	DA	1681	G	Sidechain
55	DA	1682	G	Sidechain
55	DA	1693	U	Sidechain
55	DA	1753	G	Sidechain
55	DA	1761	C	Sidechain
55	DA	1779	U	Sidechain
55	DA	1802	A	Sidechain
55	DA	1938	A	Sidechain
55	DA	2037	A	Sidechain
55	DA	2048	G	Sidechain
55	DA	2074	U	Sidechain
55	DA	2078	C	Sidechain
55	DA	221	A	Sidechain
55	DA	2250	G	Sidechain
55	DA	2266	A	Sidechain
55	DA	2267	A	Sidechain
55	DA	2282	G	Sidechain
55	DA	2328	A	Sidechain
55	DA	2375	G	Sidechain
55	DA	2382	G	Sidechain
55	DA	2405	G	Sidechain
55	DA	2468	A	Sidechain
55	DA	2481	G	Sidechain
55	DA	2497	A	Sidechain
55	DA	250	G	Sidechain
55	DA	2516	A	Sidechain
55	DA	2517	C	Sidechain
55	DA	2529	G	Sidechain
55	DA	2564	A	Sidechain
55	DA	2566	A	Sidechain
55	DA	2581	G	Sidechain
55	DA	2582	G	Sidechain
55	DA	2595	G	Sidechain
55	DA	2597	G	Sidechain
55	DA	2638	G	Sidechain
55	DA	2645	G	Sidechain
55	DA	2688	G	Sidechain
55	DA	27	G	Sidechain
55	DA	2727	A	Sidechain

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Mol	Chain	Res	Type	Group
55	DA	2732	G	Sidechain
55	DA	2848	G	Sidechain
55	DA	307	G	Sidechain
55	DA	308	G	Sidechain
55	DA	395	U	Sidechain
55	DA	452	G	Sidechain
55	DA	463	G	Sidechain
55	DA	464	U	Sidechain
55	DA	481	G	Sidechain
55	DA	512	G	Sidechain
55	DA	555	G	Sidechain
55	DA	575	A	Sidechain
55	DA	577	G	Sidechain
55	DA	58	G	Sidechain
55	DA	630	G	Sidechain
55	DA	675	A	Sidechain
55	DA	690	G	Sidechain
55	DA	700	G	Sidechain
55	DA	704	G	Sidechain
55	DA	726	G	Sidechain
55	DA	727	A	Sidechain
55	DA	728	G	Sidechain
55	DA	748	G	Sidechain
55	DA	774	G	Sidechain
55	DA	775	G	Sidechain
55	DA	800	A	Sidechain
55	DA	805	G	Sidechain
55	DA	858	G	Sidechain
55	DA	910	A	Sidechain
55	DA	956	G	Sidechain
55	DA	959	A	Sidechain
55	DA	980	A	Sidechain
55	DA	984	A	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32930	0	16591	87	0
1	BA	32908	0	16580	95	0
2	AB	1753	0	1780	11	0
2	BB	1753	0	1780	16	0
3	AC	1625	0	1696	14	0
3	BC	1625	0	1696	18	0
4	AD	1643	0	1707	13	0
4	BD	1643	0	1707	17	0
5	AE	1144	0	1185	15	0
5	BE	1105	0	1148	29	0
6	AF	862	0	864	9	0
6	BF	817	0	808	10	0
7	AG	1182	0	1238	7	0
7	BG	1182	0	1238	4	0
8	AH	979	0	1031	9	0
8	BH	979	0	1031	5	0
9	AI	1022	0	1070	6	0
9	BI	1022	0	1070	6	0
10	AJ	796	0	836	11	0
10	BJ	787	0	828	10	0
11	AK	877	0	887	14	0
11	BK	877	0	887	17	0
12	AL	957	0	1017	8	0
12	BL	957	0	1017	9	0
13	AM	884	0	941	13	0
13	BM	884	0	941	13	0
14	AN	805	0	844	9	0
14	BN	805	0	844	9	0
15	AO	714	0	734	1	0
15	BO	714	0	734	0	0
16	AP	649	0	666	3	0
16	BP	649	0	666	5	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	5	0
18	AR	456	0	478	5	0
18	BR	456	0	478	3	0
19	AS	638	0	665	7	0
19	BS	638	0	665	8	0
20	AT	670	0	719	2	0
20	BT	665	0	714	9	0
21	AU	465	0	491	2	0
21	BU	465	0	491	2	0
22	C1	444	0	458	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	D1	444	0	458	13	0
23	C2	409	0	440	5	0
23	D2	414	0	442	5	0
24	C3	377	0	418	16	0
24	D3	377	0	418	6	0
25	C4	504	0	572	13	0
25	D4	504	0	572	12	0
26	C5	302	0	340	10	0
26	D5	302	0	340	2	0
27	C0	449	0	488	4	0
27	D0	463	0	504	1	0
28	CB	2529	0	1281	4	0
28	DB	2569	0	1301	5	0
29	CC	2082	0	2154	17	0
29	DC	2082	0	2154	11	0
30	CD	1565	0	1616	16	0
31	CA	62229	0	31318	235	0
32	DD	1576	0	1627	16	0
33	CE	1552	0	1619	14	0
33	DE	1552	0	1619	11	0
34	CF	1410	0	1444	16	0
34	DF	1410	0	1444	13	0
35	CG	1323	0	1371	9	0
35	DG	1323	0	1371	9	0
36	CH	1110	0	1148	9	0
36	DH	1110	0	1148	6	0
37	CJ	979	0	1028	4	0
37	DJ	979	0	1028	5	0
38	CK	1129	0	1162	9	0
38	DK	1129	0	1162	5	0
39	CL	938	0	1012	9	0
39	DL	946	0	1023	8	0
40	CM	1053	0	1129	19	0
40	DM	1053	0	1129	15	0
41	CN	1075	0	1154	5	0
41	DN	1092	0	1177	7	0
42	CO	960	0	1000	5	0
42	DO	993	0	1034	5	0
43	CP	892	0	923	7	0
43	DP	900	0	935	9	0
44	CQ	917	0	962	7	0
44	DQ	917	0	962	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	CR	947	0	1019	13	0
45	DR	947	0	1019	9	0
46	CS	816	0	839	8	0
46	DS	816	0	839	5	0
47	CT	857	0	922	12	0
47	DT	857	0	922	10	0
48	CU	739	0	807	10	0
48	DU	739	0	807	4	0
49	CV	779	0	831	8	0
49	DV	779	0	831	5	0
50	CW	753	0	780	5	0
50	DW	753	0	780	3	0
51	CX	569	0	581	1	0
51	DX	591	0	606	5	0
52	CY	625	0	652	8	0
52	DY	625	0	652	5	0
53	CZ	501	0	531	2	0
53	DZ	501	0	531	1	0
54	DI	1023	0	1052	21	0
55	DA	62423	0	31411	171	0
56	AA	71	0	0	0	0
56	BA	43	0	0	0	0
56	CA	156	0	0	0	0
56	CB	3	0	0	0	0
56	DA	182	0	0	0	0
56	DB	9	0	0	0	0
56	DD	2	0	0	0	0
56	DM	1	0	0	0	0
56	DR	2	0	0	0	0
57	AA	13	0	18	1	0
57	BA	13	0	18	0	0
57	DA	26	0	36	2	0
57	DQ	13	0	18	0	0
57	DR	13	0	18	5	0
57	DS	13	0	18	1	0
58	AA	16	0	28	0	0
58	DA	40	0	70	5	0
58	DE	16	0	28	0	0
58	DK	8	0	14	0	0
58	DN	8	0	14	1	0
58	DS	8	0	14	0	0
58	DT	16	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	AA	24	0	48	0	0
59	DA	72	0	144	10	0
60	AA	42	0	38	0	0
60	BA	42	0	38	0	0
61	AB	1	0	0	0	0
61	C5	1	0	0	0	0
61	D5	1	0	0	0	0
62	AL	7	0	10	0	0
62	D1	7	0	10	1	0
62	D3	7	0	10	2	0
62	DA	35	0	50	1	0
62	DL	7	0	10	0	0
62	DP	7	0	10	1	0
62	DQ	7	0	10	0	0
63	D1	4	0	6	0	0
63	DA	36	0	54	2	0
63	DB	8	0	12	1	0
64	D1	10	0	14	2	0
64	D3	10	0	14	0	0
64	DA	40	0	56	5	0
64	DD	10	0	14	2	0
64	DS	10	0	14	0	0
64	DU	10	0	14	1	0
65	DA	40	0	76	4	0
66	DA	32	0	44	0	0
67	DA	12	0	12	0	0
68	DA	11	0	5	0	0
69	DA	8	0	12	1	0
70	AA	507	0	0	0	0
70	AC	4	0	0	0	0
70	AD	2	0	0	0	0
70	AE	4	0	0	0	0
70	AF	1	0	0	0	0
70	AG	1	0	0	0	0
70	AH	1	0	0	0	0
70	AJ	2	0	0	0	0
70	AK	5	0	0	0	0
70	AL	8	0	0	0	0
70	AM	4	0	0	1	0
70	AN	5	0	0	1	0
70	AO	2	0	0	0	0
70	AP	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	AR	1	0	0	0	0
70	AS	1	0	0	0	0
70	AT	2	0	0	0	0
70	AU	3	0	0	0	0
70	BA	287	0	0	1	0
70	BD	13	0	0	0	0
70	BE	1	0	0	0	0
70	BF	1	0	0	0	0
70	BK	1	0	0	0	0
70	BL	3	0	0	0	0
70	BN	2	0	0	0	0
70	BO	1	0	0	0	0
70	BP	3	0	0	0	0
70	BR	1	0	0	0	0
70	BT	4	0	0	0	0
70	BU	2	0	0	0	0
70	C3	3	0	0	1	0
70	C4	1	0	0	0	0
70	CA	694	0	0	1	0
70	CB	13	0	0	0	0
70	CC	10	0	0	0	0
70	CD	5	0	0	0	0
70	CE	6	0	0	0	0
70	CL	1	0	0	0	0
70	CM	3	0	0	0	0
70	CO	1	0	0	0	0
70	CU	3	0	0	0	0
70	CV	1	0	0	0	0
70	CW	1	0	0	0	0
70	CY	1	0	0	0	0
70	D0	25	0	0	0	0
70	D1	42	0	0	0	0
70	D2	7	0	0	0	0
70	D3	25	0	0	0	0
70	D4	32	0	0	1	0
70	D5	13	0	0	0	0
70	DA	4836	0	0	8	0
70	DB	213	0	0	0	0
70	DC	102	0	0	0	0
70	DD	105	0	0	1	0
70	DE	63	0	0	0	0
70	DF	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	DG	6	0	0	0	0
70	DH	2	0	0	0	0
70	DK	58	0	0	0	0
70	DL	51	0	0	0	0
70	DM	60	0	0	0	0
70	DN	71	0	0	0	0
70	DO	44	0	0	0	0
70	DP	35	0	0	0	0
70	DQ	27	0	0	1	0
70	DR	64	0	0	0	0
70	DS	51	0	0	0	0
70	DT	70	0	0	1	0
70	DU	17	0	0	0	0
70	DV	19	0	0	0	0
70	DW	31	0	0	0	0
70	DX	30	0	0	1	0
70	DY	9	0	0	0	0
70	DZ	7	0	0	0	0
All	All	295202	0	194489	1218	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 (1218) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C5:3:VAL:HG11	31:CA:2539:C:H5'	1.32	1.05
46:CS:14:VAL:HG21	46:CS:98:ILE:HG13	1.32	1.05
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.43	0.99
31:CA:1936:A:H2	31:CA:1943:U:H3	1.01	0.98
48:CU:28:ASN:HD21	48:CU:91:GLN:HB3	1.29	0.96
14:AN:66:GLN:HB2	70:AN:205:HOH:O	1.67	0.95
40:CM:82:LEU:HD11	40:CM:116:VAL:HG23	1.52	0.92
24:C3:7:PRO:HB2	31:CA:1309:G:H4'	1.52	0.91
46:CS:14:VAL:CG2	46:CS:98:ILE:HG13	2.00	0.90
5:AE:77:ASN:HB2	5:AE:82:GLN:NE2	1.86	0.90
40:CM:77:ILE:HD11	40:CM:108:ALA:HB1	1.55	0.89
8:BH:87:LYS:HB2	8:BH:125:ILE:HD11	1.55	0.87
22:C1:4:GLN:HA	31:CA:2615:U:C2	2.10	0.86
5:BE:77:ASN:HB2	5:BE:82:GLN:NE2	1.91	0.86
8:AH:87:LYS:HB2	8:AH:125:ILE:HD11	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2796:U:H3	31:CA:2799:A:H61	1.23	0.85
31:CA:1779:U:H5	31:CA:1784:A:N7	1.74	0.85
31:CA:1005:C:O2'	38:CK:30:THR:HG21	1.78	0.84
55:DA:2796:U:H3	55:DA:2799:A:H61	1.21	0.83
1:BA:1305:G:H21	1:BA:1332:A:H2	1.24	0.83
11:BK:88:GLY:H	11:BK:114:THR:HG22	1.43	0.82
2:BB:23:TRP:HB3	2:BB:39:HIS:CE1	2.14	0.82
1:AA:1305:G:H21	1:AA:1332:A:H2	1.23	0.81
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.61	0.81
31:CA:740:C:H5'	31:CA:1784:A:H3'	1.62	0.81
33:CE:149:ILE:HG12	33:CE:188:MET:HG2	1.62	0.81
12:BL:65:SER:HB2	12:BL:82:ILE:HD11	1.62	0.80
13:BM:114:LYS:HB3	13:BM:115:PRO:HD3	1.62	0.80
55:DA:2033:A:H5'	70:DA:4099:HOH:O	1.81	0.80
22:C1:38:HIS:HE1	31:CA:2884:U:O4	1.64	0.80
2:BB:20:THR:HA	2:BB:39:HIS:CE1	2.18	0.79
46:CS:14:VAL:HG21	46:CS:98:ILE:CG1	2.11	0.79
45:DR:20:GLN:CG	57:DR:202:PG4:H42	2.12	0.79
1:BA:9:G:H5'	5:BE:108:GLY:HA3	1.63	0.79
25:C4:60:ALA:O	40:CM:48:ARG:HD2	1.83	0.78
45:DR:20:GLN:HG3	57:DR:202:PG4:H42	1.65	0.78
55:DA:135:U:H3	55:DA:144:A:H61	1.32	0.78
35:CG:24:ILE:HD11	35:CG:43:VAL:HG11	1.66	0.77
35:DG:24:ILE:HD11	35:DG:43:VAL:HG11	1.66	0.77
41:DN:18[A]:ARG:HG2	28:DB:90:C:H5'	1.65	0.77
31:CA:135:U:H3	31:CA:144:A:H61	1.33	0.77
13:BM:22:ILE:HB	13:BM:25:VAL:CG1	2.15	0.77
55:DA:568:U:H1'	55:DA:2030:6MZ:H9C1	1.66	0.77
1:BA:664:G:H22	1:BA:741:G:H1	1.34	0.76
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.67	0.76
39:CL:38:ILE:HD11	39:CL:112:PHE:HZ	1.49	0.76
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.68	0.75
1:AA:664:G:H22	1:AA:741:G:H1	1.34	0.74
10:AJ:7:ARG:HB3	10:AJ:101:SER:HB2	1.69	0.74
4:AD:107:PHE:HB3	4:AD:145:ILE:HD11	1.70	0.74
4:BD:107:PHE:HB3	4:BD:145:ILE:HD11	1.70	0.74
13:BM:83:LEU:HD21	19:BS:65:GLU:HB2	1.70	0.74
31:CA:528:A:C2	31:CA:2043:C:H4'	2.23	0.73
3:BC:123:GLN:HB3	3:BC:128:VAL:HG21	1.69	0.73
1:AA:842:U:H4'	1:AA:843:U:OP1	1.88	0.73
25:D4:54:ASP:HB3	40:DM:57:LEU:HD22	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:522:C:H5	12:BL:50:ARG:HH12	1.37	0.73
13:BM:6:GLY:HA3	13:BM:66:GLU:HG3	1.69	0.73
1:BA:1060:U:C5	3:BC:2:GLY:HA3	2.23	0.73
55:DA:2127:G:H4'	55:DA:2128:G:OP1	1.90	0.72
1:AA:1492:A:H5"	12:AL:44:LYS:HG2	1.72	0.71
24:C3:30:VAL:HG13	31:CA:466:A:H5"	1.72	0.71
39:DL:38:ILE:HD11	39:DL:112:PHE:HZ	1.53	0.71
1:AA:73:C:HO2'	1:AA:74:A:H8	1.38	0.70
47:CT:86:MET:HB2	47:CT:96:ILE:HD11	1.74	0.70
31:CA:1936:A:H2	31:CA:1943:U:N3	1.83	0.70
55:DA:1913:A:H4'	55:DA:1913:A:OP1	1.90	0.70
55:DA:2255:G:H21	69:DA:3219:TRS:H12	1.56	0.70
31:CA:846:U:H1'	31:CA:847:U:H5	1.56	0.70
55:DA:2628:C:H5'	59:DA:3195:PUT:H12	1.73	0.69
31:CA:1478:G:H1	31:CA:1513:U:H3	1.39	0.69
54:DI:64:VAL:HG22	54:DI:69:PHE:HB2	1.75	0.69
39:DL:30:ARG:HD2	55:DA:2674:G:H4'	1.74	0.69
24:C3:19:ARG:HG3	31:CA:126:A:O5'	1.94	0.68
55:DA:1478:G:H1	55:DA:1513:U:H3	1.38	0.68
2:BB:23:TRP:HB3	2:BB:39:HIS:HE1	1.56	0.68
34:CF:36:LEU:HD21	34:CF:91:LEU:HD11	1.76	0.68
59:DA:3195:PUT:H11	70:DA:5703:HOH:O	1.94	0.68
4:BD:201:VAL:HG11	5:BE:103:THR:HB	1.76	0.67
11:BK:88:GLY:N	11:BK:114:THR:HG22	2.09	0.67
22:D1:55:ILE:HD12	42:DO:33:ILE:HD11	1.76	0.67
52:CY:4:VAL:HG22	52:CY:11:ARG:HG3	1.75	0.67
49:DV:52:LEU:HB3	49:DV:54:GLN:HB2	1.76	0.67
31:CA:45:G:H5"	31:CA:46:G:H5'	1.76	0.67
31:CA:1250:G:H5"	45:CR:6:ARG:HD3	1.77	0.67
43:DP:39:VAL:HB	43:DP:49:VAL:HG23	1.76	0.67
1:BA:73:C:HO2'	1:BA:74:A:H8	1.42	0.66
27:C0:12:SER:HB3	31:CA:988:A:P	2.35	0.66
1:BA:502:A:OP1	12:BL:115:SER:HB2	1.95	0.66
1:BA:451:A:H2'	70:BA:1701:HOH:O	1.94	0.66
40:CM:79:LEU:HD11	40:CM:112:LEU:HD12	1.77	0.66
43:DP:31:THR:HG21	28:DB:28:C:OP1	1.97	0.65
55:DA:45:G:H5"	55:DA:46:G:H5'	1.77	0.65
35:CG:80:THR:HG23	35:CG:81:GLU:H	1.60	0.65
30:CD:133:THR:HG22	31:CA:1993:U:H4'	1.78	0.65
6:AF:102:MET:HE1	18:AR:24:LYS:HB3	1.78	0.64
26:C5:3:VAL:HG11	31:CA:2539:C:C5'	2.19	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:974:G:H8	31:CA:990:A:H62	1.46	0.64
1:AA:502:A:OP1	12:AL:115:SER:HB2	1.97	0.64
12:BL:110:ARG:HB2	12:BL:119:VAL:HG21	1.78	0.64
1:AA:412:A:H3'	1:AA:413:G:H5'	1.79	0.64
1:BA:841:C:H3'	1:BA:842:U:C5'	2.27	0.64
31:CA:372:G:H5"	52:CY:61:LYS:HD3	1.78	0.64
34:DF:61:SER:HB2	34:DF:91:LEU:HD21	1.79	0.64
12:BL:43:LYS:HD2	12:BL:91:PRO:HG3	1.79	0.64
24:C3:12:ARG:HD2	24:C3:44:VAL:HG11	1.80	0.64
31:CA:2394:C:H5"	40:CM:63:LYS:HE2	1.80	0.64
22:C1:43:ILE:HG22	22:C1:49:TYR:HB2	1.81	0.63
34:CF:61:SER:HB2	34:CF:91:LEU:HD21	1.80	0.63
29:CC:29:PRO:HG2	29:CC:34:LEU:HD11	1.80	0.63
31:CA:17:G:H4'	45:CR:25:TYR:HE2	1.62	0.63
31:CA:1105:U:H2'	31:CA:1106:G:C8	2.33	0.63
17:BQ:14:SER:HB3	17:BQ:22:VAL:HG12	1.80	0.63
24:D3:7:PRO:HB2	55:DA:1309:G:H4'	1.80	0.63
39:CL:76:VAL:HG12	44:CQ:73:VAL:HB	1.81	0.63
40:DM:77:ILE:HD11	40:DM:101:ILE:CG2	2.29	0.63
55:DA:31:C:O3'	55:DA:1238:G:H5"	1.98	0.63
55:DA:1105:U:H2'	55:DA:1106:G:C8	2.34	0.63
22:C1:15:MET:HB3	31:CA:2045:C:O3'	1.98	0.63
47:CT:82:MET:HB2	47:CT:98:LYS:HB2	1.79	0.63
55:DA:2256:G:H21	57:DA:3193:PG4:H31	1.63	0.63
20:BT:9:LYS:O	20:BT:12:ILE:HG13	1.98	0.62
24:C3:30:VAL:CG1	31:CA:466:A:H5"	2.29	0.62
45:DR:20:GLN:HG2	57:DR:202:PG4:H51	1.81	0.62
55:DA:1482:G:H1'	55:DA:1509:A:H61	1.65	0.62
26:C5:3:VAL:CG1	31:CA:2539:C:H5'	2.20	0.62
31:CA:2728:U:HO2'	31:CA:2729:G:H8	1.47	0.62
29:DC:29:PRO:HG2	29:DC:34:LEU:HD11	1.82	0.62
17:AQ:17:MET:HG2	17:AQ:20:SER:HB2	1.82	0.62
22:C1:8:PRO:HG2	31:CA:1264:A:H5'	1.80	0.62
5:BE:72:ILE:HG12	5:BE:145:GLU:HG3	1.80	0.62
31:CA:328:U:O3'	49:CV:66:GLN:HG3	2.00	0.62
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	1.80	0.62
1:BA:209:U:H4'	1:BA:210:C:OP2	2.00	0.61
55:DA:788:A:H3'	59:DA:3221:PUT:H41	1.82	0.61
5:AE:77:ASN:HB2	5:AE:82:GLN:HE22	1.62	0.61
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.82	0.61
16:BP:20:VAL:HG13	16:BP:32:PHE:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:1847:A:HO2'	55:DA:1848:A:H8	1.48	0.61
19:BS:6:LYS:HD2	19:BS:7:LYS:H	1.65	0.61
22:D1:43:ILE:HG22	22:D1:49:TYR:HB2	1.83	0.61
64:DD:301:PGE:H12	55:DA:2623:G:OP1	2.01	0.61
2:BB:41:ILE:HD13	2:BB:202:GLY:HA2	1.83	0.61
36:CH:15:LEU:HD22	36:CH:15:LEU:H	1.66	0.61
31:CA:674:G:H1'	33:CE:69:ARG:HD2	1.83	0.61
45:DR:20:GLN:HG2	57:DR:202:PG4:H42	1.81	0.60
12:AL:110:ARG:HB2	12:AL:119:VAL:HG21	1.81	0.60
25:C4:13:ARG:NH1	31:CA:250:G:OP2	2.33	0.60
34:CF:31:VAL:CG1	34:CF:97:TRP:CH2	2.84	0.60
33:DE:48:THR:HG23	33:DE:88:ARG:NH1	2.16	0.60
47:DT:82:MET:HB2	47:DT:98:LYS:HB2	1.82	0.60
29:CC:17:VAL:HB	29:CC:204:VAL:HG13	1.83	0.60
48:DU:80:TRP:HB3	64:DU:101:PGE:H32	1.83	0.60
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.49	0.60
13:AM:33:ILE:HD11	13:AM:63:PHE:HE1	1.66	0.60
22:C1:25:VAL:HG13	22:C1:26:THR:H	1.67	0.60
1:BA:1323:G:H2'	1:BA:1324:A:C8	2.36	0.60
31:CA:1482:G:H1'	31:CA:1509:A:H61	1.66	0.60
47:CT:59:GLU:HA	47:CT:64:ALA:HA	1.82	0.60
1:BA:843:U:H5"	1:BA:843:U:H6	1.67	0.59
31:CA:528:A:H8	31:CA:528:A:H3'	1.67	0.59
6:AF:16:GLU:HB3	4:BD:189:SER:HA	1.83	0.59
1:BA:9:G:H4'	5:BE:109:GLY:H	1.66	0.59
31:CA:1779:U:C5	31:CA:1784:A:N7	2.64	0.59
1:AA:1238:A:H5'	1:AA:1336:C:H41	1.68	0.59
2:AB:41:ILE:HD13	2:AB:202:GLY:HA2	1.83	0.59
5:BE:104:GLY:HA3	5:BE:122:ASN:HA	1.83	0.59
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.38	0.59
31:CA:528:A:H3'	31:CA:528:A:C8	2.38	0.59
22:C1:15:MET:SD	31:CA:2045:C:H5"	2.43	0.59
45:DR:19:LYS:HB3	57:DR:202:PG4:H41	1.85	0.59
1:AA:202:G:H21	1:AA:466:A:H61	1.51	0.59
1:AA:451:A:H61	1:AA:481:G:H5'	1.67	0.59
26:C5:16:ILE:HD13	26:C5:25:VAL:HG22	1.85	0.59
33:DE:33:VAL:HG22	58:DA:3192:MPD:H12	1.84	0.59
31:CA:1847:A:HO2'	31:CA:1848:A:H8	1.48	0.58
31:CA:2728:U:O2'	31:CA:2729:G:H5"	2.04	0.58
13:BM:22:ILE:HB	13:BM:25:VAL:HG12	1.86	0.58
11:AK:34:ILE:HG12	11:AK:70:CYS:SG	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:841:C:H3'	1:BA:842:U:H5"	1.86	0.58
55:DA:2128:G:H1	55:DA:2160:C:H42	1.52	0.58
1:BA:946:A:H2'	1:BA:947:G:C8	2.38	0.58
5:BE:133:PRO:O	5:BE:137:VAL:HG12	2.02	0.58
42:CO:49:GLU:OE2	42:CO:95:THR:HG22	2.04	0.58
45:DR:31:VAL:HG13	55:DA:580:U:O3'	2.03	0.58
55:DA:12:U:H2'	55:DA:12:U:O2	2.04	0.58
1:AA:946:A:H2'	1:AA:947:G:C8	2.39	0.58
32:DD:114:LYS:HE2	55:DA:2681:C:OP2	2.03	0.58
36:CH:41:LYS:HA	36:CH:44:ILE:HG12	1.86	0.58
55:DA:1105:U:H2'	55:DA:1106:G:H8	1.68	0.58
23:C2:35:GLU:HG2	23:C2:50:LYS:HG2	1.86	0.57
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.86	0.57
29:CC:120:VAL:HG12	29:CC:134:ASN:ND2	2.19	0.57
1:BA:209:U:H2'	1:BA:209:U:O2	2.03	0.57
26:D5:16:ILE:HD13	26:D5:25:VAL:HG22	1.86	0.57
18:AR:36:SER:HA	18:AR:72:ASP:HB3	1.87	0.57
7:BG:113:ASP:HB2	7:BG:119:ARG:HG3	1.86	0.57
24:D3:4:THR:HG22	55:DA:687:C:H1'	1.87	0.57
33:DE:189:THR:HG22	33:DE:192:ALA:H	1.69	0.57
31:CA:550:C:H2'	31:CA:551:G:H5"	1.86	0.57
31:CA:1105:U:H2'	31:CA:1106:G:H8	1.68	0.57
1:AA:1492:A:C5'	12:AL:44:LYS:HG2	2.34	0.57
31:CA:310:A:H5"	49:CV:15:THR:HG23	1.86	0.57
31:CA:1703:G:H2'	31:CA:1704:C:C6	2.40	0.57
36:CH:27:ARG:HH11	52:CY:60:ASP:HA	1.70	0.57
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.87	0.57
1:BA:1238:A:H5'	1:BA:1336:C:H41	1.68	0.57
34:CF:36:LEU:HD21	34:CF:91:LEU:CD1	2.34	0.57
40:CM:82:LEU:HD11	40:CM:116:VAL:CG2	2.32	0.57
48:CU:24:MET:HG2	48:CU:29:THR:O	2.05	0.57
40:CM:28:GLY:O	40:CM:29:LYS:O	2.21	0.57
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.86	0.57
47:CT:66:ILE:HA	47:CT:69:LEU:HD22	1.87	0.57
35:DG:42:GLU:HG2	35:DG:55:ARG:HH21	1.68	0.57
36:DH:41:LYS:HA	36:DH:44:ILE:HG12	1.86	0.57
1:AA:81:A:H61	1:AA:86:G:H1	1.53	0.57
29:DC:120:VAL:HG12	29:DC:134:ASN:ND2	2.20	0.57
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.87	0.56
7:AG:22:LEU:HD12	7:AG:62:PHE:HE2	1.69	0.56
22:C1:5:GLN:HG3	31:CA:2054:A:C2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:451:A:H61	1:BA:481:G:H5'	1.69	0.56
33:CE:189:THR:HG22	33:CE:192:ALA:H	1.70	0.56
5:BE:77:ASN:HB2	5:BE:82:GLN:HE22	1.68	0.56
31:CA:2095:A:H8	31:CA:2095:A:H5"	1.69	0.56
40:DM:77:ILE:HD11	40:DM:101:ILE:HG21	1.87	0.56
55:DA:62:U:O4'	58:DA:3203:MPD:H31	2.05	0.56
1:AA:8:A:C6	4:AD:206:LYS:HB3	2.40	0.56
1:BA:1012:A:H61	1:BA:1017:U:H3	1.54	0.56
32:DD:146:ILE:HD12	32:DD:155:VAL:HG21	1.88	0.56
44:DQ:96:LYS:HE3	70:DQ:306:HOH:O	2.04	0.56
55:DA:550:C:H2'	55:DA:551:G:H5"	1.87	0.56
1:AA:1277:C:HO2'	1:AA:1279:G:H8	1.53	0.56
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.36	0.56
31:CA:2304:G:H5'	34:CF:121:SER:HB2	1.87	0.56
11:AK:67:ALA:HB2	11:AK:96:THR:HG23	1.88	0.56
23:D2:35:GLU:HG2	23:D2:50:LYS:HG2	1.86	0.56
22:C1:17:ARG:NH2	31:CA:1266:G:OP2	2.39	0.55
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.36	0.55
31:CA:2019:A:H4'	45:CR:34:VAL:HG21	1.87	0.55
41:DN:18[B]:ARG:HG3	28:DB:90:C:H5'	1.89	0.55
1:AA:1012:A:H61	1:AA:1017:U:H3	1.55	0.55
8:AH:96:MET:HE3	8:AH:130:ALA:HB1	1.88	0.55
10:AJ:5:ARG:HE	10:AJ:77:VAL:HG22	1.70	0.55
1:BA:1106:G:H5"	3:BC:172:ARG:HG3	1.87	0.55
13:BM:86:TYR:CZ	13:BM:90:ARG:HD2	2.41	0.55
31:CA:457:A:N1	31:CA:470:A:H5"	2.21	0.55
1:BA:619:U:H3	4:BD:131:ASN:HB3	1.71	0.55
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.89	0.55
24:C3:9:VAL:N	31:CA:1309:G:OP1	2.33	0.55
22:D1:8:PRO:HG2	55:DA:1264:A:H5'	1.88	0.55
35:DG:175:LYS:HG3	55:DA:2529:G:H4'	1.88	0.55
55:DA:31:C:O2'	55:DA:1238:G:H5'	2.06	0.55
8:AH:29:SER:HB3	8:AH:57:PRO:HB2	1.88	0.55
5:BE:72:ILE:HG13	5:BE:73:ASN:H	1.72	0.55
1:AA:412:A:H3'	1:AA:413:G:C5'	2.37	0.55
10:AJ:35:GLN:HB2	10:AJ:77:VAL:HB	1.88	0.55
1:BA:1151:A:HO2'	1:BA:1152:A:H8	1.53	0.55
3:BC:77:ILE:HA	3:BC:84:VAL:HG23	1.88	0.55
26:C5:1:MET:HB2	31:CA:2526:G:O2'	2.06	0.55
26:C5:36:ARG:HD3	31:CA:2742:G:OP1	2.07	0.55
48:CU:18:GLU:H	48:CU:18:GLU:CD	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:85:ASN:HB3	4:BD:88:GLU:HB2	1.89	0.55
48:CU:22:THR:HA	48:CU:25:GLU:HG2	1.87	0.55
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	1.89	0.55
20:BT:28:MET:HE1	20:BT:67:ILE:HG12	1.89	0.55
31:CA:2822:G:H2'	31:CA:2823:A:H5"	1.88	0.55
55:DA:2297:A:C8	55:DA:2297:A:H5"	2.42	0.55
25:D4:64:TYR:CE2	55:DA:242:G:H5"	2.42	0.55
13:AM:86:TYR:CZ	13:AM:90:ARG:HD2	2.41	0.54
11:BK:67:ALA:HB2	11:BK:96:THR:HG23	1.88	0.54
11:BK:89:PRO:HG3	21:BU:32:VAL:HG11	1.88	0.54
25:D4:8:ARG:HD3	55:DA:245:G:O6	2.08	0.54
31:CA:2845:U:H5"	44:CQ:52:ASN:O	2.07	0.54
64:D1:102:PGE:H42	47:DT:23:LEU:HD23	1.89	0.54
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.89	0.54
31:CA:2502:G:H5"	31:CA:2503:2MA:H5"	1.90	0.54
1:BA:108:G:H5"	1:BA:108:G:N3	2.23	0.54
44:DQ:106:LYS:HA	44:DQ:109:ARG:HD3	1.90	0.54
65:DA:3223:SPD:H92	65:DA:3223:SPD:H52	1.90	0.54
11:AK:31:ILE:HG12	11:AK:46:THR:HG22	1.88	0.54
16:BP:4:ILE:HG12	16:BP:21:VAL:HG22	1.90	0.54
45:CR:87:SER:HB3	46:CS:52:PRO:HD3	1.90	0.54
5:AE:76:LEU:HD11	5:AE:120:VAL:HG22	1.90	0.54
26:C5:17:VAL:CG1	26:C5:26:ILE:HD12	2.38	0.54
39:DL:76:VAL:CG2	55:DA:2684:U:H4'	2.37	0.54
1:AA:404:G:N7	4:AD:2:ALA:HB3	2.23	0.54
5:BE:72:ILE:HG13	5:BE:73:ASN:N	2.22	0.54
23:D2:8:LYS:HE3	55:DA:2420:C:H5"	1.89	0.54
13:AM:33:ILE:HD11	13:AM:63:PHE:CE1	2.42	0.54
22:C1:4:GLN:HB3	31:CA:2615:U:H1'	1.90	0.54
10:BJ:5:ARG:HG2	10:BJ:79:PRO:HG3	1.90	0.54
11:BK:52:PHE:HE2	11:BK:65:VAL:HG21	1.73	0.54
1:AA:108:G:N3	1:AA:108:G:H5"	2.22	0.54
5:BE:35:ALA:O	5:BE:50:TYR:O	2.26	0.54
31:CA:1394:U:H4'	31:CA:1603:A:H4'	1.90	0.54
48:DU:67:VAL:HG22	48:DU:76:ARG:HG3	1.90	0.54
1:BA:374:A:OP1	1:BA:452:A:N1	2.41	0.53
1:BA:769:G:H4'	1:BA:1513:A:H4'	1.88	0.53
5:BE:126:LYS:HG2	5:BE:128:TYR:CZ	2.44	0.53
33:CE:149:ILE:HD12	33:CE:172:ALA:HA	1.89	0.53
44:CQ:106:LYS:HA	44:CQ:109:ARG:HD3	1.90	0.53
1:AA:1144:G:H21	1:AA:1146:A:H62	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:85:ASN:HB3	4:AD:88:GLU:HB2	1.90	0.53
34:CF:31:VAL:HG11	34:CF:97:TRP:CH2	2.43	0.53
13:BM:77:ILE:HG22	13:BM:81:MET:HE2	1.90	0.53
1:AA:209:U:H4'	1:AA:210:C:OP2	2.08	0.53
31:CA:1251:C:OP2	45:CR:6:ARG:HD2	2.09	0.53
1:BA:1144:G:H21	1:BA:1146:A:H62	1.56	0.53
6:BF:45:ARG:O	6:BF:56:LYS:HA	2.08	0.53
12:BL:33:VAL:HG22	12:BL:79:VAL:HG22	1.90	0.53
36:CH:4:ILE:HD11	36:CH:44:ILE:HG22	1.90	0.53
3:BC:5:VAL:HG21	3:BC:10:ILE:HD13	1.91	0.53
8:BH:96:MET:HE2	8:BH:130:ALA:HB1	1.89	0.53
2:BB:129:LEU:HD13	2:BB:134:ALA:HB2	1.91	0.53
8:BH:29:SER:HB3	8:BH:57:PRO:HB2	1.91	0.53
11:AK:52:PHE:HE2	11:AK:65:VAL:HG21	1.73	0.53
54:DI:69:PHE:HB3	54:DI:72:LEU:HD12	1.91	0.53
55:DA:2796:U:H3	55:DA:2799:A:N6	1.97	0.53
1:AA:735:C:H5'	18:AR:60:LYS:HD3	1.91	0.53
10:AJ:42:LEU:HB2	10:AJ:71:LEU:HB3	1.91	0.53
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.90	0.53
6:BF:38:ARG:HH12	6:BF:99:ALA:HB3	1.74	0.53
44:DQ:52:ASN:O	55:DA:2845:U:H5"	2.09	0.53
2:AB:129:LEU:HD13	2:AB:134:ALA:HB2	1.91	0.53
19:AS:29:LYS:HB3	19:AS:30:PRO:HD2	1.91	0.53
10:BJ:26:VAL:HG21	10:BJ:39:PRO:HD3	1.91	0.53
31:CA:1936:A:C2	31:CA:1943:U:N3	2.59	0.53
25:C4:2:PRO:HD2	31:CA:667:U:O2	2.09	0.52
25:C4:47:LYS:NZ	40:CM:64:PHE:CE1	2.77	0.52
3:AC:5:VAL:HG21	3:AC:10:ILE:HD13	1.92	0.52
31:CA:1847:A:O2'	31:CA:1848:A:H8	1.92	0.52
6:AF:45:ARG:O	6:AF:56:LYS:HA	2.08	0.52
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	1.91	0.52
22:C1:38:HIS:CE1	31:CA:2884:U:O4	2.54	0.52
6:BF:3:HIS:H	6:BF:92:THR:HG23	1.73	0.52
31:CA:2037:A:H2'	31:CA:2038:G:C8	2.44	0.52
31:CA:2796:U:H3	31:CA:2799:A:N6	1.99	0.52
32:DD:128:ARG:HG3	70:DA:7412:HOH:O	2.09	0.52
8:AH:2:SER:HB2	8:AH:4:GLN:HE21	1.75	0.52
13:AM:71:ARG:HH21	34:DF:143:TYR:HB2	1.74	0.52
26:C5:3:VAL:HG12	31:CA:2538:C:O2'	2.10	0.52
31:CA:118:A:N3	31:CA:178:G:H1'	2.25	0.52
43:CP:100:HIS:CD2	43:CP:101:GLY:H	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DG:86:LYS:HG2	35:DG:132:VAL:HG22	1.91	0.52
23:C2:11:LEU:HD21	23:C2:34:LEU:HD23	1.91	0.52
24:C3:33:ARG:NE	31:CA:467:G:OP1	2.36	0.52
31:CA:668:A:H2'	31:CA:670:A:H62	1.75	0.52
31:CA:2297:A:C8	31:CA:2297:A:H5"	2.45	0.52
48:DU:54:GLU:HB3	48:DU:88:LYS:HD2	1.92	0.52
55:DA:74:A:H5"	55:DA:74:A:N3	2.25	0.52
65:DA:3223:SPD:H92	65:DA:3223:SPD:C5	2.40	0.52
1:AA:86:G:H21	1:AA:87:C:H41	1.58	0.52
1:BA:404:G:N7	4:BD:2:ALA:HB3	2.24	0.52
22:C1:41:HIS:HE2	31:CA:2884:U:P	2.32	0.52
6:BF:38:ARG:NH1	6:BF:99:ALA:HB3	2.24	0.52
35:CG:86:LYS:HG2	35:CG:132:VAL:HG22	1.92	0.52
1:AA:845:A:O4'	1:AA:845:A:P	2.68	0.52
1:AA:1277:C:O2'	1:AA:1279:G:H8	1.93	0.52
13:AM:77:ILE:HG22	13:AM:81:MET:HE2	1.90	0.52
22:C1:19:HIS:CE1	31:CA:2624:G:H1'	2.45	0.52
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.75	0.52
33:CE:21:ARG:HD3	33:CE:106:LYS:HB3	1.92	0.52
40:DM:79:LEU:HD11	40:DM:112:LEU:HD12	1.92	0.52
41:DN:81[B]:4D4:H9	55:DA:2496:C:OP2	2.10	0.52
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.45	0.51
10:AJ:26:VAL:HG21	10:AJ:39:PRO:HD3	1.91	0.51
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.76	0.51
11:AK:23:ILE:HD11	11:AK:86:VAL:HG13	1.92	0.51
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.92	0.51
19:BS:29:LYS:HB3	19:BS:30:PRO:HD2	1.93	0.51
31:CA:699:A:H2'	31:CA:700:G:O4'	2.10	0.51
33:DE:21:ARG:HD3	33:DE:106:LYS:HB3	1.91	0.51
29:CC:13:ARG:HD3	31:CA:728:G:H4'	1.92	0.51
43:CP:51:ALA:HB3	43:CP:78:VAL:HG13	1.92	0.51
1:BA:350:G:H5"	20:BT:3:ASN:HD22	1.76	0.51
1:BA:374:A:H5"	1:BA:452:A:N1	2.25	0.51
4:BD:48:LEU:HD21	4:BD:56:ARG:HG3	1.93	0.51
31:CA:17:G:H4'	45:CR:25:TYR:CE2	2.43	0.51
32:DD:25:THR:HG21	32:DD:193:VAL:HG22	1.92	0.51
48:CU:54:GLU:HB3	48:CU:88:LYS:HD2	1.92	0.51
54:DI:44:ALA:HB1	54:DI:95:LEU:HD11	1.91	0.51
11:BK:23:ILE:HD11	11:BK:86:VAL:HG13	1.91	0.51
25:D4:8:ARG:CD	55:DA:245:G:O6	2.59	0.51
31:CA:569:U:H5"	31:CA:821:A:C2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:1853:A:N1	55:DA:2087:G:H1'	2.25	0.51
14:AN:89:MET:HE1	14:AN:98:LYS:HD2	1.93	0.51
7:BG:111:ARG:HB3	7:BG:119:ARG:HG2	1.93	0.51
31:CA:532:A:N1	31:CA:2020:A:H1'	2.25	0.51
31:CA:1447:C:H2'	31:CA:1448:G:C8	2.46	0.51
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.92	0.51
1:BA:1218:C:H2'	1:BA:1219:A:C8	2.46	0.51
1:BA:1277:C:O2'	1:BA:1279:G:H8	1.93	0.51
22:D1:22:LEU:HD23	62:D1:103:PEG:H31	1.91	0.51
30:CD:25:THR:HG21	30:CD:193:VAL:HG22	1.93	0.51
31:CA:12:U:H2'	31:CA:12:U:O2	2.11	0.51
47:CT:69:LEU:HG	47:CT:107:VAL:HG22	1.92	0.51
39:DL:38:ILE:HD11	39:DL:112:PHE:CZ	2.42	0.51
11:AK:23:ILE:HG22	11:AK:32:VAL:HG13	1.92	0.51
25:D4:31:HIS:HB2	70:D4:103:HOH:O	2.10	0.51
30:CD:4:LEU:HD22	30:CD:101:PHE:CE2	2.45	0.51
43:DP:51:ALA:HB3	43:DP:78:VAL:HG13	1.93	0.51
5:AE:126:LYS:HG2	5:AE:128:TYR:CZ	2.46	0.51
31:CA:998:C:OP2	45:CR:58:ARG:NH2	2.44	0.51
31:CA:2025:C:H2'	31:CA:2026:U:C6	2.46	0.51
31:CA:2189:U:H2'	31:CA:2190:G:H8	1.76	0.51
25:D4:60:ALA:O	40:DM:48:ARG:HD2	2.10	0.51
30:CD:129:THR:HG23	30:CD:140:HIS:O	2.11	0.51
55:DA:1847:A:O2'	55:DA:1848:A:H8	1.93	0.51
47:CT:73:LYS:HB2	47:CT:106:VAL:HB	1.92	0.50
36:DH:4:ILE:HD11	36:DH:44:ILE:HG22	1.93	0.50
12:AL:33:VAL:HG22	12:AL:79:VAL:HG22	1.92	0.50
31:CA:784:G:H5'	31:CA:785:G:OP1	2.10	0.50
38:CK:81:ILE:HG23	38:CK:82:GLY:H	1.76	0.50
1:AA:774:G:H21	57:AA:1670:PG4:H51	1.75	0.50
5:BE:106:ILE:HD11	5:BE:124:LEU:HD23	1.93	0.50
11:BK:23:ILE:HG22	11:BK:32:VAL:HG13	1.93	0.50
20:BT:4:ILE:HA	20:BT:8:LYS:HE2	1.93	0.50
31:CA:335:C:H5"	49:CV:82:ARG:HD3	1.93	0.50
34:DF:131:GLY:HA3	55:DA:2305:U:H5"	1.94	0.50
55:DA:1026:G:H2'	55:DA:1027:A:C8	2.45	0.50
24:C3:19:ARG:NH2	31:CA:125:A:OP2	2.41	0.50
35:DG:19:ILE:HG12	35:DG:24:ILE:HG12	1.93	0.50
9:BI:19:VAL:HG22	9:BI:65:ILE:HG22	1.92	0.50
1:AA:1358:U:H3	1:AA:1363:A:H62	1.59	0.50
19:AS:15:LEU:HD13	19:AS:33:THR:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DI:57:ASN:HB3	54:DI:76:PHE:HB3	1.93	0.50
1:BA:1003:G:H21	1:BA:1005:A:H5'	1.77	0.50
14:BN:89:MET:HE1	14:BN:98:LYS:HD2	1.93	0.50
17:BQ:17:MET:HB3	17:BQ:20:SER:HB3	1.93	0.50
23:D2:25:LYS:HE2	23:D2:30:LYS:O	2.12	0.50
43:DP:31:THR:HG21	28:DB:28:C:P	2.51	0.50
3:AC:20:SER:HB3	14:AN:94:PRO:HG3	1.92	0.50
18:AR:45:THR:OG1	18:AR:47:THR:HG22	2.12	0.50
8:BH:2:SER:HB2	8:BH:4:GLN:HE21	1.76	0.50
31:CA:1638:C:H5"	31:CA:2710:C:O2'	2.12	0.50
55:DA:1536:C:H4'	55:DA:1537:G:H5"	1.93	0.50
7:AG:111:ARG:HB3	7:AG:119:ARG:HG2	1.93	0.50
11:BK:43:GLY:HA3	11:BK:74:VAL:HG12	1.93	0.50
31:CA:70:G:H5"	31:CA:112:U:O2	2.12	0.50
55:DA:914:G:H5"	55:DA:914:G:H8	1.77	0.50
9:AI:19:VAL:HG22	9:AI:65:ILE:HG22	1.93	0.49
1:BA:374:A:H5"	1:BA:452:A:C2	2.47	0.49
1:BA:735:C:H5'	18:BR:60:LYS:HD3	1.93	0.49
9:BI:57:MET:HG3	9:BI:61:LEU:HG	1.93	0.49
30:CD:99:GLU:HG2	30:CD:182:ALA:HB2	1.94	0.49
31:CA:532:A:N3	31:CA:532:A:H2'	2.26	0.49
43:DP:68:LYS:HB3	62:DP:201:PEG:H22	1.93	0.49
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.94	0.49
24:C3:24:THR:HG23	24:C3:27:GLY:H	1.77	0.49
34:CF:44:ILE:HG21	34:CF:79:ILE:HG22	1.94	0.49
55:DA:479:A:N3	55:DA:481:G:H5"	2.26	0.49
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	1.94	0.49
1:BA:202:G:O2'	1:BA:468:A:H8	1.95	0.49
7:BG:69:VAL:HG23	7:BG:100:ALA:HB1	1.94	0.49
18:BR:36:SER:HA	18:BR:72:ASP:HB3	1.93	0.49
22:D1:9:THR:HG21	55:DA:2020:A:H5'	1.94	0.49
29:CC:210:ALA:HA	29:CC:213:TRP:CE2	2.47	0.49
31:CA:2185:U:H2'	31:CA:2186:G:C8	2.46	0.49
31:CA:2445:2MG:HM21	31:CA:2449:U:O4	2.11	0.49
29:DC:227:PRO:HA	29:DC:233:GLY:HA2	1.95	0.49
41:CN:21:ALA:HB1	41:CN:100:LYS:HG2	1.94	0.49
54:DI:31:ARG:HB2	54:DI:79:PRO:HG2	1.93	0.49
55:DA:1433:A:O2'	55:DA:1434:A:H5'	2.12	0.49
29:CC:227:PRO:HA	29:CC:233:GLY:HA2	1.95	0.49
35:CG:19:ILE:HG12	35:CG:24:ILE:HG12	1.93	0.49
55:DA:2441:U:O2'	65:DA:3223:SPD:H91	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:411:A:P	4:AD:26:ARG:HH12	2.36	0.49
11:AK:84:VAL:HG21	11:AK:97:ILE:HG23	1.95	0.49
1:BA:202:G:H1	1:BA:215:C:H42	1.59	0.49
55:DA:789:A:OP1	59:DA:3221:PUT:H12	2.12	0.49
1:BA:76:G:H1	1:BA:93:U:H3	1.61	0.49
3:BC:113:ALA:O	3:BC:200:VAL:HG11	2.12	0.49
31:CA:1587:G:H2'	31:CA:1588:G:H8	1.78	0.49
12:AL:43:LYS:HE2	12:AL:89:D2T:H7	1.93	0.49
28:CB:14:U:H2'	28:CB:15:A:H2	1.76	0.49
1:AA:202:G:O2'	1:AA:468:A:H8	1.95	0.49
1:AA:736:C:H5'	6:AF:88:MET:HE2	1.94	0.49
1:AA:1003:G:H21	1:AA:1005:A:H5'	1.77	0.49
1:BA:840:C:H2'	1:BA:841:C:O4'	2.13	0.49
47:CT:4:ILE:HG12	47:CT:106:VAL:HG22	1.94	0.49
5:AE:107:ALA:HB2	5:AE:125:ALA:HB3	1.94	0.48
11:AK:34:ILE:HB	11:AK:74:VAL:HG11	1.95	0.48
3:BC:20:SER:HB3	14:BN:94:PRO:HG3	1.93	0.48
3:BC:47:LEU:HB3	3:BC:50:ALA:HB3	1.95	0.48
31:CA:479:A:N3	31:CA:481:G:H5"	2.28	0.48
31:CA:1182:G:H2'	31:CA:1183:U:O4'	2.13	0.48
32:DD:99:GLU:HG2	32:DD:182:ALA:HB2	1.94	0.48
33:CE:75:SER:O	33:CE:78:TRP:HB2	2.13	0.48
39:CL:43:ILE:HD12	39:CL:56:ASP:HB2	1.94	0.48
28:DB:84:G:H21	63:DB:211:EDO:H11	1.78	0.48
55:DA:837:C:H5	70:DA:6720:HOH:O	1.95	0.48
15:AO:82:ILE:HG21	15:AO:89:ARG:OXT	2.13	0.48
31:CA:2630:G:O4'	31:CA:2894:G:H1'	2.13	0.48
32:DD:13:ARG:NH1	70:DD:401:HOH:O	2.44	0.48
4:AD:48:LEU:HD21	4:AD:56:ARG:HG3	1.94	0.48
2:BB:73:LYS:HD2	2:BB:168:HIS:HD2	1.77	0.48
3:BC:72:ARG:HB3	3:BC:75:ILE:HG22	1.94	0.48
31:CA:2060:A:N6	33:CE:69:ARG:NH2	2.60	0.48
1:BA:736:C:H5'	6:BF:88:MET:HE2	1.94	0.48
29:CC:177:ARG:HG2	31:CA:1820:U:OP1	2.14	0.48
31:CA:914:G:H8	31:CA:914:G:H5"	1.79	0.48
31:CA:2623:G:H4'	31:CA:2825:G:H8	1.78	0.48
35:CG:80:THR:HG23	35:CG:81:GLU:N	2.24	0.48
9:AI:57:MET:HG3	9:AI:61:LEU:HG	1.94	0.48
25:C4:24:HIS:CG	40:CM:61:LEU:HD13	2.49	0.48
1:BA:677:U:H3	1:BA:713:G:H22	1.61	0.48
11:BK:30:THR:HG21	11:BK:92:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:CB:14:U:H2'	28:CB:15:A:C2	2.49	0.48
31:CA:634:C:H2'	31:CA:635:C:C6	2.49	0.48
43:DP:31:THR:HG22	43:DP:33:ARG:H	1.79	0.48
54:DI:50:VAL:HG13	54:DI:85:VAL:HG22	1.95	0.48
1:AA:413:G:H5"	1:AA:414:A:H5'	1.96	0.48
24:C3:37:LYS:O	31:CA:458:G:H2'	2.13	0.48
25:D4:64:TYR:CZ	55:DA:242:G:H5"	2.49	0.48
2:AB:20:THR:HG22	2:AB:39:HIS:CE1	2.48	0.48
11:AK:30:THR:HG21	11:AK:92:GLY:HA3	1.95	0.48
25:C4:54:ASP:HB3	40:CM:57:LEU:HD22	1.95	0.48
31:CA:247:G:H4'	31:CA:386:G:C5	2.49	0.48
39:CL:38:ILE:HD11	39:CL:112:PHE:CZ	2.38	0.48
47:DT:4:ILE:HG12	47:DT:106:VAL:HG22	1.94	0.48
47:DT:72:THR:HG21	47:DT:108:SER:HB3	1.95	0.48
5:AE:38:VAL:HG11	5:AE:114:VAL:HG22	1.96	0.48
23:D2:11:LEU:HD21	23:D2:34:LEU:HD23	1.94	0.48
40:DM:21:ARG:HA	55:DA:811:U:H2'	1.95	0.48
41:DN:41:LEU:HG	41:DN:96:ILE:HG13	1.96	0.48
7:AG:22:LEU:HD12	7:AG:62:PHE:CE2	2.48	0.48
5:BE:36:LEU:HD21	5:BE:137:VAL:HG11	1.95	0.48
22:D1:55:ILE:HD12	42:DO:33:ILE:CD1	2.44	0.48
32:DD:150[B]:MEQ:HE2	55:DA:2033:A:O5'	2.14	0.48
34:DF:44:ILE:HG21	34:DF:79:ILE:HG22	1.95	0.48
47:DT:73:LYS:HB2	47:DT:106:VAL:HB	1.95	0.48
51:DX:41[A]:ARG:HG3	55:DA:2386:A:N3	2.28	0.48
55:DA:11:C:H2'	55:DA:12:U:H5'	1.95	0.48
1:AA:542:G:H5'	4:AD:39:GLY:HA3	1.96	0.47
22:D1:25:VAL:HG11	47:DT:38:TYR:HB2	1.96	0.47
34:CF:36:LEU:HB2	34:CF:57:LEU:HD21	1.96	0.47
45:DR:6:ARG:HD3	55:DA:1250:G:H5"	1.95	0.47
55:DA:1172:C:C5	55:DA:1173:U:H1'	2.49	0.47
55:DA:1587:G:H2'	55:DA:1588:G:H8	1.79	0.47
5:AE:133:PRO:O	5:AE:137:VAL:HG13	2.14	0.47
23:C2:25:LYS:HE2	23:C2:30:LYS:O	2.14	0.47
1:BA:542:G:H5'	4:BD:39:GLY:HA3	1.96	0.47
17:BQ:76:VAL:HG12	17:BQ:77:ARG:HG3	1.97	0.47
31:CA:1364:G:P	52:CY:50:ARG:HH22	2.36	0.47
37:CJ:19:ASN:H	37:CJ:20:PRO:HD2	1.80	0.47
55:DA:1975:G:H21	64:DA:3224:PGE:C2	2.27	0.47
1:AA:1055:A:H2'	3:AC:156:ARG:HD2	1.96	0.47
6:AF:38:ARG:HE	6:AF:63:ASN:ND2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1391:U:H2'	1:BA:1392:G:C8	2.49	0.47
32:DD:8:LYS:HB2	32:DD:201:LEU:HD11	1.96	0.47
39:DL:43:ILE:HD12	39:DL:56:ASP:HB2	1.96	0.47
1:BA:1190:G:H5'	3:BC:176:HIS:NE2	2.29	0.47
32:DD:105:LYS:NZ	32:DD:106:LYS:HE3	2.30	0.47
37:DJ:103:ARG:HA	37:DJ:106:LEU:HD12	1.96	0.47
55:DA:2291:U:H2'	55:DA:2292:U:C6	2.49	0.47
11:BK:84:VAL:HG21	11:BK:97:ILE:HG23	1.97	0.47
31:CA:2185:U:H2'	31:CA:2186:G:H8	1.79	0.47
34:CF:8:TYR:HA	34:CF:12:VAL:HB	1.97	0.47
13:AM:4:ILE:HD12	13:AM:10:PRO:HG2	1.95	0.47
25:C4:25:LYS:HD3	40:CM:62:PRO:HG2	1.97	0.47
31:CA:1141:U:H4'	31:CA:1142:A:O4'	2.15	0.47
52:CY:10:LYS:HE3	52:CY:54:LYS:HG2	1.97	0.47
55:DA:789:A:OP1	59:DA:3221:PUT:C1	2.63	0.47
1:AA:269:C:H2'	1:AA:270:A:C8	2.50	0.47
22:D1:5:GLN:O	55:DA:2017:U:H4'	2.15	0.47
30:CD:26:VAL:HG21	44:CQ:5:ILE:HG12	1.97	0.47
31:CA:2030:6MZ:C2	31:CA:2499:C:H5"	2.45	0.47
34:DF:8:TYR:HA	34:DF:12:VAL:HB	1.97	0.47
34:DF:36:LEU:HB2	34:DF:57:LEU:HD21	1.96	0.47
36:DH:49:ALA:O	36:DH:53:GLU:HB3	2.15	0.47
37:DJ:19:ASN:H	37:DJ:20:PRO:HD2	1.80	0.47
43:DP:52:SER:OG	43:DP:54:VAL:HG22	2.14	0.47
49:DV:73:PHE:CE2	49:DV:75:ALA:HA	2.49	0.47
52:DY:10:LYS:HE3	52:DY:54:LYS:HG2	1.97	0.47
55:DA:644:A:H2'	55:DA:645:C:O4'	2.14	0.47
55:DA:1975:G:H21	64:DA:3224:PGE:H2	1.79	0.47
24:C3:3:ARG:HD3	31:CA:1613:G:O2'	2.15	0.47
1:BA:269:C:H2'	1:BA:270:A:C8	2.50	0.47
1:BA:846:G:H2'	1:BA:847:G:H8	1.79	0.47
30:CD:155:VAL:HG21	31:CA:2618:G:H21	1.79	0.47
31:CA:608:A:H2'	31:CA:609:A:C8	2.50	0.47
31:CA:2060:A:N6	33:CE:69:ARG:HH21	2.13	0.47
31:CA:2291:U:H2'	31:CA:2292:U:C6	2.50	0.47
32:DD:186:LEU:HD21	44:DQ:4:ILE:HG21	1.95	0.47
49:CV:74:ASN:HD22	49:CV:77:THR:H	1.63	0.47
39:DL:113:MET:HE1	39:DL:116:ILE:HD11	1.97	0.47
1:AA:677:U:H3	1:AA:713:G:H22	1.63	0.47
24:C3:7:PRO:CB	31:CA:1309:G:H4'	2.37	0.47
55:DA:1236:G:N7	59:DA:3189:PUT:H41	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C4:25:LYS:O	40:CM:62:PRO:HD2	2.15	0.47
31:CA:193:U:H5	70:CA:3372:HOH:O	1.98	0.47
31:CA:1936:A:H62	31:CA:1963:U:H3	1.60	0.47
33:CE:1:MET:HG2	33:CE:14:VAL:HG23	1.97	0.47
38:DK:69:ARG:O	38:DK:90:GLU:HB2	2.16	0.47
55:DA:1182:G:H2'	55:DA:1183:U:O4'	2.15	0.47
1:AA:310:G:H5"	16:AP:31:ARG:HB2	1.97	0.46
5:BE:57:PRO:O	5:BE:60:ILE:HG13	2.15	0.46
33:DE:176:ASP:OD2	33:DE:178:VAL:HG12	2.15	0.46
55:DA:749:A:H4'	55:DA:1271:G:N3	2.29	0.46
1:AA:73:C:O2'	1:AA:74:A:H8	1.97	0.46
1:BA:23:C:H5	1:BA:561:U:O4	1.98	0.46
1:BA:1055:A:H2'	3:BC:156:ARG:HD2	1.97	0.46
2:BB:73:LYS:HD2	2:BB:168:HIS:CD2	2.51	0.46
42:CO:47:VAL:O	42:CO:51:LEU:HD23	2.15	0.46
43:CP:31:THR:HG22	43:CP:33:ARG:H	1.79	0.46
34:DF:121:SER:HB2	55:DA:2304:G:H5'	1.96	0.46
6:AF:47:LEU:HD13	6:AF:51:ILE:HG12	1.97	0.46
31:CA:309:A:H4'	49:CV:16:GLY:HA2	1.97	0.46
31:CA:846:U:H1'	31:CA:847:U:C5	2.44	0.46
34:CF:103:LEU:HA	34:CF:107:ALA:HB3	1.97	0.46
49:CV:7:ARG:O	49:CV:25:VAL:HB	2.15	0.46
34:DF:103:LEU:HA	34:DF:107:ALA:HB3	1.97	0.46
55:DA:1180:U:H5"	55:DA:1180:U:H6	1.80	0.46
21:AU:4:ILE:HG13	21:AU:19:PHE:HA	1.97	0.46
1:BA:202:G:H21	1:BA:466:A:H61	1.62	0.46
19:BS:15:LEU:HD13	19:BS:33:THR:HG21	1.95	0.46
30:CD:152:PRO:HG3	30:CD:156:PHE:CZ	2.51	0.46
51:DX:39:ARG:NH1	70:DX:101:HOH:O	2.48	0.46
1:AA:76:G:H1	1:AA:93:U:H3	1.62	0.46
64:D1:102:PGE:H4	70:DT:313:HOH:O	2.15	0.46
30:CD:3:GLY:O	30:CD:4:LEU:HD13	2.15	0.46
30:CD:62:LYS:HE2	31:CA:2810:A:H5"	1.98	0.46
30:CD:133:THR:CG2	31:CA:1993:U:H4'	2.45	0.46
31:CA:740:C:H5'	31:CA:1784:A:C3'	2.38	0.46
40:CM:77:ILE:CD1	40:CM:108:ALA:HB1	2.36	0.46
55:DA:57:C:H2'	55:DA:58:G:O4'	2.16	0.46
1:AA:1190:G:H5'	3:AC:176:HIS:NE2	2.31	0.46
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.50	0.46
1:BA:1001:C:H2'	1:BA:1002:G:H8	1.81	0.46
21:BU:4:ILE:HG13	21:BU:19:PHE:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:219:THR:O	31:CA:1789:A:H5"	2.15	0.46
31:CA:749:A:H4'	31:CA:1271:G:N3	2.29	0.46
31:CA:1010:A:H5'	45:CR:62:ILE:CG2	2.46	0.46
31:CA:1250:G:C5'	45:CR:6:ARG:HD3	2.44	0.46
44:CQ:114:LEU:HD23	44:CQ:114:LEU:H	1.81	0.46
55:DA:102:U:H2'	55:DA:102:U:O2	2.15	0.46
29:DC:207:LYS:HB2	55:DA:729:G:C6	2.51	0.46
45:CR:58:ARG:HA	45:CR:61:TRP:CE3	2.50	0.46
48:CU:45:ALA:O	48:CU:49:LYS:HG2	2.14	0.46
52:DY:61:LYS:HD3	55:DA:372:G:H5"	1.98	0.46
17:AQ:76:VAL:HG12	17:AQ:77:ARG:HG3	1.97	0.46
23:C2:22:THR:HG21	31:CA:2419:U:H5"	1.98	0.46
1:BA:310:G:H5"	16:BP:31:ARG:HB2	1.97	0.46
1:BA:376:G:H5"	16:BP:5:ARG:HB2	1.97	0.46
1:BA:438:U:H5'	4:BD:120:HIS:HB3	1.97	0.46
24:D3:4:THR:HA	55:DA:687:C:O4'	2.14	0.46
29:CC:235:GLY:HA3	29:CC:239:ASN:HB2	1.97	0.46
31:CA:948:C:H1'	31:CA:984:A:C8	2.50	0.46
35:CG:80:THR:CG2	35:CG:81:GLU:H	2.27	0.46
40:DM:60:ARG:HD2	55:DA:2360:G:H1'	1.98	0.46
1:AA:216:U:H2'	1:AA:217:C:C6	2.50	0.46
1:BA:1496:C:H2'	1:BA:1497:G:O4'	2.16	0.46
23:D2:10:LYS:HE3	23:D2:53:LYS:O	2.16	0.46
48:CU:67:VAL:HG22	48:CU:76:ARG:HG3	1.98	0.46
1:AA:438:U:H5'	4:AD:120:HIS:HB3	1.98	0.46
1:AA:1054:C:H5"	1:AA:1054:C:H6	1.80	0.46
5:AE:57:PRO:O	5:AE:60:ILE:HG13	2.15	0.46
18:BR:27:ALA:O	18:BR:30:LYS:HG2	2.16	0.46
31:CA:694:U:OP1	31:CA:1569:A:H1'	2.15	0.46
31:CA:833:A:H2'	31:CA:834:G:C8	2.51	0.46
55:DA:722:A:H2'	55:DA:723:C:O4'	2.16	0.46
55:DA:871:U:H2'	55:DA:872:U:C6	2.51	0.46
55:DA:2070:A:H2'	55:DA:2071:A:O4'	2.16	0.46
55:DA:2800:A:C2	55:DA:2895:G:H1'	2.51	0.46
5:AE:16:ILE:HD13	5:AE:137:VAL:HG11	1.97	0.45
1:BA:846:G:H2'	1:BA:847:G:C8	2.51	0.45
9:BI:7:TYR:HE1	9:BI:18:ARG:HB2	1.80	0.45
22:D1:9:THR:CG2	55:DA:2020:A:H5'	2.46	0.45
31:CA:594:U:H2'	31:CA:595:C:C6	2.51	0.45
36:DH:104:THR:HG22	36:DH:109:GLU:HA	1.97	0.45
2:AB:97:LEU:H	2:AB:100:MET:HE3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:CD:8:LYS:HB2	30:CD:201:LEU:HD11	1.97	0.45
29:DC:177:ARG:HG2	55:DA:1820:U:OP1	2.16	0.45
29:DC:235:GLY:HA3	29:DC:239:ASN:HB2	1.98	0.45
41:CN:69:PRO:O	41:CN:93:VAL:O	2.34	0.45
55:DA:2086:U:H2'	55:DA:2087:G:C8	2.51	0.45
55:DA:2117:A:H61	55:DA:2171:A:H61	1.63	0.45
65:DA:3223:SPD:H82	70:DA:4260:HOH:O	2.16	0.45
10:AJ:52:LEU:HB2	14:AN:81:ARG:HD2	1.99	0.45
1:BA:216:U:H2'	1:BA:217:C:C6	2.51	0.45
1:BA:411:A:P	4:BD:26:ARG:HH12	2.39	0.45
1:BA:1108:G:H5"	3:BC:176:HIS:CE1	2.52	0.45
31:CA:1326:U:H2'	31:CA:1327:A:H8	1.81	0.45
37:CJ:103:ARG:HA	37:CJ:106:LEU:HD12	1.96	0.45
43:CP:31:THR:HG22	43:CP:34:HIS:H	1.81	0.45
33:DE:1:MET:HG2	33:DE:14:VAL:HG23	1.97	0.45
42:DO:9:GLN:O	42:DO:17:ARG:HD3	2.17	0.45
51:DX:37:ILE:HG21	51:DX:80:ILE:HG21	1.98	0.45
52:DY:7:VAL:HG23	52:DY:51:VAL:HG12	1.98	0.45
55:DA:2628:C:C5'	59:DA:3195:PUT:H12	2.42	0.45
1:AA:845:A:H2'	1:AA:846:G:O4'	2.17	0.45
1:AA:923:A:OP1	5:AE:26:LYS:HG2	2.16	0.45
26:C5:1:MET:HE3	31:CA:2742:G:H5"	1.96	0.45
1:BA:1053:G:N7	1:BA:1200:C:H5"	2.32	0.45
2:BB:97:LEU:H	2:BB:100:MET:HE3	1.81	0.45
2:BB:163:VAL:HG11	2:BB:173:ILE:HD11	1.99	0.45
31:CA:871:U:H2'	31:CA:872:U:C6	2.51	0.45
32:DD:152:PRO:HG3	32:DD:156:PHE:CZ	2.52	0.45
38:CK:69:ARG:O	38:CK:90:GLU:HB3	2.16	0.45
45:DR:58:ARG:HA	45:DR:61:TRP:CE3	2.51	0.45
55:DA:1133:A:N3	59:DA:3212:PUT:H22	2.32	0.45
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	1.97	0.45
1:AA:376:G:H5"	16:AP:5:ARG:HB2	1.98	0.45
27:D0:15:GLY:HA2	55:DA:969:G:O3'	2.16	0.45
31:CA:2296:U:H5	43:CP:9:ARG:NH2	2.14	0.45
33:DE:32:VAL:HG21	40:DM:6:LEU:HD13	1.99	0.45
2:AB:93:ASN:H	2:AB:93:ASN:HD22	1.65	0.45
1:BA:8:A:H1'	5:BE:108:GLY:HA2	1.97	0.45
31:CA:191:A:H2'	31:CA:192:C:C6	2.51	0.45
31:CA:722:A:H2'	31:CA:723:C:O4'	2.16	0.45
47:CT:84:ARG:HB2	47:CT:96:ILE:HB	1.99	0.45
48:CU:28:ASN:ND2	48:CU:91:GLN:HB3	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DG:103:ILE:HD11	35:DG:117:LEU:HD21	1.99	0.45
1:BA:923:A:OP1	5:BE:26:LYS:HG2	2.17	0.45
31:CA:248:G:H5'	31:CA:250:G:N7	2.31	0.45
31:CA:381:G:OP1	52:CY:18:ARG:HD3	2.16	0.45
31:CA:674:G:H1'	33:CE:69:ARG:HH11	1.82	0.45
31:CA:2544:G:H5'	31:CA:2645:G:C2	2.51	0.45
39:CL:7:MET:HE1	39:CL:44:LYS:HG3	1.98	0.45
45:CR:112:LYS:HD3	46:CS:48:LYS:HG3	1.99	0.45
43:DP:35:ILE:HG21	43:DP:71:ALA:HA	1.98	0.45
44:DQ:52:ASN:O	44:DQ:53:ARG:HD3	2.16	0.45
55:DA:136:G:H1	55:DA:143:C:H42	1.65	0.45
55:DA:1168:G:H8	55:DA:1168:G:H5"	1.81	0.45
4:AD:172:GLU:HG2	4:AD:183:LYS:HD2	1.99	0.45
8:AH:105:SER:HB2	8:AH:126:ILE:HD11	1.98	0.45
2:BB:93:ASN:HD22	2:BB:93:ASN:H	1.65	0.45
31:CA:1810:A:H2'	31:CA:1811:G:O4'	2.17	0.45
31:CA:1965:C:H5"	31:CA:1966:A:H2'	1.99	0.45
33:CE:176:ASP:OD2	33:CE:178:VAL:HG12	2.16	0.45
46:CS:49:ILE:HB	46:CS:51:VAL:O	2.17	0.45
55:DA:2609:U:C5	63:DA:3194:EDO:H12	2.52	0.45
1:AA:202:G:H1	1:AA:215:C:H42	1.64	0.45
47:CT:72:THR:HG21	47:CT:108:SER:HB3	1.98	0.45
54:DI:70:GLU:HG2	54:DI:73:LYS:HE3	1.98	0.45
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.82	0.45
25:C4:47:LYS:NZ	40:CM:64:PHE:CD1	2.75	0.45
24:D3:33:ARG:HG3	62:D3:102:PEG:H31	1.99	0.45
31:CA:278:A:N3	31:CA:278:A:H2'	2.32	0.45
31:CA:826:U:O2'	40:CM:53:GLY:HA3	2.17	0.45
31:CA:1775:U:O4	31:CA:1789:A:H2	2.00	0.45
38:DK:7:LYS:O	38:DK:11:VAL:HG23	2.17	0.45
46:DS:8:GLY:HA2	55:DA:1161:C:O2'	2.17	0.45
50:DW:38:LEU:HD21	50:DW:65:VAL:HG11	1.99	0.45
55:DA:355:U:H2'	55:DA:356:G:H8	1.82	0.45
4:BD:172:GLU:HG2	4:BD:183:LYS:HD2	1.99	0.44
31:CA:320:A:H4'	31:CA:322:A:N7	2.32	0.44
31:CA:478:A:H61	31:CA:500:G:H4'	1.81	0.44
29:DC:199:GLU:O	29:DC:202:LEU:HB2	2.17	0.44
55:DA:278:A:N3	55:DA:278:A:H2'	2.32	0.44
55:DA:612:G:H2'	55:DA:614:A:C8	2.52	0.44
55:DA:1283:G:H1'	55:DA:1329:U:O2	2.17	0.44
55:DA:1349:C:O2'	57:DA:3215:PG4:H82	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.81	0.44
22:C1:16:ARG:HA	31:CA:2046:G:C5'	2.47	0.44
1:BA:957:U:O2	1:BA:959:A:H8	2.01	0.44
1:BA:1493:A:H1'	31:CA:1913:A:H61	1.82	0.44
2:BB:68:LEU:HD11	2:BB:92:VAL:HG23	2.00	0.44
54:DI:132:TYR:H	54:DI:133:GLU:HB2	1.81	0.44
55:DA:760:G:H4'	55:DA:1776:G:OP1	2.18	0.44
1:AA:957:U:O2	1:AA:959:A:H8	2.01	0.44
1:BA:1054:C:H5"	1:BA:1054:C:H6	1.83	0.44
6:BF:47:LEU:HD13	6:BF:51:ILE:HG12	1.99	0.44
31:CA:639:U:H2'	31:CA:640:C:C6	2.52	0.44
31:CA:1556:C:H2'	31:CA:1557:C:C6	2.52	0.44
31:CA:2641:G:H5"	38:CK:78:THR:HB	1.99	0.44
29:DC:212:ARG:HD2	29:DC:216:VAL:O	2.18	0.44
34:DF:16:LEU:HD13	34:DF:29:PRO:HD2	1.99	0.44
43:DP:31:THR:HG22	43:DP:34:HIS:H	1.80	0.44
1:AA:1053:G:N7	1:AA:1200:C:H5"	2.33	0.44
2:AB:68:LEU:HD11	2:AB:92:VAL:HG23	1.99	0.44
24:C3:2:LYS:NZ	70:C3:101:HOH:O	2.49	0.44
1:BA:73:C:O2'	1:BA:74:A:H8	1.97	0.44
1:BA:1226:C:H2'	13:BM:102:THR:HB	1.99	0.44
31:CA:811:U:H2'	40:CM:21:ARG:HA	1.99	0.44
51:CX:37:ILE:HG21	51:CX:80:ILE:HG21	1.98	0.44
1:AA:9:G:H5'	5:AE:108:GLY:HA3	1.99	0.44
1:AA:864:A:H4'	5:AE:90:THR:HG23	2.00	0.44
9:AI:99:ARG:HG2	9:AI:104:VAL:HG21	1.99	0.44
13:AM:12:HIS:HB3	70:AM:302:HOH:O	2.17	0.44
22:C1:53:LYS:HE3	22:C1:56:ALA:HA	1.99	0.44
25:C4:4:ILE:HG23	31:CA:666:A:O2'	2.17	0.44
11:BK:84:VAL:HG11	11:BK:97:ILE:HG12	2.00	0.44
14:BN:31:ILE:HG23	14:BN:42:TRP:CZ2	2.53	0.44
20:BT:58:VAL:HG13	20:BT:72:ALA:HB1	1.99	0.44
31:CA:747:5MU:O2	31:CA:2014:A:H1'	2.18	0.44
31:CA:863:A:H2'	31:CA:864:G:C8	2.53	0.44
31:CA:2674:G:H4'	39:CL:30:ARG:HD2	2.00	0.44
29:DC:203:ARG:HH21	29:DC:205:LEU:HD21	1.82	0.44
34:CF:16:LEU:HD13	34:CF:29:PRO:HD2	1.98	0.44
50:CW:38:LEU:HD21	50:CW:65:VAL:HG11	1.98	0.44
33:DE:84:THR:HG21	55:DA:586:A:H5'	1.98	0.44
55:DA:1321:A:C2	64:DA:3216:PGE:H12	2.53	0.44
2:AB:129:LEU:H	2:AB:129:LEU:HG	1.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DC:13:ARG:HD3	55:DA:728:G:H4'	2.00	0.44
43:CP:35:ILE:HG21	43:CP:71:ALA:HA	1.98	0.44
55:DA:639:U:H2'	55:DA:640:C:C6	2.53	0.44
8:AH:87:LYS:HB2	8:AH:125:ILE:CD1	2.41	0.44
13:AM:17:ILE:HD12	13:AM:17:ILE:H	1.83	0.44
25:C4:13:ARG:NH1	31:CA:250:G:P	2.91	0.44
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	2.00	0.44
31:CA:659:G:H4'	33:CE:95:LYS:HD3	1.99	0.44
36:CH:104:THR:HG22	36:CH:109:GLU:HA	1.98	0.44
39:DL:7:MET:HE1	39:DL:44:LYS:HG3	2.00	0.44
54:DI:85:VAL:HG21	54:DI:90:GLY:O	2.17	0.44
55:DA:62:U:H5'	58:DA:3203:MPD:H53	2.00	0.44
55:DA:493:G:H2'	55:DA:494:G:O4'	2.18	0.44
55:DA:1831:G:H1'	64:DA:3224:PGE:H22	1.98	0.44
1:AA:1496:C:H2'	1:AA:1497:G:O4'	2.18	0.44
3:AC:21:THR:HG23	3:AC:58:GLU:HB3	1.99	0.44
11:AK:84:VAL:HG11	11:AK:97:ILE:HG12	1.99	0.44
23:C2:33:LYS:HA	23:C2:52:ALA:HB3	2.00	0.44
1:BA:1060:U:H5	3:BC:2:GLY:HA3	1.81	0.44
29:CC:199:GLU:O	29:CC:202:LEU:HB2	2.18	0.44
31:CA:2051:A:H5'	31:CA:2578:G:O4'	2.18	0.44
38:CK:7:LYS:O	38:CK:11:VAL:HG23	2.17	0.44
37:DJ:11:LEU:HD22	37:DJ:24:VAL:HG23	2.00	0.44
24:C3:7:PRO:HG3	31:CA:1612:C:H5'	2.00	0.44
1:BA:978:A:O2'	1:BA:1322:C:H5	2.00	0.44
20:BT:5:LYS:HB3	20:BT:7:ALA:H	1.82	0.44
29:CC:212:ARG:HD2	29:CC:216:VAL:O	2.18	0.44
31:CA:95:A:H4'	53:CZ:38:GLN:O	2.18	0.44
31:CA:528:A:C8	31:CA:528:A:C3'	3.00	0.44
31:CA:1469:A:H2'	31:CA:1470:A:C8	2.53	0.44
31:CA:1808:A:N1	52:CY:28:ARG:HD2	2.33	0.44
46:DS:41:ILE:HD13	46:DS:103:ALA:HA	1.99	0.44
49:DV:94:ARG:HB3	49:DV:103:ILE:HD12	1.99	0.44
17:AQ:8:LEU:HD13	17:AQ:25:ILE:HG13	1.99	0.43
4:BD:85:ASN:HA	5:BE:102:GLY:CA	2.31	0.43
14:BN:10:GLU:HG3	14:BN:63:ARG:HD2	2.00	0.43
30:CD:13:ARG:HD3	30:CD:21:SER:OG	2.18	0.43
31:CA:1274:A:N3	31:CA:1297:C:H1'	2.33	0.43
31:CA:1991:U:H2'	31:CA:1992:G:H5"	2.00	0.43
45:CR:113:ALA:O	45:CR:117:LEU:HD12	2.18	0.43
50:CW:51:GLN:HG2	50:CW:86:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:DN:42:THR:HG22	41:DN:93:VAL:HG12	1.99	0.43
1:AA:1060:U:H4'	10:AJ:53:ILE:HG23	2.00	0.43
14:AN:10:GLU:HG3	14:AN:63:ARG:HD2	2.00	0.43
14:AN:46:LEU:HA	14:AN:49:GLN:HE21	1.83	0.43
16:BP:20:VAL:CG1	16:BP:32:PHE:HB2	2.47	0.43
31:CA:355:U:H2'	31:CA:356:G:H8	1.83	0.43
34:CF:5:HIS:HB2	34:CF:97:TRP:CD1	2.53	0.43
55:DA:1394:U:H4'	55:DA:1603:A:H4'	2.00	0.43
2:AB:70:VAL:HB	2:AB:163:VAL:HG22	2.00	0.43
2:AB:163:VAL:HG11	2:AB:173:ILE:HD11	2.00	0.43
1:BA:10:A:OP2	5:BE:131:THR:HG21	2.18	0.43
1:BA:1060:U:H4'	10:BJ:53:ILE:HG23	2.00	0.43
6:BF:70:VAL:HA	6:BF:73:GLU:HG2	2.00	0.43
10:BJ:52:LEU:HB2	14:BN:81:ARG:HD2	2.00	0.43
31:CA:532:A:H4'	31:CA:533:G:C8	2.54	0.43
31:CA:2623:G:H4'	31:CA:2825:G:C8	2.53	0.43
31:CA:2688:G:H1'	31:CA:2721:A:N6	2.34	0.43
35:CG:17:VAL:HG11	35:CG:50:LEU:HD21	2.00	0.43
1:AA:604:G:H2'	1:AA:605:U:O4'	2.19	0.43
1:AA:1226:C:H2'	13:AM:102:THR:HB	2.00	0.43
12:AL:31:ARG:O	12:AL:58:THR:HG23	2.18	0.43
1:BA:1277:C:HO2'	1:BA:1279:G:H8	1.62	0.43
22:D1:53:LYS:HE3	22:D1:56:ALA:HA	2.00	0.43
34:DF:5:HIS:HB2	34:DF:97:TRP:CD1	2.54	0.43
34:DF:80:ARG:HB3	34:DF:83:TYR:CE1	2.53	0.43
55:DA:142:A:H2'	55:DA:143:C:C6	2.53	0.43
55:DA:1424:G:H21	64:DA:3213:PGE:H32	1.84	0.43
55:DA:2031:A:C6	55:DA:2498:OMC:H1'	2.53	0.43
17:AQ:15:ASP:HA	17:AQ:21:ILE:HG22	1.99	0.43
20:AT:44:LYS:H	20:AT:44:LYS:HG3	1.61	0.43
11:BK:24:HIS:HB3	11:BK:31:ILE:HG23	2.00	0.43
13:BM:54:ASP:HA	13:BM:57:ARG:HD2	2.00	0.43
17:BQ:46:VAL:HG11	17:BQ:61:ILE:CG2	2.48	0.43
30:CD:121:THR:HB	30:CD:127:PHE:CD2	2.54	0.43
31:CA:96:C:H4'	53:CZ:41:HIS:CG	2.53	0.43
31:CA:1030:C:OP2	41:CN:127:LYS:HE3	2.19	0.43
37:CJ:11:LEU:HD22	37:CJ:24:VAL:HG23	2.00	0.43
39:CL:103:VAL:O	39:CL:122:VAL:HB	2.18	0.43
42:CO:71:ARG:HG3	42:CO:71:ARG:O	2.19	0.43
49:CV:94:ARG:HB3	49:CV:103:ILE:HD12	1.99	0.43
54:DI:56:ARG:HA	55:DA:1107:G:OP1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DI:69:PHE:C	54:DI:71:CYS:H	2.27	0.43
10:AJ:10:LEU:HB2	10:AJ:72:ARG:HB2	2.00	0.43
3:BC:23:PHE:CD2	10:BJ:97:ASP:HB2	2.54	0.43
8:BH:105:SER:HB2	8:BH:126:ILE:HD11	1.99	0.43
25:D4:13:ARG:HH11	55:DA:2394:C:H5'	1.82	0.43
29:CC:225:MET:O	29:CC:233:GLY:O	2.36	0.43
31:CA:142:A:H2'	31:CA:143:C:C6	2.53	0.43
31:CA:309:A:O3'	49:CV:16:GLY:HA2	2.18	0.43
39:CL:113:MET:O	39:CL:116:ILE:HG13	2.18	0.43
46:DS:44:GLY:O	46:DS:45:GLU:HG2	2.17	0.43
54:DI:50:VAL:HG22	54:DI:85:VAL:HG13	2.00	0.43
55:DA:5:A:H2'	55:DA:6:A:C8	2.53	0.43
55:DA:191:A:H2'	55:DA:192:C:C6	2.53	0.43
55:DA:1028:A:N6	55:DA:1125:G:H2'	2.33	0.43
55:DA:2849:U:H4'	55:DA:2868:A:C2	2.54	0.43
1:BA:502:A:H2'	1:BA:503:C:O4'	2.19	0.43
31:CA:493:G:H2'	31:CA:494:G:O4'	2.18	0.43
31:CA:528:A:C2	31:CA:2042:A:H2'	2.54	0.43
31:CA:2728:U:O2'	31:CA:2729:G:H8	2.01	0.43
45:DR:51:ARG:HH22	55:DA:993:G:P	2.41	0.43
48:DU:33:LYS:HG3	48:DU:80:TRP:CE3	2.53	0.43
54:DI:27:VAL:HG13	54:DI:80:THR:HG23	2.00	0.43
55:DA:523:C:H4'	55:DA:540:C:O2	2.19	0.43
3:AC:7:PRO:HD2	3:AC:184:TYR:CD1	2.54	0.43
26:C5:17:VAL:HG12	26:C5:26:ILE:HD12	2.01	0.43
1:BA:1493:A:H8	1:BA:1493:A:OP2	2.01	0.43
4:BD:105:MET:SD	4:BD:143:VAL:HG22	2.59	0.43
31:CA:685:A:H5"	31:CA:774:G:O6	2.19	0.43
31:CA:2636:C:H2'	31:CA:2637:U:C6	2.54	0.43
40:CM:95:LEU:HD22	40:CM:100:ILE:HG12	2.00	0.43
42:CO:9:GLN:O	42:CO:17:ARG:HD3	2.17	0.43
46:CS:3:ALA:HB3	46:CS:101:ILE:HD12	2.01	0.43
34:DF:36:LEU:HD22	34:DF:154:ILE:HG12	2.01	0.43
38:DK:23:LYS:HE2	38:DK:142:ILE:OXT	2.19	0.43
55:DA:1654:A:H1'	55:DA:2823:A:H5'	2.00	0.43
6:AF:70:VAL:HA	6:AF:73:GLU:HG2	2.00	0.43
8:AH:66:PHE:CD2	8:AH:67:GLN:HG2	2.54	0.43
27:C0:53:PHE:CG	28:CB:83:G:H4'	2.54	0.43
1:BA:1152:A:H5'	10:BJ:15:HIS:HB2	2.01	0.43
5:BE:40:GLY:HA2	5:BE:45:ARG:O	2.19	0.43
5:BE:88:VAL:HG12	5:BE:93:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BM:90:ARG:HH21	13:BM:95:LEU:HB3	1.84	0.43
31:CA:83:A:H2	31:CA:103:A:N7	2.17	0.43
31:CA:1168:G:H5"	31:CA:1168:G:H8	1.83	0.43
46:DS:83:TYR:CE1	55:DA:1187:G:H5"	2.54	0.43
55:DA:2233:U:H2'	55:DA:2234:G:C8	2.54	0.43
1:AA:892:A:O2'	1:AA:1415:G:H4'	2.19	0.43
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.54	0.43
1:AA:1376:U:H2'	1:AA:1377:A:C8	2.54	0.43
30:CD:13:ARG:HH11	44:CQ:56:HIS:HA	1.84	0.43
31:CA:35:G:H2'	31:CA:36:G:O4'	2.19	0.43
31:CA:1936:A:N6	31:CA:1963:U:H3	2.16	0.43
31:CA:2642:G:H5'	38:CK:80:HIS:CG	2.53	0.43
32:DD:121:THR:HB	32:DD:127:PHE:CD2	2.54	0.43
35:DG:17:VAL:HG11	35:DG:50:LEU:HD21	2.00	0.43
41:DN:21:ALA:HB1	41:DN:100:LYS:HG2	2.00	0.43
46:DS:10:LYS:HE3	57:DS:202:PG4:H21	2.00	0.43
50:DW:51:GLN:HG2	50:DW:86:LEU:HD11	2.01	0.43
54:DI:26:VAL:HB	54:DI:83:ALA:HB3	2.01	0.43
62:DA:3200:PEG:H32	70:DA:3804:HOH:O	2.18	0.43
3:AC:151:VAL:HG12	3:AC:200:VAL:HG22	2.00	0.42
2:BB:104:TRP:O	2:BB:108:ARG:HB2	2.19	0.42
9:BI:99:ARG:HG2	9:BI:104:VAL:HG21	2.00	0.42
24:D3:29:GLN:HG2	62:D3:102:PEG:H21	2.01	0.42
29:CC:105:LEU:H	29:CC:105:LEU:HD12	1.84	0.42
31:CA:2106:U:H2'	31:CA:2107:G:H8	1.84	0.42
35:CG:103:ILE:HD11	35:CG:117:LEU:HD21	2.01	0.42
55:DA:1101:U:H2'	55:DA:1102:C:C6	2.54	0.42
55:DA:2326:C:H3'	70:DA:7772:HOH:O	2.18	0.42
1:AA:619:U:C2	4:AD:132:ILE:HD11	2.54	0.42
22:C1:4:GLN:CB	31:CA:2615:U:H1'	2.50	0.42
5:BE:81:LEU:HB3	5:BE:147:MET:SD	2.58	0.42
12:BL:80:ILE:HD12	12:BL:97:THR:HG22	2.01	0.42
31:CA:136:G:H1	31:CA:143:C:H42	1.65	0.42
31:CA:2815:C:H2'	31:CA:2816:G:O4'	2.19	0.42
32:DD:13:ARG:HD3	32:DD:21:SER:OG	2.18	0.42
38:CK:23:LYS:HE3	38:CK:142:ILE:OXT	2.20	0.42
50:DW:26:PHE:CE2	50:DW:44:HIS:HA	2.54	0.42
55:DA:1510:G:H2'	55:DA:1511:G:O4'	2.18	0.42
55:DA:2051:A:H5'	55:DA:2578:G:O4'	2.19	0.42
55:DA:2636:C:H2'	55:DA:2637:U:C6	2.53	0.42
8:AH:94:LYS:HB3	8:AH:117:ARG:HH22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BE:74:VAL:HG11	5:BE:144:LEU:HB3	2.01	0.42
22:D1:54:VAL:HG23	22:D1:55:ILE:HG12	2.00	0.42
34:CF:36:LEU:HD12	34:CF:154:ILE:HG12	2.01	0.42
36:CH:1:MET:HE3	36:CH:23:ALA:HA	2.01	0.42
48:CU:33:LYS:HG3	48:CU:80:TRP:CE3	2.55	0.42
50:CW:26:PHE:CE1	50:CW:44:HIS:HA	2.54	0.42
33:DE:48:THR:HG23	33:DE:88:ARG:HH12	1.82	0.42
42:DO:8:ARG:HD3	55:DA:1652:A:OP1	2.18	0.42
55:DA:1654:A:C1'	55:DA:2823:A:H5'	2.50	0.42
55:DA:1932:A:H2'	55:DA:1933:G:O4'	2.19	0.42
1:BA:864:A:H4'	5:BE:90:THR:HG23	2.01	0.42
2:BB:70:VAL:HB	2:BB:163:VAL:HG22	2.00	0.42
3:BC:47:LEU:HD22	3:BC:76:VAL:HG22	2.00	0.42
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	2.01	0.42
31:CA:822:G:O6	31:CA:943:A:H2	2.01	0.42
31:CA:2869:G:H2'	31:CA:2870:C:O4'	2.19	0.42
32:DD:167:ASN:O	64:DD:301:PGE:H52	2.20	0.42
46:CS:41:ILE:HD13	46:CS:103:ALA:HA	2.00	0.42
55:DA:189:G:N7	63:DA:3197:EDO:H21	2.35	0.42
1:BA:49:U:O2	1:BA:362:G:H1'	2.20	0.42
1:BA:604:G:H2'	1:BA:605:U:O4'	2.20	0.42
31:CA:1028:A:N6	31:CA:1125:G:H2'	2.34	0.42
31:CA:1430:G:H2'	31:CA:1431:A:O4'	2.19	0.42
31:CA:2060:A:H62	33:CE:69:ARG:NH2	2.18	0.42
39:CL:121:GLU:HG2	39:CL:122:VAL:HG23	2.02	0.42
3:AC:47:LEU:HD22	3:AC:76:VAL:HG22	2.01	0.42
5:AE:132:ASN:OD1	5:AE:134:ILE:HG22	2.20	0.42
2:BB:129:LEU:H	2:BB:129:LEU:HG	1.53	0.42
10:BJ:10:LEU:HB2	10:BJ:72:ARG:HB2	2.00	0.42
11:BK:25:ALA:HA	11:BK:30:THR:HG22	2.01	0.42
13:BM:11:ASP:HA	13:BM:45:ILE:HD13	2.01	0.42
13:BM:17:ILE:H	13:BM:17:ILE:HD12	1.84	0.42
25:D4:47:LYS:HE3	40:DM:64:PHE:CD1	2.55	0.42
38:CK:81:ILE:HG23	38:CK:82:GLY:N	2.35	0.42
42:DO:67:PHE:O	42:DO:71:ARG:HD2	2.20	0.42
55:DA:2445:2MG:HM21	55:DA:2449:H2U:O4	2.20	0.42
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.55	0.42
22:C1:15:MET:O	31:CA:2045:C:O2'	2.31	0.42
27:C0:31:ARG:HD3	31:CA:1158:C:H5"	2.02	0.42
28:CB:55:U:H1'	34:CF:26:MET:HG3	2.01	0.42
29:CC:57:GLY:HA2	29:CC:213:TRP:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:686:U:H2'	31:CA:788:A:N1	2.34	0.42
31:CA:1510:G:H2'	31:CA:1511:G:O4'	2.20	0.42
31:CA:2800:A:C2	31:CA:2895:G:H1'	2.54	0.42
29:DC:225:MET:O	29:DC:233:GLY:O	2.38	0.42
34:CF:138:PHE:HE1	34:CF:152:LEU:HD21	1.85	0.42
49:DV:51:ALA:O	49:DV:52:LEU:HB2	2.19	0.42
55:DA:355:U:H2'	55:DA:356:G:C8	2.55	0.42
1:AA:502:A:H2'	1:AA:503:C:O4'	2.19	0.42
5:AE:77:ASN:HB2	5:AE:82:GLN:HE21	1.74	0.42
20:AT:36:TYR:CE2	20:AT:79:LEU:HD21	2.55	0.42
1:BA:1322:C:OP1	1:BA:1322:C:O2	2.37	0.42
31:CA:2305:U:H5"	34:CF:131:GLY:HA3	2.02	0.42
36:CH:68:ARG:HB3	36:CH:134:VAL:HG21	2.02	0.42
47:CT:20:VAL:HG11	47:CT:44:ALA:HA	2.02	0.42
50:CW:86:LEU:HD13	50:CW:89:ILE:HD11	2.01	0.42
55:DA:825:A:H5"	59:DA:3222:PUT:H12	2.02	0.42
55:DA:984:A:N3	55:DA:984:A:H2'	2.34	0.42
1:AA:1322:C:P	19:AS:78:ARG:HH22	2.43	0.42
2:AB:104:TRP:O	2:AB:108:ARG:HB2	2.20	0.42
4:AD:105:MET:SD	4:AD:143:VAL:HG22	2.60	0.42
25:C4:26:HIS:HD1	31:CA:2361:G:P	2.43	0.42
1:BA:1530:G:H2'	1:BA:1531:A:C8	2.55	0.42
24:D3:2:LYS:HE2	55:DA:687:C:H5"	2.02	0.42
31:CA:796:C:H2'	31:CA:797:G:C8	2.54	0.42
36:CH:82:SER:HB2	36:CH:94:ILE:HD11	2.02	0.42
41:CN:41:LEU:HD21	41:CN:124:LEU:HD22	2.02	0.42
40:DM:109:LYS:HG2	40:DM:126:ARG:HB2	2.02	0.42
47:DT:6:LYS:HB2	55:DA:494:G:H4'	2.01	0.42
55:DA:747:5MU:O2	55:DA:2014:A:H1'	2.20	0.42
55:DA:1555:G:OP1	59:DA:3218:PUT:H41	2.20	0.42
55:DA:1794:A:H2'	55:DA:1795:C:C6	2.54	0.42
1:AA:1152:A:H5'	10:AJ:15:HIS:HB2	2.02	0.42
1:AA:1298:U:H3	7:AG:114:LYS:HA	1.85	0.42
11:AK:25:ALA:HA	11:AK:30:THR:HG22	2.02	0.42
5:BE:115:LEU:HG	5:BE:123:VAL:HG21	2.01	0.42
31:CA:1101:U:H2'	31:CA:1102:C:C6	2.54	0.42
32:DD:13:ARG:HH11	44:DQ:56:HIS:HA	1.85	0.42
33:CE:178:VAL:HG23	40:CM:3:LEU:HD21	2.02	0.42
50:CW:26:PHE:HE1	50:CW:44:HIS:HA	1.85	0.42
38:DK:7:LYS:HG2	55:DA:538:A:H4'	2.02	0.42
55:DA:320:A:H4'	55:DA:322:A:N7	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2406:A:H5'	55:DA:2406:A:C8	2.55	0.42
7:AG:72:THR:HG22	7:AG:142:HIS:CE1	2.55	0.41
24:C3:16:HIS:CD2	31:CA:464:U:O2'	2.73	0.41
1:BA:1048:G:H4'	14:BN:3:LYS:HE2	2.02	0.41
25:D4:39:LYS:O	25:D4:43:HIS:HD2	2.03	0.41
31:CA:2074:U:H2'	31:CA:2075:U:C6	2.55	0.41
31:CA:2425:A:H4'	31:CA:2426:A:O5'	2.20	0.41
3:AC:156:ARG:HD3	3:AC:193:TYR:O	2.20	0.41
19:AS:30:PRO:HB2	19:AS:50:ALA:HB2	2.03	0.41
1:BA:1141:C:O2'	1:BA:1142:G:H8	2.03	0.41
11:BK:45:ALA:HB3	11:BK:70:CYS:HB2	2.02	0.41
25:D4:8:ARG:HG3	55:DA:253:C:N4	2.36	0.41
44:CQ:52:ASN:O	44:CQ:53:ARG:HD3	2.20	0.41
48:CU:82:LYS:HD3	48:CU:84:TYR:CE1	2.55	0.41
52:DY:56:MET:HE1	55:DA:2091:C:O2'	2.20	0.41
55:DA:136:G:H1	55:DA:143:C:N4	2.18	0.41
1:AA:131:A:H2'	1:AA:132:C:C6	2.56	0.41
1:AA:302:G:O2'	1:AA:556:C:H5"	2.20	0.41
1:AA:1048:G:H4'	14:AN:3:LYS:HE2	2.01	0.41
1:AA:1108:G:H5"	3:AC:176:HIS:ND1	2.36	0.41
14:BN:31:ILE:HG23	14:BN:42:TRP:HZ2	1.85	0.41
31:CA:136:G:H1	31:CA:143:C:N4	2.19	0.41
31:CA:2339:C:H2'	31:CA:2340:A:C8	2.56	0.41
32:DD:26:VAL:HG21	44:DQ:5:ILE:HG12	2.02	0.41
55:DA:686:U:H2'	55:DA:788:A:N1	2.35	0.41
55:DA:1430:G:H2'	55:DA:1431:A:O4'	2.20	0.41
5:BE:23:LYS:HB3	5:BE:30:ILE:HG23	2.02	0.41
29:CC:221:ARG:NH1	31:CA:1789:A:OP2	2.53	0.41
31:CA:355:U:H2'	31:CA:356:G:C8	2.56	0.41
31:CA:742:A:H2'	31:CA:743:A:C8	2.55	0.41
31:CA:1794:A:H2'	31:CA:1795:C:C6	2.56	0.41
31:CA:2043:C:H5"	31:CA:2043:C:C6	2.55	0.41
31:CA:2106:U:H2'	31:CA:2107:G:C8	2.55	0.41
40:CM:123:ARG:HG3	40:CM:143:GLU:HG3	2.03	0.41
41:CN:71:LYS:HB3	41:CN:93:VAL:O	2.21	0.41
54:DI:94:ARG:HG2	54:DI:127:ALA:HA	2.02	0.41
55:DA:1202:G:H1'	58:DA:3192:MPD:HM1	2.02	0.41
55:DA:1418:G:H2'	55:DA:1579:A:N6	2.35	0.41
13:AM:95:LEU:C	13:AM:109:ARG:HG2	2.46	0.41
27:C0:14:ILE:HG21	31:CA:988:A:C6	2.56	0.41
1:BA:131:A:H2'	1:BA:132:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:429:U:H1'	1:BA:430:A:H5"	2.03	0.41
4:BD:130:VAL:HG11	4:BD:135:TYR:CG	2.55	0.41
11:BK:20:VAL:HB	11:BK:35:THR:HG23	2.02	0.41
31:CA:2114:A:N6	31:CA:2119:A:H62	2.18	0.41
36:DH:82:SER:HB2	36:DH:94:ILE:HD11	2.02	0.41
47:DT:20:VAL:HG11	47:DT:44:ALA:HA	2.03	0.41
55:DA:602:A:C6	58:DA:3190:MPD:H31	2.56	0.41
55:DA:1417:C:H5'	55:DA:1588:G:H1'	2.01	0.41
1:AA:429:U:H1'	1:AA:430:A:H5"	2.02	0.41
1:AA:1343:G:O2'	9:AI:123:ARG:HD2	2.20	0.41
13:AM:54:ASP:HA	13:AM:57:ARG:HD2	2.02	0.41
1:BA:1298:U:H3	7:BG:114:LYS:HA	1.86	0.41
14:BN:53:ARG:HH21	19:BS:37:ARG:HH22	1.69	0.41
29:CC:174:LEU:CD2	29:CC:184:VAL:HB	2.50	0.41
31:CA:2788:C:H2'	31:CA:2789:C:C6	2.55	0.41
47:CT:29:VAL:HG22	47:CT:51:LEU:HD11	2.02	0.41
52:DY:29:PHE:HB3	55:DA:396:G:H1'	2.02	0.41
54:DI:52:MET:HE1	54:DI:81:LEU:HD21	2.01	0.41
55:DA:2128:G:H1	55:DA:2160:C:N4	2.18	0.41
55:DA:2324:U:H3'	55:DA:2325:G:H5"	2.03	0.41
1:AA:439:U:H5"	4:AD:121:LYS:HD2	2.02	0.41
4:AD:170:TRP:CD2	4:AD:186:PRO:HB3	2.56	0.41
12:BL:87:VAL:HG11	12:BL:90:LEU:HD22	2.02	0.41
20:BT:44:LYS:HB3	20:BT:87:ALA:HB2	2.03	0.41
30:CD:141:ARG:HB2	31:CA:1656:C:H5"	2.01	0.41
31:CA:2095:A:H5"	31:CA:2095:A:C8	2.54	0.41
42:CO:95:THR:HG21	42:CO:113:ILE:HD11	2.02	0.41
47:CT:69:LEU:HG	47:CT:107:VAL:CG2	2.51	0.41
51:DX:41[B]:ARG:HD3	51:DX:41[B]:ARG:HA	1.94	0.41
55:DA:138:U:H5'	55:DA:139:U:H5'	2.03	0.41
55:DA:2038:G:H2'	55:DA:2039:U:O4'	2.21	0.41
1:AA:1141:C:O2'	1:AA:1142:G:H8	2.03	0.41
9:AI:19:VAL:HG11	9:AI:83:ILE:HA	2.03	0.41
1:BA:1376:U:H2'	1:BA:1377:A:C8	2.55	0.41
4:BD:170:TRP:CD2	4:BD:186:PRO:HB3	2.56	0.41
5:BE:77:ASN:HB2	5:BE:82:GLN:HE21	1.79	0.41
5:BE:82:GLN:HG2	5:BE:149:SER:HA	2.01	0.41
19:BS:30:PRO:HB2	19:BS:50:ALA:HB2	2.02	0.41
25:D4:13:ARG:NH1	55:DA:2394:C:H5'	2.36	0.41
31:CA:1722:A:N6	31:CA:1738:G:H1'	2.36	0.41
31:CA:2038:G:H2'	31:CA:2039:U:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DE:23:PHE:HE2	33:DE:25:GLU:HG3	1.86	0.41
35:DG:140:VAL:O	35:DG:144:VAL:HG23	2.20	0.41
51:DX:38:VAL:HG12	51:DX:59:LEU:HB2	2.02	0.41
55:DA:1020:A:C2	55:DA:1141:U:C2	3.08	0.41
55:DA:1515:A:H2'	55:DA:1516:G:O4'	2.20	0.41
55:DA:2097:A:H8	55:DA:2097:A:H5"	1.85	0.41
5:AE:157:ARG:CD	8:AH:43:GLU:O	2.69	0.41
6:AF:21:MET:HE2	6:AF:81:ASN:HD21	1.85	0.41
11:AK:20:VAL:HB	11:AK:35:THR:HG23	2.03	0.41
19:AS:5:LEU:H	19:AS:5:LEU:HG	1.75	0.41
1:BA:216:U:H4'	1:BA:464:U:H4'	2.02	0.41
1:BA:567:G:H2'	1:BA:568:G:O4'	2.20	0.41
1:BA:841:C:H3'	1:BA:842:U:C4'	2.51	0.41
9:BI:19:VAL:HG11	9:BI:83:ILE:HA	2.03	0.41
20:BT:67:ILE:O	20:BT:68:HIS:HB2	2.20	0.41
29:CC:107:PRO:HD2	29:CC:110:LEU:HD22	2.03	0.41
31:CA:396:G:H1'	52:CY:29:PHE:HB3	2.01	0.41
31:CA:547:A:H2'	31:CA:547:A:N3	2.36	0.41
31:CA:1636:U:H2'	31:CA:1637:A:C8	2.55	0.41
33:DE:178:VAL:HG23	40:DM:3:LEU:HD21	2.01	0.41
36:DH:68:ARG:HB3	36:DH:134:VAL:HG21	2.03	0.41
54:DI:29:ASP:HB3	54:DI:106:PHE:HB2	2.02	0.41
1:AA:831:A:H5"	2:AB:21:ARG:HD3	2.03	0.41
1:AA:1216:A:H5"	14:AN:5:SER:HB3	2.02	0.41
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.85	0.41
1:BA:439:U:H5"	4:BD:121:LYS:HD2	2.02	0.41
11:BK:34:ILE:HG12	11:BK:70:CYS:SG	2.60	0.41
20:BT:69:LYS:H	20:BT:69:LYS:HG3	1.60	0.41
31:CA:29:U:H6	31:CA:29:U:O5'	2.02	0.41
31:CA:2335:A:OP1	43:CP:13:ARG:HD2	2.21	0.41
37:CJ:49:ILE:HG13	37:CJ:55:ILE:HD13	2.03	0.41
38:DK:9:GLU:HG2	70:DA:3412:HOH:O	2.21	0.41
40:DM:74:THR:HG23	40:DM:107:PHE:HB2	2.02	0.41
40:DM:123:ARG:HG3	40:DM:143:GLU:HG3	2.02	0.41
41:DN:89:VAL:CG1	58:DN:201:MPD:HM3	2.50	0.41
54:DI:23:LEU:HD13	54:DI:89:PRO:HD3	2.03	0.41
55:DA:207:A:H2'	55:DA:208:C:O4'	2.20	0.41
55:DA:281:C:H2'	55:DA:282:A:C8	2.56	0.41
55:DA:2133:G:H21	55:DA:2158:A:N6	2.18	0.41
10:AJ:19:ASP:HA	10:AJ:22:THR:HB	2.03	0.40
22:C1:49:TYR:OH	31:CA:2883:A:OP1	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:718:A:H5'	11:BK:119:ASN:HB2	2.03	0.40
1:BA:1108:G:H5"	3:BC:176:HIS:ND1	2.36	0.40
6:BF:22:ILE:HG23	6:BF:39:LEU:HD11	2.02	0.40
22:D1:8:PRO:HD2	55:DA:1263:U:O2'	2.22	0.40
31:CA:780:G:H2'	31:CA:782:A:N7	2.36	0.40
35:CG:38:ASN:HD22	35:CG:40:ALA:HB3	1.86	0.40
35:DG:50:LEU:HD13	35:DG:72:LEU:HD23	2.02	0.40
37:DJ:14:ALA:HB3	37:DJ:17:MET:HB2	2.03	0.40
40:DM:77:ILE:CD1	40:DM:101:ILE:CG2	2.97	0.40
54:DI:132:TYR:N	54:DI:133:GLU:HB2	2.35	0.40
55:DA:839:U:H2'	55:DA:840:C:C6	2.56	0.40
55:DA:1306:C:H6	55:DA:1306:C:H5"	1.85	0.40
55:DA:2273:A:H2'	55:DA:2274:A:C8	2.55	0.40
1:AA:568:G:O6	12:AL:2:ALA:HB2	2.21	0.40
1:AA:842:U:H5"	2:BB:115:LYS:HD3	2.03	0.40
10:BJ:59:LYS:HD2	10:BJ:60:ASP:OD1	2.21	0.40
47:DT:84:ARG:HB2	47:DT:96:ILE:HB	2.02	0.40
54:DI:65:GLU:HA	54:DI:70:GLU:HG3	2.02	0.40
54:DI:120:ALA:HA	54:DI:123:ILE:HD11	2.03	0.40
55:DA:1532:A:H5"	55:DA:1532:A:H8	1.85	0.40
1:AA:268:U:H2'	1:AA:269:C:C6	2.56	0.40
11:AK:31:ILE:HG12	11:AK:46:THR:CG2	2.51	0.40
14:AN:46:LEU:HD22	19:AS:13:LEU:HG	2.02	0.40
25:C4:52:LYS:HA	25:C4:55:LEU:HD12	2.03	0.40
1:BA:1322:C:P	19:BS:78:ARG:HH22	2.43	0.40
9:BI:116:VAL:HG21	10:BJ:62:ARG:HD3	2.04	0.40
22:D1:12:LYS:HD2	22:D1:12:LYS:HA	1.86	0.40
31:CA:1418:G:H2'	31:CA:1579:A:N6	2.36	0.40
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.57	0.40
39:DL:113:MET:O	39:DL:116:ILE:HG13	2.19	0.40
40:DM:95:LEU:HD11	40:DM:125:LEU:HD21	2.03	0.40
47:DT:72:THR:CG2	47:DT:108:SER:HB3	2.52	0.40
53:DZ:56:LEU:HA	53:DZ:59:GLU:HG2	2.04	0.40
1:AA:234:C:H4'	17:AQ:66:PRO:HG3	2.03	0.40
1:AA:567:G:H2'	1:AA:568:G:O4'	2.21	0.40
1:BA:268:U:H2'	1:BA:269:C:C6	2.56	0.40
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	2.04	0.40
13:BM:95:LEU:C	13:BM:109:ARG:HG2	2.47	0.40
26:D5:32:LYS:HG2	55:DA:2478:A:H5'	2.03	0.40
31:CA:1131:G:OP1	38:CK:82:GLY:HA2	2.21	0.40
31:CA:1306:C:H5"	31:CA:1306:C:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:CH:126:GLY:H	36:CH:146:VAL:HB	1.87	0.40
45:CR:58:ARG:HH11	45:CR:62:ILE:HD11	1.86	0.40
34:DF:130:MET:HE2	34:DF:154:ILE:HD12	2.03	0.40
55:DA:2788:C:H2'	55:DA:2789:C:C6	2.57	0.40
24:C3:37:LYS:NZ	31:CA:469:G:O6	2.53	0.40
1:BA:580:C:H2'	1:BA:581:G:O4'	2.21	0.40
6:BF:78:PHE:HA	6:BF:84:VAL:HG11	2.04	0.40
12:BL:74:LEU:HD21	12:BL:80:ILE:HG21	2.03	0.40
31:CA:644:A:H2'	31:CA:645:C:O4'	2.22	0.40
31:CA:1101:U:H2'	31:CA:1102:C:H6	1.87	0.40
31:CA:2327:A:H2'	31:CA:2328:A:C8	2.57	0.40
37:DJ:49:ILE:HG13	37:DJ:55:ILE:HD13	2.03	0.40
49:DV:66:GLN:HG3	55:DA:328:U:O3'	2.22	0.40
55:DA:2339:C:H2'	55:DA:2340:A:C8	2.57	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%)	210 (95%)	9 (4%)	3 (1%)	9 24
2	BB	222/224 (99%)	211 (95%)	7 (3%)	4 (2%)	6 19
3	AC	204/206 (99%)	192 (94%)	11 (5%)	1 (0%)	24 49
3	BC	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	12 32
4	AD	203/205 (99%)	198 (98%)	5 (2%)	0	100 100
4	BD	203/205 (99%)	198 (98%)	5 (2%)	0	100 100
5	AE	153/155 (99%)	147 (96%)	5 (3%)	1 (1%)	18 40
5	BE	148/155 (96%)	132 (89%)	12 (8%)	4 (3%)	4 11
6	AF	104/106 (98%)	101 (97%)	3 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	BF	98/106 (92%)	91 (93%)	5 (5%)	2 (2%)	6 16
7	AG	149/151 (99%)	137 (92%)	11 (7%)	1 (1%)	18 40
7	BG	149/151 (99%)	140 (94%)	9 (6%)	0	100 100
8	AH	127/129 (98%)	120 (94%)	7 (6%)	0	100 100
8	BH	127/129 (98%)	119 (94%)	8 (6%)	0	100 100
9	AI	125/127 (98%)	110 (88%)	15 (12%)	0	100 100
9	BI	125/127 (98%)	110 (88%)	15 (12%)	0	100 100
10	AJ	97/99 (98%)	88 (91%)	7 (7%)	2 (2%)	5 16
10	BJ	96/99 (97%)	77 (80%)	14 (15%)	5 (5%)	1 3
11	AK	115/117 (98%)	107 (93%)	6 (5%)	2 (2%)	7 20
11	BK	115/117 (98%)	104 (90%)	9 (8%)	2 (2%)	7 20
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100 100
12	BL	120/123 (98%)	114 (95%)	5 (4%)	1 (1%)	16 37
13	AM	112/114 (98%)	103 (92%)	6 (5%)	3 (3%)	4 11
13	BM	112/114 (98%)	102 (91%)	5 (4%)	5 (4%)	2 4
14	AN	98/100 (98%)	88 (90%)	8 (8%)	2 (2%)	6 16
14	BN	98/100 (98%)	90 (92%)	6 (6%)	2 (2%)	6 16
15	AO	86/88 (98%)	84 (98%)	2 (2%)	0	100 100
15	BO	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	10 28
16	AP	80/82 (98%)	74 (92%)	6 (8%)	0	100 100
16	BP	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	4 13
17	AQ	78/80 (98%)	70 (90%)	7 (9%)	1 (1%)	9 26
17	BQ	78/80 (98%)	68 (87%)	5 (6%)	5 (6%)	1 2
18	AR	53/55 (96%)	53 (100%)	0	0	100 100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100 100
19	AS	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	9 26
19	BS	77/79 (98%)	68 (88%)	7 (9%)	2 (3%)	4 12
20	AT	84/86 (98%)	83 (99%)	1 (1%)	0	100 100
20	BT	83/86 (96%)	79 (95%)	3 (4%)	1 (1%)	10 28
21	AU	54/56 (96%)	53 (98%)	1 (2%)	0	100 100
21	BU	54/56 (96%)	53 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
22	C1	54/56 (96%)	47 (87%)	4 (7%)	3 (6%)	1 2
22	D1	54/56 (96%)	51 (94%)	3 (6%)	0	100 100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	2 5
23	D2	49/51 (96%)	48 (98%)	1 (2%)	0	100 100
24	C3	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	5 14
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100 100
25	C4	62/64 (97%)	60 (97%)	2 (3%)	0	100 100
25	D4	62/64 (97%)	60 (97%)	2 (3%)	0	100 100
26	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4 11
26	D5	36/38 (95%)	36 (100%)	0	0	100 100
27	C0	56/58 (97%)	54 (96%)	0	2 (4%)	2 6
27	D0	57/58 (98%)	56 (98%)	1 (2%)	0	100 100
29	CC	269/272 (99%)	252 (94%)	12 (4%)	5 (2%)	6 17
29	DC	269/272 (99%)	257 (96%)	10 (4%)	2 (1%)	18 40
30	CD	207/209 (99%)	201 (97%)	6 (3%)	0	100 100
32	DD	206/209 (99%)	202 (98%)	4 (2%)	0	100 100
33	CE	199/201 (99%)	191 (96%)	5 (2%)	3 (2%)	8 23
33	DE	199/201 (99%)	194 (98%)	4 (2%)	1 (0%)	24 49
34	CF	175/178 (98%)	168 (96%)	6 (3%)	1 (1%)	21 45
34	DF	175/178 (98%)	169 (97%)	5 (3%)	1 (1%)	21 45
35	CG	174/176 (99%)	162 (93%)	7 (4%)	5 (3%)	3 10
35	DG	174/176 (99%)	165 (95%)	8 (5%)	1 (1%)	21 45
36	CH	147/149 (99%)	136 (92%)	6 (4%)	5 (3%)	3 7
36	DH	147/149 (99%)	138 (94%)	6 (4%)	3 (2%)	6 16
37	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	3 9
37	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	3 9
38	CK	140/142 (99%)	135 (96%)	4 (3%)	1 (1%)	18 40
38	DK	140/142 (99%)	137 (98%)	2 (1%)	1 (1%)	18 40
39	CL	120/123 (98%)	112 (93%)	7 (6%)	1 (1%)	16 37
39	DL	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	16 37
40	CM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	5 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
40	DM	142/144 (99%)	136 (96%)	6 (4%)	0	100 100
41	CN	133/136 (98%)	125 (94%)	7 (5%)	1 (1%)	16 37
41	DN	134/136 (98%)	129 (96%)	5 (4%)	0	100 100
42	CO	118/125 (94%)	111 (94%)	5 (4%)	2 (2%)	7 20
42	DO	123/125 (98%)	116 (94%)	7 (6%)	0	100 100
43	CP	114/117 (97%)	110 (96%)	4 (4%)	0	100 100
43	DP	115/117 (98%)	112 (97%)	3 (3%)	0	100 100
44	CQ	112/114 (98%)	107 (96%)	5 (4%)	0	100 100
44	DQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	14 34
45	CR	115/117 (98%)	113 (98%)	2 (2%)	0	100 100
45	DR	115/117 (98%)	114 (99%)	1 (1%)	0	100 100
46	CS	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	3 9
46	DS	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	12 32
47	CT	108/110 (98%)	101 (94%)	5 (5%)	2 (2%)	6 17
47	DT	108/110 (98%)	106 (98%)	2 (2%)	0	100 100
48	CU	91/93 (98%)	86 (94%)	4 (4%)	1 (1%)	11 29
48	DU	91/93 (98%)	85 (93%)	6 (7%)	0	100 100
49	CV	100/103 (97%)	91 (91%)	4 (4%)	5 (5%)	1 3
49	DV	100/103 (97%)	96 (96%)	2 (2%)	2 (2%)	6 16
50	CW	92/94 (98%)	91 (99%)	1 (1%)	0	100 100
50	DW	92/94 (98%)	91 (99%)	1 (1%)	0	100 100
51	CX	73/76 (96%)	72 (99%)	1 (1%)	0	100 100
51	DX	75/76 (99%)	74 (99%)	1 (1%)	0	100 100
52	CY	75/77 (97%)	74 (99%)	1 (1%)	0	100 100
52	DY	75/77 (97%)	74 (99%)	1 (1%)	0	100 100
53	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7 20
53	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100 100
54	DI	133/135 (98%)	114 (86%)	13 (10%)	6 (4%)	2 4
All	All	11407/11635 (98%)	10791 (95%)	485 (4%)	131 (1%)	11 29

All (131) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE
3	AC	156	ARG
13	AM	5	ALA
22	C1	25	VAL
2	BB	126	PHE
3	BC	156	ARG
5	BE	51	GLY
10	BJ	38	GLY
10	BJ	91	ASP
13	BM	7	ILE
16	BP	80	LYS
20	BT	5	LYS
29	CC	158	ALA
29	CC	197	ASN
33	CE	83	VAL
35	CG	119	ALA
35	CG	175	LYS
35	CG	176	LYS
36	CH	10	ALA
37	CJ	19	ASN
38	CK	81	ILE
39	CL	35	VAL
40	CM	29	LYS
41	CN	70	ASP
42	CO	118	ARG
48	CU	88	LYS
49	CV	7	ARG
37	DJ	19	ASN
49	DV	52	LEU
10	AJ	57	VAL
13	AM	105	ASN
14	AN	38	ASP
17	AQ	82	ALA
22	C1	56	ALA
23	C2	5	ILE
23	C2	51	GLU
27	C0	4	THR
27	C0	14	ILE
3	BC	61	ALA
5	BE	110	ALA
6	BF	92	THR
6	BF	98	GLU
10	BJ	57	VAL

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Mol	Chain	Res	Type
12	BL	44	LYS
13	BM	5	ALA
13	BM	105	ASN
13	BM	114	LYS
17	BQ	70	THR
17	BQ	82	ALA
19	BS	6	LYS
29	CC	233	GLY
29	CC	253	LYS
29	DC	233	GLY
29	DC	253	LYS
33	CE	82	GLY
35	CG	46	ALA
37	CJ	25	GLY
40	CM	69	ARG
49	CV	16	GLY
49	CV	17	LYS
35	DG	46	ALA
37	DJ	25	GLY
2	AB	125	THR
2	AB	127	ASP
7	AG	56	LYS
11	AK	54	GLY
11	AK	89	PRO
13	AM	7	ILE
22	C1	26	THR
24	C3	45	SER
2	BB	125	THR
2	BB	127	ASP
5	BE	103	THR
10	BJ	95	GLY
11	BK	54	GLY
11	BK	89	PRO
14	BN	38	ASP
15	BO	88	ARG
17	BQ	17	MET
17	BQ	18	GLU
19	BS	5	LEU
29	CC	108	LYS
33	CE	6	LYS
36	CH	118	PRO
49	CV	89	ASP

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Mol	Chain	Res	Type
33	DE	6	LYS
36	DH	118	PRO
39	DL	108	ARG
46	DS	44	GLY
49	DV	89	ASP
54	DI	70	GLU
54	DI	91	ALA
54	DI	109	LYS
54	DI	130	PRO
5	AE	162	GLU
5	BE	105	ILE
10	BJ	36	VAL
13	BM	4	ILE
36	CH	9	VAL
40	CM	30	THR
42	CO	119	SER
46	CS	55	ASP
47	CT	63	GLY
36	DH	11	ASN
54	DI	88	HIS
19	AS	6	LYS
2	BB	95	ARG
14	BN	22	ALA
36	CH	8	LYS
36	CH	122	LEU
37	CJ	23	PRO
46	CS	48	LYS
46	CS	53	PHE
36	DH	122	LEU
37	DJ	23	PRO
44	DQ	105	GLY
54	DI	108	VAL
14	AN	22	ALA
16	BP	44	SER
35	CG	45	HIS
47	CT	65	ASP
49	CV	52	LEU
53	CZ	62	GLY
38	DK	83	GLY
26	C5	21	GLY
34	CF	62	GLY
37	CJ	32	GLY

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Mol	Chain	Res	Type
34	DF	62	GLY
37	DJ	32	GLY
17	BQ	35	GLY
10	AJ	33	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AB	186/186 (100%)	171 (92%)	15 (8%)	11 28
2	BB	186/186 (100%)	171 (92%)	15 (8%)	11 28
3	AC	170/170 (100%)	157 (92%)	13 (8%)	12 31
3	BC	170/170 (100%)	154 (91%)	16 (9%)	8 22
4	AD	172/172 (100%)	160 (93%)	12 (7%)	14 34
4	BD	172/172 (100%)	159 (92%)	13 (8%)	12 31
5	AE	118/118 (100%)	100 (85%)	18 (15%)	3 8
5	BE	113/118 (96%)	92 (81%)	21 (19%)	1 4
6	AF	92/92 (100%)	85 (92%)	7 (8%)	12 31
6	BF	87/92 (95%)	75 (86%)	12 (14%)	3 10
7	AG	124/124 (100%)	111 (90%)	13 (10%)	6 19
7	BG	124/124 (100%)	107 (86%)	17 (14%)	3 11
8	AH	104/104 (100%)	91 (88%)	13 (12%)	4 13
8	BH	104/104 (100%)	91 (88%)	13 (12%)	4 13
9	AI	105/105 (100%)	100 (95%)	5 (5%)	23 48
9	BI	105/105 (100%)	100 (95%)	5 (5%)	23 48
10	AJ	87/87 (100%)	80 (92%)	7 (8%)	11 28
10	BJ	86/87 (99%)	76 (88%)	10 (12%)	5 16
11	AK	90/90 (100%)	87 (97%)	3 (3%)	33 58
11	BK	90/90 (100%)	83 (92%)	7 (8%)	11 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	AL	102/102 (100%)	90 (88%)	12 (12%)	5 15
12	BL	102/102 (100%)	90 (88%)	12 (12%)	5 15
13	AM	92/92 (100%)	85 (92%)	7 (8%)	12 31
13	BM	92/92 (100%)	87 (95%)	5 (5%)	20 44
14	AN	83/83 (100%)	82 (99%)	1 (1%)	63 79
14	BN	83/83 (100%)	82 (99%)	1 (1%)	63 79
15	AO	76/76 (100%)	71 (93%)	5 (7%)	15 37
15	BO	76/76 (100%)	68 (90%)	8 (10%)	6 19
16	AP	65/65 (100%)	63 (97%)	2 (3%)	35 59
16	BP	65/65 (100%)	59 (91%)	6 (9%)	8 23
17	AQ	74/74 (100%)	67 (90%)	7 (10%)	8 22
17	BQ	74/74 (100%)	67 (90%)	7 (10%)	8 22
18	AR	48/48 (100%)	46 (96%)	2 (4%)	26 53
18	BR	48/48 (100%)	46 (96%)	2 (4%)	26 53
19	AS	70/70 (100%)	61 (87%)	9 (13%)	4 13
19	BS	70/70 (100%)	65 (93%)	5 (7%)	13 33
20	AT	65/65 (100%)	60 (92%)	5 (8%)	12 30
20	BT	65/65 (100%)	53 (82%)	12 (18%)	1 4
21	AU	48/48 (100%)	43 (90%)	5 (10%)	7 19
21	BU	48/48 (100%)	43 (90%)	5 (10%)	7 19
22	C1	47/47 (100%)	45 (96%)	2 (4%)	26 52
22	D1	47/47 (100%)	44 (94%)	3 (6%)	16 38
23	C2	45/46 (98%)	43 (96%)	2 (4%)	25 51
23	D2	45/46 (98%)	42 (93%)	3 (7%)	15 36
24	C3	38/38 (100%)	36 (95%)	2 (5%)	20 45
24	D3	38/38 (100%)	37 (97%)	1 (3%)	40 65
25	C4	51/51 (100%)	48 (94%)	3 (6%)	18 41
25	D4	51/51 (100%)	49 (96%)	2 (4%)	28 54
26	C5	34/34 (100%)	32 (94%)	2 (6%)	18 41
26	D5	34/34 (100%)	34 (100%)	0	100 100
27	C0	48/48 (100%)	42 (88%)	6 (12%)	4 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	D0	49/48 (102%)	46 (94%)	3 (6%)	17 40
29	CC	216/217 (100%)	201 (93%)	15 (7%)	14 35
29	DC	216/217 (100%)	206 (95%)	10 (5%)	24 50
30	CD	164/164 (100%)	157 (96%)	7 (4%)	26 52
32	DD	163/163 (100%)	157 (96%)	6 (4%)	30 55
33	CE	165/165 (100%)	153 (93%)	12 (7%)	13 33
33	DE	165/165 (100%)	161 (98%)	4 (2%)	43 67
34	CF	148/149 (99%)	132 (89%)	16 (11%)	6 18
34	DF	148/149 (99%)	136 (92%)	12 (8%)	11 28
35	CG	137/137 (100%)	133 (97%)	4 (3%)	37 61
35	DG	137/137 (100%)	134 (98%)	3 (2%)	45 69
36	CH	114/114 (100%)	94 (82%)	20 (18%)	2 5
36	DH	114/114 (100%)	93 (82%)	21 (18%)	1 4
37	CJ	104/104 (100%)	97 (93%)	7 (7%)	15 36
37	DJ	104/104 (100%)	97 (93%)	7 (7%)	15 36
38	CK	116/116 (100%)	111 (96%)	5 (4%)	26 52
38	DK	116/116 (100%)	113 (97%)	3 (3%)	40 65
39	CL	103/104 (99%)	97 (94%)	6 (6%)	18 41
39	DL	104/104 (100%)	97 (93%)	7 (7%)	15 36
40	CM	103/103 (100%)	96 (93%)	7 (7%)	14 35
40	DM	103/103 (100%)	97 (94%)	6 (6%)	18 41
41	CN	108/108 (100%)	98 (91%)	10 (9%)	8 23
41	DN	109/108 (101%)	104 (95%)	5 (5%)	24 50
42	CO	100/102 (98%)	94 (94%)	6 (6%)	17 40
42	DO	102/102 (100%)	98 (96%)	4 (4%)	28 54
43	CP	86/87 (99%)	77 (90%)	9 (10%)	6 19
43	DP	87/87 (100%)	81 (93%)	6 (7%)	14 35
44	CQ	99/99 (100%)	93 (94%)	6 (6%)	17 40
44	DQ	99/99 (100%)	96 (97%)	3 (3%)	36 60
45	CR	89/89 (100%)	83 (93%)	6 (7%)	15 36
45	DR	89/89 (100%)	86 (97%)	3 (3%)	32 58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	CS	84/84 (100%)	78 (93%)	6 (7%)	13 33
46	DS	84/84 (100%)	81 (96%)	3 (4%)	31 56
47	CT	93/93 (100%)	88 (95%)	5 (5%)	20 44
47	DT	93/93 (100%)	92 (99%)	1 (1%)	65 80
48	CU	80/80 (100%)	73 (91%)	7 (9%)	9 24
48	DU	80/80 (100%)	76 (95%)	4 (5%)	22 47
49	CV	83/84 (99%)	79 (95%)	4 (5%)	23 48
49	DV	83/84 (99%)	80 (96%)	3 (4%)	31 56
50	CW	78/78 (100%)	74 (95%)	4 (5%)	21 47
50	DW	78/78 (100%)	75 (96%)	3 (4%)	29 55
51	CX	56/58 (97%)	54 (96%)	2 (4%)	31 56
51	DX	58/58 (100%)	56 (97%)	2 (3%)	32 58
52	CY	67/67 (100%)	63 (94%)	4 (6%)	17 40
52	DY	67/67 (100%)	64 (96%)	3 (4%)	24 50
53	CZ	54/54 (100%)	49 (91%)	5 (9%)	8 23
53	DZ	54/54 (100%)	51 (94%)	3 (6%)	19 43
54	DI	103/103 (100%)	96 (93%)	7 (7%)	14 35
All	All	9461/9484 (100%)	8777 (93%)	684 (7%)	13 33

All (684) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	23	TRP
2	AB	44	GLU
2	AB	73	LYS
2	AB	93	ASN
2	AB	105	LYS
2	AB	125	THR
2	AB	129	LEU
2	AB	130	THR
2	AB	135	LEU
2	AB	137	ARG
2	AB	147	SER
2	AB	161	LEU
2	AB	205	ASP
2	AB	207	ILE

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Mol	Chain	Res	Type
2	AB	212	LEU
3	AC	4	LYS
3	AC	14	ILE
3	AC	16	LYS
3	AC	21	THR
3	AC	33	LEU
3	AC	46	GLU
3	AC	107	ARG
3	AC	121	THR
3	AC	175	LEU
3	AC	178	LEU
3	AC	185	ASN
3	AC	186	THR
3	AC	207	ILE
4	AD	5	LEU
4	AD	17	THR
4	AD	22	LYS
4	AD	26	ARG
4	AD	28	ILE
4	AD	50	ASP
4	AD	132	ILE
4	AD	142	VAL
4	AD	143	VAL
4	AD	172	GLU
4	AD	194	ASP
4	AD	202	GLU
5	AE	14	LYS
5	AE	26	LYS
5	AE	32	SER
5	AE	46	VAL
5	AE	71	MET
5	AE	74	VAL
5	AE	76	LEU
5	AE	81	LEU
5	AE	82	GLN
5	AE	94	VAL
5	AE	101	GLU
5	AE	106	ILE
5	AE	123	VAL
5	AE	126	LYS
5	AE	134	ILE
5	AE	137	VAL

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Mol	Chain	Res	Type
5	AE	149	SER
5	AE	159	LYS
6	AF	36	ILE
6	AF	68	GLN
6	AF	69	GLU
6	AF	71	ILE
6	AF	74	LEU
6	AF	89	VAL
6	AF	93	LYS
7	AG	22	LEU
7	AG	23	LEU
7	AG	36	LYS
7	AG	58	GLU
7	AG	59	LEU
7	AG	63	GLU
7	AG	70	ARG
7	AG	76	LYS
7	AG	83	SER
7	AG	120	LEU
7	AG	131	LYS
7	AG	133	THR
7	AG	142	HIS
8	AH	3	MET
8	AH	31	LYS
8	AH	47	GLU
8	AH	52	GLU
8	AH	54	ASP
8	AH	60	GLU
8	AH	63	LEU
8	AH	76	GLN
8	AH	90	ASP
8	AH	107	SER
8	AH	108	LYS
8	AH	117	ARG
8	AH	129	VAL
9	AI	11	ARG
9	AI	57	MET
9	AI	61	LEU
9	AI	63	LEU
9	AI	66	THR
10	AJ	6	ILE
10	AJ	8	ILE

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Mol	Chain	Res	Type
10	AJ	62	ARG
10	AJ	63	ASP
10	AJ	88	MET
10	AJ	89	ARG
10	AJ	90	LEU
11	AK	23	ILE
11	AK	55	SER
11	AK	119	ASN
12	AL	24	LEU
12	AL	40	THR
12	AL	43	LYS
12	AL	55	VAL
12	AL	62	GLU
12	AL	74	LEU
12	AL	82	ILE
12	AL	88	LYS
12	AL	90	LEU
12	AL	114	ARG
12	AL	115	SER
12	AL	121	ARG
13	AM	7	ILE
13	AM	13	LYS
13	AM	17	ILE
13	AM	27	LYS
13	AM	48	LEU
13	AM	58	ASP
13	AM	63	PHE
14	AN	31	ILE
15	AO	2	SER
15	AO	24	SER
15	AO	40	GLN
15	AO	70	LEU
15	AO	87	LEU
16	AP	18	GLN
16	AP	48	GLU
17	AQ	5	ILE
17	AQ	16	LYS
17	AQ	26	GLU
17	AQ	38	ILE
17	AQ	40	ARG
17	AQ	75	LEU
17	AQ	83	VAL

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Mol	Chain	Res	Type
18	AR	33	ILE
18	AR	47	THR
19	AS	5	LEU
19	AS	7	LYS
19	AS	11	ILE
19	AS	13	LEU
19	AS	27	ASP
19	AS	33	THR
19	AS	37	ARG
19	AS	56	GLN
19	AS	81	ARG
20	AT	15	GLU
20	AT	24	ARG
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	34	ARG
21	AU	56	HIS
22	C1	40	ARG
22	C1	52	ARG
23	C2	8	LYS
23	C2	47	VAL
24	C3	1	MET
24	C3	44	VAL
25	C4	45	ARG
25	C4	47	LYS
25	C4	52	LYS
26	C5	20	ASP
26	C5	26	ILE
27	C0	3	LYS
27	C0	4	THR
27	C0	5	ILE
27	C0	19	LYS
27	C0	36	VAL
27	C0	59	GLU
2	BB	23	TRP
2	BB	44	GLU
2	BB	73	LYS
2	BB	93	ASN

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Mol	Chain	Res	Type
2	BB	105	LYS
2	BB	125	THR
2	BB	129	LEU
2	BB	130	THR
2	BB	135	LEU
2	BB	137	ARG
2	BB	147	SER
2	BB	161	LEU
2	BB	205	ASP
2	BB	207	ILE
2	BB	212	LEU
3	BC	3	GLN
3	BC	4	LYS
3	BC	14	ILE
3	BC	16	LYS
3	BC	33	LEU
3	BC	37	PHE
3	BC	38	LYS
3	BC	46	GLU
3	BC	55	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	5	LEU
4	BD	17	THR
4	BD	22	LYS
4	BD	26	ARG
4	BD	28	ILE
4	BD	50	ASP
4	BD	142	VAL
4	BD	143	VAL
4	BD	151	LYS
4	BD	172	GLU
4	BD	173	VAL
4	BD	194	ASP
4	BD	206	LYS
5	BE	14	LYS
5	BE	24	THR

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Mol	Chain	Res	Type
5	BE	32	SER
5	BE	46	VAL
5	BE	71	MET
5	BE	76	LEU
5	BE	81	LEU
5	BE	82	GLN
5	BE	88	VAL
5	BE	94	VAL
5	BE	101	GLU
5	BE	103	THR
5	BE	114	VAL
5	BE	115	LEU
5	BE	123	VAL
5	BE	126	LYS
5	BE	134	ILE
5	BE	151	GLU
5	BE	152	MET
5	BE	157	ARG
5	BE	159	LYS
6	BF	2	ARG
6	BF	7	VAL
6	BF	14	GLN
6	BF	16	GLU
6	BF	36	ILE
6	BF	53	LYS
6	BF	68	GLN
6	BF	69	GLU
6	BF	71	ILE
6	BF	74	LEU
6	BF	89	VAL
6	BF	93	LYS
7	BG	5	ARG
7	BG	23	LEU
7	BG	36	LYS
7	BG	48	GLU
7	BG	50	LEU
7	BG	58	GLU
7	BG	59	LEU
7	BG	63	GLU
7	BG	70	ARG
7	BG	72	THR
7	BG	76	LYS

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Mol	Chain	Res	Type
7	BG	89	VAL
7	BG	120	LEU
7	BG	131	LYS
7	BG	133	THR
7	BG	142	HIS
7	BG	146	GLU
8	BH	3	MET
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	107	SER
8	BH	108	LYS
8	BH	117	ARG
8	BH	129	VAL
9	BI	11	ARG
9	BI	57	MET
9	BI	61	LEU
9	BI	63	LEU
9	BI	66	THR
10	BJ	5	ARG
10	BJ	6	ILE
10	BJ	47	GLU
10	BJ	59	LYS
10	BJ	62	ARG
10	BJ	63	ASP
10	BJ	78	GLU
10	BJ	88	MET
10	BJ	89	ARG
10	BJ	90	LEU
11	BK	18	ASP
11	BK	22	HIS
11	BK	23	ILE
11	BK	31	ILE
11	BK	38	GLN
11	BK	55	SER
11	BK	119	ASN
12	BL	24	LEU

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Mol	Chain	Res	Type
12	BL	44	LYS
12	BL	55	VAL
12	BL	58	THR
12	BL	62	GLU
12	BL	74	LEU
12	BL	82	ILE
12	BL	88	LYS
12	BL	90	LEU
12	BL	114	ARG
12	BL	115	SER
12	BL	121	ARG
13	BM	11	ASP
13	BM	16	VAL
13	BM	17	ILE
13	BM	27	LYS
13	BM	48	LEU
14	BN	26	GLU
15	BO	2	SER
15	BO	13	SER
15	BO	24	SER
15	BO	40	GLN
15	BO	64	ARG
15	BO	66	LEU
15	BO	70	LEU
15	BO	89	ARG
16	BP	18	GLN
16	BP	19	VAL
16	BP	20	VAL
16	BP	46	LYS
16	BP	48	GLU
16	BP	76	LYS
17	BQ	17	MET
17	BQ	21	ILE
17	BQ	26	GLU
17	BQ	38	ILE
17	BQ	40	ARG
17	BQ	51	ASN
17	BQ	75	LEU
18	BR	33	ILE
18	BR	47	THR
19	BS	6	LYS
19	BS	7	LYS

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Mol	Chain	Res	Type
19	BS	11	ILE
19	BS	13	LEU
19	BS	33	THR
20	BT	5	LYS
20	BT	12	ILE
20	BT	15	GLU
20	BT	27	MET
20	BT	43	ASP
20	BT	48	GLN
20	BT	54	MET
20	BT	58	VAL
20	BT	64	LYS
20	BT	67	ILE
20	BT	69	LYS
20	BT	84	ASN
21	BU	13	ASP
21	BU	16	LEU
21	BU	18	ARG
21	BU	34	ARG
21	BU	56	HIS
22	D1	26	THR
22	D1	29	SER
22	D1	52	ARG
23	D2	5	ILE
23	D2	8	LYS
23	D2	47	VAL
24	D3	1	MET
25	D4	45	ARG
25	D4	52	LYS
27	D0	10	THR
27	D0	19	LYS
27	D0	36	VAL
29	CC	3	VAL
29	CC	97	LYS
29	CC	110	LEU
29	CC	117	GLN
29	CC	120	VAL
29	CC	130	LEU
29	CC	157	SER
29	CC	168	ASP
29	CC	174	LEU
29	CC	184	VAL

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Mol	Chain	Res	Type
29	CC	195	VAL
29	CC	204	VAL
29	CC	205	LEU
29	CC	236	GLU
29	CC	252	THR
30	CD	4	LEU
30	CD	13	ARG
30	CD	18	ASP
30	CD	51	THR
30	CD	95	SER
30	CD	114	LYS
30	CD	184	ARG
29	DC	3	VAL
29	DC	70	ASN
29	DC	110	LEU
29	DC	117	GLN
29	DC	120	VAL
29	DC	130	LEU
29	DC	182	ARG
29	DC	184	VAL
29	DC	236	GLU
29	DC	252	THR
32	DD	13	ARG
32	DD	18	ASP
32	DD	51	THR
32	DD	95	SER
32	DD	114	LYS
32	DD	184	ARG
33	CE	7	ASP
33	CE	12	LEU
33	CE	25	GLU
33	CE	44	ARG
33	CE	72	SER
33	CE	83	VAL
33	CE	107	SER
33	CE	122	GLU
33	CE	127	GLU
33	CE	149	ILE
33	CE	152	GLU
33	CE	189	THR
34	CF	18	THR
34	CF	31	VAL

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Mol	Chain	Res	Type
34	CF	36	LEU
34	CF	49	LEU
34	CF	57	LEU
34	CF	72	LYS
34	CF	80	ARG
34	CF	89	VAL
34	CF	94	GLU
34	CF	106	ILE
34	CF	117	LEU
34	CF	123	ASP
34	CF	134	GLU
34	CF	141	ILE
34	CF	149	VAL
34	CF	152	LEU
35	CG	11	VAL
35	CG	18	LYS
35	CG	42	GLU
35	CG	155	GLU
36	CH	1	MET
36	CH	7	ASP
36	CH	15	LEU
36	CH	17	ASP
36	CH	21	VAL
36	CH	44	ILE
36	CH	48	GLU
36	CH	51	ARG
36	CH	53	GLU
36	CH	54	LEU
36	CH	55	GLU
36	CH	57	LYS
36	CH	62	LEU
36	CH	75	LEU
36	CH	76	GLU
36	CH	89	LYS
36	CH	112	LYS
36	CH	121	VAL
36	CH	127	GLU
36	CH	145	ASN
37	CJ	11	LEU
37	CJ	13	VAL
37	CJ	28	LEU
37	CJ	53	LEU

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Mol	Chain	Res	Type
37	CJ	55	ILE
37	CJ	101	ILE
37	CJ	113	LYS
38	CK	5	THR
38	CK	9	GLU
38	CK	30	THR
38	CK	124	VAL
38	CK	142	ILE
39	CL	35	VAL
39	CL	41	ILE
39	CL	70	ARG
39	CL	86	LEU
39	CL	98	ARG
39	CL	113	MET
40	CM	92	LEU
40	CM	93	ASN
40	CM	94	THR
40	CM	100	ILE
40	CM	103	ILE
40	CM	115	GLU
40	CM	120	VAL
41	CN	6	ARG
41	CN	14	LYS
41	CN	20	LEU
41	CN	55	ARG
41	CN	59	ARG
41	CN	75	GLU
41	CN	78	LEU
41	CN	80	VAL
41	CN	100	LYS
41	CN	126	ILE
42	CO	2	ARG
42	CO	69	ARG
42	CO	71	ARG
42	CO	76	VAL
42	CO	95	THR
42	CO	116	VAL
43	CP	18	LEU
43	CP	20	GLU
43	CP	31	THR
43	CP	38	GLN
43	CP	47	VAL

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Mol	Chain	Res	Type
43	CP	49	VAL
43	CP	56	LYS
43	CP	78	VAL
43	CP	115	LEU
44	CQ	2	SER
44	CQ	26	VAL
44	CQ	39	ARG
44	CQ	40	LEU
44	CQ	102	GLU
44	CQ	114	LEU
45	CR	5	LYS
45	CR	9	ILE
45	CR	16	LYS
45	CR	41	LYS
45	CR	51	ARG
45	CR	52	GLN
46	CS	1	MET
46	CS	12	HIS
46	CS	45	GLU
46	CS	48	LYS
46	CS	51	VAL
46	CS	102	SER
47	CT	19	LEU
47	CT	29	VAL
47	CT	69	LEU
47	CT	86	MET
47	CT	97	LEU
48	CU	2	ILE
48	CU	10	VAL
48	CU	24	MET
48	CU	30	ILE
48	CU	49	LYS
48	CU	69	ARG
48	CU	93	LEU
49	CV	28	VAL
49	CV	61	LYS
49	CV	72	ILE
49	CV	81	ASP
50	CW	1	MET
50	CW	7	GLU
50	CW	10	LYS
50	CW	66	ASP

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Mol	Chain	Res	Type
51	CX	70	GLU
51	CX	82	ILE
52	CY	25	THR
52	CY	35	SER
52	CY	48	THR
52	CY	71	LEU
53	CZ	7	ARG
53	CZ	18	LEU
53	CZ	19	LEU
53	CZ	38	GLN
53	CZ	58	ASN
33	DE	12	LEU
33	DE	107	SER
33	DE	127	GLU
33	DE	189	THR
34	DF	10	ASP
34	DF	49	LEU
34	DF	57	LEU
34	DF	72	LYS
34	DF	89	VAL
34	DF	94	GLU
34	DF	106	ILE
34	DF	117	LEU
34	DF	134	GLU
34	DF	141	ILE
34	DF	149	VAL
34	DF	152	LEU
35	DG	11	VAL
35	DG	18	LYS
35	DG	155	GLU
36	DH	1	MET
36	DH	7	ASP
36	DH	15	LEU
36	DH	17	ASP
36	DH	21	VAL
36	DH	44	ILE
36	DH	53	GLU
36	DH	54	LEU
36	DH	57	LYS
36	DH	58	LEU
36	DH	60	GLU
36	DH	62	LEU

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Mol	Chain	Res	Type
36	DH	75	LEU
36	DH	76	GLU
36	DH	89	LYS
36	DH	112	LYS
36	DH	117	LEU
36	DH	121	VAL
36	DH	127	GLU
36	DH	133	GLN
36	DH	145	ASN
37	DJ	11	LEU
37	DJ	13	VAL
37	DJ	28	LEU
37	DJ	53	LEU
37	DJ	55	ILE
37	DJ	101	ILE
37	DJ	113	LYS
38	DK	3	THR
38	DK	124	VAL
38	DK	142	ILE
39	DL	41	ILE
39	DL	70	ARG
39	DL	76	VAL
39	DL	86	LEU
39	DL	110	GLU
39	DL	113	MET
39	DL	123	LEU
40	DM	74	THR
40	DM	91	ASP
40	DM	92	LEU
40	DM	94	THR
40	DM	115	GLU
40	DM	120	VAL
41	DN	75	GLU
41	DN	80	VAL
41	DN	100	LYS
41	DN	115	GLU
41	DN	126	ILE
42	DO	2	ARG
42	DO	69	ARG
42	DO	76	VAL
42	DO	116	VAL
43	DP	1	MET

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Mol	Chain	Res	Type
43	DP	20	GLU
43	DP	31	THR
43	DP	49	VAL
43	DP	78	VAL
43	DP	115	LEU
44	DQ	26	VAL
44	DQ	40	LEU
44	DQ	102	GLU
45	DR	11	ARG
45	DR	41	LYS
45	DR	51	ARG
46	DS	1	MET
46	DS	38	VAL
46	DS	102	SER
47	DT	86	MET
48	DU	1	MET
48	DU	3	ARG
48	DU	10	VAL
48	DU	25	GLU
49	DV	28	VAL
49	DV	52	LEU
49	DV	61	LYS
50	DW	7	GLU
50	DW	53	LYS
50	DW	66	ASP
51	DX	70	GLU
51	DX	82	ILE
52	DY	25	THR
52	DY	35	SER
52	DY	37	ARG
53	DZ	7	ARG
53	DZ	19	LEU
53	DZ	38	GLN
54	DI	16	SER
54	DI	53	ARG
54	DI	59	LEU
54	DI	60	LEU
54	DI	64	VAL
54	DI	85	VAL
54	DI	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (146) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	93	ASN
2	AB	94	HIS
2	AB	120	GLN
3	AC	41	GLN
3	AC	123	GLN
3	AC	139	GLN
4	AD	41	HIS
4	AD	85	ASN
4	AD	136	GLN
5	AE	70	ASN
5	AE	77	ASN
5	AE	89	HIS
5	AE	121	HIS
5	AE	122	ASN
6	AF	17	GLN
6	AF	63	ASN
7	AG	86	GLN
7	AG	130	ASN
7	AG	142	HIS
7	AG	148	ASN
8	AH	4	GLN
8	AH	38	ASN
8	AH	67	GLN
9	AI	110	GLN
10	AJ	56	HIS
10	AJ	58	ASN
11	AK	40	ASN
11	AK	118	HIS
12	AL	77	HIS
14	AN	4	GLN
15	AO	28	GLN
15	AO	50	HIS
16	AP	40	ASN
16	AP	59	HIS
16	AP	63	GLN
20	AT	48	GLN
22	C1	6	ASN
22	C1	38	HIS
22	C1	42	HIS
23	C2	26	ASN
24	C3	26	ASN
27	C0	9	GLN
2	BB	39	HIS

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Mol	Chain	Res	Type
2	BB	93	ASN
2	BB	94	HIS
2	BB	120	GLN
2	BB	168	HIS
3	BC	123	GLN
3	BC	139	GLN
4	BD	41	HIS
4	BD	85	ASN
4	BD	131	ASN
5	BE	77	ASN
5	BE	89	HIS
5	BE	121	HIS
5	BE	122	ASN
5	BE	135	ASN
6	BF	17	GLN
6	BF	46	GLN
7	BG	130	ASN
7	BG	148	ASN
8	BH	4	GLN
8	BH	38	ASN
8	BH	67	GLN
8	BH	76	GLN
9	BI	110	GLN
10	BJ	56	HIS
11	BK	40	ASN
14	BN	4	GLN
15	BO	28	GLN
16	BP	40	ASN
16	BP	63	GLN
17	BQ	51	ASN
20	BT	3	ASN
24	D3	26	ASN
29	CC	134	ASN
29	CC	142	HIS
29	CC	260	ASN
29	DC	134	ASN
29	DC	142	HIS
32	DD	42	ASN
32	DD	49	GLN
33	CE	94	GLN
33	CE	115	GLN
33	CE	136	GLN

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Mol	Chain	Res	Type
33	CE	156	ASN
34	CF	52	ASN
35	CG	38	ASN
35	CG	73	ASN
35	CG	104	ASN
35	CG	128	GLN
36	CH	2	GLN
36	CH	18	GLN
36	CH	20	ASN
36	CH	43	ASN
36	CH	145	ASN
38	CK	58	ASN
38	CK	128	ASN
40	CM	35	HIS
41	CN	3	GLN
41	CN	13	HIS
43	CP	19	GLN
43	CP	29	HIS
43	CP	100	HIS
43	CP	104	GLN
44	CQ	41	GLN
46	CS	6	GLN
46	CS	12	HIS
46	CS	86	GLN
46	CS	87	GLN
47	CT	9	HIS
48	CU	28	ASN
49	CV	74	ASN
50	CW	75	GLN
51	CX	57	HIS
52	CY	16	ASN
52	CY	36	HIS
53	CZ	45	GLN
33	DE	90	GLN
33	DE	94	GLN
33	DE	156	ASN
35	DG	30	ASN
35	DG	101	ASN
35	DG	104	ASN
35	DG	116	GLN
35	DG	128	GLN
36	DH	2	GLN

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Mol	Chain	Res	Type
36	DH	18	GLN
36	DH	20	ASN
36	DH	145	ASN
38	DK	47	HIS
38	DK	58	ASN
38	DK	128	ASN
39	DL	93	GLN
40	DM	35	HIS
42	DO	31	HIS
43	DP	29	HIS
45	DR	81	ASN
46	DS	6	GLN
46	DS	86	GLN
49	DV	54	GLN
51	DX	46	HIS
52	DY	16	ASN
52	DY	36	HIS
54	DI	4	ASN
54	DI	122	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1533/1534 (99%)	245 (15%)	27 (1%)
1	BA	1532/1534 (99%)	251 (16%)	28 (1%)
28	CB	117/120 (97%)	11 (9%)	0
28	DB	119/120 (99%)	9 (7%)	0
31	CA	2896/2904 (99%)	443 (15%)	72 (2%)
55	DA	2884/2904 (99%)	379 (13%)	57 (1%)
All	All	9081/9116 (99%)	1338 (14%)	184 (2%)

All (1338) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G

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Mol	Chain	Res	Type
1	AA	47	C
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	69	G
1	AA	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	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	120	A
1	AA	130	A
1	AA	131	A
1	AA	137	U
1	AA	141	G
1	AA	142	G
1	AA	143	A
1	AA	144	G
1	AA	149	A
1	AA	159	G
1	AA	163	C
1	AA	168	G
1	AA	177	G
1	AA	183	C
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	250	A
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	346	G
1	AA	348	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	384	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	430	A
1	AA	436	C
1	AA	457	G
1	AA	458	U
1	AA	463	U
1	AA	466	A
1	AA	467	U
1	AA	468	A
1	AA	474	G
1	AA	481	G
1	AA	484	G

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Mol	Chain	Res	Type
1	AA	486	U
1	AA	495	A
1	AA	509	A
1	AA	511	C
1	AA	527	G7M
1	AA	531	U
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	564	C
1	AA	568	G
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	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	695	A
1	AA	702	A
1	AA	703	G
1	AA	723	U
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	814	A
1	AA	815	A
1	AA	817	C
1	AA	821	G
1	AA	828	U
1	AA	836	G
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G

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Mol	Chain	Res	Type
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	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	971	G
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	987	G
1	AA	992	U
1	AA	993	G
1	AA	1004	A
1	AA	1009	U
1	AA	1015	G
1	AA	1019	A
1	AA	1024	G
1	AA	1026	G
1	AA	1027	C
1	AA	1028	C
1	AA	1029	U
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	G
1	AA	1036	A
1	AA	1037	C
1	AA	1043	G
1	AA	1053	G
1	AA	1054	C
1	AA	1065	U
1	AA	1086	U
1	AA	1087	G
1	AA	1094	G
1	AA	1095	U
1	AA	1098	C
1	AA	1101	A
1	AA	1124	G

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Mol	Chain	Res	Type
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	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1236	A
1	AA	1238	A
1	AA	1239	A
1	AA	1256	A
1	AA	1257	A
1	AA	1260	G
1	AA	1280	A
1	AA	1281	C
1	AA	1282	C
1	AA	1286	U
1	AA	1287	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1312	G
1	AA	1317	C

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Mol	Chain	Res	Type
1	AA	1320	C
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1379	G
1	AA	1381	U
1	AA	1397	C
1	AA	1398	A
1	AA	1419	G
1	AA	1429	A
1	AA	1441	A
1	AA	1446	A
1	AA	1447	A
1	AA	1448	C
1	AA	1451	U
1	AA	1452	C
1	AA	1453	G
1	AA	1492	A
1	AA	1497	G
1	AA	1499	A
1	AA	1503	A
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1534	A
1	BA	4	U
1	BA	5	U
1	BA	6	G
1	BA	9	G
1	BA	22	G
1	BA	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

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Mol	Chain	Res	Type
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	120	A
1	BA	130	A
1	BA	131	A
1	BA	137	U
1	BA	141	G
1	BA	142	G
1	BA	143	A
1	BA	144	G
1	BA	149	A
1	BA	159	G
1	BA	163	C
1	BA	168	G
1	BA	177	G
1	BA	183	C
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	245	U
1	BA	247	G
1	BA	250	A
1	BA	251	G
1	BA	266	G

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Mol	Chain	Res	Type
1	BA	267	C
1	BA	289	G
1	BA	321	A
1	BA	328	C
1	BA	329	A
1	BA	330	C
1	BA	332	G
1	BA	346	G
1	BA	348	G
1	BA	352	C
1	BA	354	G
1	BA	367	U
1	BA	372	C
1	BA	373	A
1	BA	384	G
1	BA	398	U
1	BA	406	G
1	BA	412	A
1	BA	413	G
1	BA	414	A
1	BA	421	U
1	BA	422	C
1	BA	424	G
1	BA	429	U
1	BA	430	A
1	BA	436	C
1	BA	457	G
1	BA	458	U
1	BA	463	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	509	A
1	BA	511	C
1	BA	527	G7M
1	BA	531	U
1	BA	532	A
1	BA	533	A

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Mol	Chain	Res	Type
1	BA	547	A
1	BA	559	A
1	BA	564	C
1	BA	568	G
1	BA	572	A
1	BA	573	A
1	BA	576	C
1	BA	577	G
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	695	A
1	BA	702	A
1	BA	703	G
1	BA	723	U
1	BA	734	G
1	BA	748	G
1	BA	755	G
1	BA	777	A
1	BA	793	U
1	BA	794	A
1	BA	814	A
1	BA	815	A
1	BA	817	C
1	BA	821	G
1	BA	828	U
1	BA	836	G
1	BA	839	C
1	BA	840	C
1	BA	841	C
1	BA	842	U
1	BA	843	U
1	BA	844	G
1	BA	845	A
1	BA	846	G
1	BA	914	A
1	BA	926	G
1	BA	927	G

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Mol	Chain	Res	Type
1	BA	934	C
1	BA	935	A
1	BA	960	U
1	BA	966	2MG
1	BA	969	A
1	BA	971	G
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	1004	A
1	BA	1008	U
1	BA	1009	U
1	BA	1015	G
1	BA	1019	A
1	BA	1024	G
1	BA	1026	G
1	BA	1027	C
1	BA	1028	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	1070	U
1	BA	1086	U
1	BA	1087	G
1	BA	1094	G
1	BA	1095	U
1	BA	1098	C
1	BA	1101	A
1	BA	1124	G
1	BA	1125	U

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Mol	Chain	Res	Type
1	BA	1132	C
1	BA	1133	G
1	BA	1136	C
1	BA	1137	C
1	BA	1138	G
1	BA	1139	G
1	BA	1140	C
1	BA	1141	C
1	BA	1142	G
1	BA	1143	G
1	BA	1145	A
1	BA	1152	A
1	BA	1159	U
1	BA	1160	G
1	BA	1168	U
1	BA	1196	A
1	BA	1197	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	1280	A
1	BA	1281	C
1	BA	1282	C
1	BA	1286	U
1	BA	1287	A
1	BA	1300	G
1	BA	1302	C
1	BA	1305	G
1	BA	1312	G
1	BA	1317	C
1	BA	1320	C
1	BA	1346	A

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Mol	Chain	Res	Type
1	BA	1353	G
1	BA	1362	A
1	BA	1363	A
1	BA	1370	G
1	BA	1379	G
1	BA	1381	U
1	BA	1398	A
1	BA	1419	G
1	BA	1429	A
1	BA	1441	A
1	BA	1446	A
1	BA	1447	A
1	BA	1448	C
1	BA	1451	U
1	BA	1452	C
1	BA	1453	G
1	BA	1492	A
1	BA	1493	A
1	BA	1497	G
1	BA	1499	A
1	BA	1503	A
1	BA	1506	U
1	BA	1507	A
1	BA	1517	G
1	BA	1529	G
1	BA	1530	G
1	BA	1534	A
28	CB	9	G
28	CB	25	U
28	CB	35	C
28	CB	45	A
28	CB	56	G
28	CB	57	A
28	CB	88	C
28	CB	89	U
28	CB	90	C
28	CB	99	A
28	CB	109	A
31	CA	10	A
31	CA	14	A
31	CA	34	U
31	CA	36	G

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Mol	Chain	Res	Type
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	101	A
31	CA	102	U
31	CA	118	A
31	CA	119	A
31	CA	120	U
31	CA	138	U
31	CA	139	U
31	CA	140	C
31	CA	141	G
31	CA	142	A
31	CA	143	C
31	CA	177	G
31	CA	178	G
31	CA	196	A
31	CA	199	A
31	CA	200	U
31	CA	215	G
31	CA	216	A
31	CA	221	A
31	CA	222	A
31	CA	248	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
31	CA	279	A
31	CA	285	G
31	CA	310	A

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Mol	Chain	Res	Type
31	CA	311	A
31	CA	329	G
31	CA	330	A
31	CA	343	C
31	CA	346	A
31	CA	352	A
31	CA	353	C
31	CA	362	A
31	CA	371	A
31	CA	372	G
31	CA	385	C
31	CA	386	G
31	CA	399	U
31	CA	404	A
31	CA	405	U
31	CA	411	G
31	CA	420	C
31	CA	424	G
31	CA	425	G
31	CA	451	U
31	CA	480	A
31	CA	481	G
31	CA	491	G
31	CA	503	A
31	CA	504	A
31	CA	505	A
31	CA	508	A
31	CA	517	C
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	571	U
31	CA	573	U

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Mol	Chain	Res	Type
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	627	A
31	CA	637	A
31	CA	645	C
31	CA	647	G
31	CA	654	A
31	CA	655	A
31	CA	670	A
31	CA	684	G
31	CA	685	A
31	CA	686	U
31	CA	695	G
31	CA	717	C
31	CA	730	A
31	CA	740	C
31	CA	746	PSU
31	CA	747	5MU
31	CA	764	A
31	CA	765	C
31	CA	775	G
31	CA	776	G
31	CA	782	A
31	CA	784	G
31	CA	785	G
31	CA	792	A
31	CA	802	A
31	CA	805	G
31	CA	812	C
31	CA	819	A
31	CA	827	U
31	CA	828	U
31	CA	845	A
31	CA	846	U
31	CA	847	U
31	CA	858	G
31	CA	859	G
31	CA	878	A

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Mol	Chain	Res	Type
31	CA	883	G
31	CA	896	A
31	CA	897	C
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	973	A
31	CA	974	G
31	CA	983	A
31	CA	984	A
31	CA	985	C
31	CA	995	C
31	CA	996	A
31	CA	1012	U
31	CA	1013	C
31	CA	1022	G
31	CA	1026	G
31	CA	1033	U
31	CA	1040	A
31	CA	1045	C
31	CA	1046	A
31	CA	1047	G
31	CA	1057	A
31	CA	1061	U
31	CA	1062	G
31	CA	1069	A
31	CA	1070	A
31	CA	1083	U
31	CA	1088	A
31	CA	1089	A
31	CA	1090	A
31	CA	1091	G
31	CA	1096	A
31	CA	1097	U
31	CA	1111	A
31	CA	1112	G

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Mol	Chain	Res	Type
31	CA	1122	G
31	CA	1128	G
31	CA	1129	A
31	CA	1132	U
31	CA	1133	A
31	CA	1135	C
31	CA	1136	G
31	CA	1142	A
31	CA	1168	G
31	CA	1169	A
31	CA	1170	C
31	CA	1171	G
31	CA	1172	C
31	CA	1175	A
31	CA	1176	U
31	CA	1177	G
31	CA	1179	G
31	CA	1180	U
31	CA	1186	G
31	CA	1210	G
31	CA	1212	G
31	CA	1236	G
31	CA	1238	G
31	CA	1253	A
31	CA	1254	A
31	CA	1256	G
31	CA	1266	G
31	CA	1271	G
31	CA	1272	A
31	CA	1273	U
31	CA	1286	A
31	CA	1287	A
31	CA	1300	G
31	CA	1301	A
31	CA	1313	U
31	CA	1320	C
31	CA	1321	A
31	CA	1328	A
31	CA	1352	U
31	CA	1365	A
31	CA	1376	C
31	CA	1379	U

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Mol	Chain	Res	Type
31	CA	1380	G
31	CA	1383	A
31	CA	1391	U
31	CA	1395	A
31	CA	1416	G
31	CA	1417	C
31	CA	1419	A
31	CA	1420	A
31	CA	1428	C
31	CA	1437	C
31	CA	1452	G
31	CA	1453	A
31	CA	1460	U
31	CA	1482	G
31	CA	1490	A
31	CA	1491	G
31	CA	1493	C
31	CA	1494	A
31	CA	1497	U
31	CA	1498	C
31	CA	1509	A
31	CA	1510	G
31	CA	1515	A
31	CA	1523	U
31	CA	1532	A
31	CA	1534	U
31	CA	1535	A
31	CA	1536	C
31	CA	1537	G
31	CA	1565	C
31	CA	1566	A
31	CA	1569	A
31	CA	1578	U
31	CA	1583	A
31	CA	1585	C
31	CA	1607	C
31	CA	1608	A
31	CA	1647	U
31	CA	1648	U
31	CA	1649	G
31	CA	1674	G
31	CA	1695	G

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Mol	Chain	Res	Type
31	CA	1715	G
31	CA	1729	U
31	CA	1730	C
31	CA	1731	G
31	CA	1732	C
31	CA	1738	G
31	CA	1744	A
31	CA	1750	G
31	CA	1764	C
31	CA	1773	A
31	CA	1782	U
31	CA	1800	C
31	CA	1801	A
31	CA	1808	A
31	CA	1816	C
31	CA	1822	C
31	CA	1829	A
31	CA	1869	G
31	CA	1870	C
31	CA	1871	A
31	CA	1872	A
31	CA	1873	G
31	CA	1900	A
31	CA	1906	G
31	CA	1907	G
31	CA	1914	C
31	CA	1929	G
31	CA	1930	G
31	CA	1931	U
31	CA	1937	A
31	CA	1938	A
31	CA	1955	U
31	CA	1967	C
31	CA	1970	A
31	CA	1972	G
31	CA	1991	U
31	CA	1993	U
31	CA	1997	C
31	CA	2022	U
31	CA	2023	C
31	CA	2031	A
31	CA	2033	A

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Mol	Chain	Res	Type
31	CA	2035	G
31	CA	2036	C
31	CA	2043	C
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	2096	C
31	CA	2100	G
31	CA	2102	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
31	CA	2118	U
31	CA	2119	A
31	CA	2123	G
31	CA	2124	G
31	CA	2125	G
31	CA	2126	A
31	CA	2127	G
31	CA	2128	G
31	CA	2131	U
31	CA	2132	U
31	CA	2133	G
31	CA	2146	C
31	CA	2147	A
31	CA	2157	G
31	CA	2158	A
31	CA	2159	G
31	CA	2160	C
31	CA	2162	G
31	CA	2164	C

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Mol	Chain	Res	Type
31	CA	2165	C
31	CA	2171	A
31	CA	2172	U
31	CA	2173	A
31	CA	2174	C
31	CA	2178	C
31	CA	2183	A
31	CA	2190	G
31	CA	2198	A
31	CA	2203	U
31	CA	2204	G
31	CA	2211	A
31	CA	2225	A
31	CA	2226	C
31	CA	2238	G
31	CA	2239	G
31	CA	2259	U
31	CA	2268	A
31	CA	2280	G
31	CA	2282	G
31	CA	2283	C
31	CA	2287	A
31	CA	2305	U
31	CA	2311	A
31	CA	2322	A
31	CA	2326	C
31	CA	2327	A
31	CA	2333	A
31	CA	2335	A
31	CA	2345	G
31	CA	2347	C
31	CA	2350	C
31	CA	2354	C
31	CA	2361	G
31	CA	2383	G
31	CA	2385	C
31	CA	2388	A
31	CA	2402	U
31	CA	2403	C
31	CA	2406	A
31	CA	2423	U
31	CA	2424	C

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Mol	Chain	Res	Type
31	CA	2425	A
31	CA	2426	A
31	CA	2429	G
31	CA	2430	A
31	CA	2435	A
31	CA	2441	U
31	CA	2448	A
31	CA	2465	C
31	CA	2476	A
31	CA	2491	U
31	CA	2502	G
31	CA	2505	G
31	CA	2518	A
31	CA	2529	G
31	CA	2535	G
31	CA	2547	A
31	CA	2554	U
31	CA	2556	C
31	CA	2566	A
31	CA	2567	G
31	CA	2573	C
31	CA	2578	G
31	CA	2582	G
31	CA	2585	U
31	CA	2603	G
31	CA	2609	U
31	CA	2613	U
31	CA	2629	U
31	CA	2630	G
31	CA	2646	C
31	CA	2661	G
31	CA	2663	G
31	CA	2681	C
31	CA	2682	A
31	CA	2689	U
31	CA	2690	U
31	CA	2714	G
31	CA	2718	G
31	CA	2726	A
31	CA	2744	G
31	CA	2748	A
31	CA	2769	U

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Mol	Chain	Res	Type
31	CA	2778	A
31	CA	2791	G
31	CA	2794	C
31	CA	2799	A
31	CA	2820	A
31	CA	2835	A
31	CA	2836	U
31	CA	2849	U
31	CA	2850	A
31	CA	2861	U
31	CA	2865	U
31	CA	2867	G
31	CA	2883	A
31	CA	2884	U
31	CA	2886	A
31	CA	2887	A
31	CA	2891	U
31	CA	2903	U
31	CA	2904	U
28	DB	25	U
28	DB	35	C
28	DB	45	A
28	DB	56	G
28	DB	57	A
28	DB	88	C
28	DB	89	U
28	DB	90	C
28	DB	109	A
55	DA	10	A
55	DA	12	U
55	DA	34	U
55	DA	46	G
55	DA	63	A
55	DA	71	A
55	DA	74	A
55	DA	75	G
55	DA	80	G
55	DA	84	A
55	DA	101	A
55	DA	102	U
55	DA	118	A
55	DA	119	A

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Mol	Chain	Res	Type
55	DA	120	U
55	DA	138	U
55	DA	139	U
55	DA	140	C
55	DA	141	G
55	DA	142	A
55	DA	143	C
55	DA	196	A
55	DA	199	A
55	DA	200	U
55	DA	215	G
55	DA	216	A
55	DA	221	A
55	DA	222	A
55	DA	248	G
55	DA	265	A
55	DA	266	G
55	DA	272	A
55	DA	276	U
55	DA	277	G
55	DA	278	A
55	DA	279	A
55	DA	285	G
55	DA	302	C
55	DA	311	A
55	DA	329	G
55	DA	330	A
55	DA	343	C
55	DA	346	A
55	DA	352	A
55	DA	353	C
55	DA	362	A
55	DA	370	G
55	DA	372	G
55	DA	386	G
55	DA	399	U
55	DA	411	G
55	DA	412	A
55	DA	420	C
55	DA	424	G
55	DA	425	G
55	DA	451	U

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Mol	Chain	Res	Type
55	DA	480	A
55	DA	481	G
55	DA	491	G
55	DA	504	A
55	DA	505	A
55	DA	508	A
55	DA	531	C
55	DA	532	A
55	DA	543	G
55	DA	544	C
55	DA	546	U
55	DA	547	A
55	DA	548	G
55	DA	549	G
55	DA	550	C
55	DA	551	G
55	DA	563	A
55	DA	573	U
55	DA	575	A
55	DA	586	A
55	DA	603	A
55	DA	613	A
55	DA	614	A
55	DA	615	U
55	DA	627	A
55	DA	637	A
55	DA	645	C
55	DA	647	G
55	DA	654	A
55	DA	655	A
55	DA	686	U
55	DA	717	C
55	DA	730	A
55	DA	746	PSU
55	DA	747	5MU
55	DA	764	A
55	DA	765	C
55	DA	775	G
55	DA	776	G
55	DA	782	A
55	DA	784	G
55	DA	785	G

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Mol	Chain	Res	Type
55	DA	790	U
55	DA	792	A
55	DA	805	G
55	DA	812	C
55	DA	827	U
55	DA	828	U
55	DA	858	G
55	DA	859	G
55	DA	860	U
55	DA	878	A
55	DA	883	G
55	DA	885	C
55	DA	896	A
55	DA	897	C
55	DA	910	A
55	DA	914	G
55	DA	915	C
55	DA	927	A
55	DA	931	U
55	DA	932	U
55	DA	946	C
55	DA	961	C
55	DA	974	G
55	DA	983	A
55	DA	984	A
55	DA	985	C
55	DA	996	A
55	DA	1012	U
55	DA	1013	C
55	DA	1022	G
55	DA	1026	G
55	DA	1033	U
55	DA	1040	A
55	DA	1047	G
55	DA	1057	A
55	DA	1061	U
55	DA	1062	G
55	DA	1069	A
55	DA	1070	A
55	DA	1083	U
55	DA	1088	A
55	DA	1089	A

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Mol	Chain	Res	Type
55	DA	1090	A
55	DA	1091	G
55	DA	1096	A
55	DA	1097	U
55	DA	1112	G
55	DA	1128	G
55	DA	1129	A
55	DA	1132	U
55	DA	1133	A
55	DA	1135	C
55	DA	1136	G
55	DA	1142	A
55	DA	1143	A
55	DA	1168	G
55	DA	1172	C
55	DA	1174	U
55	DA	1175	A
55	DA	1176	U
55	DA	1177	G
55	DA	1180	U
55	DA	1187	G
55	DA	1237	A
55	DA	1238	G
55	DA	1253	A
55	DA	1254	A
55	DA	1256	G
55	DA	1271	G
55	DA	1272	A
55	DA	1273	U
55	DA	1300	G
55	DA	1301	A
55	DA	1329	U
55	DA	1352	U
55	DA	1365	A
55	DA	1379	U
55	DA	1383	A
55	DA	1391	U
55	DA	1416	G
55	DA	1417	C
55	DA	1427	A
55	DA	1428	C
55	DA	1434	A

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Mol	Chain	Res	Type
55	DA	1435	G
55	DA	1452	G
55	DA	1453	A
55	DA	1460	U
55	DA	1482	G
55	DA	1490	A
55	DA	1491	G
55	DA	1493	C
55	DA	1494	A
55	DA	1497	U
55	DA	1498	C
55	DA	1508	A
55	DA	1509	A
55	DA	1510	G
55	DA	1515	A
55	DA	1523	U
55	DA	1532	A
55	DA	1534	U
55	DA	1535	A
55	DA	1536	C
55	DA	1537	G
55	DA	1566	A
55	DA	1569	A
55	DA	1578	U
55	DA	1583	A
55	DA	1585	C
55	DA	1607	C
55	DA	1608	A
55	DA	1616	A
55	DA	1647	U
55	DA	1648	U
55	DA	1649	G
55	DA	1674	G
55	DA	1715	G
55	DA	1729	U
55	DA	1730	C
55	DA	1731	G
55	DA	1732	C
55	DA	1738	G
55	DA	1744	A
55	DA	1764	C
55	DA	1773	A

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Mol	Chain	Res	Type
55	DA	1782	U
55	DA	1800	C
55	DA	1801	A
55	DA	1808	A
55	DA	1816	C
55	DA	1829	A
55	DA	1869	G
55	DA	1870	C
55	DA	1871	A
55	DA	1872	A
55	DA	1873	G
55	DA	1906	G
55	DA	1907	G
55	DA	1913	A
55	DA	1914	C
55	DA	1929	G
55	DA	1930	G
55	DA	1931	U
55	DA	1937	A
55	DA	1938	A
55	DA	1955	U
55	DA	1965	C
55	DA	1967	C
55	DA	1970	A
55	DA	1972	G
55	DA	1991	U
55	DA	1993	U
55	DA	1997	C
55	DA	2023	C
55	DA	2031	A
55	DA	2033	A
55	DA	2043	C
55	DA	2055	C
55	DA	2056	G
55	DA	2060	A
55	DA	2061	G
55	DA	2062	A
55	DA	2069	G7M
55	DA	2097	A
55	DA	2098	U
55	DA	2100	G
55	DA	2102	G

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Mol	Chain	Res	Type
55	DA	2105	U
55	DA	2111	U
55	DA	2112	G
55	DA	2113	U
55	DA	2116	G
55	DA	2117	A
55	DA	2118	U
55	DA	2119	A
55	DA	2120	G
55	DA	2123	G
55	DA	2125	G
55	DA	2126	A
55	DA	2128	G
55	DA	2131	U
55	DA	2132	U
55	DA	2133	G
55	DA	2134	A
55	DA	2135	A
55	DA	2145	C
55	DA	2146	C
55	DA	2148	G
55	DA	2158	A
55	DA	2159	G
55	DA	2160	C
55	DA	2161	C
55	DA	2162	G
55	DA	2163	A
55	DA	2164	C
55	DA	2165	C
55	DA	2167	U
55	DA	2168	G
55	DA	2169	A
55	DA	2170	A
55	DA	2171	A
55	DA	2172	U
55	DA	2173	A
55	DA	2177	C
55	DA	2178	C
55	DA	2179	C
55	DA	2181	U
55	DA	2183	A
55	DA	2185	U

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Mol	Chain	Res	Type
55	DA	2190	G
55	DA	2198	A
55	DA	2204	G
55	DA	2211	A
55	DA	2225	A
55	DA	2238	G
55	DA	2239	G
55	DA	2268	A
55	DA	2283	C
55	DA	2286	G
55	DA	2287	A
55	DA	2305	U
55	DA	2308	G
55	DA	2311	A
55	DA	2312	U
55	DA	2324	U
55	DA	2325	G
55	DA	2333	A
55	DA	2335	A
55	DA	2347	C
55	DA	2383	G
55	DA	2385	C
55	DA	2402	U
55	DA	2403	C
55	DA	2406	A
55	DA	2407	A
55	DA	2423	U
55	DA	2424	C
55	DA	2425	A
55	DA	2431	U
55	DA	2435	A
55	DA	2441	U
55	DA	2448	A
55	DA	2476	A
55	DA	2491	U
55	DA	2502	G
55	DA	2505	G
55	DA	2518	A
55	DA	2529	G
55	DA	2535	G
55	DA	2547	A
55	DA	2556	C

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Mol	Chain	Res	Type
55	DA	2566	A
55	DA	2567	G
55	DA	2573	C
55	DA	2574	G
55	DA	2585	U
55	DA	2603	G
55	DA	2609	U
55	DA	2613	U
55	DA	2629	U
55	DA	2630	G
55	DA	2661	G
55	DA	2663	G
55	DA	2689	U
55	DA	2690	U
55	DA	2714	G
55	DA	2726	A
55	DA	2744	G
55	DA	2748	A
55	DA	2765	A
55	DA	2778	A
55	DA	2791	G
55	DA	2798	U
55	DA	2799	A
55	DA	2811	G
55	DA	2820	A
55	DA	2821	A
55	DA	2836	U
55	DA	2867	G
55	DA	2891	U

All (184) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	70	U
1	AA	88	U
1	AA	89	U
1	AA	209	U
1	AA	413	G
1	AA	429	U
1	AA	485	U
1	AA	576	C

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Mol	Chain	Res	Type
1	AA	653	U
1	AA	702	A
1	AA	793	U
1	AA	841	C
1	AA	842	U
1	AA	884	U
1	AA	992	U
1	AA	1086	U
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1225	A
1	AA	1281	C
1	AA	1299	A
1	AA	1397	C
1	AA	1447	A
1	AA	1452	C
1	BA	5	U
1	BA	70	U
1	BA	86	G
1	BA	89	U
1	BA	209	U
1	BA	429	U
1	BA	485	U
1	BA	576	C
1	BA	653	U
1	BA	702	A
1	BA	793	U
1	BA	842	U
1	BA	844	G
1	BA	884	U
1	BA	992	U
1	BA	1008	U
1	BA	1086	U
1	BA	1137	C
1	BA	1139	G
1	BA	1140	C
1	BA	1141	C
1	BA	1225	A
1	BA	1281	C
1	BA	1299	A

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Mol	Chain	Res	Type
1	BA	1362	A
1	BA	1397	C
1	BA	1447	A
1	BA	1452	C
31	CA	83	A
31	CA	101	A
31	CA	138	U
31	CA	141	G
31	CA	177	G
31	CA	196	A
31	CA	199	A
31	CA	221	A
31	CA	271	G
31	CA	278	A
31	CA	310	A
31	CA	345	A
31	CA	403	U
31	CA	404	A
31	CA	451	U
31	CA	503	A
31	CA	506	G
31	CA	555	G
31	CA	620	G
31	CA	764	A
31	CA	784	G
31	CA	846	U
31	CA	973	A
31	CA	984	A
31	CA	1045	C
31	CA	1046	A
31	CA	1061	U
31	CA	1069	A
31	CA	1070	A
31	CA	1088	A
31	CA	1089	A
31	CA	1128	G
31	CA	1141	U
31	CA	1253	A
31	CA	1286	A
31	CA	1300	G
31	CA	1320	C
31	CA	1329	U

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Mol	Chain	Res	Type
31	CA	1379	U
31	CA	1452	G
31	CA	1490	A
31	CA	1497	U
31	CA	1509	A
31	CA	1535	A
31	CA	1536	C
31	CA	1607	C
31	CA	1647	U
31	CA	1730	C
31	CA	1786	A
31	CA	1870	C
31	CA	1871	A
31	CA	2035	G
31	CA	2095	A
31	CA	2119	A
31	CA	2126	A
31	CA	2146	C
31	CA	2157	G
31	CA	2164	C
31	CA	2225	A
31	CA	2282	G
31	CA	2286	G
31	CA	2326	C
31	CA	2423	U
31	CA	2425	A
31	CA	2430	A
31	CA	2680	U
31	CA	2681	C
31	CA	2778	A
31	CA	2779	U
31	CA	2797	U
31	CA	2849	U
31	CA	2873	A
55	DA	138	U
55	DA	141	G
55	DA	199	A
55	DA	271	G
55	DA	278	A
55	DA	370	G
55	DA	403	U
55	DA	503	A

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Mol	Chain	Res	Type
55	DA	620	G
55	DA	764	A
55	DA	784	G
55	DA	859	G
55	DA	961	C
55	DA	984	A
55	DA	1061	U
55	DA	1069	A
55	DA	1070	A
55	DA	1087	G
55	DA	1088	A
55	DA	1089	A
55	DA	1128	G
55	DA	1141	U
55	DA	1142	A
55	DA	1175	A
55	DA	1253	A
55	DA	1286	A
55	DA	1300	G
55	DA	1320	C
55	DA	1490	A
55	DA	1497	U
55	DA	1509	A
55	DA	1535	A
55	DA	1607	C
55	DA	1647	U
55	DA	1730	C
55	DA	1870	C
55	DA	1871	A
55	DA	1936	A
55	DA	2097	A
55	DA	2119	A
55	DA	2127	G
55	DA	2146	C
55	DA	2157	G
55	DA	2158	A
55	DA	2164	C
55	DA	2172	U
55	DA	2286	G
55	DA	2311	A
55	DA	2324	U
55	DA	2406	A

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Mol	Chain	Res	Type
55	DA	2423	U
55	DA	2501	C
55	DA	2585	U
55	DA	2681	C
55	DA	2797	U
55	DA	2798	U
55	DA	2873	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
55	5MU	DA	1939	55	19,22,23	0.34	0	27,32,35	0.41	0
1	5MC	BA	1407	1	19,22,23	0.32	0	26,32,35	0.44	0
55	5MU	DA	747	55	19,22,23	0.46	0	27,32,35	0.44	0
31	OMG	CA	2251	31	23,26,27	0.38	0	32,38,41	0.41	0
31	PSU	CA	746	31,56	18,21,22	0.63	1 (5%)	21,30,33	0.44	0
55	OMG	DA	2251	55	23,26,27	0.40	0	32,38,41	0.51	0
1	MA6	AA	1519	1	23,26,27	0.50	0	33,38,41	1.28	4 (12%)
1	2MG	AA	1207	1	23,26,27	0.25	0	33,38,41	0.43	0
31	PSU	CA	2457	31	18,21,22	0.45	0	21,30,33	0.47	0
31	6MZ	CA	2030	31	22,25,26	0.43	0	29,36,39	0.59	1 (3%)
31	5MU	CA	747	31	19,22,23	0.34	0	27,32,35	0.39	0
31	5MU	CA	1939	31	19,22,23	0.48	0	27,32,35	0.41	0
55	2MG	DA	2445	55	23,26,27	0.53	0	33,38,41	0.52	0
55	3TD	DA	1915	55	19,22,23	0.54	0	23,32,35	0.86	1 (4%)
1	4OC	BA	1402	1	20,23,24	0.42	0	25,32,35	0.51	0
1	G7M	AA	527	1	23,26,27	0.69	0	34,39,42	1.48	4 (11%)
55	PSU	DA	2580	55	18,21,22	0.78	1 (5%)	21,30,33	0.69	0
31	1MG	CA	745	31	23,26,27	1.03	1 (4%)	33,39,42	0.64	1 (3%)
1	PSU	BA	516	1	18,21,22	0.40	0	21,30,33	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
55	H2U	DA	2449	55	18,21,22	0.47	0	19,30,33	0.50	0
1	MA6	BA	1519	1	23,26,27	0.44	0	33,38,41	1.27	4 (12%)
55	2MG	DA	1835	55	23,26,27	0.32	0	33,38,41	0.41	0
1	UR3	AA	1498	1	19,22,23	0.29	0	26,32,35	0.35	0
55	PSU	DA	2504	55	18,21,22	0.63	0	21,30,33	0.45	0
12	D2T	AL	89	12	8,9,10	1.33	1 (12%)	6,11,13	0.68	0
1	2MG	BA	1516	1	23,26,27	0.40	0	33,38,41	0.56	0
1	MA6	AA	1518	1	23,26,27	0.50	0	33,38,41	1.01	3 (9%)
31	PSU	CA	2580	31	18,21,22	0.41	0	21,30,33	0.68	1 (4%)
55	PSU	DA	2457	55	18,21,22	0.42	0	21,30,33	0.43	0
31	6MZ	CA	1618	31	22,25,26	0.43	0	29,36,39	0.77	1 (3%)
55	2MA	DA	2503	55,56	22,25,26	0.73	0	32,37,40	1.87	6 (18%)
55	PSU	DA	2605	55	18,21,22	0.40	0	21,30,33	0.56	0
41	4D4	DN	81[B]	-	9,11,12	1.49	1 (11%)	7,13,15	2.64	2 (28%)
1	UR3	BA	1498	1	19,22,23	0.50	0	26,32,35	0.83	1 (3%)
32	MEQ	DD	150[B]	32	8,9,10	1.97	1 (12%)	5,10,12	1.71	1 (20%)
31	2MA	CA	2503	31	22,25,26	0.74	1 (4%)	32,37,40	1.89	6 (18%)
55	6MZ	DA	2030	55	22,25,26	0.56	0	29,36,39	0.48	0
1	2MG	BA	966	1	23,26,27	0.25	0	33,38,41	0.38	0
1	5MC	BA	967	1	19,22,23	0.27	0	26,32,35	0.36	0
1	MA6	BA	1518	1	23,26,27	0.46	0	33,38,41	1.03	4 (12%)
55	PSU	DA	746	55,56	18,21,22	0.98	2 (11%)	21,30,33	0.50	0
31	OMU	CA	2552	31	19,22,23	0.32	0	25,31,34	0.31	0
55	OMU	DA	2552	55	19,22,23	0.33	0	25,31,34	0.36	0
55	1MG	DA	745	55	23,26,27	1.12	1 (4%)	33,39,42	0.70	1 (3%)
31	2MG	CA	2445	31	23,26,27	0.43	0	33,38,41	0.47	0
31	PSU	CA	2605	31	18,21,22	0.33	0	21,30,33	0.57	0
1	2MG	AA	1516	1	23,26,27	0.44	0	33,38,41	0.59	0
41	4D4	CN	81	41	9,11,12	2.09	2 (22%)	7,13,15	2.62	2 (28%)
55	PSU	DA	1911	55	18,21,22	0.30	0	21,30,33	0.39	0
55	OMC	DA	2498	55,56	19,22,23	0.41	0	25,31,34	0.56	0
1	G7M	BA	527	1	23,26,27	0.73	0	34,39,42	1.82	5 (14%)
55	6MZ	DA	1618	55	22,25,26	0.57	0	29,36,39	1.20	1 (3%)
55	PSU	DA	1917	55	18,21,22	0.41	0	21,30,33	0.50	0
1	2MG	BA	1207	1	23,26,27	0.31	0	33,38,41	0.46	0
31	2MG	CA	1835	31	23,26,27	0.37	0	33,38,41	0.38	0
1	5MC	AA	1407	1	19,22,23	0.34	0	26,32,35	0.46	0
31	PSU	CA	1911	31	18,21,22	0.27	0	21,30,33	0.40	0
55	5MC	DA	1962	55	19,22,23	0.46	0	26,32,35	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	2MG	AA	966	1	23,26,27	0.32	0	33,38,41	0.47	0
41	4D4	DN	81[A]	-	9,11,12	2.24	2 (22%)	7,13,15	2.37	2 (28%)
31	OMC	CA	2498	31,56	19,22,23	0.45	0	25,31,34	0.47	0
55	G7M	DA	2069	55	23,26,27	0.56	0	34,39,42	1.21	4 (11%)
55	PSU	DA	955	55	18,21,22	0.62	1 (5%)	21,30,33	0.64	0
1	5MC	AA	967	1	19,22,23	0.29	0	26,32,35	0.37	0
31	3TD	CA	1915	31	19,22,23	0.50	0	23,32,35	0.80	1 (4%)
32	MEQ	DD	150[A]	32	8,9,10	0.56	0	5,10,12	0.45	0
31	PSU	CA	1917	31	18,21,22	0.34	0	21,30,33	0.44	0
1	PSU	AA	516	56,1	18,21,22	0.27	0	21,30,33	0.45	0
55	PSU	DA	2604	55	18,21,22	0.55	0	21,30,33	0.65	0
1	4OC	AA	1402	1	20,23,24	0.30	0	25,32,35	0.52	0
12	D2T	BL	89	12	8,9,10	0.83	0	6,11,13	0.66	0
31	G7M	CA	2069	31	23,26,27	0.65	1 (4%)	34,39,42	1.38	4 (11%)
31	PSU	CA	955	31	18,21,22	0.30	0	21,30,33	0.53	0
31	5MC	CA	1962	31	19,22,23	0.24	0	26,32,35	0.37	0
31	PSU	CA	2504	31	18,21,22	0.40	0	21,30,33	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	DA	1939	55	-	0/7/25/26	0/2/2/2
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
55	5MU	DA	747	55	-	0/7/25/26	0/2/2/2
31	OMG	CA	2251	31	-	1/9/27/28	0/3/3/3
31	PSU	CA	746	31,56	-	2/7/25/26	0/2/2/2
55	OMG	DA	2251	55	-	1/9/27/28	0/3/3/3
1	MA6	AA	1519	1	-	0/11/29/30	0/3/3/3
1	2MG	AA	1207	1	-	0/9/27/28	0/3/3/3
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
31	6MZ	CA	2030	31	-	1/9/27/28	0/3/3/3
31	5MU	CA	747	31	-	0/7/25/26	0/2/2/2
31	5MU	CA	1939	31	-	0/7/25/26	0/2/2/2
55	2MG	DA	2445	55	-	0/9/27/28	0/3/3/3
55	3TD	DA	1915	55	-	0/7/25/26	0/2/2/2
1	4OC	BA	1402	1	-	0/9/29/30	0/2/2/2
1	G7M	AA	527	1	-	2/7/25/26	0/3/3/3
55	PSU	DA	2580	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	1MG	CA	745	31	-	0/7/25/26	0/3/3/3
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
55	H2U	DA	2449	55	-	1/7/38/39	0/2/2/2
1	MA6	BA	1519	1	-	0/11/29/30	0/3/3/3
55	2MG	DA	1835	55	-	2/9/27/28	0/3/3/3
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
55	PSU	DA	2504	55	-	1/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	2/7/12/14	-
1	2MG	BA	1516	1	-	0/9/27/28	0/3/3/3
1	MA6	AA	1518	1	-	0/11/29/30	0/3/3/3
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
55	PSU	DA	2457	55	-	0/7/25/26	0/2/2/2
31	6MZ	CA	1618	31	-	0/9/27/28	0/3/3/3
55	2MA	DA	2503	55,56	-	1/7/25/26	0/3/3/3
55	PSU	DA	2605	55	-	0/7/25/26	0/2/2/2
41	4D4	DN	81[B]	-	-	2/11/12/14	-
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
32	MEQ	DD	150[B]	32	-	4/8/9/11	-
31	2MA	CA	2503	31	-	1/7/25/26	0/3/3/3
55	6MZ	DA	2030	55	-	2/9/27/28	0/3/3/3
1	2MG	BA	966	1	-	0/9/27/28	0/3/3/3
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
1	MA6	BA	1518	1	-	0/11/29/30	0/3/3/3
55	PSU	DA	746	55,56	-	2/7/25/26	0/2/2/2
31	OMU	CA	2552	31	-	1/9/27/28	0/2/2/2
55	OMU	DA	2552	55	-	1/9/27/28	0/2/2/2
55	1MG	DA	745	55	-	0/7/25/26	0/3/3/3
31	2MG	CA	2445	31	-	0/9/27/28	0/3/3/3
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3
41	4D4	CN	81	41	-	1/11/12/14	-
55	PSU	DA	1911	55	-	0/7/25/26	0/2/2/2
55	OMC	DA	2498	55,56	-	0/9/27/28	0/2/2/2
1	G7M	BA	527	1	-	2/7/25/26	0/3/3/3
55	6MZ	DA	1618	55	-	0/9/27/28	0/3/3/3
55	PSU	DA	1917	55	-	0/7/25/26	0/2/2/2
1	2MG	BA	1207	1	-	0/9/27/28	0/3/3/3
31	2MG	CA	1835	31	-	2/9/27/28	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MC	DA	1962	55	-	2/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/9/27/28	0/3/3/3
41	4D4	DN	81[A]	-	-	0/11/12/14	-
31	OMC	CA	2498	31,56	-	0/9/27/28	0/2/2/2
55	G7M	DA	2069	55	-	1/7/25/26	0/3/3/3
55	PSU	DA	955	55	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
32	MEQ	DD	150[A]	32	-	3/8/9/11	-
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	56,1	-	0/7/25/26	0/2/2/2
55	PSU	DA	2604	55	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
12	D2T	BL	89	12	-	4/7/12/14	-
31	G7M	CA	2069	31	-	1/7/25/26	0/3/3/3
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
31	5MC	CA	1962	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2504	31	-	1/7/25/26	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	DN	81[A]	4D4	CZ-NE	6.08	1.45	1.33
41	CN	81	4D4	CZ-NE	5.59	1.44	1.33
32	DD	150[B]	MEQ	CB-CA	5.36	1.61	1.53
31	CA	745	1MG	C2-N1	4.46	1.45	1.37
55	DA	745	1MG	C2-N1	4.41	1.45	1.37
41	DN	81[B]	4D4	CZ-NE	3.85	1.40	1.33
12	AL	89	D2T	CB-SB	2.80	1.85	1.82
55	DA	746	PSU	O4'-C1'	-2.76	1.40	1.43
41	DN	81[A]	4D4	CZ-NH1	2.58	1.43	1.34
55	DA	2580	PSU	O4'-C1'	-2.54	1.40	1.43
41	CN	81	4D4	CZ-NH1	2.53	1.43	1.34
55	DA	746	PSU	C2'-C1'	-2.53	1.50	1.53
31	CA	746	PSU	O4'-C1'	-2.34	1.40	1.43
31	CA	2503	2MA	C6-N1	2.22	1.38	1.35
31	CA	2069	G7M	C1'-N9	-2.05	1.41	1.47
55	DA	955	PSU	C2'-C1'	-2.03	1.51	1.53

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	CA	2503	2MA	N6-C6-N1	8.25	128.16	117.03
55	DA	2503	2MA	N6-C6-N1	8.10	127.96	117.03
1	BA	527	G7M	C6-C5-N7	-6.31	124.27	132.17
55	DA	1618	6MZ	C9-N6-C6	6.11	128.52	122.85
41	CN	81	4D4	NE-CZ-NH2	5.78	130.60	120.67
41	DN	81[B]	4D4	NE-CZ-NH2	5.64	130.36	120.67
41	DN	81[A]	4D4	NE-CZ-NH2	5.27	129.72	120.67
1	BA	527	G7M	O4'-C1'-N9	4.81	119.26	108.36
31	CA	2069	G7M	C6-C5-N7	-4.73	126.25	132.17
1	AA	527	G7M	C6-C5-N7	-4.34	126.73	132.17
1	AA	527	G7M	O4'-C1'-N9	4.17	117.80	108.36
1	AA	1519	MA6	C4-C5-C6	-4.11	111.66	115.91
1	BA	1519	MA6	C4-C5-C6	-4.08	111.69	115.91
31	CA	2069	G7M	C5-C4-N3	-4.07	120.47	128.15
31	CA	2503	2MA	C2-N1-C6	4.03	124.29	118.10
1	AA	1519	MA6	N1-C6-N6	-3.92	112.08	116.86
1	AA	527	G7M	C4-C5-N7	-3.89	101.31	107.67
1	BA	527	G7M	C5-C4-N3	-3.84	120.89	128.15
1	BA	1519	MA6	N1-C6-N6	-3.83	112.19	116.86
55	DA	2503	2MA	C2-N1-C6	3.82	123.97	118.10
32	DD	150[B]	MEQ	CB-CG-CD	3.80	121.54	113.06
41	DN	81[B]	4D4	NH1-CZ-NE	-3.79	110.65	119.27
55	DA	2069	G7M	C6-C5-N7	-3.78	127.43	132.17
1	BA	527	G7M	C4-C5-N7	-3.71	101.59	107.67
55	DA	2069	G7M	C5-C4-N3	-3.44	121.66	128.15
31	CA	2069	G7M	C4-C5-N7	-3.43	102.06	107.67
41	CN	81	4D4	NH1-CZ-NE	-3.36	111.64	119.27
55	DA	1915	3TD	C1'-C5-C4	3.34	122.68	117.61
1	BA	1518	MA6	C4-C5-C6	-3.13	112.67	115.91
1	BA	1498	UR3	C4-N3-C2	-3.13	122.06	124.58
31	CA	1915	3TD	C1'-C5-C4	3.11	122.32	117.61
1	BA	527	G7M	C6-C5-C4	-3.08	113.67	119.01
31	CA	1618	6MZ	C9-N6-C6	3.06	125.69	122.85
1	AA	1518	MA6	C4-C5-C6	-2.93	112.88	115.91
55	DA	2069	G7M	C4-C5-N7	-2.88	102.95	107.67
31	CA	2503	2MA	C5-C6-N1	-2.87	114.43	118.90
41	DN	81[A]	4D4	NH1-CZ-NE	-2.83	112.83	119.27
1	AA	1519	MA6	C5-C6-N1	2.77	124.29	118.55
1	BA	1519	MA6	C5-C6-N1	2.69	124.14	118.55
1	AA	527	G7M	C6-C5-C4	-2.69	114.35	119.01
1	BA	1519	MA6	C6-C5-N7	2.65	137.66	133.43
1	AA	1519	MA6	C6-C5-N7	2.63	137.63	133.43
55	DA	2503	2MA	C5-C6-N1	-2.53	114.96	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	DA	2503	2MA	C5-C6-N6	-2.51	117.08	123.29
31	CA	2503	2MA	C5-C6-N6	-2.37	117.41	123.29
55	DA	2503	2MA	CM2-C2-N3	2.37	120.67	117.13
31	CA	2069	G7M	O4'-C1'-N9	2.30	113.58	108.36
55	DA	2503	2MA	N3-C2-N1	-2.28	121.74	125.77
1	BA	1518	MA6	C5-C6-N1	2.26	123.23	118.55
1	AA	1518	MA6	C5-C6-N1	2.24	123.21	118.55
31	CA	2030	6MZ	C9-N6-C6	2.22	124.91	122.85
31	CA	2503	2MA	N3-C2-N1	-2.19	121.90	125.77
31	CA	745	1MG	C6-C5-C4	-2.13	117.56	119.97
1	AA	1518	MA6	C5-C6-N6	-2.12	121.97	125.33
55	DA	745	1MG	O4'-C4'-C3'	-2.11	100.97	105.15
31	CA	2580	PSU	O4'-C1'-C2'	2.10	108.06	105.15
31	CA	2503	2MA	CM2-C2-N3	2.07	120.23	117.13
1	BA	1518	MA6	C6-C5-N7	2.07	136.75	133.43
55	DA	2069	G7M	O4'-C1'-N9	2.07	113.06	108.36
1	BA	1518	MA6	N1-C6-N6	-2.06	114.34	116.86

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	O4'-C4'-C5'-O5'
12	AL	89	D2T	SB-CB-CG-OD2
1	BA	527	G7M	O4'-C4'-C5'-O5'
12	BL	89	D2T	CG-CB-SB-CB1
12	BL	89	D2T	CA-CB-CG-OD1
12	BL	89	D2T	CA-CB-CG-OD2
31	CA	2251	OMG	C1'-C2'-O2'-CM2
32	DD	150[B]	MEQ	N-CA-CB-CG
32	DD	150[B]	MEQ	C-CA-CB-CG
41	DN	81[B]	4D4	CA-CB-CG-CD
1	AA	527	G7M	C3'-C4'-C5'-O5'
1	BA	527	G7M	C3'-C4'-C5'-O5'
32	DD	150[A]	MEQ	OE1-CD-CG-CB
32	DD	150[A]	MEQ	NE2-CD-CG-CB
41	DN	81[B]	4D4	OB-CB-CG-CD
55	DA	2030	6MZ	O4'-C4'-C5'-O5'
55	DA	2030	6MZ	C3'-C4'-C5'-O5'
32	DD	150[A]	MEQ	CA-CB-CG-CD
31	CA	1835	2MG	O4'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1

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Mol	Chain	Res	Type	Atoms
31	CA	1835	2MG	C3'-C4'-C5'-O5'
55	DA	2069	G7M	C4'-C5'-O5'-P
55	DA	1835	2MG	C3'-C4'-C5'-O5'
55	DA	2503	2MA	C4'-C5'-O5'-P
55	DA	1835	2MG	O4'-C4'-C5'-O5'
32	DD	150[B]	MEQ	OE1-CD-NE2-CE
31	CA	2030	6MZ	O4'-C4'-C5'-O5'
31	CA	2069	G7M	C4'-C5'-O5'-P
32	DD	150[B]	MEQ	CA-CB-CG-CD
31	CA	2503	2MA	C4'-C5'-O5'-P
31	CA	2504	PSU	O4'-C4'-C5'-O5'
41	CN	81	4D4	CG-CD-NE-CZ
12	BL	89	D2T	SB-CB-CG-OD2
55	DA	2251	OMG	C1'-C2'-O2'-CM2
31	CA	746	PSU	O4'-C1'-C5-C6
55	DA	746	PSU	O4'-C1'-C5-C6
31	CA	2552	OMU	C3'-C2'-O2'-CM2
55	DA	2504	PSU	O4'-C4'-C5'-O5'
31	CA	746	PSU	C2'-C1'-C5-C6
55	DA	746	PSU	C2'-C1'-C5-C6
55	DA	2552	OMU	C3'-C2'-O2'-CM2
55	DA	1962	5MC	O4'-C4'-C5'-O5'
55	DA	2449	H2U	C4'-C5'-O5'-P
55	DA	1962	5MC	O4'-C1'-N1-C6

There are no ring outliers.

16 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	DA	747	5MU	1	0
1	AA	1519	MA6	1	0
31	CA	2030	6MZ	2	0
31	CA	747	5MU	1	0
55	DA	2445	2MG	1	0
55	DA	2449	H2U	1	0
1	BA	1519	MA6	1	0
12	AL	89	D2T	1	0
1	AA	1518	MA6	1	0
41	DN	81[B]	4D4	1	0
32	DD	150[B]	MEQ	1	0
31	CA	2503	2MA	1	0
55	DA	2030	6MZ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	BA	1518	MA6	1	0
31	CA	2445	2MG	1	0
55	DA	2498	OMC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 554 ligands modelled in this entry, 472 are monoatomic - leaving 82 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	MPD	DS	203	-	7,7,7	0.42	0	9,10,10	0.73	0
58	MPD	DT	202	-	7,7,7	0.75	0	9,10,10	0.43	0
65	SPD	DA	3187	-	9,9,9	0.16	0	8,8,8	0.43	0
58	MPD	DA	3203	-	7,7,7	0.83	0	9,10,10	0.65	0
63	EDO	DA	3198	-	3,3,3	0.61	0	2,2,2	0.39	0
58	MPD	DA	3209	-	7,7,7	0.63	0	9,10,10	0.41	0
62	PEG	DA	3217	-	6,6,6	0.30	0	5,5,5	0.08	0
58	MPD	AA	1676	-	7,7,7	0.54	0	9,10,10	0.45	0
62	PEG	DA	3226	-	6,6,6	0.43	0	5,5,5	0.27	0
59	PUT	DA	3195	-	5,5,5	0.32	0	4,4,4	0.55	0
59	PUT	DA	3218	-	5,5,5	0.13	0	4,4,4	0.09	0
63	EDO	DA	3003	-	3,3,3	0.71	0	2,2,2	0.17	0
58	MPD	DA	3190	-	7,7,7	0.44	0	9,10,10	0.51	0
57	PG4	DS	202	-	12,12,12	0.47	0	11,11,11	0.43	0
67	ACY	DA	3201	-	3,3,3	0.97	0	3,3,3	0.93	0
58	MPD	AA	1671	-	7,7,7	0.64	0	9,10,10	0.50	0
62	PEG	DL	201	-	6,6,6	0.13	0	5,5,5	0.11	0
58	MPD	DA	3192	-	7,7,7	0.63	0	9,10,10	0.83	0
58	MPD	DA	3206	-	7,7,7	0.94	1 (14%)	9,10,10	0.55	0
62	PEG	AL	201	-	6,6,6	0.25	0	5,5,5	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
63	EDO	DA	3207	-	3,3,3	0.65	0	2,2,2	0.21	0
63	EDO	DA	3004	-	3,3,3	0.67	0	2,2,2	0.17	0
58	MPD	DK	201	-	7,7,7	0.68	0	9,10,10	0.24	0
59	PUT	DA	3002	-	5,5,5	0.20	0	4,4,4	0.07	0
68	GUN	DA	3210	-	12,12,12	0.69	0	15,17,17	0.47	0
58	MPD	DN	201	-	7,7,7	1.01	1 (14%)	9,10,10	0.63	0
63	EDO	DA	3197	-	3,3,3	0.59	0	2,2,2	0.27	0
58	MPD	DE	302	-	7,7,7	0.83	0	9,10,10	0.52	0
62	PEG	DP	201	-	6,6,6	0.29	0	5,5,5	0.16	0
67	ACY	DA	3191	-	3,3,3	1.01	0	3,3,3	0.90	0
59	PUT	DA	3188	-	5,5,5	0.44	0	4,4,4	0.28	0
64	PGE	DA	3224	-	9,9,9	0.24	0	8,8,8	0.17	0
57	PG4	DA	3193	-	12,12,12	0.30	0	11,11,11	0.43	0
62	PEG	DA	3199	-	6,6,6	0.30	0	5,5,5	0.20	0
59	PUT	DA	3189	-	5,5,5	0.47	0	4,4,4	0.45	0
59	PUT	DA	3204	-	5,5,5	0.35	0	4,4,4	0.30	0
59	PUT	DA	3211	-	5,5,5	0.31	0	4,4,4	0.20	0
59	PUT	AA	1673	-	5,5,5	0.15	0	4,4,4	0.15	0
64	PGE	DA	3216	-	9,9,9	0.14	0	8,8,8	0.25	0
63	EDO	DB	210	-	3,3,3	0.54	0	2,2,2	0.27	0
59	PUT	AA	1675	-	5,5,5	0.20	0	4,4,4	0.23	0
67	ACY	DA	3196	-	3,3,3	1.43	1 (33%)	3,3,3	0.84	0
63	EDO	D1	101	-	3,3,3	0.61	0	2,2,2	0.18	0
62	PEG	D1	103	-	6,6,6	0.43	0	5,5,5	0.15	0
65	SPD	DA	3205	-	9,9,9	0.24	0	8,8,8	0.19	0
59	PUT	DA	3221	-	5,5,5	0.45	0	4,4,4	0.66	0
57	PG4	DQ	202	-	12,12,12	0.15	0	11,11,11	0.16	0
65	SPD	DA	3223	-	9,9,9	0.17	0	8,8,8	0.69	0
63	EDO	DA	3208	-	3,3,3	0.53	0	2,2,2	0.34	0
60	T1C	BA	1643	56	45,45,45	1.02	3 (6%)	56,72,72	1.55	6 (10%)
64	PGE	D1	102	-	9,9,9	0.30	0	8,8,8	0.30	0
64	PGE	DS	201	-	9,9,9	0.48	0	8,8,8	0.48	0
63	EDO	DB	211	-	3,3,3	0.54	0	2,2,2	0.22	0
59	PUT	DA	3212	-	5,5,5	0.37	0	4,4,4	0.33	0
62	PEG	DQ	201	-	6,6,6	0.21	0	5,5,5	0.15	0
64	PGE	DU	101	-	9,9,9	0.25	0	8,8,8	0.37	0
59	PUT	AA	1672	-	5,5,5	0.22	0	4,4,4	0.19	0
57	PG4	DA	3215	-	12,12,12	0.16	0	11,11,11	0.13	0
62	PEG	DA	3200	-	6,6,6	0.52	0	5,5,5	0.28	0
57	PG4	DR	202	-	12,12,12	0.43	0	11,11,11	0.54	0
66	1PE	DA	3202	-	15,15,15	0.35	0	14,14,14	0.40	0
62	PEG	DA	3225	-	6,6,6	0.50	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
59	PUT	DA	3184	-	5,5,5	0.23	0	4,4,4	0.16	0
65	SPD	DA	3183	-	9,9,9	0.12	0	8,8,8	0.20	0
63	EDO	DA	3001	-	3,3,3	0.78	0	2,2,2	0.15	0
57	PG4	BA	1642	-	12,12,12	0.20	0	11,11,11	0.22	0
59	PUT	AA	1674	-	5,5,5	0.15	0	4,4,4	0.14	0
60	T1C	AA	1677	56	45,45,45	1.06	4 (8%)	56,72,72	1.61	5 (8%)
64	PGE	DA	3186	-	9,9,9	0.35	0	8,8,8	0.56	0
62	PEG	D3	102	-	6,6,6	0.33	0	5,5,5	0.24	0
58	MPD	DE	301	-	7,7,7	0.79	0	9,10,10	0.81	0
64	PGE	DA	3213	-	9,9,9	0.16	0	8,8,8	0.18	0
64	PGE	DD	301	-	9,9,9	0.29	0	8,8,8	0.33	0
63	EDO	DA	3194	-	3,3,3	0.60	0	2,2,2	0.12	0
69	TRS	DA	3219	-	7,7,7	0.35	0	9,9,9	0.36	0
64	PGE	D3	101	-	9,9,9	0.29	0	8,8,8	0.23	0
63	EDO	DA	3214	-	3,3,3	0.61	0	2,2,2	0.28	0
58	MPD	DT	201	-	7,7,7	0.57	0	9,10,10	0.19	0
59	PUT	DA	3222	-	5,5,5	0.30	0	4,4,4	0.29	0
59	PUT	DA	3220	-	5,5,5	0.18	0	4,4,4	0.14	0
66	1PE	DA	3185	-	15,15,15	0.16	0	14,14,14	0.15	0
57	PG4	AA	1670	-	12,12,12	0.26	0	11,11,11	0.41	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	DS	203	-	-	0/5/5/5	-
58	MPD	DT	202	-	-	3/5/5/5	-
65	SPD	DA	3187	-	-	0/7/7/7	-
58	MPD	DA	3203	-	-	1/5/5/5	-
63	EDO	DA	3198	-	-	1/1/1/1	-
58	MPD	DA	3209	-	-	1/5/5/5	-
62	PEG	DA	3217	-	-	3/4/4/4	-
58	MPD	AA	1676	-	-	1/5/5/5	-
62	PEG	DA	3226	-	-	0/4/4/4	-
59	PUT	DA	3195	-	-	1/3/3/3	-
59	PUT	DA	3218	-	-	0/3/3/3	-
63	EDO	DA	3003	-	-	0/1/1/1	-
58	MPD	DA	3190	-	-	2/5/5/5	-
57	PG4	DS	202	-	-	2/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	MPD	AA	1671	-	-	1/5/5/5	-
62	PEG	DL	201	-	-	2/4/4/4	-
58	MPD	DA	3192	-	-	2/5/5/5	-
58	MPD	DA	3206	-	-	2/5/5/5	-
62	PEG	AL	201	-	-	2/4/4/4	-
63	EDO	DA	3207	-	-	0/1/1/1	-
63	EDO	DA	3004	-	-	0/1/1/1	-
58	MPD	DK	201	-	-	2/5/5/5	-
59	PUT	DA	3002	-	-	0/3/3/3	-
68	GUN	DA	3210	-	-	-	0/2/2/2
58	MPD	DN	201	-	-	3/5/5/5	-
63	EDO	DA	3197	-	-	0/1/1/1	-
58	MPD	DE	302	-	-	1/5/5/5	-
62	PEG	DP	201	-	-	2/4/4/4	-
59	PUT	DA	3188	-	-	0/3/3/3	-
64	PGE	DA	3224	-	-	4/7/7/7	-
57	PG4	DA	3193	-	-	8/10/10/10	-
62	PEG	DA	3199	-	-	3/4/4/4	-
59	PUT	DA	3189	-	-	0/3/3/3	-
59	PUT	DA	3204	-	-	1/3/3/3	-
59	PUT	DA	3211	-	-	0/3/3/3	-
59	PUT	AA	1673	-	-	0/3/3/3	-
64	PGE	DA	3216	-	-	4/7/7/7	-
63	EDO	DB	210	-	-	0/1/1/1	-
59	PUT	AA	1675	-	-	1/3/3/3	-
63	EDO	D1	101	-	-	0/1/1/1	-
62	PEG	D1	103	-	-	1/4/4/4	-
65	SPD	DA	3205	-	-	5/7/7/7	-
59	PUT	DA	3221	-	-	1/3/3/3	-
57	PG4	DQ	202	-	-	1/10/10/10	-
65	SPD	DA	3223	-	-	4/7/7/7	-
63	EDO	DA	3208	-	-	0/1/1/1	-
60	T1C	BA	1643	56	-	11/22/80/80	0/4/4/4
64	PGE	D1	102	-	-	4/7/7/7	-
64	PGE	DS	201	-	-	3/7/7/7	-
63	EDO	DB	211	-	-	0/1/1/1	-
59	PUT	DA	3212	-	-	1/3/3/3	-
62	PEG	DQ	201	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	PGE	DU	101	-	-	4/7/7/7	-
59	PUT	AA	1672	-	-	0/3/3/3	-
57	PG4	DA	3215	-	-	4/10/10/10	-
62	PEG	DA	3200	-	-	3/4/4/4	-
57	PG4	DR	202	-	-	6/10/10/10	-
66	1PE	DA	3202	-	-	8/13/13/13	-
62	PEG	DA	3225	-	-	2/4/4/4	-
59	PUT	DA	3184	-	-	0/3/3/3	-
65	SPD	DA	3183	-	-	1/7/7/7	-
63	EDO	DA	3001	-	-	1/1/1/1	-
57	PG4	BA	1642	-	-	0/10/10/10	-
59	PUT	AA	1674	-	-	0/3/3/3	-
60	T1C	AA	1677	56	-	8/22/80/80	0/4/4/4
64	PGE	DA	3186	-	-	4/7/7/7	-
62	PEG	D3	102	-	-	2/4/4/4	-
58	MPD	DE	301	-	-	5/5/5/5	-
64	PGE	DA	3213	-	-	3/7/7/7	-
64	PGE	DD	301	-	-	4/7/7/7	-
63	EDO	DA	3194	-	-	1/1/1/1	-
69	TRS	DA	3219	-	-	0/9/9/9	-
64	PGE	D3	101	-	-	2/7/7/7	-
63	EDO	DA	3214	-	-	0/1/1/1	-
58	MPD	DT	201	-	-	2/5/5/5	-
59	PUT	DA	3222	-	-	1/3/3/3	-
59	PUT	DA	3220	-	-	0/3/3/3	-
66	1PE	DA	3185	-	-	5/13/13/13	-
57	PG4	AA	1670	-	-	4/10/10/10	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	1643	T1C	C4-C3	3.40	1.58	1.51
60	AA	1677	T1C	C4-C3	3.00	1.57	1.51
60	AA	1677	T1C	C7-C61	2.77	1.43	1.40
60	BA	1643	T1C	C7-C61	2.66	1.43	1.40
60	BA	1643	T1C	C7-N7	2.63	1.49	1.42
60	AA	1677	T1C	C7-N7	2.56	1.49	1.42
58	DN	201	MPD	C3-C2	2.22	1.60	1.54
60	AA	1677	T1C	C4-N4	2.17	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	DA	3196	ACY	OXT-C	2.14	1.40	1.30
58	DA	3206	MPD	C3-C2	2.08	1.60	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	BA	1643	T1C	C92-N92-C93	6.95	124.57	115.77
60	AA	1677	T1C	C92-N92-C93	6.82	124.40	115.77
60	AA	1677	T1C	C61-C6-C51	-4.93	106.59	113.12
60	BA	1643	T1C	C8-C9-C10	-4.80	115.88	120.53
60	AA	1677	T1C	C8-C9-C10	-4.33	116.33	120.53
60	BA	1643	T1C	C61-C6-C51	-3.48	108.52	113.12
60	AA	1677	T1C	C1A-C10-C9	2.70	123.65	118.98
60	AA	1677	T1C	C6-C61-C1A	2.50	122.38	118.13
60	BA	1643	T1C	C5-C41-C4	-2.45	110.20	113.73
60	BA	1643	T1C	C91-C92-N92	-2.25	107.92	113.21
60	BA	1643	T1C	C1A-C10-C9	2.21	122.81	118.98

There are no chirality outliers.

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AA	1676	MPD	C2-C3-C4-O4
58	DE	301	MPD	C1-C2-C3-C4
58	DE	301	MPD	O2-C2-C3-C4
58	DE	301	MPD	C2-C3-C4-O4
58	DE	301	MPD	C2-C3-C4-C5
58	DN	201	MPD	CM-C2-C3-C4
58	DT	202	MPD	C2-C3-C4-C5
58	DA	3190	MPD	C2-C3-C4-O4
58	DA	3190	MPD	C2-C3-C4-C5
60	AA	1677	T1C	C95-C93-N92-C92
60	AA	1677	T1C	C96-C93-N92-C92
60	BA	1643	T1C	C1-C2-C21-O21
60	BA	1643	T1C	C1-C2-C21-N21
57	DR	202	PG4	O3-C5-C6-O4
66	DA	3202	1PE	OH6-C15-C25-OH5
65	DA	3205	SPD	C3-C4-C5-N6
64	DA	3213	PGE	O2-C3-C4-O3
60	AA	1677	T1C	C94-C93-N92-C92
57	DR	202	PG4	O2-C3-C4-O3
57	DA	3193	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
64	DA	3186	PGE	O3-C5-C6-O4
66	DA	3202	1PE	OH4-C13-C23-OH3
57	DS	202	PG4	O4-C7-C8-O5
66	DA	3185	1PE	OH2-C12-C22-OH3
57	DQ	202	PG4	O1-C1-C2-O2
64	DU	101	PGE	O3-C5-C6-O4
60	BA	1643	T1C	C92-C91-N9-C9
59	DA	3195	PUT	C1-C2-C3-C4
64	DS	201	PGE	O3-C5-C6-O4
65	DA	3205	SPD	C4-C5-N6-C7
65	DA	3205	SPD	C8-C7-N6-C5
62	D1	103	PEG	O2-C3-C4-O4
62	DL	201	PEG	O2-C3-C4-O4
62	DA	3199	PEG	O2-C3-C4-O4
64	DA	3186	PGE	O1-C1-C2-O2
64	DA	3224	PGE	O3-C5-C6-O4
66	DA	3202	1PE	OH2-C12-C22-OH3
63	DA	3194	EDO	O1-C1-C2-O2
60	BA	1643	T1C	O91-C91-N9-C9
59	DA	3204	PUT	C1-C2-C3-C4
65	DA	3205	SPD	C2-C3-C4-C5
62	DA	3200	PEG	O2-C3-C4-O4
64	DA	3224	PGE	O1-C1-C2-O2
64	DD	301	PGE	O2-C3-C4-O3
59	DA	3222	PUT	C1-C2-C3-C4
62	DA	3217	PEG	O2-C3-C4-O4
57	DR	202	PG4	C5-C6-O4-C7
59	DA	3212	PUT	C1-C2-C3-C4
57	DR	202	PG4	C6-C5-O3-C4
64	DU	101	PGE	O1-C1-C2-O2
62	DP	201	PEG	C1-C2-O2-C3
57	DA	3193	PG4	C1-C2-O2-C3
62	DL	201	PEG	C4-C3-O2-C2
57	AA	1670	PG4	C4-C3-O2-C2
62	AL	201	PEG	C1-C2-O2-C3
64	D3	101	PGE	C3-C4-O3-C5
66	DA	3185	1PE	C12-C22-OH3-C23
57	DA	3215	PG4	C1-C2-O2-C3
57	DA	3215	PG4	C3-C4-O3-C5
57	AA	1670	PG4	C3-C4-O3-C5
62	DA	3200	PEG	C1-C2-O2-C3
64	DA	3213	PGE	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
57	DA	3193	PG4	C4-C3-O2-C2
62	DA	3199	PEG	O1-C1-C2-O2
62	DA	3217	PEG	O1-C1-C2-O2
64	DD	301	PGE	O3-C5-C6-O4
62	DA	3199	PEG	C1-C2-O2-C3
65	DA	3223	SPD	C4-C5-N6-C7
66	DA	3202	1PE	C16-C26-OH6-C15
62	DA	3225	PEG	C1-C2-O2-C3
62	DA	3225	PEG	C4-C3-O2-C2
62	DP	201	PEG	C4-C3-O2-C2
66	DA	3202	1PE	C12-C22-OH3-C23
57	DR	202	PG4	C4-C3-O2-C2
57	DA	3215	PG4	C8-C7-O4-C6
64	DD	301	PGE	C4-C3-O2-C2
57	AA	1670	PG4	C5-C6-O4-C7
66	DA	3185	1PE	C16-C26-OH6-C15
57	AA	1670	PG4	O1-C1-C2-O2
58	DA	3203	MPD	O2-C2-C3-C4
62	DA	3200	PEG	C4-C3-O2-C2
58	DE	302	MPD	C2-C3-C4-O4
58	DA	3192	MPD	C2-C3-C4-O4
60	BA	1643	T1C	O91-C91-C92-N92
58	DE	301	MPD	CM-C2-C3-C4
58	DN	201	MPD	C1-C2-C3-C4
58	DT	201	MPD	C1-C2-C3-C4
60	BA	1643	T1C	C3-C2-C21-N21
66	DA	3185	1PE	C24-C14-OH5-C25
64	DA	3224	PGE	C1-C2-O2-C3
60	BA	1643	T1C	C3-C2-C21-O21
64	DA	3216	PGE	C3-C4-O3-C5
62	DA	3217	PEG	C1-C2-O2-C3
60	AA	1677	T1C	C91-C92-N92-C93
60	BA	1643	T1C	C91-C92-N92-C93
59	AA	1675	PUT	C1-C2-C3-C4
64	DA	3216	PGE	C4-C3-O2-C2
65	DA	3205	SPD	N6-C7-C8-C9
63	DA	3001	EDO	O1-C1-C2-O2
64	DA	3224	PGE	C3-C4-O3-C5
58	DA	3192	MPD	C2-C3-C4-C5
60	AA	1677	T1C	O91-C91-N9-C9
57	DA	3193	PG4	C3-C4-O3-C5
57	DR	202	PG4	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
59	DA	3221	PUT	C1-C2-C3-C4
64	D1	102	PGE	O3-C5-C6-O4
65	DA	3223	SPD	C3-C4-C5-N6
62	AL	201	PEG	C4-C3-O2-C2
63	DA	3198	EDO	O1-C1-C2-O2
64	DA	3186	PGE	C3-C4-O3-C5
64	D1	102	PGE	C3-C4-O3-C5
60	BA	1643	T1C	N9-C91-C92-N92
64	DS	201	PGE	C6-C5-O3-C4
66	DA	3202	1PE	C15-C25-OH5-C14
57	DA	3193	PG4	C6-C5-O3-C4
64	D1	102	PGE	C4-C3-O2-C2
64	DU	101	PGE	C6-C5-O3-C4
64	DA	3186	PGE	C4-C3-O2-C2
57	DS	202	PG4	O2-C3-C4-O3
57	DA	3193	PG4	C8-C7-O4-C6
57	DA	3193	PG4	O4-C7-C8-O5
64	DD	301	PGE	C3-C4-O3-C5
65	DA	3183	SPD	C8-C7-N6-C5
64	DA	3216	PGE	C1-C2-O2-C3
62	D3	102	PEG	C1-C2-O2-C3
65	DA	3223	SPD	C8-C7-N6-C5
64	DU	101	PGE	O2-C3-C4-O3
57	DA	3215	PG4	O1-C1-C2-O2
62	DQ	201	PEG	O1-C1-C2-O2
66	DA	3185	1PE	C13-C23-OH3-C22
64	D3	101	PGE	C4-C3-O2-C2
57	DA	3193	PG4	O2-C3-C4-O3
64	DA	3216	PGE	O2-C3-C4-O3
60	AA	1677	T1C	C61-C7-N7-C72
58	DK	201	MPD	O2-C2-C3-C4
58	DT	202	MPD	O2-C2-C3-C4
58	DA	3206	MPD	O2-C2-C3-C4
60	AA	1677	T1C	C92-C91-N9-C9
62	D3	102	PEG	O1-C1-C2-O2
58	AA	1671	MPD	C2-C3-C4-O4
58	DK	201	MPD	C2-C3-C4-O4
58	DN	201	MPD	C2-C3-C4-O4
58	DT	202	MPD	C2-C3-C4-O4
58	DA	3209	MPD	C2-C3-C4-O4
62	DQ	201	PEG	C1-C2-O2-C3
60	BA	1643	T1C	C61-C7-N7-C71

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Mol	Chain	Res	Type	Atoms
60	BA	1643	T1C	C61-C7-N7-C72
58	DT	201	MPD	CM-C2-C3-C4
58	DA	3206	MPD	CM-C2-C3-C4
66	DA	3202	1PE	C14-C24-OH4-C13
60	AA	1677	T1C	C61-C7-N7-C71
65	DA	3223	SPD	C7-C8-C9-N10
64	DS	201	PGE	O2-C3-C4-O3
64	D1	102	PGE	O2-C3-C4-O3
64	DA	3213	PGE	O1-C1-C2-O2
66	DA	3202	1PE	OH5-C14-C24-OH4

There are no ring outliers.

30 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	DA	3203	MPD	2	0
59	DA	3195	PUT	3	0
59	DA	3218	PUT	1	0
58	DA	3190	MPD	1	0
57	DS	202	PG4	1	0
58	DA	3192	MPD	2	0
58	DN	201	MPD	1	0
63	DA	3197	EDO	1	0
62	DP	201	PEG	1	0
64	DA	3224	PGE	3	0
57	DA	3193	PG4	1	0
59	DA	3189	PUT	1	0
64	DA	3216	PGE	1	0
62	D1	103	PEG	1	0
59	DA	3221	PUT	3	0
65	DA	3223	SPD	4	0
64	D1	102	PGE	2	0
63	DB	211	EDO	1	0
59	DA	3212	PUT	1	0
64	DU	101	PGE	1	0
57	DA	3215	PG4	1	0
62	DA	3200	PEG	1	0
57	DR	202	PG4	5	0
62	D3	102	PEG	2	0
64	DA	3213	PGE	1	0
64	DD	301	PGE	2	0
63	DA	3194	EDO	1	0

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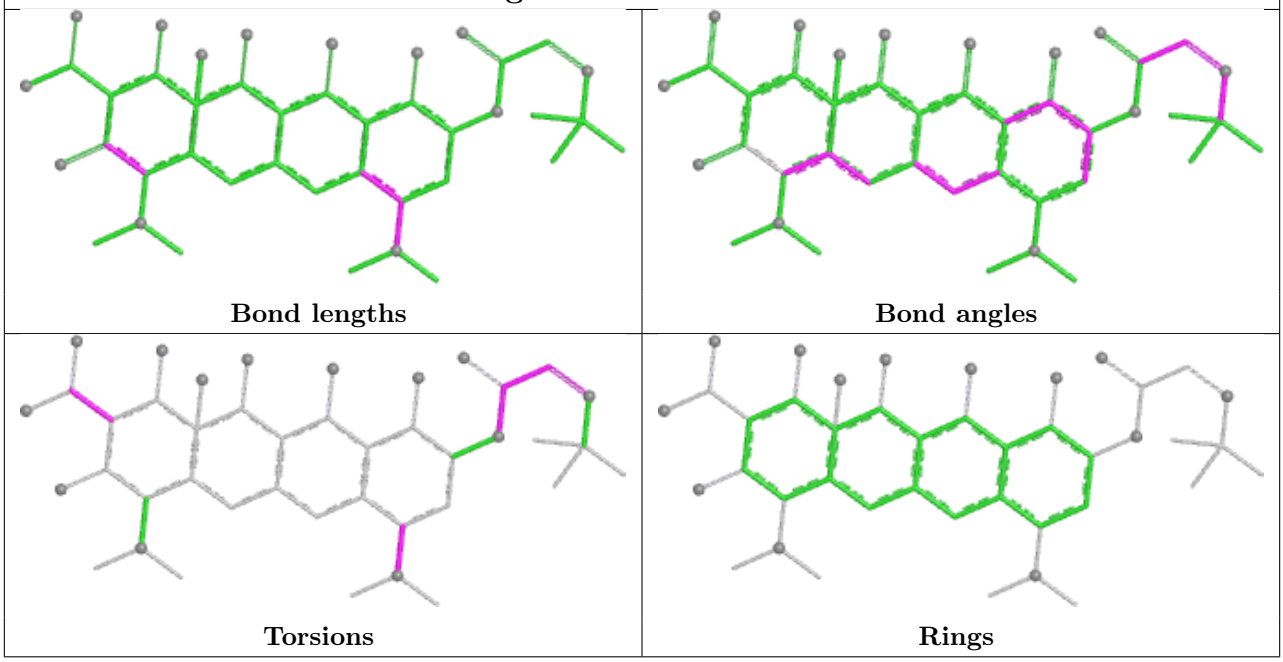
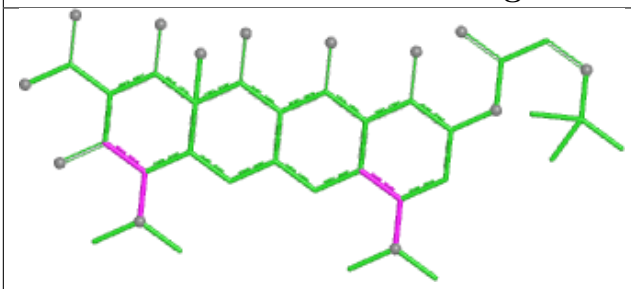
Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	DA	3219	TRS	1	0
59	DA	3222	PUT	1	0
57	AA	1670	PG4	1	0

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

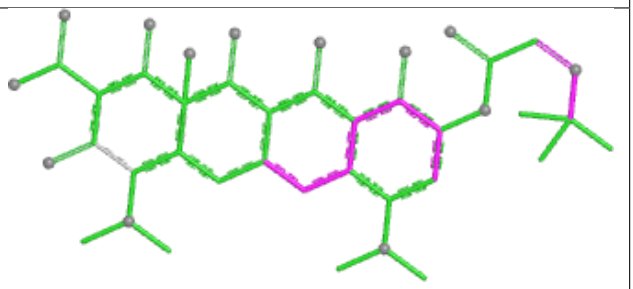
Ligand T1C BA 1643



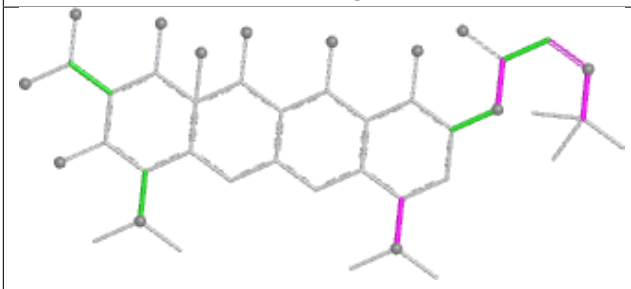
Ligand T1C AA 1677



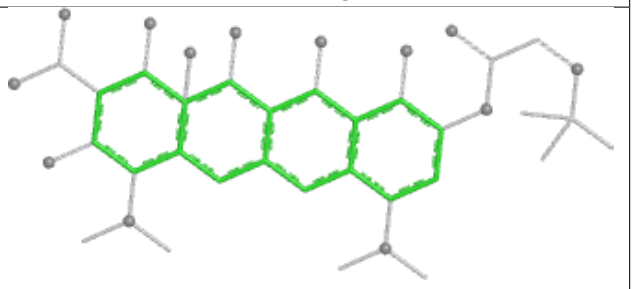
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.74	136 (8%) 15 14	46, 105, 241, 293	0
1	BA	1522/1534 (99%)	1.26	309 (20%) 3 2	61, 140, 279, 284	0
2	AB	224/224 (100%)	1.24	42 (18%) 3 3	83, 127, 202, 270	0
2	BB	224/224 (100%)	1.40	45 (20%) 3 2	99, 144, 211, 261	0
3	AC	206/206 (100%)	1.04	23 (11%) 10 9	80, 108, 141, 163	0
3	BC	206/206 (100%)	1.57	58 (28%) 1 1	115, 151, 190, 231	0
4	AD	205/205 (100%)	0.95	20 (9%) 13 12	64, 103, 131, 154	0
4	BD	205/205 (100%)	0.64	10 (4%) 35 29	61, 81, 107, 131	0
5	AE	155/155 (100%)	0.83	21 (13%) 7 6	67, 91, 133, 169	0
5	BE	150/155 (96%)	1.23	25 (16%) 4 4	77, 97, 144, 227	0
6	AF	106/106 (100%)	0.86	10 (9%) 14 12	82, 105, 128, 142	0
6	BF	100/106 (94%)	0.88	6 (6%) 27 23	86, 121, 146, 154	0
7	AG	151/151 (100%)	1.38	34 (22%) 2 2	107, 137, 166, 179	0
7	BG	151/151 (100%)	1.93	69 (45%) 0 0	147, 202, 218, 228	0
8	AH	129/129 (100%)	0.85	16 (12%) 8 8	71, 91, 118, 136	0
8	BH	129/129 (100%)	1.37	22 (17%) 4 3	91, 116, 150, 168	0
9	AI	127/127 (100%)	1.61	37 (29%) 1 1	96, 132, 169, 200	0
9	BI	127/127 (100%)	2.18	59 (46%) 0 0	138, 176, 209, 229	0
10	AJ	99/99 (100%)	1.80	33 (33%) 1 1	94, 121, 153, 168	0
10	BJ	98/99 (98%)	2.04	46 (46%) 0 0	141, 171, 197, 207	0
11	AK	117/117 (100%)	1.27	19 (16%) 4 4	68, 112, 147, 163	0
11	BK	117/117 (100%)	1.36	24 (20%) 2 2	83, 116, 148, 168	0
12	AL	122/123 (99%)	0.76	12 (9%) 13 12	55, 72, 104, 132	0
12	BL	122/123 (99%)	1.45	33 (27%) 1 1	79, 97, 118, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	114/114 (100%)	1.81	45 (39%) 1 0	106, 131, 182, 202	0
13	BM	114/114 (100%)	1.81	41 (35%) 1 1	203, 237, 245, 249	0
14	AN	100/100 (100%)	1.95	45 (45%) 0 0	90, 117, 206, 215	0
14	BN	100/100 (100%)	2.05	55 (55%) 0 0	132, 181, 239, 250	0
15	AO	88/88 (100%)	0.93	10 (11%) 10 9	72, 94, 112, 132	0
15	BO	88/88 (100%)	1.14	12 (13%) 7 6	79, 112, 132, 150	0
16	AP	82/82 (100%)	0.96	6 (7%) 21 18	67, 86, 121, 139	0
16	BP	82/82 (100%)	2.37	53 (64%) 0 0	94, 111, 157, 166	0
17	AQ	80/80 (100%)	0.83	4 (5%) 34 28	70, 86, 119, 143	0
17	BQ	80/80 (100%)	1.75	29 (36%) 1 1	100, 128, 151, 156	0
18	AR	55/55 (100%)	1.09	7 (12%) 8 7	79, 99, 135, 164	0
18	BR	55/55 (100%)	1.10	6 (10%) 10 9	80, 96, 129, 157	0
19	AS	79/79 (100%)	1.81	29 (36%) 1 1	103, 119, 156, 164	0
19	BS	79/79 (100%)	1.97	30 (37%) 1 0	215, 232, 243, 251	0
20	AT	86/86 (100%)	1.26	11 (12%) 7 7	70, 85, 120, 133	0
20	BT	85/86 (98%)	2.29	48 (56%) 0 0	108, 128, 165, 179	0
21	AU	56/56 (100%)	1.15	7 (12%) 8 7	83, 123, 159, 172	0
21	BU	56/56 (100%)	1.08	8 (14%) 6 6	80, 106, 149, 160	0
22	C1	56/56 (100%)	2.95	37 (66%) 0 0	110, 150, 178, 195	0
22	D1	56/56 (100%)	0.73	1 (1%) 67 59	26, 46, 71, 102	0
23	C2	50/51 (98%)	2.13	23 (46%) 0 0	133, 148, 161, 183	0
23	D2	51/51 (100%)	0.97	9 (17%) 4 3	55, 69, 95, 110	0
24	C3	46/46 (100%)	3.04	41 (89%) 0 0	108, 117, 127, 138	0
24	D3	46/46 (100%)	0.60	3 (6%) 25 21	38, 46, 61, 104	0
25	C4	64/64 (100%)	3.43	55 (85%) 0 0	112, 130, 142, 148	0
25	D4	64/64 (100%)	0.69	2 (3%) 51 44	36, 44, 53, 68	0
26	C5	38/38 (100%)	2.32	22 (57%) 0 0	108, 122, 133, 143	0
26	D5	38/38 (100%)	0.76	2 (5%) 32 27	43, 54, 68, 91	0
27	C0	58/58 (100%)	2.32	31 (53%) 0 0	104, 121, 140, 143	0
27	D0	58/58 (100%)	0.85	5 (8%) 16 14	29, 40, 57, 72	2 (3%)
28	CB	118/120 (98%)	1.29	17 (14%) 6 5	140, 195, 250, 254	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DB	120/120 (100%)	-0.10	0 100 100	33, 60, 99, 143	0
29	CC	271/272 (99%)	2.16	119 (43%) 0 0	88, 119, 152, 165	0
29	DC	271/272 (99%)	0.38	16 (5%) 28 23	31, 57, 83, 96	0
30	CD	209/209 (100%)	2.44	124 (59%) 0 0	103, 134, 170, 190	0
31	CA	2876/2904 (99%)	1.90	1177 (40%) 0 0	73, 178, 274, 295	0
32	DD	208/209 (99%)	-0.08	3 (1%) 73 67	22, 41, 69, 91	0
33	CE	201/201 (100%)	2.39	112 (55%) 0 0	119, 167, 201, 218	0
33	DE	201/201 (100%)	0.31	3 (1%) 72 65	31, 59, 101, 141	0
34	CF	177/178 (99%)	1.47	37 (20%) 2 2	204, 217, 226, 233	0
34	DF	177/178 (99%)	0.75	5 (2%) 55 47	58, 84, 125, 138	0
35	CG	176/176 (100%)	1.53	44 (25%) 2 1	140, 181, 219, 228	0
35	DG	176/176 (100%)	0.52	8 (4%) 38 31	49, 73, 99, 128	0
36	CH	149/149 (100%)	1.31	26 (17%) 4 3	86, 156, 175, 183	0
36	DH	149/149 (100%)	1.40	33 (22%) 2 2	79, 157, 193, 208	0
37	CJ	134/134 (100%)	1.98	54 (40%) 0 0	236, 253, 264, 272	0
37	DJ	134/134 (100%)	2.16	63 (47%) 0 0	204, 229, 238, 246	0
38	CK	142/142 (100%)	2.30	74 (52%) 0 0	105, 129, 168, 221	0
38	DK	142/142 (100%)	-0.19	2 (1%) 73 67	25, 37, 61, 75	0
39	CL	122/123 (99%)	1.64	43 (35%) 1 1	95, 116, 149, 167	0
39	DL	123/123 (100%)	0.01	1 (0%) 82 78	30, 46, 71, 109	0
40	CM	144/144 (100%)	2.78	98 (68%) 0 0	113, 163, 214, 236	0
40	DM	144/144 (100%)	0.52	13 (9%) 15 13	21, 58, 88, 117	0
41	CN	135/136 (99%)	1.89	52 (38%) 1 0	98, 119, 150, 189	0
41	DN	135/136 (99%)	-0.17	0 100 100	20, 43, 69, 88	1 (0%)
42	CO	120/125 (96%)	2.56	74 (61%) 0 0	110, 132, 155, 186	0
42	DO	125/125 (100%)	-0.08	1 (0%) 82 78	29, 39, 68, 111	0
43	CP	116/117 (99%)	1.44	26 (22%) 2 2	147, 171, 185, 189	0
43	DP	117/117 (100%)	0.42	2 (1%) 69 62	47, 60, 87, 97	0
44	CQ	114/114 (100%)	1.84	41 (35%) 1 1	108, 126, 156, 172	0
44	DQ	114/114 (100%)	0.03	1 (0%) 81 76	34, 52, 82, 114	0
45	CR	117/117 (100%)	2.70	71 (60%) 0 0	98, 138, 174, 199	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
45	DR	117/117 (100%)	-0.14	1 (0%) 81 76	23, 33, 48, 70	0
46	CS	103/103 (100%)	2.48	55 (53%) 0 0	114, 143, 185, 201	0
46	DS	103/103 (100%)	0.01	2 (1%) 66 58	26, 45, 71, 93	0
47	CT	110/110 (100%)	2.67	81 (73%) 0 0	109, 137, 180, 193	0
47	DT	110/110 (100%)	-0.01	2 (1%) 67 59	21, 36, 60, 118	0
48	CU	93/93 (100%)	2.60	62 (66%) 0 0	131, 156, 184, 194	0
48	DU	93/93 (100%)	0.68	5 (5%) 31 26	37, 60, 114, 130	0
49	CV	102/103 (99%)	2.72	68 (66%) 0 0	119, 167, 203, 213	0
49	DV	102/103 (99%)	0.45	5 (4%) 35 29	47, 64, 112, 144	0
50	CW	94/94 (100%)	1.36	17 (18%) 3 3	125, 145, 165, 170	0
50	DW	94/94 (100%)	0.22	2 (2%) 63 55	38, 56, 80, 92	0
51	CX	75/76 (98%)	2.03	32 (42%) 0 0	111, 134, 148, 178	0
51	DX	76/76 (100%)	0.29	2 (2%) 57 49	20, 45, 69, 107	1 (1%)
52	CY	77/77 (100%)	2.22	45 (58%) 0 0	103, 122, 147, 168	0
52	DY	77/77 (100%)	0.37	2 (2%) 57 49	37, 59, 92, 108	0
53	CZ	62/62 (100%)	2.18	35 (56%) 0 0	134, 171, 184, 195	0
53	DZ	62/62 (100%)	0.73	3 (4%) 35 30	52, 75, 111, 132	0
54	DI	135/135 (100%)	1.90	49 (36%) 1 1	82, 158, 202, 211	1 (0%)
55	DA	2873/2904 (98%)	-0.10	122 (4%) 40 33	18, 48, 215, 300	11 (0%)
All	All	20634/20751 (99%)	1.15	4716 (22%) 2 2	18, 116, 247, 300	16 (0%)

All (4716) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	C1	2	ALA	12.3
29	CC	241	GLY	11.0
29	CC	242	LYS	10.4
9	BI	16	ALA	9.9
48	CU	43	ILE	9.6
49	CV	31	SER	9.4
38	CK	81	ILE	9.1
22	C1	3	VAL	9.0
25	C4	37	ALA	8.4
20	BT	4	ILE	8.2
29	CC	240	PHE	8.1

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Mol	Chain	Res	Type	RSRZ
40	CM	80	SER	8.1
31	CA	1984	G	8.0
46	CS	81	LYS	8.0
31	CA	2383	G	7.9
25	C4	39	LYS	7.9
1	AA	121	U	7.6
45	CR	35	ALA	7.6
29	CC	234	GLY	7.6
33	CE	73	ILE	7.4
22	C1	5	GLN	7.3
18	BR	20	GLU	7.3
31	CA	2363	G	7.2
33	CE	32	VAL	7.0
23	C2	24	THR	7.0
49	CV	5	ILE	7.0
12	AL	124	ALA	7.0
10	BJ	41	PRO	6.9
33	CE	104	ALA	6.8
48	CU	36	LYS	6.7
45	CR	8	VAL	6.7
9	BI	68	LYS	6.7
24	C3	1	MET	6.7
24	C3	42	LEU	6.7
40	DM	104	GLN	6.7
31	CA	931	U	6.6
29	CC	223	THR	6.6
30	CD	6	GLY	6.6
38	CK	42	ALA	6.6
7	AG	5	ARG	6.5
25	C4	40	ARG	6.5
25	C4	36	LYS	6.5
45	CR	17	ILE	6.5
31	CA	331	C	6.4
45	CR	9	ILE	6.4
49	CV	35	ILE	6.4
42	CO	46	ARG	6.4
46	CS	78	ARG	6.4
40	CM	92	LEU	6.4
22	C1	7	LYS	6.4
40	CM	30	THR	6.4
25	C4	41	LYS	6.4
45	CR	18	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
20	BT	72	ALA	6.3
40	CM	114	GLY	6.3
31	CA	1216	G	6.3
41	CN	17	ASN	6.3
46	CS	80	ARG	6.3
37	DJ	54	PRO	6.3
25	C4	3	LYS	6.2
31	CA	2891	U	6.2
46	CS	96	VAL	6.2
9	BI	14	SER	6.2
40	CM	81	ASP	6.2
31	CA	2666	C	6.2
48	CU	62	VAL	6.2
40	CM	35	HIS	6.1
10	BJ	8	ILE	6.1
27	C0	29	LEU	6.1
40	CM	27	LEU	6.1
45	CR	28	ARG	6.0
13	AM	33	ILE	6.0
46	CS	88	GLY	6.0
29	CC	233	GLY	6.0
49	CV	80	ALA	6.0
49	CV	36	VAL	6.0
40	CM	53	GLY	5.9
31	CA	12	U	5.9
30	CD	154	LYS	5.9
17	BQ	29	VAL	5.9
55	DA	2172	U	5.9
33	CE	67	ARG	5.9
18	BR	51	TYR	5.8
30	CD	8	LYS	5.8
29	CC	239	ASN	5.8
46	CS	82	HIS	5.8
55	DA	654	A	5.8
25	C4	15	LYS	5.8
23	C2	22	THR	5.8
48	CU	61	LEU	5.8
25	C4	28	ASN	5.8
31	CA	327	G	5.8
31	CA	1215	G	5.8
13	AM	19	LEU	5.8
9	BI	128	SER	5.8

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Mol	Chain	Res	Type	RSRZ
55	DA	2886[A]	A	5.8
2	AB	30	PHE	5.7
20	BT	67	ILE	5.7
29	CC	245	VAL	5.7
31	CA	329	G	5.7
1	BA	983	A	5.7
46	CS	75	VAL	5.7
49	CV	13	VAL	5.7
1	AA	1281	C	5.7
29	CC	236	GLU	5.7
40	CM	100	ILE	5.7
31	CA	1217	U	5.7
53	CZ	32	ALA	5.7
45	CR	37	GLN	5.7
42	CO	105	GLY	5.7
47	CT	86	MET	5.7
33	CE	164	LEU	5.7
10	BJ	74	VAL	5.7
33	CE	33	VAL	5.7
30	CD	132	ALA	5.6
20	BT	64	LYS	5.6
40	CM	101	ILE	5.6
3	BC	155	GLY	5.6
2	BB	34	ALA	5.6
8	BH	2	SER	5.6
13	AM	30	SER	5.6
31	CA	183	C	5.6
45	CR	6	ARG	5.6
39	CL	122	VAL	5.6
22	C1	6	ASN	5.6
1	AA	984	C	5.5
29	CC	9	THR	5.5
3	BC	197	GLY	5.5
1	BA	1305	G	5.5
21	AU	36	GLU	5.5
2	AB	139	ARG	5.5
25	C4	29	LEU	5.5
47	CT	97	LEU	5.5
40	CM	72	ALA	5.5
54	DI	2	ALA	5.5
30	CD	200	ASP	5.5
44	DQ	2	SER	5.5

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Mol	Chain	Res	Type	RSRZ
1	BA	196	A	5.5
44	CQ	95	ALA	5.5
33	CE	62	GLN	5.5
45	CR	33	ARG	5.5
40	CM	19	LEU	5.4
30	CD	144	GLY	5.4
52	CY	49	LEU	5.4
31	CA	1647	U	5.4
29	CC	212	ARG	5.4
29	CC	232	HIS	5.4
33	CE	63	LYS	5.4
21	BU	57	ALA	5.4
13	BM	96	PRO	5.4
16	BP	57	ILE	5.4
37	DJ	13	VAL	5.3
25	C4	4	ILE	5.3
33	CE	134	LEU	5.3
31	CA	1644	C	5.3
27	C0	24	LEU	5.3
33	CE	175	ILE	5.3
38	CK	84	ILE	5.3
47	CT	47	VAL	5.3
29	CC	8	PRO	5.3
31	CA	1213	A	5.3
37	DJ	12	GLN	5.3
4	AD	21	LEU	5.3
30	CD	10	GLY	5.3
40	CM	71	ALA	5.2
19	BS	49	ILE	5.2
24	C3	4	THR	5.2
9	AI	17	ALA	5.2
33	CE	36	ALA	5.2
31	CA	514	A	5.2
41	CN	73	ILE	5.2
1	BA	222	C	5.2
45	CR	29	SER	5.2
30	CD	146	ILE	5.2
33	CE	77	ILE	5.2
49	CV	39	ILE	5.2
9	BI	116	VAL	5.2
29	CC	228	VAL	5.2
40	CM	29	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
47	CT	85	ILE	5.2
20	BT	63	ALA	5.2
31	CA	411	G	5.1
40	DM	102	GLY	5.1
54	DI	126	LEU	5.1
51	CX	55	ARG	5.1
37	DJ	138	LEU	5.1
15	AO	69	TYR	5.1
40	CM	75	ALA	5.1
46	CS	83	TYR	5.1
30	CD	26	VAL	5.1
29	DC	240	PHE	5.1
44	CQ	84	ILE	5.1
46	CS	84	ARG	5.1
31	CA	386	G	5.1
31	CA	512	G	5.1
31	CA	1238	G	5.1
17	BQ	70	THR	5.1
51	CX	63	ALA	5.1
55	DA	1061	U	5.1
24	D3	46	LYS	5.0
3	BC	196	ILE	5.0
13	AM	99	GLY	5.0
1	BA	633	G	5.0
46	CS	73	LYS	5.0
10	AJ	74	VAL	5.0
37	DJ	55	ILE	5.0
41	CN	97	GLN	5.0
37	DJ	24	VAL	5.0
49	CV	67	VAL	5.0
8	AH	2	SER	5.0
7	BG	62	PHE	5.0
7	AG	23	LEU	5.0
11	AK	129	VAL	5.0
33	CE	178	VAL	5.0
54	DI	72	LEU	5.0
1	BA	211	G	4.9
31	CA	68	G	4.9
31	CA	412	A	4.9
31	CA	829	A	4.9
48	CU	83	ALA	4.9
30	CD	9	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
40	CM	15	ALA	4.9
54	DI	93	ALA	4.9
1	BA	202	G	4.9
16	BP	52	LEU	4.9
24	C3	31	LEU	4.9
14	AN	21	PHE	4.9
21	AU	37	PHE	4.9
14	BN	47	LYS	4.9
45	CR	38	ALA	4.9
31	CA	2172	U	4.9
37	CJ	74	PRO	4.9
33	CE	96	VAL	4.9
45	CR	11	ARG	4.9
1	AA	1171	A	4.9
34	CF	156	ILE	4.9
29	CC	248	TRP	4.9
7	AG	4	ARG	4.9
40	CM	36	LYS	4.9
45	CR	25	TYR	4.9
35	CG	172	LYS	4.8
29	CC	12	GLY	4.8
11	BK	47	ALA	4.8
49	CV	3	ALA	4.8
42	CO	36	THR	4.8
31	CA	326	G	4.8
31	CA	1983	G	4.8
2	AB	136	MET	4.8
37	CJ	13	VAL	4.8
9	BI	127	PHE	4.8
42	CO	21	PHE	4.8
16	BP	17	TYR	4.8
33	CE	30	GLN	4.8
45	CR	44	GLN	4.8
20	BT	5	LYS	4.8
55	DA	2120	G	4.8
47	CT	82	MET	4.8
29	CC	255	LYS	4.8
29	CC	220	VAL	4.8
38	CK	47	HIS	4.8
1	BA	632	U	4.8
55	DA	277	G	4.8
33	CE	81	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
30	CD	138	LEU	4.7
31	CA	1214	A	4.7
31	CA	2691	C	4.7
33	CE	55	SER	4.7
47	CT	43	ALA	4.7
26	C5	10	LEU	4.7
37	CJ	11	LEU	4.7
31	CA	1026	G	4.7
45	CR	13	ARG	4.7
40	CM	42	SER	4.7
46	CS	77	PHE	4.7
22	C1	4	GLN	4.7
24	C3	7	PRO	4.7
42	CO	25	ALA	4.7
45	CR	30	ARG	4.7
31	CA	1986	C	4.7
31	CA	2364	C	4.7
7	BG	93	PRO	4.7
29	CC	238	ARG	4.7
23	C2	21	TYR	4.7
46	DS	26	ASP	4.7
40	CM	84	LYS	4.7
33	CE	72	SER	4.7
7	BG	65	ALA	4.7
9	BI	17	ALA	4.7
9	BI	125	PRO	4.7
25	C4	60	ALA	4.7
31	CA	930	G	4.7
30	CD	126	ASN	4.7
40	CM	52	GLY	4.7
31	CA	125	A	4.7
36	CH	27	ARG	4.7
47	CT	99	ARG	4.7
25	C4	14	PHE	4.6
47	CT	83	LYS	4.6
42	CO	1	MET	4.6
7	BG	134	ALA	4.6
16	BP	27	ALA	4.6
9	BI	124	ARG	4.6
37	CJ	24	VAL	4.6
43	CP	103	VAL	4.6
1	BA	108	G	4.6

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Mol	Chain	Res	Type	RSRZ
1	AA	1126	U	4.6
16	BP	54	LEU	4.6
51	CX	33	ALA	4.6
19	BS	35	SER	4.6
33	CE	75	SER	4.6
9	BI	67	VAL	4.6
31	CA	328	U	4.6
36	CH	132	PHE	4.6
9	BI	121	ALA	4.6
38	CK	93	ILE	4.6
51	CX	54	GLY	4.6
30	CD	122	VAL	4.6
25	C4	38	THR	4.6
42	CO	20	MET	4.6
19	BS	71	LEU	4.6
31	CA	667	U	4.6
40	CM	79	LEU	4.6
33	CE	69	ARG	4.6
1	BA	948	C	4.6
1	BA	260	G	4.6
48	CU	46	ALA	4.6
54	DI	40	GLU	4.6
41	CN	36	VAL	4.6
29	CC	30	PHE	4.5
30	CD	133	THR	4.5
37	CJ	80	LEU	4.5
37	DJ	53	LEU	4.5
47	CT	46	LEU	4.5
1	AA	1030	U	4.5
1	AA	1240	U	4.5
31	CA	330	A	4.5
31	CA	1205	A	4.5
37	CJ	129	ILE	4.5
29	CC	249	GLY	4.5
40	CM	83	ALA	4.5
48	CU	47	VAL	4.5
45	CR	22	LYS	4.5
1	BA	203	G	4.5
31	CA	1271	G	4.5
24	C3	27	GLY	4.5
30	CD	198	GLY	4.5
31	CA	1234	U	4.5

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Mol	Chain	Res	Type	RSRZ
38	CK	66	GLY	4.5
49	CV	32	GLY	4.5
40	CM	51	GLU	4.5
8	BH	110	VAL	4.5
30	CD	62	LYS	4.5
30	CD	142	VAL	4.5
36	CH	83	LYS	4.5
49	CV	70	VAL	4.5
1	AA	983	A	4.5
31	CA	2800	A	4.5
31	CA	815	C	4.5
54	DI	38	MET	4.5
3	BC	175	LEU	4.5
54	DI	59	LEU	4.5
29	CC	243	HIS	4.5
29	CC	48	ARG	4.5
31	CA	1250	G	4.5
18	AR	51	TYR	4.5
42	CO	113	ILE	4.5
1	BA	4	U	4.5
16	BP	20	VAL	4.5
19	AS	58	VAL	4.5
26	C5	3	VAL	4.5
31	CA	810	U	4.5
30	CD	156	PHE	4.5
33	CE	50	ALA	4.5
49	CV	33	LYS	4.5
1	BA	212	G	4.5
29	CC	27	GLY	4.5
31	CA	1826	G	4.5
45	CR	39	VAL	4.5
43	CP	48	LEU	4.5
48	CU	32	LEU	4.5
31	CA	53	A	4.5
31	CA	1275	A	4.5
33	CE	131	THR	4.4
33	CE	34	ALA	4.4
1	BA	121	U	4.4
31	CA	776	G	4.4
31	CA	801	G	4.4
31	CA	1068	G	4.4
49	CV	29	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
29	CC	52	ARG	4.4
47	CT	11	ARG	4.4
6	BF	100	SER	4.4
37	DJ	135	SER	4.4
19	BS	33	THR	4.4
31	CA	2346	A	4.4
34	CF	65	PRO	4.4
35	CG	157	TYR	4.4
47	CT	105	VAL	4.4
1	BA	186	C	4.4
30	CD	130	GLN	4.4
10	BJ	52	LEU	4.4
41	CN	40	ARG	4.4
52	CY	30	LEU	4.4
9	AI	129	LYS	4.4
14	BN	97	LYS	4.4
25	C4	25	LYS	4.4
1	AA	1127	G	4.4
23	D2	54	ILE	4.4
31	CA	75	G	4.4
37	DJ	129	ILE	4.4
46	CS	27	ILE	4.4
45	CR	34	VAL	4.4
31	CA	1134	A	4.4
41	CN	16	ARG	4.4
1	BA	634	C	4.4
29	CC	61	ALA	4.4
54	DI	83	ALA	4.4
12	BL	4	VAL	4.4
1	BA	1242	G	4.4
2	AB	132	LYS	4.4
27	C0	56	LYS	4.4
40	CM	107	PHE	4.4
3	BC	30	ALA	4.3
29	CC	227	PRO	4.4
5	BE	91	GLY	4.3
23	C2	23	THR	4.3
46	CS	76	LYS	4.3
31	CA	1202	G	4.3
31	CA	508	A	4.3
1	BA	1243	C	4.3
19	BS	76	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
21	AU	57	ALA	4.3
31	CA	1985	C	4.3
48	CU	34	VAL	4.3
30	CD	129	THR	4.3
1	BA	223	A	4.3
10	AJ	75	ASP	4.3
38	CK	48	VAL	4.3
42	CO	48	VAL	4.3
25	C4	61	CYS	4.3
40	CM	34	GLY	4.3
30	CD	201	LEU	4.3
41	CN	41	LEU	4.3
3	AC	207	ILE	4.3
29	CC	210	ALA	4.3
30	CD	155	VAL	4.3
31	CA	2614	A	4.3
49	DV	56	GLY	4.3
31	CA	805	G	4.3
31	CA	1374	G	4.3
25	C4	22	PHE	4.3
16	BP	4	ILE	4.3
55	DA	1172	C	4.3
12	BL	86	ARG	4.3
19	BS	12	ASP	4.3
33	CE	177	PRO	4.3
29	CC	202	LEU	4.3
38	CK	109	LEU	4.3
20	BT	13	GLN	4.2
31	CA	1235	G	4.2
31	CA	1236	G	4.2
33	CE	80	SER	4.2
40	CM	23	ILE	4.2
49	CV	30	SER	4.2
31	CA	2362	C	4.2
43	CP	30	ARG	4.2
46	CS	79	ARG	4.2
49	CV	83	VAL	4.2
25	C4	33	LEU	4.2
12	BL	3	THR	4.2
24	C3	24	THR	4.2
13	BM	22	ILE	4.2
29	CC	37	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
31	CA	513	A	4.2
36	CH	91	PHE	4.2
13	BM	86	TYR	4.2
43	DP	1	MET	4.2
20	BT	76	LYS	4.2
38	CK	111	LYS	4.2
31	CA	2455	G	4.2
31	CA	2525	G	4.2
14	BN	11	VAL	4.2
27	C0	18	PRO	4.2
29	CC	231	PRO	4.2
10	BJ	42	LEU	4.2
31	CA	1518	C	4.2
2	BB	67	ILE	4.2
10	AJ	58	ASN	4.2
1	AA	1148	U	4.2
1	AA	1170	A	4.2
45	CR	5	LYS	4.2
52	CY	54	LYS	4.2
25	C4	57	LEU	4.2
36	DH	12	LEU	4.2
42	CO	47	VAL	4.2
37	CJ	76	ALA	4.2
29	CC	47	GLY	4.2
7	BG	106	GLU	4.2
31	CA	26	G	4.2
31	CA	455	C	4.2
31	CA	765	C	4.2
31	CA	2627	G	4.2
31	CA	2667	C	4.2
51	CX	62	LYS	4.2
2	BB	187	VAL	4.2
30	CD	65	ALA	4.2
7	AG	42	ILE	4.2
1	AA	962	C	4.1
30	CD	7	LYS	4.1
31	CA	343	C	4.1
40	CM	18	ARG	4.1
52	CY	16	ASN	4.1
25	C4	7	VAL	4.1
37	CJ	28	LEU	4.1
42	CO	44	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
48	CU	10	VAL	4.1
31	CA	1325	U	4.1
34	CF	76	GLY	4.1
14	BN	60	GLN	4.1
10	BJ	50	THR	4.1
31	CA	1764	C	4.1
30	CD	4	LEU	4.1
31	CA	30	G	4.1
33	CE	101	TYR	4.1
3	BC	171	GLY	4.1
24	C3	17	GLY	4.1
37	CJ	55	ILE	4.1
37	DJ	117	MET	4.1
1	AA	199	A	4.1
9	BI	129	LYS	4.1
25	C4	35	LYS	4.1
31	CA	515	A	4.1
55	DA	613	A	4.1
37	DJ	76	ALA	4.1
37	DJ	133	ALA	4.1
31	CA	2067	G	4.1
31	CA	2615	U	4.1
47	CT	103	ILE	4.1
31	CA	377	G	4.1
31	CA	408	G	4.1
1	BA	250	A	4.1
3	BC	26	THR	4.1
54	DI	131	THR	4.1
29	CC	213	TRP	4.1
30	CD	31	ALA	4.1
27	C0	32	ILE	4.1
29	CC	265	LYS	4.1
41	CN	99	GLY	4.1
46	CS	49	ILE	4.1
31	CA	2833	U	4.1
31	CA	577	G	4.1
1	BA	263	A	4.0
31	CA	2406	A	4.0
52	CY	47	VAL	4.0
22	C1	8	PRO	4.0
40	CM	56	PRO	4.0
22	C1	21	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
45	CR	27	ALA	4.0
46	DS	103	ALA	4.0
7	BG	36	LYS	4.0
9	BI	31	ASN	4.0
29	CC	209	GLY	4.0
37	CJ	122	ILE	4.0
49	CV	12	ILE	4.0
45	CR	59	GLN	4.0
46	CS	87	GLN	4.0
23	C2	36	LEU	4.0
27	C0	10	THR	4.0
54	DI	128	THR	4.0
3	BC	118	ASP	4.0
16	BP	2	VAL	4.0
36	CH	130	VAL	4.0
52	CY	31	PRO	4.0
1	AA	963	G	4.0
30	CD	160	LYS	4.0
31	CA	1537	G	4.0
42	CO	19	ALA	4.0
1	AA	1019	A	4.0
45	CR	3	ARG	4.0
27	C0	17	LEU	4.0
11	AK	84	VAL	4.0
30	CD	121	THR	4.0
31	CA	240	C	4.0
31	CA	1606	C	4.0
33	CE	196	VAL	4.0
45	CR	31	VAL	4.0
48	CU	60	THR	4.0
29	CC	229	ASP	4.0
49	CV	26	LYS	4.0
13	BM	32	ALA	4.0
9	AI	28	ILE	4.0
10	BJ	100	ILE	4.0
11	AK	110	ILE	4.0
1	AA	1306	A	4.0
31	CA	2358	A	4.0
31	CA	1770	G	4.0
13	BM	89	LEU	4.0
19	BS	15	LEU	4.0
37	DJ	106	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
33	CE	52	VAL	4.0
31	CA	767	U	4.0
35	CG	171	THR	4.0
29	CC	247	PRO	4.0
11	BK	21	ALA	4.0
12	AL	2	ALA	4.0
12	BL	2	ALA	4.0
31	CA	335	C	4.0
29	CC	46	ASN	4.0
31	CA	575	A	4.0
30	CD	137	SER	4.0
31	CA	46	G	4.0
31	CA	2890	G	4.0
39	CL	35	VAL	4.0
29	CC	225	MET	4.0
22	C1	43	ILE	3.9
9	BI	119	ARG	3.9
31	CA	816	C	3.9
30	CD	118	PHE	3.9
14	AN	97	LYS	3.9
11	BK	86	VAL	3.9
33	CE	31	VAL	3.9
47	CT	20	VAL	3.9
52	CY	35	SER	3.9
55	DA	1084	A	3.9
42	CO	109	PRO	3.9
1	AA	951	G	3.9
31	CA	180	G	3.9
31	CA	1210	G	3.9
1	BA	1307	U	3.9
31	CA	1779	U	3.9
37	DJ	96	ASP	3.9
40	CM	45	GLY	3.9
49	CV	20	GLY	3.9
33	CE	200	LEU	3.9
42	CO	10	LEU	3.9
44	CQ	97	LEU	3.9
13	AM	105	ASN	3.9
51	CX	44	LYS	3.9
34	CF	31	VAL	3.9
2	BB	40	ILE	3.9
45	CR	10	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
40	CM	49	GLY	3.9
1	BA	79	G	3.9
16	BP	12	LYS	3.9
30	CD	186	LEU	3.9
55	DA	1062	G	3.9
29	CC	250	VAL	3.9
31	CA	433	C	3.9
31	CA	2248	C	3.9
48	DU	70	HIS	3.9
37	DJ	35	ILE	3.9
51	CX	36	ILE	3.9
3	BC	119	SER	3.9
30	CD	192	ALA	3.9
30	CD	199	SER	3.9
44	CQ	85	SER	3.9
48	CU	35	ALA	3.9
5	BE	140	THR	3.9
7	BG	133	THR	3.9
1	BA	1151	A	3.9
31	CA	675	A	3.9
38	CK	79	GLY	3.9
13	BM	27	LYS	3.9
40	CM	106	GLU	3.9
3	AC	39	VAL	3.9
29	CC	216	VAL	3.9
30	CD	150	GLN	3.9
31	CA	124	G	3.9
42	CO	18	GLN	3.9
19	AS	9	PRO	3.9
25	C4	2	PRO	3.9
25	C4	43	HIS	3.9
37	CJ	23	PRO	3.9
19	AS	39	THR	3.9
22	D1	27	SER	3.9
10	BJ	59	LYS	3.8
26	C5	21	GLY	3.8
40	CM	14	LYS	3.8
4	BD	11	LEU	3.8
20	BT	86	LEU	3.8
37	CJ	79	LEU	3.8
53	CZ	14	LEU	3.8
1	AA	1236	A	3.8

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Mol	Chain	Res	Type	RSRZ
31	CA	666	A	3.8
30	CD	131	ASP	3.8
1	BA	982	U	3.8
9	AI	110	GLN	3.8
20	BT	60	ARG	3.8
40	CM	21	ARG	3.8
40	DM	101	ILE	3.8
1	AA	1305	G	3.8
31	CA	245	G	3.8
31	CA	1136	G	3.8
14	BN	16	LEU	3.8
41	CN	2	LEU	3.8
53	CZ	18	LEU	3.8
53	CZ	57	LEU	3.8
1	BA	962	C	3.8
31	CA	16	C	3.8
31	CA	421	C	3.8
38	CK	105	VAL	3.8
46	CS	86	GLN	3.8
20	BT	68	HIS	3.8
22	C1	12	LYS	3.8
41	CN	84	LYS	3.8
14	BN	96	LEU	3.8
19	BS	13	LEU	3.8
30	CD	151	THR	3.8
40	CM	3	LEU	3.8
41	CN	78	LEU	3.8
22	C1	18	SER	3.8
37	CJ	128	SER	3.8
40	CM	25	SER	3.8
12	BL	70	GLU	3.8
1	BA	104	G	3.8
31	CA	1300	G	3.8
42	CO	24	MET	3.8
31	CA	565	C	3.8
7	AG	7	ILE	3.8
31	CA	241	A	3.8
38	CK	97	PRO	3.8
47	CT	48	LYS	3.8
53	CZ	15	ASN	3.8
7	AG	8	GLY	3.8
9	BI	117	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
37	DJ	118	THR	3.8
9	AI	20	PHE	3.8
48	DU	1	MET	3.8
47	CT	101	SER	3.8
54	DI	24	SER	3.8
29	CC	3	VAL	3.8
46	CS	20	VAL	3.8
47	CT	84	ARG	3.8
45	CR	90	ILE	3.8
1	AA	1128	C	3.8
1	BA	266	G	3.8
31	CA	54	G	3.8
30	CD	23	PRO	3.8
31	CA	61	C	3.8
31	CA	257	C	3.8
31	CA	325	G	3.8
31	CA	379	G	3.8
24	C3	2	LYS	3.8
25	C4	46	PRO	3.8
31	CA	394	C	3.8
31	CA	1185	G	3.8
31	CA	1645	G	3.8
31	CA	2027	G	3.8
31	CA	2502	G	3.8
1	AA	1364	U	3.8
31	CA	1396	U	3.8
9	BI	108	ALA	3.8
52	CY	24	ALA	3.8
8	BH	32	LEU	3.8
37	DJ	80	LEU	3.8
40	CM	26	GLY	3.8
5	BE	157	ARG	3.7
22	C1	54	VAL	3.7
26	C5	22	VAL	3.7
30	CD	203	VAL	3.7
10	AJ	6	ILE	3.7
20	BT	83	ILE	3.7
44	CQ	4	ILE	3.7
20	AT	20	HIS	3.7
42	CO	39	PRO	3.7
42	CO	111	ALA	3.7
1	AA	961	U	3.7

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Mol	Chain	Res	Type	RSRZ
2	AB	42	ASN	3.7
29	CC	205	LEU	3.7
31	CA	2045	C	3.7
1	BA	1386	G	3.7
31	CA	1	G	3.7
31	CA	1252	G	3.7
31	CA	1622	G	3.7
31	CA	2032	G	3.7
1	AA	959	A	3.7
31	CA	2665	A	3.7
9	BI	11	ARG	3.7
29	CC	221	ARG	3.7
45	CR	64	ARG	3.7
13	AM	25	VAL	3.7
37	CJ	58	VAL	3.7
47	CT	29	VAL	3.7
45	CR	65	ILE	3.7
47	CT	81	SER	3.7
12	BL	15	LYS	3.7
30	CD	123	LYS	3.7
37	CJ	56	PRO	3.7
14	AN	71	HIS	3.7
33	CE	39	ALA	3.7
33	CE	172	ALA	3.7
38	CK	133	ALA	3.7
46	CS	28	ALA	3.7
38	CK	44	TYR	3.7
7	AG	82	GLY	3.7
38	CK	119	PHE	3.7
52	CY	15	GLY	3.7
1	AA	1277	C	3.7
31	CA	1233	C	3.7
31	CA	1958	C	3.7
31	CA	2050	C	3.7
31	CA	2174	C	3.7
31	CA	2260	C	3.7
1	BA	1024	G	3.7
31	CA	2056	G	3.7
2	BB	132	LYS	3.7
26	C5	2	LYS	3.7
31	CA	941	A	3.7
42	CO	40	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
42	CO	116	VAL	3.7
44	CQ	110	ILE	3.7
49	CV	59	VAL	3.7
20	BT	6	SER	3.7
9	BI	126	GLN	3.7
14	BN	4	GLN	3.7
30	CD	162	ALA	3.7
33	CE	135	ALA	3.7
38	CK	74	TYR	3.7
21	BU	37	PHE	3.7
45	CR	26	GLY	3.7
14	BN	12	LYS	3.7
48	CU	81	LYS	3.7
49	CV	24	LYS	3.7
49	CV	77	THR	3.7
31	CA	1289	C	3.7
31	CA	1350	C	3.7
37	CJ	9	VAL	3.7
40	DM	103	ILE	3.7
49	CV	65	ILE	3.7
31	CA	764	A	3.7
31	CA	2453	A	3.7
31	CA	799	G	3.7
42	CO	27	SER	3.7
40	CM	38	GLN	3.7
42	CO	9	GLN	3.7
46	CS	6	GLN	3.7
13	BM	106	ALA	3.7
33	CE	78	TRP	3.7
3	BC	2	GLY	3.7
25	C4	56	GLY	3.7
29	DC	239	ASN	3.7
33	CE	57	LYS	3.7
10	BJ	76	ILE	3.7
13	AM	16	VAL	3.7
26	C5	26	ILE	3.7
31	CA	355	U	3.7
31	CA	387	U	3.7
52	CY	4	VAL	3.7
10	AJ	55	PRO	3.6
29	CC	244	PRO	3.6
31	CA	11	C	3.6

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Mol	Chain	Res	Type	RSRZ
31	CA	225	C	3.6
40	CM	8	PRO	3.6
39	CL	3	GLN	3.6
1	BA	609	A	3.6
1	BA	974	A	3.6
31	CA	219	A	3.6
31	CA	1598	A	3.6
48	CU	41	ALA	3.6
1	AA	973	G	3.6
31	CA	1380	G	3.6
31	CA	1992	G	3.6
31	CA	2107	G	3.6
33	CE	60	TRP	3.6
40	CM	39	LYS	3.6
40	CM	78	ARG	3.6
42	CO	11	ASN	3.6
42	CO	23	ASN	3.6
3	BC	162	ILE	3.6
50	CW	89	ILE	3.6
51	DX	10	THR	3.6
31	CA	2629	U	3.6
42	CO	28	LEU	3.6
19	BS	66	MET	3.6
27	D0	2[A]	ALA	3.6
40	CM	40	SER	3.6
1	BA	631	C	3.6
55	DA	2165	C	3.6
9	BI	120	LYS	3.6
40	CM	64	PHE	3.6
30	CD	80	TRP	3.6
47	CT	74	ILE	3.6
49	CV	103	ILE	3.6
54	DI	11	ILE	3.6
1	BA	201	G	3.6
1	BA	1370	G	3.6
31	CA	51	G	3.6
31	CA	619	G	3.6
31	CA	1643	G	3.6
31	CA	2895	G	3.6
55	DA	2123	G	3.6
7	BG	49	THR	3.6
13	BM	19	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
48	CU	93	LEU	3.6
53	CZ	6	LEU	3.6
55	DA	846[A]	U	3.6
30	CD	75	ALA	3.6
38	CK	6	ALA	3.6
50	CW	22	ALA	3.6
14	AN	5	SER	3.6
20	BT	69	LYS	3.6
29	CC	28	LYS	3.6
49	CV	44	LYS	3.6
16	BP	30	GLY	3.6
30	CD	166	GLY	3.6
40	CM	11	GLY	3.6
47	CT	79	GLY	3.6
31	CA	2347	C	3.6
31	CA	1307	A	3.6
9	AI	104	VAL	3.6
35	CG	169	VAL	3.6
54	DI	55	VAL	3.6
13	AM	86	TYR	3.6
47	CT	37	THR	3.6
22	C1	28	LEU	3.6
33	CE	143	LEU	3.6
38	CK	46	PRO	3.6
31	CA	248	G	3.6
31	CA	914	G	3.6
31	CA	989	G	3.6
31	CA	1168	G	3.6
31	CA	2245	U	3.6
55	DA	2141	G	3.6
16	BP	7	ALA	3.6
25	C4	5	LYS	3.6
30	CD	119	ALA	3.6
37	DJ	14	ALA	3.6
30	CD	139	SER	3.6
27	C0	15	GLY	3.6
40	CM	24	GLY	3.6
22	C1	55	ILE	3.6
14	AN	101	TRP	3.6
42	CO	29	VAL	3.6
46	CS	51	VAL	3.6
46	CS	72	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	AA	1097	C	3.6
1	BA	234	C	3.6
3	AC	168	TYR	3.6
19	AS	33	THR	3.6
23	C2	34	LEU	3.6
30	CD	136	ASN	3.6
31	CA	222	A	3.6
31	CA	504	A	3.6
31	CA	2706	A	3.6
37	DJ	79	LEU	3.6
55	DA	1847	A	3.6
38	CK	40	HIS	3.5
48	CU	19	LYS	3.5
33	CE	182	ALA	3.5
52	CY	28	ARG	3.5
1	AA	1233	G	3.5
1	BA	1355	G	3.5
31	CA	291	G	3.5
31	CA	2410	G	3.5
31	CA	2618	G	3.5
45	CR	57	PHE	3.5
41	CN	63	ILE	3.5
51	CX	37	ILE	3.5
26	C5	7	VAL	3.5
51	CX	23	VAL	3.5
51	CX	56	ASP	3.5
2	AB	27	MET	3.5
29	CC	34	LEU	3.5
37	CJ	138	LEU	3.5
14	BN	98	LYS	3.5
29	CC	246	THR	3.5
47	CT	100	THR	3.5
1	BA	194	C	3.5
31	CA	128	C	3.5
31	CA	413	C	3.5
31	CA	676	A	3.5
31	CA	2088	A	3.5
31	CA	2628	C	3.5
13	AM	101	ARG	3.5
19	AS	55	ARG	3.5
31	CA	67	U	3.5
31	CA	2713	U	3.5

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Mol	Chain	Res	Type	RSRZ
26	C5	23	ILE	3.5
40	CM	20	GLY	3.5
42	CO	97	ILE	3.5
48	CU	30	ILE	3.5
51	CX	13	GLY	3.5
51	CX	17	GLU	3.5
31	CA	729	G	3.5
31	CA	2382	G	3.5
33	CE	133	LEU	3.5
40	CM	55	MET	3.5
9	BI	66	THR	3.5
29	CC	86	ASN	3.5
35	CG	156	PRO	3.5
24	C3	35	ARG	3.5
30	CD	128	ARG	3.5
32	DD	54	ALA	3.5
49	CV	75	ALA	3.5
53	DZ	63	ALA	3.5
1	BA	984	C	3.5
31	CA	979	A	3.5
31	CA	994	C	3.5
31	CA	1262	A	3.5
16	AP	4	ILE	3.5
46	CS	35	PHE	3.5
52	CY	64	ILE	3.5
31	CA	2384	U	3.5
54	DI	90	GLY	3.5
34	CF	25	VAL	3.5
37	CJ	140	VAL	3.5
2	AB	135	LEU	3.5
10	AJ	54	SER	3.5
37	CJ	106	LEU	3.5
48	CU	7	LEU	3.5
44	CQ	94	LYS	3.5
10	BJ	60	ASP	3.5
12	BL	117	TYR	3.5
33	CE	79	ARG	3.5
38	CK	34	ARG	3.5
10	BJ	58	ASN	3.5
35	CG	80	THR	3.5
19	AS	75	ALA	3.5
24	C3	23	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
31	CA	583	G	3.5
31	CA	1193	G	3.5
31	CA	1444	G	3.5
27	C0	9	GLN	3.5
19	AS	49	ILE	3.5
29	CC	49	ILE	3.5
54	DI	106	PHE	3.5
31	CA	354	A	3.5
3	BC	52	VAL	3.5
24	C3	9	VAL	3.5
31	CA	584	C	3.5
31	CA	623	C	3.5
31	CA	995	C	3.5
31	CA	1600	C	3.5
31	CA	1646	C	3.5
31	CA	2089	C	3.5
47	CT	71	VAL	3.5
55	DA	2174	C	3.5
1	BA	1126	U	3.5
2	AB	114	LEU	3.5
31	CA	1460	U	3.5
31	CA	1778	U	3.5
33	CE	138	LEU	3.5
42	CO	56	LYS	3.5
42	CO	98	LEU	3.5
45	CR	109	LEU	3.5
49	CV	14	LEU	3.5
49	CV	17	LYS	3.5
37	CJ	54	PRO	3.5
22	C1	49	TYR	3.5
29	CC	251	GLN	3.4
30	CD	127	PHE	3.4
44	CQ	59	PHE	3.4
1	BA	1371	G	3.4
31	CA	55	G	3.4
31	CA	1131	G	3.4
31	CA	1195	G	3.4
31	CA	1653	G	3.4
7	AG	32	VAL	3.4
23	D2	16	GLY	3.4
50	CW	48	MET	3.4
7	BG	50	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
29	CC	18	LYS	3.4
37	DJ	28	LEU	3.4
40	CM	61	LEU	3.4
8	AH	91	GLU	3.4
17	BQ	63	GLU	3.4
42	CO	43	GLU	3.4
44	CQ	27	GLU	3.4
1	BA	195	A	3.4
31	CA	616	A	3.4
31	CA	1253	A	3.4
31	CA	390	U	3.4
31	CA	1771	C	3.4
7	BG	4	ARG	3.4
7	BG	5	ARG	3.4
10	AJ	7	ARG	3.4
14	AN	53	ARG	3.4
19	AS	3	ARG	3.4
16	BP	60	TRP	3.4
38	CK	71	ASP	3.4
16	BP	50	THR	3.4
40	DM	74	THR	3.4
47	CT	45	VAL	3.4
48	CU	87	LEU	3.4
53	CZ	53	VAL	3.4
35	DG	173	GLU	3.4
1	BA	165	G	3.4
1	BA	1432	G	3.4
16	BP	51	ARG	3.4
18	AR	73	ARG	3.4
31	CA	375	G	3.4
31	CA	618	G	3.4
31	CA	1248	G	3.4
31	CA	1358	G	3.4
1	AA	994	A	3.4
1	AA	1492	A	3.4
9	BI	23	PRO	3.4
13	AM	96	PRO	3.4
31	CA	615	U	3.4
31	CA	1373	A	3.4
9	BI	15	SER	3.4
31	CA	105	C	3.4
31	CA	336	C	3.4

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Mol	Chain	Res	Type	RSRZ
31	CA	587	C	3.4
31	CA	2815	C	3.4
29	CC	230	HIS	3.4
29	DC	243	HIS	3.4
35	CG	40	ALA	3.4
47	CT	21	ALA	3.4
22	C1	9	THR	3.4
36	DH	25	TYR	3.4
13	BM	4	ILE	3.4
16	AP	39	PHE	3.4
27	C0	53	PHE	3.4
40	CM	13	LYS	3.4
46	CS	71	LYS	3.4
10	AJ	73	LEU	3.4
49	CV	49	VAL	3.4
52	CY	18	ARG	3.4
26	C5	31	PRO	3.4
31	CA	665	U	3.4
1	AA	1020	G	3.4
27	C0	20	HIS	3.4
30	CD	134	HIS	3.4
1	BA	65	A	3.4
1	BA	975	A	3.4
1	BA	1304	G	3.4
1	BA	1435	G	3.4
9	AI	16	ALA	3.4
37	DJ	128	SER	3.4
31	CA	256	A	3.4
31	CA	332	A	3.4
31	CA	407	G	3.4
31	CA	1239	G	3.4
31	CA	2892	G	3.4
3	BC	182	ILE	3.4
10	AJ	53	ILE	3.4
35	DG	114	ASP	3.4
41	CN	96	ILE	3.4
1	AA	948	C	3.4
1	BA	1141	C	3.4
1	BA	1302	C	3.4
29	DC	242	LYS	3.4
31	CA	57	C	3.4
38	CK	72	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
39	CL	67	LYS	3.4
41	CN	22	GLN	3.4
54	DI	96	PHE	3.4
16	BP	26	ASN	3.4
49	CV	27	ASN	3.4
10	AJ	42	LEU	3.4
37	CJ	53	LEU	3.4
38	CK	82	GLY	3.4
17	BQ	40	ARG	3.4
38	CK	9	GLU	3.4
40	CM	41	ARG	3.4
40	CM	59	ARG	3.4
47	CT	87	PRO	3.4
22	C1	19	HIS	3.4
38	CK	94	ALA	3.4
39	CL	33	ALA	3.4
13	BM	21	SER	3.4
31	CA	448	U	3.4
31	CA	1406	U	3.4
31	CA	1599	U	3.4
37	CJ	10	LYS	3.4
37	DJ	109	ILE	3.4
48	CU	33	LYS	3.4
48	CU	74	ILE	3.4
5	BE	103	THR	3.4
7	AG	62	PHE	3.4
24	C3	6	GLN	3.4
37	CJ	73	THR	3.4
52	CY	14	THR	3.4
52	CY	48	THR	3.4
1	BA	1201	A	3.4
31	CA	668	A	3.4
38	CK	49	ASP	3.4
14	BN	46	LEU	3.3
25	C4	44	LEU	3.3
1	AA	1140	C	3.3
29	CC	254	GLY	3.3
29	DC	233	GLY	3.3
31	CA	389	G	3.3
31	CA	953	G	3.3
37	CJ	57	VAL	3.3
39	CL	24	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
49	CV	25	VAL	3.3
53	CZ	50	VAL	3.3
40	CM	102	GLY	3.3
49	CV	38	GLY	3.3
55	DA	2152	G	3.3
31	CA	236	C	3.3
31	CA	510	C	3.3
31	CA	581	C	3.3
31	CA	968	C	3.3
29	CC	217	ARG	3.3
41	CN	72	PRO	3.3
7	AG	39	ALA	3.3
7	BG	76	LYS	3.3
9	BI	44	ALA	3.3
26	C5	18	LYS	3.3
30	CD	57	ALA	3.3
35	CG	175	LYS	3.3
33	CE	119	ILE	3.3
38	CK	55	ILE	3.3
45	CR	14	HIS	3.3
39	CL	7	MET	3.3
39	CL	22	ILE	3.3
46	CS	36	ALA	3.3
53	CZ	30	MET	3.3
1	BA	1235	U	3.3
29	DC	252	THR	3.3
31	CA	29	U	3.3
39	CL	28	SER	3.3
25	C4	55	LEU	3.3
33	CE	159	LEU	3.3
46	CS	22	LEU	3.3
30	CD	37	VAL	3.3
36	CH	108	VAL	3.3
46	CS	63	VAL	3.3
22	C1	16	ARG	3.3
26	C5	38	GLY	3.3
37	DJ	94	ASN	3.3
31	CA	1156	A	3.3
31	CA	1654	A	3.3
31	CA	2059	A	3.3
55	DA	2163	A	3.3
3	AC	188	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	BA	135	C	3.3
31	CA	246	C	3.3
31	CA	1092	C	3.3
31	CA	1135	C	3.3
31	CA	2452	C	3.3
31	CA	333	G	3.3
31	CA	2692	G	3.3
44	CQ	22	PRO	3.3
55	DA	548	G	3.3
33	CE	74	LYS	3.3
9	AI	21	ILE	3.3
37	DJ	114	ALA	3.3
16	BP	6	LEU	3.3
54	DI	95	LEU	3.3
33	CE	65	THR	3.3
47	CT	39	THR	3.3
1	BA	1049	U	3.3
5	BE	46	VAL	3.3
6	BF	91	ARG	3.3
7	BG	64	VAL	3.3
9	BI	48	VAL	3.3
31	CA	906	U	3.3
51	CX	41	ARG	3.3
10	AJ	60	ASP	3.3
33	CE	168	ASP	3.3
36	CH	92	GLY	3.3
41	CN	23	GLY	3.3
47	CT	94	ASP	3.3
54	DI	36	ASP	3.3
31	CA	472	A	3.3
55	DA	2176	A	3.3
49	CV	21	LYS	3.3
24	C3	36	ALA	3.3
42	CO	55	ALA	3.3
54	DI	111	ALA	3.3
1	BA	102	G	3.3
1	BA	380	G	3.3
31	CA	27	G	3.3
31	CA	376	G	3.3
31	CA	669	G	3.3
33	CE	85	PHE	3.3
37	CJ	69	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
37	DJ	38	PHE	3.3
3	BC	39	VAL	3.3
3	BC	198	VAL	3.3
33	CE	49	ARG	3.3
33	CE	173	THR	3.3
41	CN	24	THR	3.3
43	CP	27	VAL	3.3
53	CZ	23	ARG	3.3
29	CC	235	GLY	3.3
50	CW	15	GLY	3.3
1	BA	1025	U	3.3
54	DI	84	TYR	3.3
41	CN	71	LYS	3.3
5	AE	164	ILE	3.3
11	BK	110	ILE	3.3
20	BT	12	ILE	3.3
29	CC	135	ILE	3.3
31	CA	182	A	3.3
31	CA	218	A	3.3
31	CA	311	A	3.3
31	CA	1359	A	3.3
31	CA	2435	A	3.3
41	CN	65	ILE	3.3
27	C0	34	HIS	3.3
36	DH	63	ALA	3.3
41	CN	52	ALA	3.3
42	CO	3	HIS	3.3
8	BH	121	LEU	3.3
24	C3	10	LEU	3.3
30	CD	175	LEU	3.3
1	BA	175	C	3.3
1	BA	381	C	3.3
1	BA	470	C	3.3
31	CA	786	C	3.3
31	CA	1251	C	3.3
43	CP	7	ARG	3.3
6	AF	89	VAL	3.3
3	BC	44	THR	3.3
30	CD	135	GLY	3.3
31	CA	117	G	3.3
31	CA	356	G	3.3
31	CA	410	G	3.3

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Mol	Chain	Res	Type	RSRZ
31	CA	907	G	3.3
31	CA	1767	G	3.3
47	CT	38	TYR	3.2
1	AA	1049	U	3.2
22	C1	20	ASP	3.2
31	CA	224	U	3.2
31	CA	1769	U	3.2
31	CA	2743	U	3.2
30	CD	167	ASN	3.2
38	CK	110	PRO	3.2
34	CF	67	ILE	3.2
45	CR	40	ILE	3.2
43	CP	14	ALA	3.2
48	CU	45	ALA	3.2
1	AA	974	A	3.2
1	BA	1117	A	3.2
1	BA	1236	A	3.2
1	BA	1289	A	3.2
12	BL	50	ARG	3.2
16	BP	32	PHE	3.2
31	CA	590	A	3.2
16	BP	36	VAL	3.2
33	CE	83	VAL	3.2
1	BA	63	C	3.2
31	CA	680	C	3.2
31	CA	1349	C	3.2
31	CA	2000	C	3.2
23	C2	10	LYS	3.2
20	AT	23	SER	3.2
1	BA	457	G	3.2
12	BL	91	PRO	3.2
13	BM	10	PRO	3.2
30	CD	152	PRO	3.2
31	CA	234	U	3.2
31	CA	235	U	3.2
55	DA	2797	U	3.2
3	AC	162	ILE	3.2
11	AK	97	ILE	3.2
17	BQ	21	ILE	3.2
12	BL	24	LEU	3.2
25	C4	65	ALA	3.2
40	DM	95	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
47	CT	44	ALA	3.2
25	C4	42	ARG	3.2
16	BP	16	PHE	3.2
38	CK	100	VAL	3.2
12	BL	69	GLY	3.2
30	CD	116	LYS	3.2
31	CA	52	A	3.2
31	CA	342	A	3.2
31	CA	480	A	3.2
31	CA	482	A	3.2
31	CA	1084	A	3.2
29	CC	219	THR	3.2
34	CF	131	GLY	3.2
17	AQ	53	CYS	3.2
48	CU	42	GLU	3.2
1	AA	1320	C	3.2
1	BA	267	C	3.2
1	BA	322	C	3.2
1	BA	330	C	3.2
1	BA	352	C	3.2
1	BA	1237	C	3.2
31	CA	2300	C	3.2
14	BN	54	ASP	3.2
37	CJ	59	ILE	3.2
31	CA	1825	U	3.2
31	CA	2068	U	3.2
31	CA	2334	U	3.2
42	CO	107	ASN	3.2
4	AD	117	LEU	3.2
11	AK	102	ALA	3.2
14	BN	8	ALA	3.2
19	BS	31	LEU	3.2
34	CF	103	LEU	3.2
40	CM	6	LEU	3.2
19	AS	74	PHE	3.2
28	CB	98	G	3.2
31	CA	188	G	3.2
31	CA	242	G	3.2
31	CA	312	G	3.2
31	CA	535	G	3.2
31	CA	1106	G	3.2
31	CA	1266	G	3.2

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Mol	Chain	Res	Type	RSRZ
31	CA	1277	G	3.2
45	CR	106	PHE	3.2
55	DA	549	G	3.2
22	C1	25	VAL	3.2
23	C2	47	VAL	3.2
33	CE	47	LYS	3.2
41	CN	118	LYS	3.2
42	CO	5	LYS	3.2
50	CW	87	GLN	3.2
13	BM	99	GLY	3.2
2	AB	46	THR	3.2
15	AO	25	THR	3.2
1	BA	389	A	3.2
1	BA	1280	A	3.2
24	D3	1	MET	3.2
29	CC	194	GLU	3.2
31	CA	1067	A	3.2
31	CA	2020	A	3.2
14	BN	93	ILE	3.2
22	C1	27	SER	3.2
9	BI	107	ASP	3.2
7	BG	124	LEU	3.2
18	AR	29	LEU	3.2
20	BT	66	LEU	3.2
31	CA	33	C	3.2
31	CA	1208	C	3.2
31	CA	2616	C	3.2
38	CK	25	LEU	3.2
41	CN	55	ARG	3.2
42	CO	22	ARG	3.2
42	CO	51	LEU	3.2
42	CO	83	LEU	3.2
45	CR	60	LEU	3.2
19	BS	14	HIS	3.2
31	CA	431	U	3.2
31	CA	2871	U	3.2
54	DI	25	ALA	3.2
7	AG	26	PHE	3.2
24	C3	18	PHE	3.2
3	BC	66	VAL	3.2
9	AI	13	LYS	3.2
11	BK	14	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
35	CG	162	VAL	3.2
38	CK	39	LYS	3.2
42	CO	60	VAL	3.2
48	CU	31	VAL	3.2
51	CX	38	VAL	3.2
54	DI	33	VAL	3.2
1	BA	265	G	3.2
25	C4	9	GLY	3.2
31	CA	808	G	3.2
31	CA	1381	G	3.2
31	CA	2409	G	3.2
31	CA	2677	G	3.2
31	CA	2693	G	3.2
55	DA	879	G	3.2
55	DA	2124	G	3.2
2	BB	136	MET	3.2
14	BN	70	PRO	3.2
33	CE	76	PRO	3.2
43	CP	87	ILE	3.2
1	AA	1201	A	3.1
1	BA	174	A	3.1
1	BA	325	A	3.1
31	CA	1129	A	3.1
31	CA	2820	A	3.1
11	AK	13	ARG	3.1
16	BP	74	LEU	3.1
20	AT	6	SER	3.1
40	CM	82	LEU	3.1
48	CU	73	ARG	3.1
42	CO	104	ALA	3.1
43	CP	6	ALA	3.1
5	AE	86	LYS	3.1
9	BI	100	LYS	3.1
10	BJ	30	LYS	3.1
23	C2	53	LYS	3.1
24	C3	25	LYS	3.1
47	CT	6	LYS	3.1
1	AA	1031	C	3.1
10	BJ	84	VAL	3.1
11	BK	84	VAL	3.1
13	AM	97	VAL	3.1
31	CA	1015	U	3.1

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Mol	Chain	Res	Type	RSRZ
31	CA	1161	C	3.1
31	CA	1326	U	3.1
31	CA	1375	U	3.1
31	CA	2073	C	3.1
31	CA	2402	U	3.1
31	CA	2522	U	3.1
3	BC	64	ILE	3.1
13	AM	112	PRO	3.1
20	BT	57	ILE	3.1
25	C4	63	PRO	3.1
1	BA	331	G	3.1
30	CD	125	TRP	3.1
31	CA	250	G	3.1
31	CA	317	G	3.1
31	CA	2732	G	3.1
41	CN	20	LEU	3.1
41	CN	95	LEU	3.1
47	CT	23	LEU	3.1
54	DI	41	LEU	3.1
42	CO	112	TYR	3.1
14	AN	3	LYS	3.1
14	BN	7	LYS	3.1
20	BT	9	LYS	3.1
23	C2	37	LYS	3.1
29	CC	112	ALA	3.1
33	CE	179	SER	3.1
37	DJ	10	LYS	3.1
40	DM	96	LYS	3.1
48	CU	66	LYS	3.1
1	BA	1251	A	3.1
5	AE	19	ASN	3.1
31	CA	505	A	3.1
31	CA	1378	A	3.1
31	CA	1548	A	3.1
31	CA	1552	A	3.1
31	CA	1805	A	3.1
3	BC	200	VAL	3.1
36	DH	78	VAL	3.1
1	BA	185	U	3.1
31	CA	1865	U	3.1
30	CD	158	GLY	3.1
31	CA	31	C	3.1

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Mol	Chain	Res	Type	RSRZ
31	CA	393	C	3.1
31	CA	426	C	3.1
31	CA	673	C	3.1
31	CA	2626	C	3.1
49	CV	78	GLY	3.1
3	BC	192	THR	3.1
42	CO	52	ILE	3.1
47	CT	96	ILE	3.1
10	AJ	43	PRO	3.1
30	CD	143	PRO	3.1
17	BQ	8	LEU	3.1
29	CC	33	LEU	3.1
29	CC	261	LYS	3.1
12	BL	23	ALA	3.1
29	CC	211	ALA	3.1
39	CL	32	TYR	3.1
54	DI	112	ALA	3.1
33	DE	165	HIS	3.1
52	CY	34	HIS	3.1
9	BI	104	VAL	3.1
10	BJ	54	SER	3.1
1	AA	971	G	3.1
1	BA	134	G	3.1
1	BA	213	G	3.1
19	BS	51	VAL	3.1
31	CA	481	G	3.1
31	CA	830	G	3.1
31	CA	1339	G	3.1
31	CA	1382	G	3.1
37	DJ	78	VAL	3.1
42	CO	13	ASN	3.1
42	CO	106	ASP	3.1
48	CU	59	ASN	3.1
1	AA	1016	A	3.1
31	CA	626	A	3.1
31	CA	631	A	3.1
31	CA	1616	A	3.1
31	CA	2126	A	3.1
5	AE	111	MET	3.1
1	BA	458	U	3.1
31	CA	2249	U	3.1
31	CA	2491	U	3.1

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Mol	Chain	Res	Type	RSRZ
39	CL	68	GLY	3.1
40	CM	22	GLY	3.1
20	AT	32	ILE	3.1
38	CK	103	ILE	3.1
42	CO	34	ILE	3.1
1	BA	1245	C	3.1
7	BG	59	LEU	3.1
14	BN	9	ARG	3.1
31	CA	1639	C	3.1
37	CJ	126	THR	3.1
42	CO	103	ARG	3.1
55	DA	2153	C	3.1
27	C0	27	LEU	3.1
4	AD	31	LYS	3.1
25	C4	23	LYS	3.1
33	CE	130	LYS	3.1
39	CL	66	LYS	3.1
45	CR	41	LYS	3.1
13	AM	15	ALA	3.1
36	CH	23	ALA	3.1
23	D2	42	VAL	3.1
30	CD	60	VAL	3.1
37	DJ	58	VAL	3.1
41	CN	12	MET	3.1
12	AL	92	GLY	3.1
29	DC	241	GLY	3.1
33	CE	42	GLY	3.1
35	CG	108	GLY	3.1
1	AA	1441	A	3.1
1	BA	942	G	3.1
1	BA	1356	G	3.1
31	CA	23	G	3.1
31	CA	320	A	3.1
31	CA	443	A	3.1
31	CA	536	G	3.1
31	CA	1237	A	3.1
31	CA	2238	G	3.1
55	DA	1077	A	3.1
55	DA	1087	G	3.1
55	DA	1171	G	3.1
1	AA	4	U	3.1
1	BA	137	U	3.1

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Mol	Chain	Res	Type	RSRZ
8	BH	126	ILE	3.1
31	CA	1199	U	3.1
24	C3	3	ARG	3.1
29	DC	247	PRO	3.1
38	CK	106	LYS	3.1
43	CP	32	PRO	3.1
52	CY	22	LEU	3.1
13	AM	104	THR	3.1
27	C0	23	THR	3.1
11	BK	67	ALA	3.0
31	CA	129	C	3.1
31	CA	143	C	3.1
31	CA	385	C	3.1
2	AB	14	VAL	3.0
9	AI	39	PHE	3.0
24	C3	5	PHE	3.0
37	CJ	38	PHE	3.0
52	DY	20	HIS	3.0
39	CL	57	VAL	3.0
48	CU	58	VAL	3.0
38	CK	118	MET	3.0
12	BL	5	ASN	3.0
46	CS	7	SER	3.0
45	CR	52	GLN	3.0
46	CS	50	GLY	3.0
12	BL	14	ARG	3.0
22	C1	17	ARG	3.0
30	CD	77	ARG	3.0
42	CO	2	ARG	3.0
14	AN	96	LEU	3.0
16	BP	46	LYS	3.0
41	CN	14	LYS	3.0
42	CO	114	GLU	3.0
47	CT	16	LYS	3.0
1	BA	1252	A	3.0
31	CA	150	U	3.0
31	CA	392	U	3.0
31	CA	984	A	3.0
31	CA	1785	A	3.0
31	CA	2689	U	3.0
31	CA	2850	A	3.0
31	CA	2250	G	3.0

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Mol	Chain	Res	Type	RSRZ
31	CA	2802	G	3.0
7	BG	43	VAL	3.0
10	BJ	51	VAL	3.0
21	BU	19	PHE	3.0
22	C1	42	HIS	3.0
33	CE	92	HIS	3.0
40	CM	50	PHE	3.0
47	CT	9	HIS	3.0
1	AA	1001	C	3.0
1	BA	136	C	3.0
16	AP	17	TYR	3.0
31	CA	445	C	3.0
31	CA	1461	C	3.0
31	CA	2021	C	3.0
31	CA	2066	C	3.0
14	AN	80	SER	3.0
36	DH	11	ASN	3.0
47	CT	34	ASP	3.0
15	AO	62	GLN	3.0
9	BI	114	LYS	3.0
13	BM	98	ARG	3.0
29	DC	235	GLY	3.0
44	CQ	105	GLY	3.0
40	CM	17	LYS	3.0
40	CM	70	LYS	3.0
40	CM	105	ILE	3.0
48	CU	72	GLN	3.0
30	CD	187	LEU	3.0
35	CG	33	LEU	3.0
52	CY	33	LEU	3.0
3	AC	105	GLU	3.0
1	BA	208	U	3.0
31	CA	803	U	3.0
31	CA	2324	U	3.0
55	DA	2585	U	3.0
1	AA	1000	A	3.0
1	BA	262	A	3.0
20	BT	73	ALA	3.0
31	CA	582	A	3.0
31	CA	599	A	3.0
31	CA	1572	A	3.0
35	CG	59	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
40	CM	113	ALA	3.0
45	CR	99	ALA	3.0
2	BB	126	PHE	3.0
38	CK	89	PHE	3.0
1	AA	1015	G	3.0
1	BA	187	G	3.0
1	BA	1343	G	3.0
31	CA	491	G	3.0
31	CA	561	G	3.0
31	CA	993	G	3.0
31	CA	1361	G	3.0
1	BA	221	C	3.0
1	BA	328	C	3.0
1	BA	1369	C	3.0
12	AL	15	LYS	3.0
14	AN	31	ILE	3.0
23	C2	38	LYS	3.0
24	C3	14	ARG	3.0
28	CB	63	C	3.0
31	CA	201	C	3.0
31	CA	610	C	3.0
31	CA	1278	C	3.0
31	CA	1612	C	3.0
31	CA	2178	C	3.0
38	CK	83	GLY	3.0
40	CM	16	GLY	3.0
40	CM	33	ARG	3.0
42	CO	12	ARG	3.0
45	CR	15	LYS	3.0
47	CT	98	LYS	3.0
53	CZ	44	LYS	3.0
55	DA	143	C	3.0
24	C3	26	ASN	3.0
19	AS	71	LEU	3.0
22	C1	22	LEU	3.0
29	DC	272	SER	3.0
33	CE	93	SER	3.0
33	CE	109	LEU	3.0
37	DJ	11	LEU	3.0
45	CR	91	ASP	3.0
29	DC	236	GLU	3.0
39	CL	94	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
8	BH	55	THR	3.0
7	AG	116	MET	3.0
13	AM	32	ALA	3.0
27	C0	50	ALA	3.0
44	CQ	108	ALA	3.0
55	DA	1078	U	3.0
17	BQ	23	VAL	3.0
41	CN	93	VAL	3.0
46	CS	12	HIS	3.0
1	AA	958	A	3.0
1	AA	1332	A	3.0
28	CB	29	A	3.0
31	CA	127	A	3.0
31	CA	227	A	3.0
31	CA	804	A	3.0
31	CA	1272	A	3.0
31	CA	1276	A	3.0
3	BC	193	TYR	3.0
38	CK	2	LYS	3.0
3	BC	94	ILE	3.0
3	BC	120	ILE	3.0
8	BH	36	ILE	3.0
10	AJ	8	ILE	3.0
19	AS	37	ARG	3.0
40	CM	58	TYR	3.0
39	CL	41	ILE	3.0
42	CO	8	ARG	3.0
47	CT	18	ARG	3.0
9	AI	35	LEU	3.0
30	CD	3	GLY	3.0
30	CD	120	GLY	3.0
33	CE	56	GLY	3.0
34	CF	93	GLY	3.0
42	CO	115	LEU	3.0
53	CZ	21	LEU	3.0
53	CZ	28	LEU	3.0
53	CZ	37	LEU	3.0
1	BA	1222	G	3.0
31	CA	60	G	3.0
31	CA	259	G	3.0
31	CA	396	G	3.0
31	CA	409	G	3.0

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Mol	Chain	Res	Type	RSRZ
31	CA	539	G	3.0
31	CA	831	G	3.0
31	CA	1377	G	3.0
55	DA	1091	G	3.0
13	BM	46	SER	3.0
1	AA	1282	C	3.0
1	BA	985	C	3.0
31	CA	1314	C	3.0
31	CA	1547	C	3.0
17	BQ	42	THR	3.0
18	BR	71	THR	3.0
33	CE	43	THR	3.0
40	CM	9	ALA	3.0
40	CM	74	THR	3.0
40	CM	117	THR	3.0
52	CY	56	MET	3.0
3	BC	173	VAL	3.0
19	BS	58	VAL	3.0
30	CD	5	VAL	3.0
36	DH	29	PHE	3.0
38	CK	124	VAL	3.0
1	BA	961	U	3.0
31	CA	2904	U	3.0
30	CD	157	LYS	2.9
35	DG	44	LYS	2.9
47	CT	90	LYS	2.9
51	CX	24	LYS	2.9
1	BA	66	A	2.9
1	BA	109	A	2.9
29	CC	54	ILE	2.9
31	CA	422	A	2.9
31	CA	457	A	2.9
31	CA	1393	A	2.9
31	CA	2051	A	2.9
31	CA	2058	A	2.9
29	CC	41	GLY	2.9
38	CK	36	LEU	2.9
38	CK	115	GLY	2.9
54	DI	60	LEU	2.9
2	BB	201	PRO	2.9
29	CC	260	ASN	2.9
19	BS	4	SER	2.9

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Mol	Chain	Res	Type	RSRZ
39	CL	37	ASP	2.9
31	CA	664	G	2.9
31	CA	1324	G	2.9
31	CA	1360	G	2.9
31	CA	2230	G	2.9
31	CA	2444	G	2.9
31	CA	2697	G	2.9
1	BA	207	C	2.9
1	BA	379	C	2.9
1	BA	1303	C	2.9
25	C4	27	ALA	2.9
31	CA	678	C	2.9
31	CA	854	C	2.9
41	CN	79	ALA	2.9
2	BB	163	VAL	2.9
8	BH	104	VAL	2.9
9	BI	20	PHE	2.9
29	CC	268	VAL	2.9
37	DJ	9	VAL	2.9
1	AA	950	U	2.9
7	AG	109	ARG	2.9
7	BG	109	ARG	2.9
42	CO	4	ARG	2.9
7	BG	12	ILE	2.9
10	BJ	71	LEU	2.9
42	CO	38	LEU	2.9
2	BB	98	GLY	2.9
25	D4	20	GLY	2.9
1	BA	101	A	2.9
10	BJ	39	PRO	2.9
21	AU	2	PRO	2.9
31	CA	788	A	2.9
31	CA	2267	A	2.9
31	CA	2412	A	2.9
31	CA	2882	A	2.9
50	CW	27	PRO	2.9
55	DA	1085	A	2.9
55	DA	1420	A	2.9
12	AL	5	ASN	2.9
2	BB	147	SER	2.9
8	BH	3	MET	2.9
33	CE	70	SER	2.9

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Mol	Chain	Res	Type	RSRZ
40	CM	1	MET	2.9
2	BB	92	VAL	2.9
14	AN	2	ALA	2.9
3	BC	37	PHE	2.9
5	AE	120	VAL	2.9
5	BE	120	VAL	2.9
9	AI	127	PHE	2.9
10	AJ	57	VAL	2.9
11	BK	121	CYS	2.9
19	AS	51	VAL	2.9
19	AS	60	VAL	2.9
33	CE	37	ALA	2.9
38	CK	64	VAL	2.9
47	CT	17	VAL	2.9
54	DI	26	VAL	2.9
13	BM	103	LYS	2.9
20	BT	44	LYS	2.9
23	D2	10	LYS	2.9
26	C5	32	LYS	2.9
46	CS	85	LYS	2.9
47	CT	73	LYS	2.9
52	CY	25	THR	2.9
1	AA	934	C	2.9
1	BA	110	C	2.9
1	BA	210	C	2.9
1	BA	483	C	2.9
1	BA	1217	C	2.9
25	C4	30	ARG	2.9
31	CA	76	C	2.9
31	CA	208	C	2.9
31	CA	209	C	2.9
31	CA	456	C	2.9
31	CA	517	C	2.9
31	CA	2175	C	2.9
31	CA	2827	C	2.9
1	BA	105	G	2.9
31	CA	254	G	2.9
31	CA	684	G	2.9
31	CA	1288	G	2.9
31	CA	1430	G	2.9
31	CA	2239	G	2.9
31	CA	2801	G	2.9

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Mol	Chain	Res	Type	RSRZ
31	CA	2808	G	2.9
29	CC	64	ILE	2.9
49	CV	72	ILE	2.9
31	CA	588	U	2.9
31	CA	1390	U	2.9
31	CA	1880	U	2.9
53	CZ	43	LEU	2.9
55	DA	1060	U	2.9
17	BQ	73	TRP	2.9
30	CD	44	GLY	2.9
39	CL	26	GLY	2.9
40	CM	44	GLY	2.9
48	CU	90	GLY	2.9
29	DC	251	GLN	2.9
47	CT	15	GLN	2.9
9	AI	125	PRO	2.9
14	BN	57	PRO	2.9
41	CN	98	PRO	2.9
6	AF	16	GLU	2.9
31	CA	2872	A	2.9
45	CR	72	ASN	2.9
5	BE	114	VAL	2.9
7	BG	137	LYS	2.9
8	BH	130	ALA	2.9
10	AJ	61	ALA	2.9
13	BM	18	ALA	2.9
19	BS	17	LYS	2.9
24	C3	20	ALA	2.9
27	C0	51	VAL	2.9
33	CE	161	ALA	2.9
40	CM	108	ALA	2.9
44	CQ	92	VAL	2.9
45	CR	78	LYS	2.9
47	CT	10	ALA	2.9
48	CU	20	ALA	2.9
49	CV	43	LYS	2.9
51	CX	60	PHE	2.9
2	BB	35	ARG	2.9
37	DJ	39	CYS	2.9
46	CS	90	ARG	2.9
37	DJ	122	ILE	2.9
39	CL	2	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
11	AK	100	LEU	2.9
18	BR	67	LEU	2.9
42	CO	54	LEU	2.9
47	CT	19	LEU	2.9
53	CZ	22	LEU	2.9
1	BA	1203	C	2.9
1	AA	1235	U	2.9
1	BA	1125	U	2.9
13	AM	26	GLY	2.9
22	C1	14	GLY	2.9
23	C2	4	GLY	2.9
31	CA	1200	C	2.9
31	CA	1319	C	2.9
31	CA	1774	C	2.9
31	CA	288	U	2.9
31	CA	832	U	2.9
31	CA	1827	U	2.9
31	CA	1855	U	2.9
35	CG	82	GLY	2.9
37	DJ	137	GLY	2.9
40	CM	37	GLY	2.9
55	DA	1094	U	2.9
1	BA	1026	G	2.9
31	CA	380	G	2.9
31	CA	446	G	2.9
31	CA	488	G	2.9
31	CA	1332	G	2.9
31	CA	1573	G	2.9
31	CA	2029	G	2.9
31	CA	2061	G	2.9
31	CA	2269	G	2.9
31	CA	2599	G	2.9
31	CA	2816	G	2.9
49	CV	66	GLN	2.9
33	CE	89	PRO	2.9
35	CG	151	TYR	2.9
50	CW	57	TYR	2.9
27	C0	6	LYS	2.9
51	CX	75	LYS	2.9
20	BT	70	ASN	2.9
7	BG	33	ASP	2.9
7	BG	51	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
7	BG	61	ALA	2.9
7	BG	128	ALA	2.9
10	BJ	91	ASP	2.9
33	CE	28	VAL	2.9
38	CK	60	ASP	2.9
39	CL	83	ALA	2.9
41	CN	116	ALA	2.9
48	CU	85	VAL	2.9
49	CV	2	ALA	2.9
14	BN	5	SER	2.9
1	BA	1275	A	2.9
9	AI	124	ARG	2.9
9	BI	81	HIS	2.9
30	CD	59	ARG	2.9
40	CM	12	SER	2.9
31	CA	91	A	2.9
31	CA	118	A	2.9
31	CA	677	A	2.9
31	CA	877	A	2.9
31	CA	1085	A	2.9
31	CA	1169	A	2.9
31	CA	1566	A	2.9
31	CA	2837	A	2.9
42	CO	64	ARG	2.9
38	CK	45	THR	2.9
54	DI	58	THR	2.9
3	AC	78	GLY	2.8
2	AB	6	MET	2.8
6	AF	88	MET	2.8
26	C5	1	MET	2.8
30	CD	148	GLN	2.8
1	BA	1341	U	2.8
1	BA	1364	U	2.8
31	CA	444	C	2.8
31	CA	1305	C	2.8
31	CA	1870	C	2.8
33	CE	35	TYR	2.8
33	CE	132	LYS	2.8
44	CQ	29	LYS	2.8
45	CR	16	LYS	2.8
1	BA	64	G	2.8
3	AC	151	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
3	BC	137	ALA	2.8
10	BJ	57	VAL	2.8
16	BP	25	ARG	2.8
23	C2	52	ALA	2.8
31	CA	215	G	2.8
31	CA	289	G	2.8
31	CA	388	G	2.8
31	CA	1368	G	2.8
31	CA	1721	G	2.8
31	CA	1811	G	2.8
31	CA	2780	G	2.8
36	DH	74	ALA	2.8
37	CJ	70	VAL	2.8
38	CK	67	ASN	2.8
38	CK	134	ALA	2.8
55	DA	141	G	2.8
55	DA	1056	G	2.8
55	DA	2121	G	2.8
30	CD	141	ARG	2.8
7	BG	142	HIS	2.8
10	BJ	73	LEU	2.8
13	AM	4	ILE	2.8
24	C3	43	THR	2.8
30	CD	25	THR	2.8
37	CJ	109	ILE	2.8
40	CM	67	THR	2.8
31	CA	144	A	2.8
31	CA	391	A	2.8
31	CA	528	A	2.8
31	CA	1762	A	2.8
31	CA	1981	A	2.8
31	CA	2070	A	2.8
8	AH	3	MET	2.8
15	BO	62	GLN	2.8
19	BS	9	PRO	2.8
12	BL	30	LYS	2.8
30	CD	55	LYS	2.8
33	CE	139	LYS	2.8
1	AA	1017	U	2.8
25	C4	64	TYR	2.8
1	AA	1141	C	2.8
1	BA	106	C	2.8

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Mol	Chain	Res	Type	RSRZ
1	BA	623	C	2.8
1	BA	1209	C	2.8
5	AE	161	VAL	2.8
7	AG	94	VAL	2.8
13	AM	109	ARG	2.8
20	BT	24	ARG	2.8
30	CD	29	VAL	2.8
30	CD	69	ALA	2.8
30	CD	193	VAL	2.8
31	CA	237	C	2.8
31	CA	1006	C	2.8
31	CA	2055	C	2.8
36	CH	84	ALA	2.8
54	DI	75	ALA	2.8
33	CE	183	PHE	2.8
49	CV	85	PHE	2.8
51	CX	45	PHE	2.8
19	AS	53	ASN	2.8
47	CT	7	HIS	2.8
47	CT	40	ASN	2.8
7	BG	47	LEU	2.8
13	AM	83	LEU	2.8
11	AK	30	THR	2.8
11	BK	30	THR	2.8
14	BN	56	SER	2.8
25	C4	17	THR	2.8
31	CA	185	G	2.8
31	CA	308	G	2.8
31	CA	442	G	2.8
31	CA	474	G	2.8
31	CA	798	G	2.8
31	CA	1331	G	2.8
31	CA	1341	G	2.8
31	CA	2812	G	2.8
1	BA	306	A	2.8
31	CA	453	A	2.8
31	CA	608	A	2.8
31	CA	800	A	2.8
31	CA	1528	A	2.8
31	CA	1938	A	2.8
31	CA	2587	A	2.8
6	AF	93	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
25	C4	52	LYS	2.8
29	CC	5	LYS	2.8
35	CG	176	LYS	2.8
52	CY	26	LYS	2.8
11	BK	64	GLN	2.8
33	CE	90	GLN	2.8
54	DI	130	PRO	2.8
3	AC	82	GLU	2.8
11	BK	68	GLU	2.8
3	BC	156	ARG	2.8
7	BG	69	VAL	2.8
10	BJ	26	VAL	2.8
10	BJ	98	VAL	2.8
11	AK	86	VAL	2.8
13	AM	23	TYR	2.8
16	BP	21	VAL	2.8
35	CG	152	ARG	2.8
38	CK	116	ARG	2.8
45	CR	45	TYR	2.8
31	CA	1443	U	2.8
31	CA	1971	U	2.8
31	CA	2387	U	2.8
52	CY	13	VAL	2.8
52	CY	67	VAL	2.8
4	AD	182	PHE	2.8
5	BE	118	ALA	2.8
7	BG	46	ALA	2.8
11	BK	27	PHE	2.8
14	BN	29	ALA	2.8
14	BN	73	PHE	2.8
20	BT	22	ALA	2.8
32	DD	209	ALA	2.8
49	CV	64	ALA	2.8
53	CZ	61	ALA	2.8
55	DA	138	U	2.8
37	DJ	67	PHE	2.8
42	CO	102	PHE	2.8
3	BC	33	LEU	2.8
11	BK	22	HIS	2.8
27	C0	25	LEU	2.8
27	C0	48	ILE	2.8
41	CN	124	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
49	CV	45	HIS	2.8
1	BA	1112	C	2.8
7	BG	15	ASP	2.8
28	CB	28	C	2.8
31	CA	32	C	2.8
31	CA	69	C	2.8
31	CA	435	C	2.8
31	CA	791	C	2.8
31	CA	2501	C	2.8
34	DF	113	ASP	2.8
51	DX	56	ASP	2.8
14	BN	32	SER	2.8
14	BN	80	SER	2.8
35	CG	36	THR	2.8
22	C1	15	MET	2.8
19	BS	21	LYS	2.8
30	CD	38	LYS	2.8
10	AJ	38	GLY	2.8
35	DG	120	GLY	2.8
1	AA	933	G	2.8
1	AA	1331	G	2.8
1	BA	1385	G	2.8
31	CA	15	G	2.8
31	CA	88	G	2.8
31	CA	530	G	2.8
31	CA	774	G	2.8
31	CA	777	G	2.8
31	CA	1356	G	2.8
31	CA	1429	G	2.8
31	CA	1873	G	2.8
31	CA	2597	G	2.8
1	AA	1130	A	2.8
1	BA	959	A	2.8
31	CA	996	A	2.8
55	DA	2170	A	2.8
9	AI	130	ARG	2.8
10	BJ	7	ARG	2.8
45	CR	92	ARG	2.8
48	CU	80	TRP	2.8
2	BB	217	VAL	2.8
14	BN	45	VAL	2.8
30	CD	50	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
14	AN	22	ALA	2.8
16	AP	16	PHE	2.8
41	CN	56	ALA	2.8
42	CO	68	ALA	2.8
45	CR	47	TYR	2.8
49	DV	2	ALA	2.8
50	CW	82	TYR	2.8
52	CY	29	PHE	2.8
1	BA	103	U	2.8
3	BC	207	ILE	2.8
12	BL	81	LEU	2.8
31	CA	2081	U	2.8
31	CA	2233	U	2.8
31	CA	2240	U	2.8
31	CA	2690	U	2.8
33	CE	153	LEU	2.8
35	CG	103	ILE	2.8
35	CG	148	LEU	2.8
41	CN	126	ILE	2.8
42	CO	65	LEU	2.8
55	DA	2167	U	2.8
2	BB	130	THR	2.8
14	AN	54	ASP	2.8
13	AM	27	LYS	2.8
30	CD	171	THR	2.8
37	DJ	132	THR	2.8
1	AA	1149	C	2.8
31	CA	378	C	2.8
31	CA	806	C	2.8
31	CA	1290	C	2.8
31	CA	1437	C	2.8
31	CA	1454	C	2.8
31	CA	1806	C	2.8
31	CA	1997	C	2.8
31	CA	2096	C	2.8
40	CM	68	SER	2.8
33	CE	103	GLY	2.8
19	AS	56	GLN	2.7
37	CJ	12	GLN	2.7
3	BC	91	VAL	2.7
7	BG	141	VAL	2.7
1	AA	441	A	2.7

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Mol	Chain	Res	Type	RSRZ
1	BA	149	A	2.7
1	BA	1016	A	2.7
16	BP	65	ALA	2.7
1	BA	1244	G	2.7
1	BA	1387	G	2.7
29	CC	266	PHE	2.7
31	CA	217	A	2.7
31	CA	384	A	2.7
31	CA	501	A	2.7
31	CA	1367	A	2.7
31	CA	1475	G	2.7
31	CA	1631	G	2.7
31	CA	2035	G	2.7
31	CA	2046	G	2.7
31	CA	2209	G	2.7
31	CA	2428	G	2.7
31	CA	2630	G	2.7
31	CA	2682	A	2.7
37	DJ	63	ALA	2.7
31	CA	2803	G	2.7
47	CT	75	PHE	2.7
55	DA	1089	A	2.7
7	BG	23	LEU	2.7
13	BM	33	ILE	2.7
14	AN	30	ILE	2.7
30	CD	27	ILE	2.7
42	CO	79	LEU	2.7
43	CP	40	ILE	2.7
55	DA	1093	G	2.7
14	BN	71	HIS	2.7
24	C3	16	HIS	2.7
1	BA	1183	U	2.7
31	CA	2585	U	2.7
5	BE	23	LYS	2.7
24	C3	22	MET	2.7
38	CK	1	MET	2.7
48	CU	1	MET	2.7
49	CV	47	LYS	2.7
8	AH	38	ASN	2.7
7	AG	38	THR	2.7
25	C4	6	THR	2.7
36	DH	79	THR	2.7

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Mol	Chain	Res	Type	RSRZ
11	BK	123	PRO	2.7
38	CK	113	PRO	2.7
14	AN	13	ARG	2.7
15	BO	58	ARG	2.7
33	CE	61	ARG	2.7
40	CM	69	ARG	2.7
47	DT	110	ARG	2.7
1	AA	470	C	2.7
1	AA	985	C	2.7
1	BA	183	C	2.7
31	CA	37	C	2.7
31	CA	211	C	2.7
31	CA	267	C	2.7
31	CA	679	C	2.7
31	CA	1178	C	2.7
31	CA	1270	C	2.7
31	CA	1351	C	2.7
46	CS	23	GLU	2.7
55	DA	2150	C	2.7
25	C4	58	VAL	2.7
36	DH	144	VAL	2.7
40	CM	85	VAL	2.7
40	CM	110	VAL	2.7
45	CR	4	VAL	2.7
46	CS	33	VAL	2.7
10	BJ	102	LEU	2.7
13	BM	95	LEU	2.7
17	BQ	75	LEU	2.7
22	C1	24	ALA	2.7
51	CX	21	LEU	2.7
54	DI	92	ALA	2.7
40	CM	77	ILE	2.7
45	CR	94	ILE	2.7
3	BC	168	TYR	2.7
33	CE	165	HIS	2.7
43	CP	99	TYR	2.7
25	C4	12	LYS	2.7
31	CA	432	A	2.7
31	CA	1551	A	2.7
31	CA	2054	A	2.7
31	CA	2764	A	2.7
53	CZ	54	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	AA	201	G	2.7
1	AA	540	G	2.7
1	AA	1018	G	2.7
1	AA	1354	U	2.7
1	BA	933	G	2.7
1	BA	1116	U	2.7
1	BA	1331	G	2.7
1	BA	1436	U	2.7
31	CA	189	G	2.7
31	CA	193	U	2.7
31	CA	252	G	2.7
31	CA	425	G	2.7
31	CA	1166	G	2.7
31	CA	1240	U	2.7
31	CA	2125	G	2.7
31	CA	2128	G	2.7
55	DA	12	U	2.7
55	DA	2166	U	2.7
55	DA	2186	G	2.7
55	DA	2885[A]	G	2.7
9	BI	9	THR	2.7
33	CE	53	THR	2.7
2	BB	33	GLY	2.7
20	BT	65	GLY	2.7
21	AU	13	ASP	2.7
7	AG	2	PRO	2.7
14	BN	55	SER	2.7
20	BT	10	ARG	2.7
36	CH	136	SER	2.7
38	CK	35	ARG	2.7
38	CK	37	ARG	2.7
48	CU	12	ARG	2.7
48	CU	76	ARG	2.7
7	BG	135	VAL	2.7
17	BQ	46	VAL	2.7
25	C4	50	VAL	2.7
29	DC	250	VAL	2.7
1	AA	1096	C	2.7
1	AA	1325	C	2.7
23	C2	48	ILE	2.7
30	CD	96	ILE	2.7
31	CA	509	C	2.7

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Mol	Chain	Res	Type	RSRZ
31	CA	961	C	2.7
31	CA	1574	C	2.7
31	CA	2443	C	2.7
31	CA	2456	C	2.7
33	CE	118	LEU	2.7
34	CF	152	LEU	2.7
52	CY	53	ALA	2.7
19	BS	7	LYS	2.7
45	CR	54	LYS	2.7
48	CU	44	LYS	2.7
49	CV	61	LYS	2.7
51	CX	53	CYS	2.7
3	BC	42	TYR	2.7
9	BI	64	TYR	2.7
12	BL	96	HIS	2.7
34	DF	83	TYR	2.7
1	AA	1299	A	2.7
31	CA	793	A	2.7
31	CA	1353	A	2.7
1	BA	261	U	2.7
20	AT	24	ARG	2.7
29	CC	50	THR	2.7
31	CA	1066	U	2.7
31	CA	1201	U	2.7
31	CA	1340	U	2.7
31	CA	2079	U	2.7
31	CA	2231	U	2.7
31	CA	2680	U	2.7
31	CA	2903	U	2.7
37	CJ	132	THR	2.7
38	DK	95	ARG	2.7
41	CN	18	ARG	2.7
45	CR	23	GLY	2.7
46	CS	32	THR	2.7
52	CY	17	ASN	2.7
36	DH	92	GLY	2.7
2	BB	82	ASP	2.7
47	CT	80	PRO	2.7
1	BA	1461	G	2.7
2	AB	44	GLU	2.7
14	AN	66	GLN	2.7
31	CA	7	G	2.7

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Mol	Chain	Res	Type	RSRZ
31	CA	406	G	2.7
31	CA	473	G	2.7
31	CA	1137	G	2.7
31	CA	1160	G	2.7
31	CA	1212	G	2.7
31	CA	1642	G	2.7
31	CA	2110	G	2.7
31	CA	2405	G	2.7
31	CA	2688	G	2.7
55	DA	2110	G	2.7
30	CD	30	GLU	2.7
37	CJ	78	VAL	2.7
37	CJ	130	GLU	2.7
3	BC	12	LEU	2.7
3	BC	43	LEU	2.7
7	BG	22	LEU	2.7
10	AJ	10	LEU	2.7
13	AM	56	LEU	2.7
19	AS	41	PHE	2.7
20	BT	87	ALA	2.7
27	C0	44	ILE	2.7
33	CE	201	ALA	2.7
40	CM	73	ILE	2.7
44	CQ	58	ALA	2.7
51	CX	26	PHE	2.7
13	AM	44	LYS	2.7
14	AN	7	LYS	2.7
44	CQ	111	LYS	2.7
48	CU	9	LYS	2.7
33	CE	100	MET	2.7
1	BA	307	C	2.7
20	BT	36	TYR	2.7
31	CA	420	C	2.7
31	CA	660	C	2.7
31	CA	1656	C	2.7
31	CA	2427	C	2.7
31	CA	2619	C	2.7
10	AJ	62	ARG	2.7
14	AN	63	ARG	2.7
15	AO	72	ARG	2.7
29	CC	14	ARG	2.7
3	AC	74	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
29	CC	218	PRO	2.7
30	CD	61	THR	2.7
34	CF	23	ASN	2.7
40	CM	65	GLY	2.7
53	CZ	16	THR	2.7
1	AA	472	U	2.7
1	AA	935	A	2.7
1	AA	1169	A	2.7
1	AA	1318	A	2.7
1	BA	1362	A	2.7
31	CA	14	A	2.7
31	CA	65	U	2.7
31	CA	73	A	2.7
31	CA	197	A	2.7
31	CA	324	A	2.7
31	CA	415	A	2.7
31	CA	423	A	2.7
31	CA	866	A	2.7
31	CA	1029	A	2.7
31	CA	1679	A	2.7
31	CA	1758	U	2.7
16	BP	23	ASP	2.7
14	AN	4	GLN	2.7
40	CM	54	GLN	2.7
2	AB	70	VAL	2.7
13	BM	60	VAL	2.7
27	C0	55	VAL	2.7
29	CC	172	VAL	2.7
35	CG	76	VAL	2.7
40	CM	46	VAL	2.7
3	BC	10	ILE	2.6
5	AE	15	LEU	2.7
6	BF	39	LEU	2.7
7	BG	7	ILE	2.6
10	BJ	46	LYS	2.6
27	C0	7	ILE	2.6
29	CC	259	SER	2.7
27	C0	21	LYS	2.6
30	CD	202	ILE	2.6
33	CE	147	LEU	2.7
37	DJ	59	ILE	2.6
37	DJ	66	SER	2.7

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Mol	Chain	Res	Type	RSRZ
44	CQ	57	SER	2.7
47	CT	33	LEU	2.7
49	CV	41	LEU	2.7
51	CX	78	LYS	2.6
37	CJ	14	ALA	2.6
1	BA	100	G	2.6
1	BA	112	G	2.6
1	BA	198	G	2.6
1	BA	484	G	2.6
31	CA	258	G	2.6
31	CA	297	G	2.6
31	CA	489	G	2.6
31	CA	1309	G	2.6
31	CA	1627	G	2.6
31	CA	1903	G	2.6
31	CA	2127	G	2.6
34	CF	130	MET	2.6
41	CN	82	MET	2.6
16	BP	8	ARG	2.6
38	CK	120	ARG	2.6
47	CT	92	ARG	2.6
31	CA	22	C	2.6
31	CA	239	C	2.6
31	CA	672	C	2.6
31	CA	1615	C	2.6
31	CA	1658	C	2.6
31	CA	2047	C	2.6
31	CA	2214	C	2.6
31	CA	2902	C	2.6
19	BS	48	THR	2.6
37	CJ	60	THR	2.6
38	CK	3	THR	2.6
13	BM	105	ASN	2.6
24	C3	13	ASN	2.6
2	AB	142	GLU	2.6
3	AC	206	GLU	2.6
13	AM	43	VAL	2.6
21	AU	16	LEU	2.6
23	D2	38	LYS	2.6
31	CA	641	U	2.6
35	CG	10	VAL	2.6
43	CP	4	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
46	CS	24	LYS	2.6
48	DU	56	GLU	2.6
49	CV	46	GLN	2.6
49	CV	79	LYS	2.6
55	DA	653	U	2.6
1	AA	977	A	2.6
1	AA	1014	A	2.6
1	BA	78	A	2.6
1	BA	151	A	2.6
1	BA	172	A	2.6
9	AI	72	ILE	2.6
13	AM	73	ILE	2.6
13	BM	45	ILE	2.6
31	CA	111	A	2.6
31	CA	223	A	2.6
31	CA	503	A	2.6
31	CA	1322	A	2.6
31	CA	2851	A	2.6
31	CA	2873	A	2.6
37	CJ	101	ILE	2.6
55	DA	2135	A	2.6
9	AI	121	ALA	2.6
14	AN	55	SER	2.6
33	CE	23	PHE	2.6
37	DJ	18	ALA	2.6
40	CM	98	ALA	2.6
45	CR	87	SER	2.6
48	CU	27	SER	2.6
30	CD	67	HIS	2.6
44	CQ	56	HIS	2.6
1	BA	346	G	2.6
1	BA	1347	G	2.6
7	BG	78	ARG	2.6
10	BJ	62	ARG	2.6
28	CB	85	G	2.6
31	CA	600	G	2.6
31	CA	656	G	2.6
31	CA	942	G	2.6
31	CA	974	G	2.6
31	CA	1218	G	2.6
31	CA	1279	G	2.6
31	CA	1371	G	2.6

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Mol	Chain	Res	Type	RSRZ
31	CA	1743	G	2.6
31	CA	2578	G	2.6
31	CA	2668	G	2.6
31	CA	2885	G	2.6
44	CQ	99	TYR	2.6
55	DA	2125	G	2.6
7	AG	93	PRO	2.6
26	D5	38	GLY	2.6
29	CC	11	PRO	2.6
1	AA	330	C	2.6
1	BA	1352	C	2.6
2	BB	131	LYS	2.6
6	BF	92	THR	2.6
9	BI	60	LYS	2.6
10	AJ	80	THR	2.6
20	BT	71	LYS	2.6
3	BC	195	VAL	2.6
5	BE	135	ASN	2.6
7	BG	27	VAL	2.6
30	CD	149	ASN	2.6
31	CA	238	C	2.6
31	CA	353	C	2.6
31	CA	550	C	2.6
31	CA	634	C	2.6
31	CA	1167	C	2.6
31	CA	1879	C	2.6
31	CA	2078	C	2.6
33	CE	169	VAL	2.6
40	CM	89	VAL	2.6
47	CT	107	VAL	2.6
53	CZ	19	LEU	2.6
55	DA	1104	C	2.6
49	CV	58	ILE	2.6
53	CZ	17	GLU	2.6
1	AA	1326	U	2.6
3	BC	34	ASP	2.6
11	BK	85	MET	2.6
29	CC	132	MET	2.6
31	CA	1209	U	2.6
31	CA	1982	U	2.6
31	CA	2847	U	2.6
38	CK	92	MET	2.6

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Mol	Chain	Res	Type	RSRZ
51	CX	15	ASP	2.6
3	BC	117	ALA	2.6
20	BT	7	ALA	2.6
34	CF	100	PHE	2.6
35	CG	109	PHE	2.6
41	CN	21	ALA	2.6
44	CQ	43	PHE	2.6
44	CQ	49	ALA	2.6
47	CT	32	ALA	2.6
49	DV	51	ALA	2.6
55	DA	1065	U	2.6
1	BA	80	A	2.6
1	BA	482	A	2.6
14	AN	56	SER	2.6
31	CA	1609	A	2.6
31	CA	2170	A	2.6
55	DA	1070	A	2.6
55	DA	1090	A	2.6
55	DA	1095	A	2.6
10	BJ	72	ARG	2.6
6	AF	42	TRP	2.6
9	AI	74	GLY	2.6
16	BP	49	GLY	2.6
23	D2	18	GLY	2.6
37	DJ	131	GLY	2.6
10	AJ	59	LYS	2.6
33	CE	58	LYS	2.6
41	CN	133	LYS	2.6
47	CT	42	LYS	2.6
1	AA	685	G	2.6
9	BI	55	VAL	2.6
10	BJ	44	THR	2.6
15	BO	57	LEU	2.6
24	C3	30	VAL	2.6
31	CA	1093	G	2.6
31	CA	1311	G	2.6
31	CA	1346	G	2.6
31	CA	1823	G	2.6
31	CA	2624	G	2.6
37	CJ	139	VAL	2.6
38	CK	78	THR	2.6
47	CT	69	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
21	BU	36	GLU	2.6
25	C4	59	ILE	2.6
29	CC	104	ILE	2.6
55	DA	1063	G	2.6
14	AN	6	MET	2.6
16	BP	18	GLN	2.6
29	CC	153	GLN	2.6
30	CD	28	GLU	2.6
53	CZ	45	GLN	2.6
8	BH	116	ALA	2.6
37	DJ	110	ALA	2.6
1	BA	972	C	2.6
31	CA	184	C	2.6
31	CA	268	C	2.6
31	CA	985	C	2.6
31	CA	1323	C	2.6
31	CA	1732	C	2.6
31	CA	1768	C	2.6
31	CA	2422	C	2.6
46	CS	55	ASP	2.6
55	DA	1092	C	2.6
31	CA	1709	U	2.6
29	CC	10	SER	2.6
36	DH	136	SER	2.6
43	CP	9	ARG	2.6
1	BA	949	A	2.6
31	CA	126	A	2.6
31	CA	181	A	2.6
31	CA	1226	A	2.6
31	CA	2015	A	2.6
31	CA	2602	A	2.6
9	BI	26	GLY	2.6
13	AM	94	GLY	2.6
14	AN	57	PRO	2.6
27	D0	3[A]	LYS	2.6
29	CC	253	LYS	2.6
30	CD	153	GLY	2.6
41	CN	19	GLY	2.6
47	CT	26	GLY	2.6
47	CT	63	GLY	2.6
14	AN	46	LEU	2.6
33	CE	105	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
47	CT	36	LEU	2.6
5	BE	30	ILE	2.6
5	BE	131	THR	2.6
7	BG	105	VAL	2.6
9	BI	72	ILE	2.6
14	BN	6	MET	2.6
16	BP	42	ILE	2.6
16	BP	67	ILE	2.6
20	AT	58	VAL	2.6
30	CD	207	VAL	2.6
33	CE	84	THR	2.6
35	CG	144	VAL	2.6
37	CJ	49	ILE	2.6
37	DJ	71	THR	2.6
39	CL	76	VAL	2.6
47	CT	104	THR	2.6
48	CU	22	THR	2.6
40	DM	106	GLU	2.6
47	CT	31	GLN	2.6
2	BB	166	ALA	2.6
13	AM	2	ALA	2.6
30	CD	185	ASN	2.6
33	CE	26	ALA	2.6
47	CT	93	ALA	2.6
52	CY	38	PHE	2.6
1	BA	1260	G	2.5
31	CA	24	G	2.5
31	CA	220	G	2.5
31	CA	381	G	2.5
31	CA	597	G	2.5
31	CA	617	G	2.5
31	CA	1206	G	2.5
31	CA	1464	G	2.5
31	CA	1619	G	2.5
31	CA	2744	G	2.5
55	DA	2138	G	2.5
1	BA	1189	U	2.5
26	C5	19	ARG	2.5
29	CC	270	ARG	2.5
31	CA	25	U	2.5
31	CA	1033	U	2.5
51	CX	25	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	AA	1098	C	2.5
1	BA	1412	C	2.5
14	AN	100	SER	2.5
28	CB	90	C	2.5
31	CA	130	C	2.5
31	CA	151	C	2.5
31	CA	179	C	2.5
31	CA	671	C	2.5
31	CA	1708	C	2.5
31	CA	1957	C	2.5
55	DA	1072	C	2.5
55	DA	2175	C	2.5
4	AD	206	LYS	2.5
16	BP	13	LYS	2.5
1	BA	532	A	2.5
1	BA	1441	A	2.5
9	AI	23	PRO	2.5
16	BP	15	PRO	2.5
31	CA	104	A	2.5
31	CA	401	A	2.5
31	CA	654	A	2.5
31	CA	792	A	2.5
31	CA	1133	A	2.5
34	CF	84	PRO	2.5
34	CF	97	TRP	2.5
41	CN	92	TRP	2.5
4	BD	21	LEU	2.5
10	BJ	87	LEU	2.5
41	CN	33	LEU	2.5
2	AB	151	ILE	2.5
4	AD	123	ILE	2.5
5	AE	137	VAL	2.5
7	BG	73	VAL	2.5
9	AI	79	ILE	2.5
10	BJ	40	ILE	2.5
11	AK	113	VAL	2.5
14	AN	34	VAL	2.5
19	BS	19	VAL	2.5
33	CE	167	VAL	2.5
39	CL	69	VAL	2.5
41	CN	89	VAL	2.5
47	CT	24	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
47	CT	76	VAL	2.5
47	DT	82	MET	2.5
48	CU	2	ILE	2.5
13	BM	108	THR	2.5
14	AN	67	THR	2.5
36	CH	133	GLN	2.5
44	CQ	25	THR	2.5
10	AJ	49	PHE	2.5
36	DH	91	PHE	2.5
52	CY	6	GLN	2.5
13	BM	40	ALA	2.5
52	DY	46	PHE	2.5
24	C3	41	ARG	2.5
29	CC	101	ARG	2.5
6	AF	37	HIS	2.5
1	AA	632	U	2.5
1	BA	1159	U	2.5
9	AI	120	LYS	2.5
20	BT	33	LYS	2.5
31	CA	34	U	2.5
31	CA	82	U	2.5
31	CA	958	U	2.5
31	CA	1224	U	2.5
31	CA	1352	U	2.5
44	CQ	106	LYS	2.5
1	AA	413	G	2.5
1	AA	733	G	2.5
1	AA	1142	G	2.5
1	BA	204	G	2.5
1	BA	326	G	2.5
1	BA	1057	G	2.5
1	BA	1221	G	2.5
1	BA	1241	G	2.5
31	CA	313	G	2.5
31	CA	372	G	2.5
31	CA	549	G	2.5
31	CA	585	G	2.5
31	CA	1296	G	2.5
31	CA	1369	G	2.5
31	CA	1719	G	2.5
55	DA	1731	G	2.5
1	BA	936	C	2.5

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Mol	Chain	Res	Type	RSRZ
1	BA	1320	C	2.5
31	CA	66	C	2.5
31	CA	106	C	2.5
31	CA	198	C	2.5
31	CA	758	C	2.5
31	CA	1261	C	2.5
31	CA	1320	C	2.5
31	CA	2717	C	2.5
2	BB	148	LEU	2.5
4	AD	9	LEU	2.5
6	AF	61	LEU	2.5
8	AH	93	PRO	2.5
8	BH	122	GLY	2.5
25	C4	18	GLY	2.5
29	CC	105	LEU	2.5
5	AE	18	VAL	2.5
7	AG	141	VAL	2.5
9	BI	79	ILE	2.5
12	BL	107	VAL	2.5
13	BM	25	VAL	2.5
14	BN	14	VAL	2.5
17	BQ	78	VAL	2.5
37	DJ	139	VAL	2.5
38	CK	53	TYR	2.5
42	CO	76	VAL	2.5
44	CQ	73	VAL	2.5
46	CS	59	ILE	2.5
53	CZ	11	VAL	2.5
54	DI	123	ILE	2.5
34	CF	128	TYR	2.5
45	CR	32	TYR	2.5
1	AA	1280	A	2.5
1	BA	1204	A	2.5
1	BA	1418	A	2.5
28	CB	101	A	2.5
31	CA	149	A	2.5
31	CA	207	A	2.5
31	CA	244	A	2.5
31	CA	532	A	2.5
31	CA	574	A	2.5
31	CA	878	A	2.5
31	CA	983	A	2.5

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Mol	Chain	Res	Type	RSRZ
31	CA	1194	A	2.5
31	CA	2003	A	2.5
31	CA	2247	A	2.5
31	CA	2741	A	2.5
14	BN	77	PHE	2.5
30	CD	35	THR	2.5
33	CE	124	PHE	2.5
8	BH	35	ALA	2.5
9	AI	44	ALA	2.5
16	BP	22	ALA	2.5
34	CF	119	ALA	2.5
37	CJ	133	ALA	2.5
41	CN	121	ALA	2.5
54	DI	91	ALA	2.5
2	BB	103	ASN	2.5
20	BT	3	ASN	2.5
29	DC	238	ARG	2.5
49	CV	40	ASN	2.5
4	AD	174	ASP	2.5
7	AG	25	LYS	2.5
14	AN	47	LYS	2.5
43	CP	2	ASP	2.5
45	CR	93	LYS	2.5
47	CT	49	LYS	2.5
1	AA	85	U	2.5
1	AA	471	U	2.5
1	AA	1025	U	2.5
9	AI	128	SER	2.5
30	CD	97	SER	2.5
31	CA	591	U	2.5
31	CA	686	U	2.5
31	CA	1379	U	2.5
31	CA	2449	U	2.5
42	CO	15	SER	2.5
3	AC	43	LEU	2.5
3	BC	178	LEU	2.5
4	BD	19	LEU	2.5
13	AM	10	PRO	2.5
16	BP	41	PRO	2.5
38	CK	122	LEU	2.5
7	AG	12	ILE	2.5
20	BT	42	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
25	C4	32	ILE	2.5
51	CX	80	ILE	2.5
54	DI	82	ILE	2.5
7	BG	80	VAL	2.5
30	CD	98	VAL	2.5
36	CH	138	VAL	2.5
52	CY	51	VAL	2.5
1	BA	1342	C	2.5
31	CA	264	C	2.5
31	CA	440	C	2.5
1	BA	1190	G	2.5
9	AI	64	TYR	2.5
31	CA	1117	C	2.5
31	CA	1526	C	2.5
55	DA	1064	C	2.5
55	DA	2178	C	2.5
28	CB	102	G	2.5
31	CA	98	G	2.5
31	CA	186	G	2.5
31	CA	1087	G	2.5
31	CA	1364	G	2.5
31	CA	2004	G	2.5
31	CA	2057	G	2.5
31	CA	2294	G	2.5
31	CA	2631	G	2.5
31	CA	2877	G	2.5
2	AB	130	THR	2.5
7	BG	98	ALA	2.5
16	BP	81	ALA	2.5
22	C1	23	THR	2.5
27	C0	8	THR	2.5
33	CE	94	GLN	2.5
38	CK	4	PHE	2.5
38	CK	70	THR	2.5
1	AA	1239	A	2.5
1	AA	1287	A	2.5
1	BA	1110	A	2.5
1	BA	1150	A	2.5
13	BM	87	ARG	2.5
19	BS	3	ARG	2.5
31	CA	196	A	2.5
31	CA	454	A	2.5

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Mol	Chain	Res	Type	RSRZ
31	CA	1626	A	2.5
31	CA	1808	A	2.5
31	CA	2019	A	2.5
31	CA	2171	A	2.5
36	DH	97	ARG	2.5
48	CU	6	ARG	2.5
55	DA	142	A	2.5
29	CC	143	ASN	2.5
50	CW	14	LYS	2.5
52	CY	32	ASN	2.5
53	CZ	27	ASN	2.5
54	DI	88	HIS	2.5
34	DF	56	ASP	2.5
53	DZ	49	ASP	2.5
9	AI	63	LEU	2.5
22	C1	39	LEU	2.5
46	CS	25	LEU	2.5
54	DI	3	LEU	2.5
5	BE	119	GLY	2.5
10	AJ	33	GLY	2.5
10	AJ	100	ILE	2.5
19	AS	35	SER	2.5
22	C1	11	SER	2.5
38	CK	8	PRO	2.5
41	CN	69	PRO	2.5
31	CA	72	U	2.5
31	CA	99	U	2.5
31	CA	434	U	2.5
31	CA	566	U	2.5
31	CA	827	U	2.5
31	CA	2034	U	2.5
36	CH	24	GLY	2.5
37	DJ	86	ILE	2.5
39	CL	43	ILE	2.5
47	CT	35	ILE	2.5
7	BG	32	VAL	2.5
7	BG	87	VAL	2.5
8	AH	110	VAL	2.5
29	CC	120	VAL	2.5
53	CZ	46	VAL	2.5
54	DI	12	VAL	2.5
2	BB	96	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
8	BH	86	TYR	2.5
32	DD	99	GLU	2.5
35	CG	58	TYR	2.5
40	CM	10	GLU	2.5
44	CQ	74	PHE	2.5
2	BB	120	GLN	2.5
2	BB	139	ARG	2.5
8	AH	76	GLN	2.5
15	BO	28	GLN	2.5
1	AA	207	C	2.5
1	BA	334	C	2.5
1	BA	1218	C	2.5
1	BA	1281	C	2.5
7	BG	72	THR	2.5
11	AK	111	THR	2.5
14	BN	50	THR	2.5
16	BP	3	THR	2.5
34	CF	54	ALA	2.5
35	CG	46	ALA	2.5
37	DJ	77	ALA	2.5
38	CK	50	THR	2.5
39	CL	104	THR	2.5
45	CR	12	ALA	2.5
45	CR	21	ALA	2.5
31	CA	316	C	2.5
31	CA	318	C	2.5
31	CA	687	C	2.5
31	CA	740	C	2.5
31	CA	1306	C	2.5
31	CA	1605	C	2.5
31	CA	2699	C	2.5
31	CA	2712	C	2.5
43	CP	17	LYS	2.5
46	CS	48	LYS	2.5
52	CY	77	LYS	2.5
55	DA	885	C	2.5
1	AA	1353	G	2.5
1	BA	57	G	2.5
1	BA	191	G	2.5
1	BA	259	G	2.5
1	BA	1050	G	2.5
1	BA	1064	G	2.5

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Mol	Chain	Res	Type	RSRZ
1	BA	1353	G	2.5
31	CA	338	G	2.5
31	CA	690	G	2.5
31	CA	759	G	2.5
31	CA	1197	G	2.5
31	CA	1337	G	2.5
31	CA	1875	G	2.5
31	CA	2012	G	2.5
31	CA	2276	G	2.5
55	DA	1059	G	2.5
55	DA	1074	G	2.5
55	DA	2140	G	2.5
1	BA	630	A	2.5
1	BA	1145	A	2.5
3	AC	176	HIS	2.5
31	CA	279	A	2.5
31	CA	447	A	2.5
31	CA	911	A	2.5
31	CA	1008	A	2.5
31	CA	1287	A	2.5
31	CA	1525	A	2.5
31	CA	2274	A	2.5
31	CA	2411	A	2.5
31	CA	2530	A	2.5
31	CA	2887	A	2.5
40	CM	93	ASN	2.5
55	DA	1722	A	2.5
9	BI	54	LEU	2.4
20	AT	28	MET	2.4
29	CC	146	MET	2.4
10	AJ	25	ILE	2.4
14	BN	52	PRO	2.4
26	D5	26	ILE	2.4
34	CF	34	ILE	2.4
43	CP	8	ILE	2.4
44	CQ	5	ILE	2.4
52	CY	12	PRO	2.4
3	BC	154	SER	2.4
4	BD	153	SER	2.4
7	BG	94	VAL	2.4
19	AS	67	VAL	2.4
33	CE	64	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
29	CC	272	SER	2.4
1	BA	268	U	2.4
1	BA	989	U	2.4
31	CA	276	U	2.4
31	CA	1624	U	2.4
31	CA	1864	U	2.4
31	CA	2244	U	2.4
7	AG	10	ARG	2.4
12	BL	9	ARG	2.4
23	C2	51	GLU	2.4
24	C3	34	ARG	2.4
30	CD	124	ARG	2.4
39	CL	112	PHE	2.4
9	BI	13	LYS	2.4
13	AM	13	LYS	2.4
13	AM	31	LYS	2.4
14	BN	20	TYR	2.4
16	BP	82	ALA	2.4
30	CD	159	LYS	2.4
33	CE	128	ALA	2.4
36	CH	89	LYS	2.4
36	DH	10	ALA	2.4
42	CO	61	ALA	2.4
47	CT	64	ALA	2.4
7	BG	38	THR	2.4
12	BL	58	THR	2.4
13	AM	102	THR	2.4
42	CO	70	THR	2.4
1	AA	1317	C	2.4
1	BA	1120	C	2.4
31	CA	398	C	2.4
31	CA	418	C	2.4
31	CA	516	C	2.4
31	CA	946	C	2.4
31	CA	1295	C	2.4
31	CA	1357	C	2.4
31	CA	2006	C	2.4
31	CA	2232	C	2.4
55	DA	2161	C	2.4
29	CC	90	ASN	2.4
5	AE	115	LEU	2.4
7	AG	66	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
9	BI	118	LEU	2.4
33	CE	180	LEU	2.4
31	CA	382	A	2.4
31	CA	609	A	2.4
31	CA	781	A	2.4
31	CA	1354	A	2.4
31	CA	1395	A	2.4
31	CA	1597	A	2.4
55	DA	1073	A	2.4
1	AA	86	G	2.4
1	BA	378	G	2.4
7	BG	2	PRO	2.4
8	BH	90	ASP	2.4
31	CA	214	G	2.4
31	CA	400	G	2.4
31	CA	771	G	2.4
31	CA	1225	G	2.4
31	CA	2216	G	2.4
40	CM	62	PRO	2.4
45	CR	98	ILE	2.4
48	DU	2	ILE	2.4
4	AD	25	VAL	2.4
7	AG	69	VAL	2.4
9	AI	40	GLY	2.4
10	AJ	36	VAL	2.4
13	BM	97	VAL	2.4
14	BN	34	VAL	2.4
16	BP	19	VAL	2.4
33	CE	187	VAL	2.4
47	CT	106	VAL	2.4
4	AD	73	ARG	2.4
9	AI	14	SER	2.4
14	BN	69	ARG	2.4
29	CC	38	SER	2.4
39	CL	117	SER	2.4
1	BA	173	U	2.4
1	BA	1240	U	2.4
3	BC	167	TRP	2.4
16	BP	39	PHE	2.4
19	AS	7	LYS	2.4
31	CA	102	U	2.4
31	CA	870	U	2.4

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Mol	Chain	Res	Type	RSRZ
31	CA	932	U	2.4
31	CA	1258	U	2.4
31	CA	1466	U	2.4
31	CA	1621	U	2.4
31	CA	1648	U	2.4
43	CP	97	PHE	2.4
15	AO	9	ALA	2.4
35	CG	150	ALA	2.4
52	CY	73	ALA	2.4
54	DI	44	ALA	2.4
14	AN	50	THR	2.4
27	C0	4	THR	2.4
29	CC	15	HIS	2.4
3	AC	178	LEU	2.4
14	AN	74	LEU	2.4
14	BN	51	LEU	2.4
48	CU	50	LEU	2.4
52	CY	23	ASN	2.4
10	BJ	53	ILE	2.4
10	BJ	79	PRO	2.4
13	BM	77	ILE	2.4
14	BN	82	ILE	2.4
37	DJ	74	PRO	2.4
38	CK	142	ILE	2.4
46	CS	52	PRO	2.4
47	CT	4	ILE	2.4
1	AA	995	C	2.4
1	BA	95	C	2.4
1	BA	176	C	2.4
1	BA	934	C	2.4
31	CA	485	C	2.4
31	CA	2072	C	2.4
31	CA	2620	C	2.4
39	CL	84	CYS	2.4
2	AB	221	VAL	2.4
5	AE	136	VAL	2.4
7	AG	6	VAL	2.4
17	AQ	83	VAL	2.4
25	C4	21	GLY	2.4
27	C0	46	GLY	2.4
30	CD	189	VAL	2.4
36	DH	16	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
37	DJ	25	GLY	2.4
1	BA	607	A	2.4
1	BA	1274	A	2.4
1	BA	1363	A	2.4
31	CA	428	A	2.4
31	CA	1365	A	2.4
31	CA	1773	A	2.4
31	CA	2392	A	2.4
2	AB	143	LYS	2.4
13	AM	103	LYS	2.4
15	AO	89	ARG	2.4
24	C3	28	ARG	2.4
34	CF	30	ARG	2.4
45	CR	53	ARG	2.4
47	CT	95	ARG	2.4
53	DZ	2	LYS	2.4
1	AA	200	G	2.4
1	AA	203	G	2.4
1	AA	1026	G	2.4
1	BA	68	G	2.4
1	BA	168	G	2.4
1	BA	391	G	2.4
1	BA	1253	G	2.4
10	BJ	49	PHE	2.4
31	CA	45	G	2.4
31	CA	107	G	2.4
31	CA	263	G	2.4
31	CA	969	G	2.4
31	CA	1628	G	2.4
31	CA	1863	G	2.4
47	CT	30	SER	2.4
49	CV	98	SER	2.4
55	DA	1068	G	2.4
14	AN	29	ALA	2.4
20	AT	62	ALA	2.4
22	C1	56	ALA	2.4
1	AA	1307	U	2.4
31	CA	511	U	2.4
31	CA	562	U	2.4
31	CA	2092	U	2.4
31	CA	2419	U	2.4
31	CA	2438	U	2.4

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Mol	Chain	Res	Type	RSRZ
31	CA	2695	U	2.4
18	BR	70	TYR	2.4
29	CC	62	TYR	2.4
34	CF	35	THR	2.4
48	CU	39	THR	2.4
15	AO	51	HIS	2.4
25	C4	26	HIS	2.4
48	CU	15	HIS	2.4
8	BH	59	LEU	2.4
19	AS	5	LEU	2.4
23	C2	11	LEU	2.4
39	CL	8	LEU	2.4
23	C2	9	ILE	2.4
37	CJ	35	ILE	2.4
43	CP	35	ILE	2.4
13	AM	8	ASN	2.4
33	CE	24	ASN	2.4
39	CL	102	PRO	2.4
44	CQ	66	ASN	2.4
5	AE	21	VAL	2.4
13	BM	43	VAL	2.4
7	AG	78	ARG	2.4
9	BI	122	ARG	2.4
9	BI	130	ARG	2.4
13	BM	44	LYS	2.4
13	BM	85	CYS	2.4
20	BT	8	LYS	2.4
25	D4	18	GLY	2.4
33	CE	146	VAL	2.4
36	DH	3	VAL	2.4
46	CS	54	VAL	2.4
52	CY	7	VAL	2.4
29	CC	43	ARG	2.4
29	CC	256	LYS	2.4
30	CD	83	ARG	2.4
30	CD	105	LYS	2.4
42	CO	63	ARG	2.4
45	CR	84	LYS	2.4
45	CR	114	LYS	2.4
48	CU	68	LYS	2.4
52	CY	57	ARG	2.4
1	BA	67	C	2.4

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Mol	Chain	Res	Type	RSRZ
1	BA	308	C	2.4
1	BA	995	C	2.4
31	CA	1399	C	2.4
31	CA	1752	C	2.4
31	CA	1760	C	2.4
31	CA	2874	C	2.4
1	AA	263	A	2.4
1	AA	1092	A	2.4
1	BA	1021	A	2.4
15	AO	43	PHE	2.4
17	BQ	37	PHE	2.4
28	CB	99	A	2.4
31	CA	255	A	2.4
31	CA	685	A	2.4
31	CA	689	A	2.4
31	CA	783	A	2.4
31	CA	802	A	2.4
31	CA	1254	A	2.4
31	CA	1453	A	2.4
31	CA	1655	A	2.4
31	CA	2060	A	2.4
31	CA	2062	A	2.4
31	CA	2765	A	2.4
49	CV	95	PHE	2.4
34	CF	32	GLU	2.4
46	CS	37	GLU	2.4
55	DA	1080	A	2.4
12	BL	26	ALA	2.4
13	AM	18	ALA	2.4
16	BP	11	ALA	2.4
33	CE	68	ALA	2.4
33	CE	160	ALA	2.4
37	CJ	114	ALA	2.4
47	CT	54	ALA	2.4
53	CZ	33	ALA	2.4
10	BJ	99	GLN	2.4
13	AM	100	GLN	2.4
30	CD	145	SER	2.4
35	CG	143	GLN	2.4
36	DH	82	SER	2.4
19	BS	34	TRP	2.4
45	CR	61	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	BA	252	U	2.4
1	BA	610	U	2.4
1	BA	941	G	2.4
1	BA	1312	G	2.4
1	BA	1439	G	2.4
2	BB	213	TYR	2.4
5	BE	24	THR	2.4
31	CA	506	G	2.4
31	CA	533	G	2.4
31	CA	598	U	2.4
31	CA	674	G	2.4
31	CA	1124	G	2.4
31	CA	1203	U	2.4
31	CA	1661	G	2.4
31	CA	2526	G	2.4
31	CA	2722	G	2.4
31	CA	2742	G	2.4
31	CA	2838	G	2.4
31	CA	2884	U	2.4
34	CF	26	MET	2.4
39	CL	1	MET	2.4
39	CL	65	THR	2.4
55	DA	2107	G	2.4
55	DA	2423	U	2.4
2	BB	97	LEU	2.4
7	BG	13	LEU	2.4
44	CQ	100	LEU	2.4
2	BB	164	ILE	2.4
9	BI	65	ILE	2.4
17	BQ	55	ILE	2.4
46	CS	101	ILE	2.4
7	BG	16	PRO	2.4
37	DJ	20	PRO	2.4
49	DV	48	PRO	2.4
2	AB	178	ASN	2.3
4	AD	121	LYS	2.3
7	BG	89	VAL	2.3
14	AN	11	VAL	2.3
20	BT	34	LYS	2.3
27	C0	19	LYS	2.3
29	CC	59	LYS	2.3
35	CG	15	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
36	CH	21	VAL	2.3
37	DJ	57	VAL	2.3
49	CV	4	LYS	2.3
49	CV	11	VAL	2.3
54	DI	85	VAL	2.3
16	BP	37	GLY	2.3
7	BG	151	PHE	2.3
17	BQ	64	CYS	2.3
19	AS	10	PHE	2.3
48	CU	37	ASP	2.3
7	BG	150	ALA	2.3
12	AL	70	GLU	2.3
20	BT	17	ALA	2.3
27	D0	39	GLU	2.3
38	CK	98	GLU	2.3
40	DM	75	ALA	2.3
44	CQ	34	GLU	2.3
48	CU	18	GLU	2.3
50	CW	6	ALA	2.3
1	BA	193	C	2.3
1	BA	233	C	2.3
4	AD	40	GLN	2.3
31	CA	109	C	2.3
31	CA	302	C	2.3
31	CA	812	C	2.3
31	CA	865	C	2.3
31	CA	1229	C	2.3
31	CA	1447	C	2.3
31	CA	2527	C	2.3
31	CA	2755	C	2.3
31	CA	2830	C	2.3
1	AA	1289	A	2.3
1	BA	71	A	2.3
1	BA	889	A	2.3
1	BA	1377	A	2.3
19	AS	66	MET	2.3
31	CA	477	A	2.3
31	CA	614	A	2.3
31	CA	1027	A	2.3
31	CA	1301	A	2.3
31	CA	1496	A	2.3
31	CA	2814	A	2.3

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Mol	Chain	Res	Type	RSRZ
35	CG	62	TRP	2.3
55	DA	144	A	2.3
9	BI	87	LEU	2.3
11	AK	22	HIS	2.3
13	AM	14	HIS	2.3
14	AN	27	LEU	2.3
19	AS	77	THR	2.3
20	BT	80	THR	2.3
29	CC	83	TYR	2.3
30	CD	79	LEU	2.3
34	CF	117	LEU	2.3
36	DH	75	LEU	2.3
39	CL	86	LEU	2.3
40	CM	95	LEU	2.3
48	CU	84	TYR	2.3
53	CZ	56	LEU	2.3
1	BA	981	U	2.3
31	CA	50	U	2.3
31	CA	1963	U	2.3
55	DA	1105	U	2.3
55	DA	2130	U	2.3
55	DA	2151	U	2.3
55	DA	2796	U	2.3
13	BM	7	ILE	2.3
38	CK	54	ILE	2.3
47	CT	55	ILE	2.3
19	BS	30	PRO	2.3
35	CG	112	PRO	2.3
1	AA	1222	G	2.3
1	BA	293	G	2.3
1	BA	351	G	2.3
1	BA	953	G	2.3
1	BA	973	G	2.3
8	AH	39	VAL	2.3
31	CA	81	G	2.3
31	CA	630	G	2.3
31	CA	1862	G	2.3
31	CA	2120	G	2.3
31	CA	2190	G	2.3
31	CA	2625	G	2.3
31	CA	2894	G	2.3
48	CU	53	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	AB	98	GLY	2.3
7	AG	81	GLY	2.3
29	CC	73	GLY	2.3
29	CC	119	GLY	2.3
30	CD	78	GLY	2.3
30	CD	147	GLY	2.3
35	CG	78	GLY	2.3
37	DJ	52	GLY	2.3
40	CM	43	GLY	2.3
2	AB	69	PHE	2.3
16	BP	38	PHE	2.3
36	CH	47	PHE	2.3
46	CS	53	PHE	2.3
36	DH	87	GLU	2.3
44	CQ	44	GLU	2.3
45	DR	49	ASP	2.3
3	BC	71	ALA	2.3
8	AH	130	ALA	2.3
13	BM	2	ALA	2.3
29	CC	6	CYS	2.3
45	CR	42	ALA	2.3
49	CV	71	ALA	2.3
2	AB	49	MET	2.3
23	D2	45	GLN	2.3
30	CD	161	MET	2.3
4	AD	119	SER	2.3
9	BI	61	LEU	2.3
9	BI	98	LEU	2.3
12	BL	7	LEU	2.3
13	BM	48	LEU	2.3
19	AS	15	LEU	2.3
24	C3	15	SER	2.3
44	CQ	114	LEU	2.3
54	DI	117	LEU	2.3
17	BQ	45	HIS	2.3
1	BA	55	A	2.3
1	BA	1067	A	2.3
8	AH	85	ILE	2.3
17	BQ	25	ILE	2.3
19	BS	79	THR	2.3
23	C2	29	THR	2.3
30	CD	52	THR	2.3

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Mol	Chain	Res	Type	RSRZ
31	CA	145	C	2.3
31	CA	357	C	2.3
31	CA	486	C	2.3
31	CA	531	C	2.3
31	CA	1370	C	2.3
31	CA	2896	C	2.3
36	DH	125	THR	2.3
49	CV	15	THR	2.3
55	DA	1493	C	2.3
31	CA	84	A	2.3
31	CA	507	A	2.3
31	CA	661	A	2.3
31	CA	849	A	2.3
31	CA	1427	A	2.3
55	DA	2887[A]	A	2.3
14	AN	23	LYS	2.3
14	BN	3	LYS	2.3
23	C2	33	LYS	2.3
48	CU	82	LYS	2.3
1	BA	467	U	2.3
12	AL	9	ARG	2.3
14	BN	63	ARG	2.3
20	BT	56	PRO	2.3
29	CC	13	ARG	2.3
31	CA	1249	U	2.3
45	CR	50	ARG	2.3
55	DA	139	U	2.3
30	CD	63	PRO	2.3
2	AB	217	VAL	2.3
2	BB	107	VAL	2.3
9	AI	111	VAL	2.3
9	AI	116	VAL	2.3
24	C3	44	VAL	2.3
30	CD	73	VAL	2.3
41	CN	101	VAL	2.3
54	DI	27	VAL	2.3
33	DE	20	GLY	2.3
42	CO	101	GLY	2.3
49	CV	69	ASN	2.3
9	BI	103	PHE	2.3
35	CG	83	PHE	2.3
41	CN	117	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	BA	107	G	2.3
1	BA	251	G	2.3
1	BA	1139	G	2.3
5	AE	162	GLU	2.3
7	AG	106	GLU	2.3
15	BO	26	GLU	2.3
19	AS	22	ALA	2.3
24	C3	40	ALA	2.3
31	CA	168	G	2.3
31	CA	295	G	2.3
31	CA	682	G	2.3
31	CA	695	G	2.3
31	CA	809	G	2.3
31	CA	1232	G	2.3
31	CA	1355	G	2.3
31	CA	1524	G	2.3
31	CA	1718	G	2.3
31	CA	1814	G	2.3
31	CA	2121	G	2.3
31	CA	2237	G	2.3
31	CA	2633	G	2.3
31	CA	2782	G	2.3
31	CA	2828	G	2.3
36	DH	137	GLU	2.3
30	CD	43	ASP	2.3
2	BB	89	GLN	2.3
2	BB	135	LEU	2.3
3	BC	144	LEU	2.3
10	BJ	90	LEU	2.3
15	AO	57	LEU	2.3
15	BO	31	LEU	2.3
33	CE	3	LEU	2.3
48	DU	93	LEU	2.3
7	BG	104	ILE	2.3
7	BG	110	LYS	2.3
8	BH	14	ILE	2.3
14	AN	32	SER	2.3
15	AO	11	ILE	2.3
22	C1	37	LYS	2.3
25	C4	16	LYS	2.3
26	C5	28	SER	2.3
29	CC	39	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
37	DJ	101	ILE	2.3
38	CK	15	TRP	2.3
38	CK	101	ILE	2.3
42	CO	99	LYS	2.3
46	CS	92	TRP	2.3
14	BN	53	ARG	2.3
15	BO	72	ARG	2.3
34	CF	8	TYR	2.3
46	CS	13	ARG	2.3
47	CT	25	ARG	2.3
49	CV	82	ARG	2.3
52	CY	3	ARG	2.3
1	AA	210	C	2.3
1	AA	949	A	2.3
1	BA	1208	C	2.3
1	BA	1306	A	2.3
1	BA	1317	C	2.3
26	C5	25	VAL	2.3
28	CB	97	C	2.3
30	CD	170	VAL	2.3
1	BA	1354	U	2.3
1	BA	1368	A	2.3
2	BB	70	VAL	2.3
7	AG	43	VAL	2.3
7	BG	75	VAL	2.3
10	AJ	98	VAL	2.3
10	BJ	77	VAL	2.3
31	CA	4	U	2.3
31	CA	113	U	2.3
31	CA	216	A	2.3
31	CA	624	C	2.3
31	CA	821	A	2.3
31	CA	1493	C	2.3
31	CA	2091	C	2.3
31	CA	2726	A	2.3
31	CA	2860	A	2.3
31	CA	2870	C	2.3
40	CM	120	VAL	2.3
31	CA	1083	U	2.3
31	CA	1255	U	2.3
31	CA	1467	U	2.3
31	CA	1513	U	2.3

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Mol	Chain	Res	Type	RSRZ
31	CA	2265	U	2.3
55	DA	276	U	2.3
29	CC	169	GLY	2.3
37	DJ	119	GLY	2.3
14	BN	21	PHE	2.3
36	DH	47	PHE	2.3
54	DI	76	PHE	2.3
2	AB	75	ALA	2.3
17	BQ	82	ALA	2.3
20	BT	47	ALA	2.3
30	CD	168	GLU	2.3
45	CR	2	ALA	2.3
10	BJ	64	GLN	2.3
19	BS	5	LEU	2.3
48	CU	11	LEU	2.3
48	CU	48	GLN	2.3
49	CV	18	ASP	2.3
12	BL	88	LYS	2.3
24	C3	37	LYS	2.3
30	CD	190	LYS	2.3
44	CQ	37	LYS	2.3
49	CV	97	LYS	2.3
1	AA	76	G	2.3
1	AA	1241	G	2.3
1	BA	148	G	2.3
1	BA	177	G	2.3
1	BA	200	G	2.3
2	AB	164	ILE	2.3
10	BJ	6	ILE	2.3
13	AM	45	ILE	2.3
27	C0	14	ILE	2.3
31	CA	85	G	2.3
31	CA	194	G	2.3
31	CA	205	G	2.3
31	CA	468	G	2.3
31	CA	954	G	2.3
31	CA	1099	G	2.3
31	CA	2391	G	2.3
31	CA	2454	G	2.3
31	CA	2686	G	2.3
35	CG	115	HIS	2.3
38	DK	80	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
39	CL	99	ILE	2.3
55	DA	883	G	2.3
13	AM	113	ARG	2.3
14	AN	58	SER	2.3
14	AN	59	ARG	2.3
17	BQ	72	SER	2.3
19	BS	37	ARG	2.3
24	C3	33	ARG	2.3
27	C0	11	ARG	2.3
29	CC	257	THR	2.3
33	CE	150	THR	2.3
39	CL	105	ARG	2.3
47	CT	8	ARG	2.3
48	CU	78	SER	2.3
3	BC	5	VAL	2.3
8	AH	95	VAL	2.3
12	BL	8	VAL	2.3
13	AM	64	VAL	2.3
13	BM	65	VAL	2.3
19	BS	23	VAL	2.3
23	D2	43	VAL	2.3
30	CD	194	PRO	2.3
34	CF	40	VAL	2.3
39	CL	103	VAL	2.3
48	CU	63	VAL	2.3
10	AJ	95	GLY	2.3
11	BK	88	GLY	2.3
37	CJ	99	GLY	2.3
41	CN	15	GLY	2.3
1	AA	1125	U	2.3
1	BA	154	U	2.3
1	BA	1023	U	2.3
31	CA	395	U	2.3
31	CA	1391	U	2.3
31	CA	2016	U	2.3
55	DA	1081	U	2.3
1	AA	964	A	2.2
1	AA	1302	C	2.2
1	BA	60	A	2.2
1	BA	205	A	2.2
1	BA	372	C	2.2
1	BA	1411	C	2.2

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Mol	Chain	Res	Type	RSRZ
1	BA	1448	C	2.2
2	AB	162	PHE	2.2
11	AK	27	PHE	2.2
31	CA	79	C	2.2
31	CA	294	A	2.2
31	CA	374	A	2.2
31	CA	972	A	2.2
31	CA	988	A	2.2
31	CA	1603	A	2.2
31	CA	1625	C	2.2
31	CA	2031	A	2.2
31	CA	2082	A	2.2
33	CE	158	PHE	2.2
49	CV	96	PHE	2.2
3	BC	99	ALA	2.2
12	AL	62	GLU	2.2
27	D0	50	ALA	2.2
29	CC	89	ALA	2.2
30	CD	196	ALA	2.2
30	CD	209	ALA	2.2
36	CH	11	ASN	2.2
43	CP	26	LEU	2.2
43	CP	106	LEU	2.2
4	AD	148	LYS	2.2
4	BD	206	LYS	2.2
25	C4	54	ASP	2.2
50	CW	90	ASP	2.2
3	BC	75	ILE	2.2
13	BM	73	ILE	2.2
35	CG	77	ILE	2.2
36	DH	80	ILE	2.2
46	CS	74	ILE	2.2
50	CW	30	ILE	2.2
2	BB	108	ARG	2.2
4	BD	44	ARG	2.2
11	BK	13	ARG	2.2
25	C4	24	HIS	2.2
38	CK	80	HIS	2.2
45	CR	51	ARG	2.2
47	CT	88	ARG	2.2
52	CY	11	ARG	2.2
13	AM	85	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	BC	165	THR	2.2
12	AL	3	THR	2.2
14	AN	42	TRP	2.2
2	BB	210	VAL	2.2
5	AE	74	VAL	2.2
7	AG	41	SER	2.2
9	AI	19	VAL	2.2
9	BI	96	SER	2.2
10	BJ	55	PRO	2.2
8	BH	128	TYR	2.2
24	C3	8	SER	2.2
35	CG	74	SER	2.2
37	CJ	75	PRO	2.2
38	CK	65	THR	2.2
37	DJ	140	VAL	2.2
38	CK	56	VAL	2.2
44	CQ	46	VAL	2.2
48	CU	57	VAL	2.2
52	CY	78	TYR	2.2
1	AA	1050	G	2.2
1	AA	1260	G	2.2
1	BA	220	G	2.2
1	BA	1142	G	2.2
1	BA	1438	G	2.2
31	CA	17	G	2.2
31	CA	39	G	2.2
31	CA	551	G	2.2
31	CA	559	G	2.2
31	CA	622	G	2.2
31	CA	681	G	2.2
31	CA	775	G	2.2
31	CA	938	G	2.2
31	CA	997	G	2.2
31	CA	1245	G	2.2
31	CA	1256	G	2.2
31	CA	2087	G	2.2
31	CA	2277	G	2.2
31	CA	2429	G	2.2
31	CA	2523	G	2.2
31	CA	2831	G	2.2
31	CA	2848	G	2.2
55	DA	2116	G	2.2

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Mol	Chain	Res	Type	RSRZ
3	AC	2	GLY	2.2
5	BE	109	GLY	2.2
7	BG	34	GLY	2.2
11	AK	90	GLY	2.2
14	BN	68	GLY	2.2
14	BN	78	GLY	2.2
39	CL	27	GLY	2.2
46	CS	8	GLY	2.2
3	AC	29	PHE	2.2
6	AF	90	MET	2.2
11	AK	85	MET	2.2
30	CD	82	PHE	2.2
43	CP	117	PHE	2.2
1	AA	1286	U	2.2
1	BA	1065	U	2.2
1	BA	1121	U	2.2
31	CA	321	U	2.2
31	CA	397	U	2.2
31	CA	459	U	2.2
31	CA	499	U	2.2
31	CA	567	U	2.2
31	CA	1113	U	2.2
31	CA	1180	U	2.2
31	CA	1856	U	2.2
31	CA	2348	U	2.2
55	DA	2109	U	2.2
11	BK	102	ALA	2.2
14	AN	8	ALA	2.2
14	BN	2	ALA	2.2
33	CE	86	ALA	2.2
44	CQ	91	ALA	2.2
1	BA	977	A	2.2
1	BA	1249	C	2.2
1	BA	1375	A	2.2
2	AB	10	LEU	2.2
1	AA	1172	C	2.2
1	BA	132	C	2.2
1	BA	290	C	2.2
17	BQ	43	LYS	2.2
17	BQ	44	LEU	2.2
17	BQ	67	LEU	2.2
19	BS	47	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	1007	C	2.2
31	CA	1175	A	2.2
31	CA	1302	A	2.2
36	CH	75	LEU	2.2
36	DH	15	LEU	2.2
51	CX	32	LEU	2.2
28	CB	30	C	2.2
28	CB	62	C	2.2
31	CA	210	C	2.2
31	CA	249	C	2.2
31	CA	337	C	2.2
31	CA	2359	C	2.2
31	CA	2507	C	2.2
11	BK	97	ILE	2.2
14	BN	30	ILE	2.2
18	AR	21	ILE	2.2
50	CW	29	ILE	2.2
2	BB	21	ARG	2.2
3	AC	127	ARG	2.2
5	BE	112	ARG	2.2
13	BM	109	ARG	2.2
18	AR	43	ARG	2.2
18	AR	74	HIS	2.2
24	C3	39	ARG	2.2
49	CV	6	ARG	2.2
49	CV	22	ARG	2.2
54	DI	61	ARG	2.2
2	AB	210	VAL	2.2
2	BB	20	THR	2.2
12	AL	4	VAL	2.2
22	C1	44	THR	2.2
29	CC	17	VAL	2.2
29	CC	29	PRO	2.2
30	CD	172	VAL	2.2
30	CD	197	THR	2.2
33	CE	126	VAL	2.2
33	CE	186	VAL	2.2
34	CF	157	THR	2.2
36	CH	31	VAL	2.2
36	CH	110	VAL	2.2
48	CU	67	VAL	2.2
49	CV	34	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
54	DI	77	VAL	2.2
13	BM	74	SER	2.2
3	BC	159	GLY	2.2
5	AE	91	GLY	2.2
9	BI	69	GLY	2.2
37	CJ	25	GLY	2.2
44	CQ	23	GLY	2.2
5	AE	96	MET	2.2
30	CD	68	PHE	2.2
2	AB	128	LYS	2.2
2	BB	174	LYS	2.2
1	BA	61	G	2.2
1	BA	230	G	2.2
1	BA	890	G	2.2
2	AB	169	GLU	2.2
2	BB	134	ALA	2.2
9	BI	112	GLU	2.2
13	AM	48	LEU	2.2
14	AN	26	GLU	2.2
14	BN	48	LEU	2.2
16	BP	43	ALA	2.2
26	C5	5	ALA	2.2
31	CA	628	G	2.2
31	CA	638	G	2.2
31	CA	757	G	2.2
31	CA	1139	G	2.2
31	CA	1538	G	2.2
31	CA	2140	G	2.2
31	CA	2621	G	2.2
33	CE	112	LEU	2.2
36	DH	64	ALA	2.2
37	DJ	15	ALA	2.2
38	CK	63	ALA	2.2
39	CL	16	ALA	2.2
40	DM	92	LEU	2.2
43	CP	63	LYS	2.2
31	CA	187	G	2.2
42	DO	123	GLU	2.2
47	CT	89	ALA	2.2
54	DI	100	ALA	2.2
31	CA	596	U	2.2
55	DA	1058	U	2.2

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Mol	Chain	Res	Type	RSRZ
55	DA	1963	U	2.2
55	DA	2137	U	2.2
14	AN	43	ASN	2.2
29	CC	45	ASN	2.2
2	BB	173	ILE	2.2
4	BD	40	GLN	2.2
5	AE	93	ARG	2.2
5	BE	72	ILE	2.2
9	BI	32	GLN	2.2
12	BL	12	ARG	2.2
16	BP	63	GLN	2.2
17	BQ	5	ILE	2.2
40	CM	2	ARG	2.2
40	CM	111	ILE	2.2
42	CO	45	ARG	2.2
44	CQ	64	ILE	2.2
45	CR	80	ILE	2.2
53	CZ	31	GLN	2.2
53	CZ	48	ARG	2.2
1	BA	702	A	2.2
1	AA	396	C	2.2
1	AA	754	C	2.2
1	BA	932	C	2.2
30	CD	140	HIS	2.2
31	CA	13	A	2.2
31	CA	56	A	2.2
31	CA	226	A	2.2
31	CA	309	A	2.2
31	CA	404	A	2.2
31	CA	429	A	2.2
31	CA	430	A	2.2
31	CA	632	A	2.2
31	CA	633	A	2.2
31	CA	1937	A	2.2
31	CA	2266	A	2.2
31	CA	2835	A	2.2
31	CA	314	C	2.2
31	CA	772	C	2.2
31	CA	817	C	2.2
31	CA	838	C	2.2
31	CA	915	C	2.2
31	CA	1005	C	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	1291	C	2.2
31	CA	1499	C	2.2
31	CA	1881	C	2.2
31	CA	2145	C	2.2
31	CA	2275	C	2.2
31	CA	2573	C	2.2
31	CA	2710	C	2.2
39	DL	29	HIS	2.2
47	CT	60	HIS	2.2
55	DA	1052	C	2.2
55	DA	2164	C	2.2
49	CV	81	ASP	2.2
2	AB	4	VAL	2.2
5	BE	25	VAL	2.2
9	AI	55	VAL	2.2
12	BL	98	VAL	2.2
17	BQ	22	VAL	2.2
17	BQ	32	PRO	2.2
20	BT	35	VAL	2.2
29	CC	204	VAL	2.2
33	CE	48	THR	2.2
41	CN	74	THR	2.2
47	CT	3	THR	2.2
39	CL	21	CYS	2.2
7	BG	44	TYR	2.2
9	BI	40	GLY	2.2
17	BQ	14	SER	2.2
18	AR	23	TYR	2.2
21	AU	38	TYR	2.2
37	DJ	89	GLY	2.2
37	DJ	125	MET	2.2
46	CS	69	GLY	2.2
53	CZ	10	SER	2.2
6	BF	93	LYS	2.2
7	BG	35	LYS	2.2
12	BL	116	LYS	2.2
20	BT	31	PHE	2.2
34	CF	138	PHE	2.2
39	CL	44	LYS	2.2
45	CR	101	PHE	2.2
13	BM	80	LEU	2.2
35	CG	107	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	AB	140	GLU	2.2
2	BB	145	GLU	2.2
3	BC	161	GLU	2.2
4	AD	122	ALA	2.2
13	BM	41	GLU	2.2
14	BN	15	ALA	2.2
14	BN	99	ALA	2.2
15	BO	19	ALA	2.2
30	CD	64	GLU	2.2
34	CF	55	ALA	2.2
37	CJ	27	ALA	2.2
37	CJ	83	ALA	2.2
37	DJ	115	ALA	2.2
38	CK	43	GLU	2.2
48	CU	4	GLU	2.2
18	BR	21	ILE	2.2
23	C2	5	ILE	2.2
38	CK	95	ARG	2.2
39	CL	31	ARG	2.2
40	CM	47	ARG	2.2
40	DM	105	ILE	2.2
1	AA	218	U	2.2
1	BA	1420	U	2.2
14	BN	62	ASN	2.2
31	CA	999	U	2.2
55	DA	1173	U	2.2
55	DA	1174	U	2.2
1	AA	1371	G	2.2
1	BA	46	G	2.2
31	CA	175	G	2.2
31	CA	498	G	2.2
31	CA	760	G	2.2
31	CA	770	G	2.2
31	CA	1227	G	2.2
31	CA	1407	G	2.2
31	CA	1601	G	2.2
31	CA	2083	G	2.2
31	CA	2242	G	2.2
31	CA	2708	G	2.2
31	CA	2709	G	2.2
4	AD	129	VAL	2.2
10	AJ	79	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
14	AN	45	VAL	2.2
16	BP	53	ASP	2.2
20	BT	58	VAL	2.2
29	CC	4	VAL	2.2
31	CA	10	A	2.2
31	CA	38	A	2.2
31	CA	1690	A	2.2
31	CA	2632	A	2.2
31	CA	2721	A	2.2
35	CG	8	PRO	2.2
35	CG	113	VAL	2.2
36	DH	9	VAL	2.2
44	CQ	26	VAL	2.2
45	CR	97	ASP	2.2
47	CT	50	VAL	2.2
55	DA	1098	A	2.2
1	BA	979	C	2.2
1	BA	1366	C	2.2
31	CA	269	C	2.2
31	CA	334	C	2.2
31	CA	540	C	2.2
31	CA	611	C	2.2
31	CA	1607	C	2.2
31	CA	1934	C	2.2
55	DA	225	C	2.2
24	D3	4	THR	2.2
3	BC	38	LYS	2.2
5	BE	108	GLY	2.2
25	C4	47	LYS	2.2
25	C4	53	GLY	2.2
30	CD	163	GLY	2.2
34	CF	72	LYS	2.2
45	CR	7	GLY	2.2
48	CU	26	LYS	2.2
49	CV	16	GLY	2.2
50	CW	25	LYS	2.2
50	DW	67	GLY	2.2
8	BH	45	PHE	2.2
42	CO	87	PHE	2.2
42	CO	94	TYR	2.2
7	BG	66	LEU	2.2
8	BH	40	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
15	BO	67	LEU	2.2
20	BT	79	LEU	2.2
22	C1	29	SER	2.2
30	CD	21	SER	2.2
36	CH	15	LEU	2.2
5	AE	110	ALA	2.2
7	AG	61	ALA	2.2
10	AJ	12	ALA	2.2
11	BK	94	GLU	2.2
35	CG	32	GLU	2.2
43	CP	20	GLU	2.2
49	CV	37	GLU	2.2
14	BN	31	ILE	2.1
16	BP	5	ARG	2.1
14	BN	66	GLN	2.1
43	CP	38	GLN	2.1
1	AA	96	U	2.1
1	BA	209	U	2.1
1	BA	218	U	2.1
16	BP	9	HIS	2.1
31	CA	135	U	2.1
31	CA	589	U	2.1
31	CA	1183	U	2.1
31	CA	1956	U	2.1
31	CA	2321	U	2.1
31	CA	2696	U	2.1
39	CL	29	HIS	2.1
39	CL	82	ASN	2.1
50	CW	24	ASN	2.1
5	BE	18	VAL	2.1
7	BG	71	PRO	2.1
8	AH	103	VAL	2.1
11	AK	16	VAL	2.1
12	BL	28	PRO	2.1
21	BU	6	VAL	2.1
30	CD	178	VAL	2.1
35	CG	92	VAL	2.1
38	CK	62	VAL	2.1
49	CV	55	PRO	2.1
29	CC	66	ASP	2.1
37	CJ	96	ASP	2.1
1	AA	1039	G	2.1

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Mol	Chain	Res	Type	RSRZ
1	BA	292	G	2.1
1	BA	1184	G	2.1
1	BA	1233	G	2.1
2	BB	66	LYS	2.1
7	BG	149	LYS	2.1
1	BA	935	A	2.1
1	BA	1285	A	2.1
1	BA	1431	A	2.1
1	BA	1447	A	2.1
2	AB	71	GLY	2.1
12	BL	64	THR	2.1
19	BS	63	THR	2.1
23	D2	53	LYS	2.1
29	CC	26	LYS	2.1
31	CA	74	A	2.1
31	CA	199	A	2.1
31	CA	203	A	2.1
31	CA	212	G	2.1
31	CA	232	G	2.1
31	CA	315	G	2.1
31	CA	319	G	2.1
31	CA	613	A	2.1
31	CA	833	A	2.1
31	CA	1051	G	2.1
31	CA	1246	A	2.1
31	CA	1425	G	2.1
31	CA	1494	A	2.1
31	CA	1828	G	2.1
31	CA	1854	A	2.1
31	CA	2040	G	2.1
36	CH	35	LYS	2.1
36	DH	89	LYS	2.1
31	CA	2071	A	2.1
31	CA	2093	G	2.1
31	CA	2148	G	2.1
31	CA	2434	A	2.1
31	CA	2542	A	2.1
31	CA	2705	A	2.1
31	CA	2729	G	2.1
39	CL	42	THR	2.1
46	CS	10	LYS	2.1
49	CV	91	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	2886	A	2.1
40	CM	28	GLY	2.1
51	CX	34	GLY	2.1
55	DA	1067	A	2.1
55	DA	1086	A	2.1
55	DA	1103	A	2.1
1	AA	215	C	2.1
1	AA	1234	C	2.1
1	BA	1322	C	2.1
1	BA	1533	C	2.1
2	AB	129	LEU	2.1
5	BE	115	LEU	2.1
11	BK	77	TYR	2.1
28	CB	91	C	2.1
31	CA	192	C	2.1
31	CA	560	C	2.1
31	CA	692	C	2.1
31	CA	876	C	2.1
31	CA	944	C	2.1
31	CA	1330	C	2.1
31	CA	1362	C	2.1
31	CA	2521	C	2.1
31	CA	2579	C	2.1
35	CG	50	LEU	2.1
36	CH	29	PHE	2.1
36	DH	6	LEU	2.1
49	CV	73	PHE	2.1
51	CX	79	PHE	2.1
41	CN	103	TYR	2.1
9	AI	15	SER	2.1
13	AM	106	ALA	2.1
16	AP	27	ALA	2.1
16	BP	58	ALA	2.1
20	BT	11	ALA	2.1
37	CJ	63	ALA	2.1
40	DM	72	ALA	2.1
14	BN	81	ARG	2.1
44	CQ	93	ARG	2.1
45	CR	58	ARG	2.1
2	AB	111	ILE	2.1
8	AH	125	ILE	2.1
11	AK	23	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
11	BK	107	ILE	2.1
16	BP	33	ILE	2.1
30	CD	48	ILE	2.1
33	CE	148	ILE	2.1
9	BI	5	GLN	2.1
29	CC	60	GLN	2.1
33	CE	115	GLN	2.1
20	BT	75	HIS	2.1
29	CC	226	ASN	2.1
1	AA	837	U	2.1
1	BA	133	U	2.1
1	BA	229	U	2.1
1	BA	1286	U	2.1
3	BC	116	VAL	2.1
7	BG	6	VAL	2.1
9	BI	58	VAL	2.1
11	BK	124	PRO	2.1
15	BO	75	VAL	2.1
27	C0	36	VAL	2.1
31	CA	419	U	2.1
31	CA	2028	U	2.1
34	CF	176	PRO	2.1
37	CJ	61	VAL	2.1
37	DJ	26	PRO	2.1
50	CW	84	PRO	2.1
54	DI	108	VAL	2.1
9	AI	68	LYS	2.1
40	CM	63	LYS	2.1
22	C1	46	ASP	2.1
29	DC	234	GLY	2.1
33	CE	71	GLY	2.1
36	CH	85	GLY	2.1
42	CO	7	GLY	2.1
2	AB	126	PHE	2.1
2	AB	148	LEU	2.1
45	CR	95	LEU	2.1
52	CY	46	PHE	2.1
14	BN	101	TRP	2.1
1	BA	321	A	2.1
7	BG	39	ALA	2.1
8	AH	86	TYR	2.1
12	AL	14	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
14	BN	59	ARG	2.1
19	BS	80	TYR	2.1
24	C3	19	ARG	2.1
24	C3	21	ARG	2.1
29	CC	177	ARG	2.1
31	CA	71	A	2.1
31	CA	233	A	2.1
31	CA	1247	A	2.1
31	CA	1321	A	2.1
31	CA	1789	A	2.1
31	CA	2033	A	2.1
31	CA	2119	A	2.1
31	CA	2433	A	2.1
31	CA	2448	A	2.1
31	CA	2572	A	2.1
31	CA	2883	A	2.1
33	DE	201	ALA	2.1
36	DH	56	ALA	2.1
42	CO	96	ARG	2.1
55	DA	878	A	2.1
55	DA	2154	A	2.1
1	AA	947	G	2.1
1	BA	94	G	2.1
1	BA	1032	G	2.1
4	BD	15	GLU	2.1
29	CC	124	ILE	2.1
31	CA	36	G	2.1
31	CA	132	G	2.1
31	CA	230	G	2.1
31	CA	350	G	2.1
31	CA	450	G	2.1
31	CA	476	G	2.1
31	CA	537	G	2.1
31	CA	659	G	2.1
31	CA	1310	G	2.1
31	CA	1514	G	2.1
31	CA	1517	G	2.1
31	CA	1623	G	2.1
31	CA	1972	G	2.1
31	CA	2010	G	2.1
31	CA	2201	G	2.1
31	CA	2854	G	2.1

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Mol	Chain	Res	Type	RSRZ
33	CE	149	ILE	2.1
47	CT	78	GLU	2.1
55	DA	1071	G	2.1
55	DA	1875	G	2.1
55	DA	2112	G	2.1
1	AA	990	C	2.1
1	BA	58	C	2.1
31	CA	1257	C	2.1
31	CA	1428	C	2.1
31	CA	1462	C	2.1
31	CA	1638	C	2.1
31	CA	2001	C	2.1
31	CA	2179	C	2.1
31	CA	2338	C	2.1
31	CA	2606	C	2.1
31	CA	2676	C	2.1
31	CA	2681	C	2.1
12	BL	6	GLN	2.1
14	AN	60	GLN	2.1
20	AT	61	GLN	2.1
25	C4	31	HIS	2.1
3	AC	195	VAL	2.1
16	BP	71	VAL	2.1
2	AB	201	PRO	2.1
4	AD	22	LYS	2.1
4	AD	74	ASN	2.1
7	BG	97	ASN	2.1
16	AP	41	PRO	2.1
20	BT	16	LYS	2.1
33	CE	185	LYS	2.1
35	CG	158	LYS	2.1
36	DH	41	LYS	2.1
37	DJ	136	MET	2.1
41	CN	8	LYS	2.1
1	AA	208	U	2.1
1	AA	1183	U	2.1
31	CA	1394	U	2.1
31	CA	1602	U	2.1
31	CA	2296	U	2.1
31	CA	2698	U	2.1
31	CA	2707	U	2.1
55	DA	1066	U	2.1

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Mol	Chain	Res	Type	RSRZ
2	AB	144	LEU	2.1
3	BC	111	LEU	2.1
3	BC	158	GLY	2.1
5	BE	144	LEU	2.1
8	AH	32	LEU	2.1
8	BH	5	ASP	2.1
9	AI	107	ASP	2.1
13	BM	83	LEU	2.1
3	AC	191	THR	2.1
3	AC	192	THR	2.1
10	BJ	69	THR	2.1
14	BN	18	ASP	2.1
15	BO	3	LEU	2.1
20	AT	86	LEU	2.1
34	CF	20	PHE	2.1
35	DG	47	ASP	2.1
36	CH	12	LEU	2.1
37	CJ	131	GLY	2.1
37	DJ	42	PHE	2.1
41	CN	25	ASP	2.1
49	DV	52	LEU	2.1
52	CY	68	LEU	2.1
25	C4	34	THR	2.1
53	CZ	26	PHE	2.1
54	DI	39	THR	2.1
7	BG	95	ARG	2.1
14	AN	69	ARG	2.1
14	AN	81	ARG	2.1
25	C4	13	ARG	2.1
3	AC	103	ILE	2.1
3	BC	55	ILE	2.1
4	BD	132	ILE	2.1
6	AF	95	ALA	2.1
10	BJ	34	ALA	2.1
24	C3	32	ALA	2.1
6	AF	69	GLU	2.1
40	CM	76	GLU	2.1
43	DP	55	GLU	2.1
44	CQ	68	GLU	2.1
46	CS	70	GLU	2.1
1	BA	44	A	2.1
1	BA	1357	A	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	483	A	2.1
31	CA	739	A	2.1
31	CA	1089	A	2.1
31	CA	1591	A	2.1
31	CA	1772	A	2.1
31	CA	2241	A	2.1
37	CJ	21	SER	2.1
52	CY	52	SER	2.1
55	DA	1057	A	2.1
55	DA	2119	A	2.1
55	DA	2211	A	2.1
1	AA	1220	G	2.1
1	BA	377	G	2.1
1	BA	481	G	2.1
1	BA	705	G	2.1
1	BA	1013	G	2.1
2	AB	92	VAL	2.1
7	AG	27	VAL	2.1
7	AG	105	VAL	2.1
7	BG	11	LYS	2.1
10	AJ	84	VAL	2.1
15	BO	12	VAL	2.1
19	AS	19	VAL	2.1
21	BU	49	LYS	2.1
23	C2	25	LYS	2.1
28	CB	11	C	2.1
23	C2	42	VAL	2.1
29	CC	16	VAL	2.1
31	CA	363	G	2.1
31	CA	370	G	2.1
31	CA	465	G	2.1
31	CA	518	G	2.1
31	CA	649	G	2.1
31	CA	823	C	2.1
31	CA	1297	C	2.1
31	CA	1348	C	2.1
31	CA	1404	C	2.1
31	CA	1667	G	2.1
31	CA	2583	G	2.1
31	CA	2735	G	2.1
31	CA	2852	G	2.1
31	CA	2862	G	2.1

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Mol	Chain	Res	Type	RSRZ
42	CO	78	LYS	2.1
42	CO	110	MET	2.1
46	CS	47	VAL	2.1
48	CU	55	VAL	2.1
55	DA	1738	G	2.1
55	DA	2133	G	2.1
33	CE	59	PRO	2.1
2	BB	57	LEU	2.1
2	BB	157	LEU	2.1
19	AS	31	LEU	2.1
27	D0	25	LEU	2.1
33	CE	27	LEU	2.1
1	BA	96	U	2.1
1	BA	1148	U	2.1
1	BA	1205	U	2.1
3	BC	203	PHE	2.1
10	BJ	95	GLY	2.1
13	BM	94	GLY	2.1
17	BQ	28	PHE	2.1
31	CA	399	U	2.1
31	CA	688	U	2.1
31	CA	2137	U	2.1
34	CF	126	GLY	2.1
50	CW	91	PHE	2.1
51	CX	22	GLY	2.1
55	DA	1083	U	2.1
3	AC	31	ASP	2.1
9	BI	18	ARG	2.1
10	AJ	50	THR	2.1
12	BL	40	THR	2.1
13	AM	11	ASP	2.1
17	AQ	27	ARG	2.1
22	C1	50	ARG	2.1
25	C4	8	ARG	2.1
26	C5	12	ARG	2.1
30	CD	108	ASP	2.1
35	CG	84	THR	2.1
36	DH	124	THR	2.1
37	CJ	112	THR	2.1
38	CK	10	THR	2.1
42	CO	58	ASP	2.1
43	CP	13	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
49	CV	102	THR	2.1
54	DI	7	ASP	2.1
7	BG	29	ILE	2.1
9	AI	108	ALA	2.1
10	BJ	25	ILE	2.1
11	AK	31	ILE	2.1
33	CE	108	ILE	2.1
35	DG	24	ILE	2.1
40	DM	71	ALA	2.1
43	CP	59	ALA	2.1
53	CZ	51	ALA	2.1
5	AE	128	TYR	2.1
5	AE	92	SER	2.0
26	C5	8	LYS	2.0
26	C5	9	LYS	2.0
27	C0	12	SER	2.0
34	DF	72	LYS	2.0
44	CQ	38	LYS	2.0
48	CU	70	HIS	2.0
1	AA	539	A	2.0
1	BA	59	A	2.0
1	BA	1288	A	2.0
11	BK	129	VAL	2.0
21	BU	32	VAL	2.0
31	CA	103	A	2.0
31	CA	213	A	2.0
31	CA	322	A	2.0
31	CA	466	A	2.0
31	CA	526	A	2.0
31	CA	1308	A	2.0
31	CA	1439	A	2.0
31	CA	1677	A	2.0
31	CA	2013	A	2.0
31	CA	2430	A	2.0
31	CA	2810	A	2.0
55	DA	2108	A	2.0
55	DA	2171	A	2.0
29	DC	218	PRO	2.0
37	CJ	22	PRO	2.0
1	BA	264	C	2.0
1	BA	1325	C	2.0
1	BA	1367	C	2.0

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Mol	Chain	Res	Type	RSRZ
6	BF	74	LEU	2.0
7	AG	59	LEU	2.0
7	BG	68	ASN	2.0
8	AH	121	LEU	2.0
8	BH	21	ASN	2.0
10	AJ	71	LEU	2.0
21	BU	29	LEU	2.0
29	CC	93	LEU	2.0
31	CA	484	C	2.0
31	CA	640	C	2.0
31	CA	1451	C	2.0
31	CA	1498	C	2.0
31	CA	1604	C	2.0
31	CA	2044	C	2.0
31	CA	2215	C	2.0
31	CA	2416	C	2.0
34	CF	36	LEU	2.0
34	CF	127	ASN	2.0
51	CX	50	ASN	2.0
55	DA	897	C	2.0
1	AA	198	G	2.0
1	AA	202	G	2.0
1	AA	752	G	2.0
1	AA	1278	G	2.0
1	BA	69	G	2.0
1	BA	97	G	2.0
1	BA	138	G	2.0
1	BA	319	G	2.0
1	BA	1442	G	2.0
7	BG	111	ARG	2.0
10	BJ	38	GLY	2.0
16	BP	10	GLY	2.0
19	AS	61	PHE	2.0
23	C2	44	ARG	2.0
24	C3	12	ARG	2.0
26	C5	36	ARG	2.0
31	CA	48	G	2.0
31	CA	467	G	2.0
31	CA	493	G	2.0
31	CA	768	G	2.0
31	CA	1041	G	2.0
31	CA	1807	G	2.0

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Mol	Chain	Res	Type	RSRZ
31	CA	2038	G	2.0
31	CA	2235	G	2.0
31	CA	2293	G	2.0
31	CA	2361	G	2.0
31	CA	2414	G	2.0
31	CA	2825	G	2.0
36	DH	95	GLY	2.0
40	CM	66	PHE	2.0
44	CQ	109	ARG	2.0
55	DA	2136	G	2.0
55	DA	2168	G	2.0
1	AA	1009	U	2.0
1	AA	1205	U	2.0
1	BA	471	U	2.0
1	BA	1202	U	2.0
1	BA	1321	U	2.0
17	BQ	74	THR	2.0
20	AT	80	THR	2.0
2	BB	167	ASP	2.0
3	BC	101	ILE	2.0
5	BE	80	THR	2.0
9	BI	28	ILE	2.0
10	BJ	75	ASP	2.0
29	CC	267	ILE	2.0
31	CA	292	U	2.0
31	CA	1263	U	2.0
31	CA	2236	U	2.0
31	CA	2783	U	2.0
35	CG	131	ILE	2.0
40	CM	103	ILE	2.0
40	CM	118	THR	2.0
47	CT	72	THR	2.0
14	BN	36	ALA	2.0
42	CO	41	ALA	2.0
54	DI	135	ALA	2.0
4	AD	113	GLU	2.0
52	CY	76	GLU	2.0
3	BC	79	LYS	2.0
4	AD	204	TYR	2.0
9	BI	7	TYR	2.0
19	AS	80	TYR	2.0
29	CC	7	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
50	DW	34	LYS	2.0
41	CN	136	MET	2.0
2	BB	39	HIS	2.0
4	BD	125	VAL	2.0
5	BE	56	VAL	2.0
20	BT	48	GLN	2.0
30	CD	36	GLN	2.0
34	CF	132	VAL	2.0
35	DG	111	HIS	2.0
36	DH	108	VAL	2.0
37	DJ	70	VAL	2.0
39	CL	5	GLN	2.0
46	CS	14	VAL	2.0
46	CS	58	VAL	2.0
47	CT	102	HIS	2.0
51	CX	40	GLN	2.0
52	CY	2	SER	2.0
53	CZ	25	GLN	2.0
53	CZ	40	SER	2.0
37	DJ	56	PRO	2.0
1	AA	412	A	2.0
1	AA	1368	A	2.0
1	BA	1250	A	2.0
2	AB	68	LEU	2.0
2	BB	129	LEU	2.0
5	BE	36	LEU	2.0
7	AG	124	LEU	2.0
9	AI	87	LEU	2.0
9	BI	35	LEU	2.0
31	CA	83	A	2.0
31	CA	265	A	2.0
31	CA	492	A	2.0
31	CA	845	A	2.0
31	CA	975	A	2.0
31	CA	1244	A	2.0
31	CA	1640	A	2.0
31	CA	2336	A	2.0
53	CZ	42	LEU	2.0
55	DA	2142	A	2.0
3	BC	164	ARG	2.0
10	AJ	45	ARG	2.0
16	BP	29	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
35	DG	170	ARG	2.0
36	CH	123	ARG	2.0
17	BQ	35	GLY	2.0
20	BT	51	PHE	2.0
51	CX	42	GLY	2.0
52	CY	63	GLY	2.0
1	BA	188	C	2.0
1	BA	314	C	2.0
1	BA	1132	C	2.0
1	BA	1234	C	2.0
1	BA	1314	C	2.0
1	BA	1344	C	2.0
7	BG	42	ILE	2.0
9	AI	65	ILE	2.0
11	AK	116	ILE	2.0
13	AM	7	ILE	2.0
28	CB	60	C	2.0
31	CA	837	C	2.0
31	CA	1386	C	2.0
31	CA	1790	C	2.0
31	CA	2200	C	2.0
31	CA	2462	C	2.0
12	AL	13	ALA	2.0
12	BL	97	THR	2.0
13	AM	35	ALA	2.0
17	AQ	82	ALA	2.0
26	C5	29	ALA	2.0
37	DJ	68	THR	2.0
40	CM	97	ALA	2.0
45	CR	96	ALA	2.0
1	AA	1002	G	2.0
1	AA	1139	G	2.0
1	AA	1276	G	2.0
1	BA	31	G	2.0
1	BA	127	G	2.0
1	BA	318	G	2.0
1	BA	976	G	2.0
1	BA	1220	G	2.0
5	AE	163	GLU	2.0
10	BJ	11	LYS	2.0
12	BL	44	LYS	2.0
16	BP	34	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
20	BT	59	ASP	2.0
28	CB	74	U	2.0
28	CB	82	U	2.0
31	CA	90	U	2.0
31	CA	293	U	2.0
31	CA	828	U	2.0
31	CA	1438	U	2.0
31	CA	1657	U	2.0
31	CA	1781	U	2.0
31	CA	2408	U	2.0
34	CF	113	ASP	2.0
22	C1	32	LYS	2.0
31	CA	58	G	2.0
31	CA	108	G	2.0
31	CA	123	G	2.0
54	DI	47	GLU	2.0
55	DA	2155	U	2.0
31	CA	662	G	2.0
31	CA	956	G	2.0
31	CA	1107	G	2.0
31	CA	1441	G	2.0
31	CA	1455	G	2.0
31	CA	1465	G	2.0
31	CA	1568	G	2.0
31	CA	1763	G	2.0
31	CA	1824	G	2.0
31	CA	1980	G	2.0
31	CA	2053	G	2.0
31	CA	2355	G	2.0
31	CA	2367	G	2.0
31	CA	2607	G	2.0
31	CA	2669	G	2.0
31	CA	2811	G	2.0
31	CA	2839	G	2.0
31	CA	2846	G	2.0
38	CK	85	LYS	2.0
2	AB	9	MET	2.0
7	BG	103	TRP	2.0
3	AC	184	TYR	2.0
9	BI	19	VAL	2.0
34	DF	89	VAL	2.0
41	CN	80	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
48	CU	16	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	2MG	BA	966	24/25	0.59	0.15	153,160,171,171	0
1	5MC	BA	967	21/22	0.63	0.17	153,164,167,167	0
1	2MG	BA	1207	24/25	0.63	0.13	158,161,165,168	0
31	PSU	CA	1911	20/21	0.72	0.11	123,137,138,139	0
31	PSU	CA	1917	20/21	0.73	0.12	119,125,134,135	0
31	2MA	CA	2503	23/24	0.76	0.23	110,115,118,118	0
31	PSU	CA	2457	20/21	0.77	0.17	106,107,108,109	0
31	3TD	CA	1915	21/22	0.77	0.10	150,155,157,157	0
31	PSU	CA	746	20/21	0.78	0.15	120,123,126,127	0
31	PSU	CA	2580	20/21	0.78	0.15	102,105,109,109	0
1	PSU	BA	516	20/21	0.81	0.13	88,99,102,104	0
31	PSU	CA	2504	20/21	0.81	0.18	98,108,110,111	0
31	6MZ	CA	1618	23/24	0.81	0.18	136,143,148,149	0
31	PSU	CA	955	20/21	0.82	0.16	107,112,115,115	0
55	3TD	DA	1915	21/22	0.83	0.12	103,106,112,113	0
41	4D4	CN	81	12/13	0.83	0.16	112,122,143,143	0
31	6MZ	CA	2030	23/24	0.84	0.17	108,114,116,117	0
1	2MG	AA	966	24/25	0.86	0.14	95,98,107,108	0
1	2MG	AA	1207	24/25	0.86	0.12	114,118,121,124	0
31	G7M	CA	2069	24/25	0.86	0.20	109,112,115,116	0
31	OMG	CA	2251	24/25	0.86	0.15	90,95,100,101	0
55	PSU	DA	1917	20/21	0.86	0.11	74,82,90,90	0
12	D2T	AL	89	10/11	0.86	0.16	66,71,78,78	0
55	PSU	DA	1911	20/21	0.87	0.11	78,88,91,91	0
31	1MG	CA	745	24/25	0.87	0.15	106,113,118,121	0
31	OMU	CA	2552	21/22	0.87	0.24	91,96,100,101	0
12	D2T	BL	89	10/11	0.87	0.17	86,88,94,95	0
31	5MU	CA	747	21/22	0.88	0.14	126,128,130,131	0
1	UR3	BA	1498	21/22	0.88	0.12	89,93,97,98	0
31	OMC	CA	2498	21/22	0.89	0.17	97,102,104,106	0
1	PSU	AA	516	20/21	0.89	0.13	88,92,97,97	0
1	5MC	BA	1407	21/22	0.89	0.14	100,109,114,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	2MG	CA	1835	24/25	0.90	0.14	74,76,78,78	0
31	2MG	CA	2445	24/25	0.90	0.17	105,110,112,113	0
31	5MU	CA	1939	21/22	0.90	0.15	75,79,81,82	0
31	PSU	CA	2605	20/21	0.91	0.12	82,84,86,87	0
1	5MC	AA	967	21/22	0.91	0.13	90,106,107,108	0
31	5MC	CA	1962	21/22	0.91	0.12	72,78,79,82	0
1	2MG	BA	1516	24/25	0.91	0.12	82,90,99,100	0
1	G7M	BA	527	24/25	0.91	0.10	75,80,83,84	0
1	G7M	AA	527	24/25	0.92	0.11	63,67,73,74	0
32	MEQ	DD	150[B]	10/11	0.93	0.14	27,32,45,50	10
1	MA6	BA	1518	24/25	0.93	0.12	84,88,95,96	0
1	4OC	BA	1402	22/23	0.93	0.10	78,81,84,85	0
1	UR3	AA	1498	21/22	0.93	0.10	64,68,72,73	0
32	MEQ	DD	150[A]	10/11	0.93	0.14	14,23,32,32	10
1	MA6	BA	1519	24/25	0.94	0.12	84,87,91,92	0
1	MA6	AA	1518	24/25	0.95	0.10	60,61,62,64	0
1	5MC	AA	1407	21/22	0.95	0.09	60,61,63,64	0
55	PSU	DA	2604	20/21	0.95	0.09	37,42,54,55	0
1	2MG	AA	1516	24/25	0.95	0.09	58,61,62,63	0
41	4D4	DN	81[A]	12/13	0.95	0.14	33,38,53,55	9
41	4D4	DN	81[B]	12/13	0.95	0.14	27,32,34,35	9
55	2MG	DA	1835	24/25	0.96	0.08	49,55,56,56	0
1	4OC	AA	1402	22/23	0.96	0.08	61,68,72,73	0
55	5MU	DA	1939	21/22	0.96	0.10	35,38,40,43	0
55	5MC	DA	1962	21/22	0.96	0.11	43,46,50,52	0
55	OMU	DA	2552	21/22	0.97	0.10	33,37,39,43	0
1	MA6	AA	1519	24/25	0.97	0.09	61,62,70,71	0
55	PSU	DA	2605	20/21	0.97	0.07	35,41,43,44	0
55	OMG	DA	2251	24/25	0.98	0.07	29,33,35,39	0
55	2MG	DA	2445	24/25	0.98	0.09	25,29,33,34	0
55	H2U	DA	2449	20/21	0.98	0.08	27,30,36,39	0
55	PSU	DA	2457	20/21	0.98	0.07	25,29,31,35	0
55	2MA	DA	2503	23/24	0.98	0.06	33,36,39,43	0
55	PSU	DA	2504	20/21	0.98	0.12	33,41,49,52	0
55	PSU	DA	955	20/21	0.98	0.07	27,28,32,35	0
55	PSU	DA	2580	20/21	0.98	0.07	25,30,33,35	0
55	6MZ	DA	1618	23/24	0.98	0.06	25,30,32,35	0
55	PSU	DA	746	20/21	0.98	0.06	28,32,36,38	0
55	5MU	DA	747	21/22	0.98	0.06	28,31,37,38	0
55	6MZ	DA	2030	23/24	0.98	0.07	24,28,32,39	0
55	G7M	DA	2069	24/25	0.98	0.07	26,35,36,37	0
55	OMC	DA	2498	21/22	0.99	0.07	20,27,31,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	1MG	DA	745	24/25	0.99	0.06	28,31,33,38	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3110	1/1	-0.27	0.42	188,188,188,188	0
56	MG	CA	3130	1/1	-0.07	0.44	141,141,141,141	0
56	MG	CA	3132	1/1	-0.05	0.38	152,152,152,152	0
56	MG	CA	3146	1/1	-0.02	0.25	247,247,247,247	0
56	MG	CA	3140	1/1	0.07	0.26	147,147,147,147	0
56	MG	AA	1622	1/1	0.17	0.36	130,130,130,130	0
56	MG	CA	3061	1/1	0.18	0.20	274,274,274,274	0
56	MG	CA	3123	1/1	0.22	0.25	188,188,188,188	0
56	MG	BA	1640	1/1	0.24	0.49	156,156,156,156	0
56	MG	BA	1636	1/1	0.24	0.37	172,172,172,172	0
56	MG	CA	3141	1/1	0.26	0.50	109,109,109,109	0
56	MG	CA	3142	1/1	0.26	0.34	133,133,133,133	0
56	MG	CA	3139	1/1	0.26	0.42	139,139,139,139	0
56	MG	CA	3007	1/1	0.27	0.12	257,257,257,257	0
56	MG	CA	3126	1/1	0.30	0.35	136,136,136,136	0
56	MG	CA	3077	1/1	0.30	0.20	252,252,252,252	0
56	MG	CA	3124	1/1	0.32	0.23	202,202,202,202	0
56	MG	CA	3154	1/1	0.33	0.39	155,155,155,155	0
56	MG	CA	3111	1/1	0.34	0.37	159,159,159,159	0
56	MG	BA	1641	1/1	0.39	0.21	140,140,140,140	0
56	MG	AA	1606	1/1	0.39	0.61	120,120,120,120	0
56	MG	CA	3032	1/1	0.39	0.17	269,269,269,269	0
56	MG	BA	1603	1/1	0.40	0.13	261,261,261,261	0
56	MG	DA	3145	1/1	0.42	0.29	101,101,101,101	0
56	MG	CA	3038	1/1	0.44	0.17	268,268,268,268	0
56	MG	CA	3075	1/1	0.46	0.24	253,253,253,253	0
56	MG	CA	3005	1/1	0.46	0.23	253,253,253,253	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3124	1/1	0.47	0.63	114,114,114,114	0
56	MG	CA	3122	1/1	0.47	0.38	136,136,136,136	0
56	MG	CA	3034	1/1	0.48	0.23	256,256,256,256	0
56	MG	CA	3108	1/1	0.49	0.42	109,109,109,109	0
56	MG	CA	3129	1/1	0.49	0.37	141,141,141,141	0
56	MG	AA	1609	1/1	0.49	0.39	107,107,107,107	0
56	MG	CA	3002	1/1	0.50	0.21	259,259,259,259	0
56	MG	CA	3104	1/1	0.50	0.20	263,263,263,263	0
56	MG	DA	3168	1/1	0.50	0.24	108,108,108,108	0
56	MG	CA	3107	1/1	0.51	0.47	106,106,106,106	0
56	MG	AA	1608	1/1	0.51	0.46	119,119,119,119	0
56	MG	CA	3060	1/1	0.52	0.17	242,242,242,242	0
56	MG	BA	1639	1/1	0.53	0.27	106,106,106,106	0
56	MG	CA	3117	1/1	0.56	0.47	109,109,109,109	0
56	MG	CA	3026	1/1	0.56	0.26	197,197,197,197	0
56	MG	CA	3133	1/1	0.56	0.41	140,140,140,140	0
56	MG	CA	3031	1/1	0.56	0.14	127,127,127,127	0
56	MG	CA	3092	1/1	0.57	0.15	202,202,202,202	0
56	MG	AA	1628	1/1	0.57	0.18	142,142,142,142	0
56	MG	CA	3135	1/1	0.57	0.28	104,104,104,104	0
56	MG	AA	1661	1/1	0.57	0.17	190,190,190,190	0
56	MG	CA	3121	1/1	0.57	0.39	101,101,101,101	0
56	MG	CA	3014	1/1	0.57	0.22	262,262,262,262	0
56	MG	BA	1606	1/1	0.58	0.21	251,251,251,251	0
56	MG	CA	3008	1/1	0.58	0.20	179,179,179,179	0
56	MG	CA	3010	1/1	0.58	0.19	231,231,231,231	0
56	MG	CA	3145	1/1	0.59	0.30	75,75,75,75	0
56	MG	CA	3056	1/1	0.59	0.58	100,100,100,100	0
56	MG	DA	3180	1/1	0.59	0.23	97,97,97,97	0
56	MG	CA	3003	1/1	0.60	0.31	284,284,284,284	0
56	MG	CA	3112	1/1	0.62	0.28	110,110,110,110	0
56	MG	CA	3113	1/1	0.62	0.45	94,94,94,94	0
56	MG	CA	3115	1/1	0.62	0.34	108,108,108,108	0
56	MG	CA	3155	1/1	0.62	0.24	204,204,204,204	0
56	MG	CA	3134	1/1	0.63	0.25	204,204,204,204	0
56	MG	CA	3156	1/1	0.63	0.15	246,246,246,246	0
67	ACY	DA	3196	4/4	0.63	0.24	75,79,79,80	0
56	MG	CA	3033	1/1	0.64	0.30	200,200,200,200	0
56	MG	CA	3109	1/1	0.65	0.24	93,93,93,93	0
56	MG	AA	1611	1/1	0.65	0.26	113,113,113,113	0
56	MG	AA	1614	1/1	0.65	0.28	131,131,131,131	0
56	MG	AA	1603	1/1	0.65	0.43	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3152	1/1	0.66	0.23	215,215,215,215	0
56	MG	BA	1630	1/1	0.66	0.17	221,221,221,221	0
56	MG	CA	3105	1/1	0.66	0.19	254,254,254,254	0
56	MG	AA	1679	1/1	0.67	0.17	189,189,189,189	0
56	MG	CA	3131	1/1	0.67	0.29	111,111,111,111	0
56	MG	CA	3149	1/1	0.67	0.39	92,92,92,92	0
56	MG	CA	3118	1/1	0.67	0.39	90,90,90,90	0
56	MG	CA	3099	1/1	0.67	0.20	235,235,235,235	0
56	MG	CA	3073	1/1	0.67	0.21	260,260,260,260	0
56	MG	CA	3106	1/1	0.68	0.30	103,103,103,103	0
56	MG	CA	3119	1/1	0.68	0.34	134,134,134,134	0
56	MG	CA	3072	1/1	0.68	0.13	272,272,272,272	0
56	MG	BA	1604	1/1	0.68	0.13	182,182,182,182	0
56	MG	AA	1654	1/1	0.68	0.25	252,252,252,252	0
56	MG	BA	1625	1/1	0.68	0.15	274,274,274,274	0
56	MG	DA	3134	1/1	0.69	0.25	78,78,78,78	0
56	MG	DA	3139	1/1	0.69	0.91	64,64,64,64	1
56	MG	CA	3028	1/1	0.69	0.15	283,283,283,283	0
56	MG	DA	3159	1/1	0.69	0.33	80,80,80,80	0
56	MG	CA	3047	1/1	0.69	0.31	240,240,240,240	0
56	MG	CA	3116	1/1	0.69	0.42	89,89,89,89	0
56	MG	CA	3138	1/1	0.69	0.32	103,103,103,103	0
56	MG	DA	3162	1/1	0.70	0.19	64,64,64,64	0
56	MG	CA	3150	1/1	0.70	0.32	82,82,82,82	0
56	MG	DA	3153	1/1	0.70	0.42	100,100,100,100	0
59	PUT	AA	1672	6/6	0.70	0.44	110,112,114,114	0
56	MG	BA	1624	1/1	0.70	0.12	275,275,275,275	0
56	MG	BA	1623	1/1	0.71	0.20	235,235,235,235	0
56	MG	CA	3125	1/1	0.71	0.32	141,141,141,141	0
56	MG	CA	3067	1/1	0.72	0.14	289,289,289,289	0
56	MG	CA	3054	1/1	0.72	0.11	140,140,140,140	0
56	MG	DA	3178	1/1	0.72	0.36	101,101,101,101	0
56	MG	AA	1601	1/1	0.72	0.54	104,104,104,104	0
56	MG	CA	3148	1/1	0.72	0.67	86,86,86,86	1
56	MG	DA	3161	1/1	0.72	0.25	78,78,78,78	0
58	MPD	DE	301	8/8	0.73	0.22	102,104,107,109	0
56	MG	AA	1624	1/1	0.73	0.23	93,93,93,93	0
56	MG	CA	3006	1/1	0.73	0.12	227,227,227,227	0
56	MG	DB	209	1/1	0.74	0.33	80,80,80,80	0
56	MG	CA	3120	1/1	0.74	0.17	195,195,195,195	0
56	MG	AA	1616	1/1	0.74	0.51	88,88,88,88	0
56	MG	DB	207	1/1	0.75	0.29	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3128	1/1	0.75	0.25	87,87,87,87	0
56	MG	CA	3147	1/1	0.75	0.99	91,91,91,91	1
56	MG	AA	1615	1/1	0.75	0.29	90,90,90,90	0
63	EDO	DA	3004	4/4	0.76	0.28	107,107,108,109	0
64	PGE	D1	102	10/10	0.76	0.26	95,96,100,100	0
56	MG	DA	3179	1/1	0.76	0.20	102,102,102,102	0
68	GUN	DA	3210	11/11	0.76	0.20	71,73,74,74	0
56	MG	AA	1642	1/1	0.77	0.20	165,165,165,165	0
56	MG	DA	3131	1/1	0.77	0.25	87,87,87,87	0
56	MG	CA	3009	1/1	0.77	0.21	248,248,248,248	0
56	MG	CA	3071	1/1	0.77	0.09	207,207,207,207	0
56	MG	DA	3143	1/1	0.77	0.45	95,95,95,95	0
56	MG	BA	1627	1/1	0.77	0.23	129,129,129,129	0
56	MG	DA	3147	1/1	0.77	0.22	89,89,89,89	0
69	TRS	DA	3219	8/8	0.77	0.21	98,99,102,104	0
56	MG	CA	3143	1/1	0.78	0.22	107,107,107,107	0
58	MPD	DE	302	8/8	0.78	0.29	96,97,98,98	0
56	MG	CA	3022	1/1	0.78	0.24	188,188,188,188	0
62	PEG	DQ	201	7/7	0.78	0.20	107,109,110,110	0
56	MG	AA	1625	1/1	0.78	0.21	78,78,78,78	0
56	MG	AA	1647	1/1	0.78	0.15	202,202,202,202	0
56	MG	CA	3083	1/1	0.78	0.18	241,241,241,241	0
56	MG	CA	3090	1/1	0.78	0.13	215,215,215,215	0
56	MG	CA	3021	1/1	0.78	0.38	278,278,278,278	0
56	MG	BA	1644	1/1	0.79	0.16	97,97,97,97	0
56	MG	DR	203	1/1	0.79	0.20	111,111,111,111	0
59	PUT	AA	1674	6/6	0.79	0.32	98,99,100,100	0
56	MG	DA	3163	1/1	0.79	0.34	84,84,84,84	0
56	MG	AA	1619	1/1	0.79	0.26	92,92,92,92	0
56	MG	AA	1602	1/1	0.79	0.30	88,88,88,88	0
56	MG	CA	3093	1/1	0.79	0.13	123,123,123,123	0
56	MG	DA	3128	1/1	0.79	0.43	78,78,78,78	0
56	MG	CA	3080	1/1	0.79	0.21	186,186,186,186	0
56	MG	AA	1660	1/1	0.80	0.16	286,286,286,286	0
56	MG	CA	3094	1/1	0.80	0.21	159,159,159,159	0
56	MG	DA	3171	1/1	0.80	0.14	82,82,82,82	0
58	MPD	DT	201	8/8	0.80	0.26	73,82,84,86	0
56	MG	AA	1605	1/1	0.80	0.46	99,99,99,99	0
56	MG	CB	203	1/1	0.80	0.10	155,155,155,155	0
56	MG	DA	3170	1/1	0.81	0.20	73,73,73,73	0
62	PEG	DA	3225	7/7	0.81	0.32	62,65,70,70	0
56	MG	CA	3068	1/1	0.81	0.15	253,253,253,253	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MPD	DN	201	8/8	0.81	0.17	87,89,92,93	0
64	PGE	D3	101	10/10	0.81	0.22	87,88,88,88	0
56	MG	CA	3076	1/1	0.81	0.13	213,213,213,213	0
67	ACY	DA	3201	4/4	0.81	0.29	60,64,64,66	0
56	MG	DA	3154	1/1	0.81	0.43	59,59,59,59	0
56	MG	CA	3062	1/1	0.81	0.18	237,237,237,237	0
59	PUT	AA	1675	6/6	0.82	0.22	90,92,93,93	0
56	MG	CA	3013	1/1	0.82	0.11	135,135,135,135	0
56	MG	DA	3122	1/1	0.82	0.35	80,80,80,80	0
56	MG	AA	1664	1/1	0.82	0.11	186,186,186,186	0
56	MG	DA	3167	1/1	0.82	0.24	75,75,75,75	0
56	MG	DA	3126	1/1	0.82	0.28	76,76,76,76	0
56	MG	CA	3018	1/1	0.82	0.14	133,133,133,133	0
58	MPD	DA	3203	8/8	0.82	0.23	96,99,102,104	0
56	MG	CA	3063	1/1	0.82	0.25	207,207,207,207	0
56	MG	CA	3078	1/1	0.82	0.17	195,195,195,195	0
56	MG	DA	3138	1/1	0.83	0.35	89,89,89,89	0
56	MG	BA	1609	1/1	0.83	0.12	194,194,194,194	0
60	T1C	BA	1643	42/42	0.83	0.17	169,175,185,185	0
62	PEG	DP	201	7/7	0.83	0.16	94,94,99,100	0
57	PG4	DR	202	13/13	0.83	0.22	61,63,75,75	0
57	PG4	DA	3215	13/13	0.83	0.20	95,103,104,104	0
56	MG	AA	1618	1/1	0.83	0.42	91,91,91,91	0
56	MG	CA	3127	1/1	0.83	0.31	85,85,85,85	0
56	MG	DB	206	1/1	0.83	0.20	102,102,102,102	0
56	MG	CA	3039	1/1	0.83	0.12	153,153,153,153	0
58	MPD	DT	202	8/8	0.83	0.30	87,88,89,91	0
56	MG	DA	3132	1/1	0.83	0.46	77,77,77,77	0
56	MG	CA	3059	1/1	0.83	0.21	147,147,147,147	0
56	MG	AA	1623	1/1	0.84	0.22	85,85,85,85	0
56	MG	DA	3173	1/1	0.84	0.30	81,81,81,81	0
56	MG	CA	3082	1/1	0.84	0.27	160,160,160,160	0
59	PUT	AA	1673	6/6	0.84	0.22	125,126,127,128	0
56	MG	AA	1617	1/1	0.84	0.32	98,98,98,98	0
56	MG	AA	1665	1/1	0.84	0.11	168,168,168,168	0
59	PUT	DA	3204	6/6	0.84	0.24	66,66,70,71	0
59	PUT	DA	3221	6/6	0.84	0.20	44,48,50,50	0
57	PG4	AA	1670	13/13	0.84	0.15	80,92,101,102	0
62	PEG	D3	102	7/7	0.84	0.54	72,74,83,84	0
62	PEG	AL	201	7/7	0.85	0.17	74,78,85,85	0
56	MG	CA	3057	1/1	0.85	0.12	132,132,132,132	0
56	MG	CA	3151	1/1	0.85	0.36	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3130	1/1	0.85	0.39	87,87,87,87	0
62	PEG	DA	3199	7/7	0.85	0.22	60,64,69,70	0
56	MG	DA	3182	1/1	0.85	0.27	73,73,73,73	0
56	MG	BA	1614	1/1	0.85	0.16	147,147,147,147	0
57	PG4	BA	1642	13/13	0.85	0.16	96,102,107,107	0
57	PG4	DQ	202	13/13	0.85	0.13	64,66,71,72	0
65	SPD	DA	3205	10/10	0.85	0.28	75,81,84,85	0
56	MG	CB	201	1/1	0.85	0.10	166,166,166,166	0
56	MG	CA	3055	1/1	0.85	0.14	195,195,195,195	0
56	MG	DA	3155	1/1	0.85	0.34	74,74,74,74	0
56	MG	AA	1621	1/1	0.85	0.30	83,83,83,83	0
56	MG	DA	3133	1/1	0.86	0.33	78,78,78,78	0
56	MG	CA	3064	1/1	0.86	0.18	267,267,267,267	0
56	MG	DA	3123	1/1	0.86	0.39	77,77,77,77	0
62	PEG	DA	3217	7/7	0.86	0.32	89,93,98,99	0
56	MG	CA	3058	1/1	0.86	0.15	135,135,135,135	0
63	EDO	DA	3003	4/4	0.86	0.31	64,64,66,67	0
56	MG	CA	3048	1/1	0.86	0.12	107,107,107,107	0
56	MG	DA	3127	1/1	0.86	0.36	62,62,62,62	0
56	MG	BA	1629	1/1	0.86	0.19	157,157,157,157	0
56	MG	AA	1604	1/1	0.86	0.31	82,82,82,82	0
56	MG	AA	1626	1/1	0.86	0.25	111,111,111,111	0
56	MG	DA	3176	1/1	0.86	0.32	93,93,93,93	0
58	MPD	DK	201	8/8	0.86	0.15	93,94,95,95	0
56	MG	BA	1638	1/1	0.86	0.49	110,110,110,110	0
56	MG	CA	3097	1/1	0.87	0.14	125,125,125,125	0
57	PG4	DA	3193	13/13	0.87	0.21	63,65,76,77	0
56	MG	CA	3088	1/1	0.87	0.08	88,88,88,88	0
56	MG	DD	303	1/1	0.87	0.18	66,66,66,66	0
59	PUT	DA	3189	6/6	0.87	0.17	47,48,49,49	0
56	MG	CA	3004	1/1	0.87	0.20	223,223,223,223	0
56	MG	BA	1612	1/1	0.87	0.16	137,137,137,137	0
60	T1C	AA	1677	42/42	0.87	0.14	89,96,109,110	0
65	SPD	DA	3183	10/10	0.87	0.18	57,63,66,66	0
56	MG	AA	1612	1/1	0.87	0.30	81,81,81,81	0
56	MG	CA	3065	1/1	0.87	0.14	122,122,122,122	0
62	PEG	D1	103	7/7	0.87	0.29	56,60,61,62	0
56	MG	DA	3063	1/1	0.87	0.17	222,222,222,222	0
56	MG	DA	3112	1/1	0.87	0.29	293,293,293,293	0
56	MG	DA	3151	1/1	0.88	0.10	58,58,58,58	0
56	MG	CA	3101	1/1	0.88	0.08	149,149,149,149	0
56	MG	DA	3172	1/1	0.88	0.31	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3024	1/1	0.88	0.11	141,141,141,141	0
56	MG	DA	3125	1/1	0.88	0.64	83,83,83,83	0
63	EDO	DB	210	4/4	0.88	0.20	85,85,85,86	0
63	EDO	DB	211	4/4	0.88	0.17	73,73,74,75	0
59	PUT	DA	3195	6/6	0.88	0.29	51,53,62,65	0
56	MG	CA	3137	1/1	0.88	0.28	168,168,168,168	0
63	EDO	DA	3194	4/4	0.88	0.23	51,56,59,60	0
59	PUT	DA	3211	6/6	0.88	0.23	65,66,72,74	0
56	MG	CA	3037	1/1	0.88	0.19	235,235,235,235	0
64	PGE	DS	201	10/10	0.88	0.16	56,66,68,69	0
64	PGE	DU	101	10/10	0.88	0.16	64,72,83,83	0
64	PGE	DA	3213	10/10	0.88	0.16	84,86,90,90	0
56	MG	CA	3084	1/1	0.88	0.13	208,208,208,208	0
56	MG	AA	1630	1/1	0.88	0.10	134,134,134,134	0
56	MG	BA	1633	1/1	0.88	0.14	235,235,235,235	0
56	MG	DA	3148	1/1	0.88	0.24	115,115,115,115	0
58	MPD	DA	3206	8/8	0.88	0.22	89,93,94,94	0
62	PEG	DL	201	7/7	0.88	0.16	65,69,76,78	0
56	MG	CA	3023	1/1	0.89	0.11	150,150,150,150	0
64	PGE	DD	301	10/10	0.89	0.26	63,67,72,73	0
58	MPD	DA	3190	8/8	0.89	0.17	91,92,93,94	0
63	EDO	D1	101	4/4	0.89	0.11	67,67,68,68	0
56	MG	DA	3166	1/1	0.89	0.19	90,90,90,90	0
64	PGE	DA	3224	10/10	0.89	0.21	74,81,83,83	0
56	MG	AA	1607	1/1	0.89	0.36	92,92,92,92	0
56	MG	AA	1657	1/1	0.89	0.22	162,162,162,162	0
66	1PE	DA	3202	16/16	0.89	0.16	60,63,65,65	0
59	PUT	DA	3218	6/6	0.89	0.21	75,77,80,81	0
56	MG	CA	3040	1/1	0.89	0.09	126,126,126,126	0
63	EDO	DA	3208	4/4	0.89	0.30	98,99,100,101	0
56	MG	AA	1669	1/1	0.89	0.15	118,118,118,118	0
56	MG	CA	3081	1/1	0.90	0.12	134,134,134,134	0
56	MG	AA	1636	1/1	0.90	0.11	97,97,97,97	0
56	MG	DA	3136	1/1	0.90	0.09	92,92,92,92	0
59	PUT	DA	3220	6/6	0.90	0.19	92,92,94,95	0
56	MG	CA	3049	1/1	0.90	0.15	100,100,100,100	0
56	MG	AA	1678	1/1	0.90	0.19	74,74,74,74	0
56	MG	CA	3016	1/1	0.90	0.18	148,148,148,148	0
61	ZN	AB	301	1/1	0.90	0.07	209,209,209,209	0
56	MG	DA	3129	1/1	0.90	0.49	60,60,60,60	0
66	1PE	DA	3185	16/16	0.90	0.15	44,53,71,72	0
56	MG	DA	3118	1/1	0.90	0.24	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3001	1/1	0.90	0.26	299,299,299,299	0
63	EDO	DA	3198	4/4	0.90	0.25	56,57,58,59	0
56	MG	CA	3020	1/1	0.90	0.09	103,103,103,103	0
63	EDO	DA	3214	4/4	0.90	0.20	77,78,79,79	0
56	MG	DA	3164	1/1	0.91	0.24	72,72,72,72	0
59	PUT	DA	3222	6/6	0.91	0.18	50,54,55,55	0
56	MG	DA	3165	1/1	0.91	0.27	69,69,69,69	0
56	MG	DA	3150	1/1	0.91	0.12	59,59,59,59	0
58	MPD	DA	3192	8/8	0.91	0.31	79,79,82,83	0
56	MG	CA	3091	1/1	0.91	0.09	96,96,96,96	0
56	MG	AA	1613	1/1	0.91	0.47	85,85,85,85	0
56	MG	DA	3169	1/1	0.91	0.34	73,73,73,73	0
56	MG	CA	3136	1/1	0.91	0.29	105,105,105,105	0
57	PG4	DS	202	13/13	0.91	0.11	43,51,59,61	0
56	MG	BA	1617	1/1	0.91	0.06	126,126,126,126	0
59	PUT	DA	3184	6/6	0.91	0.26	42,48,50,51	0
62	PEG	DA	3200	7/7	0.91	0.28	55,58,65,65	0
56	MG	DA	3144	1/1	0.91	0.14	65,65,65,65	0
65	SPD	DA	3223	10/10	0.91	0.16	40,44,54,55	0
58	MPD	AA	1671	8/8	0.91	0.20	101,103,104,106	0
62	PEG	DA	3226	7/7	0.91	0.16	58,59,65,67	0
56	MG	BA	1618	1/1	0.91	0.11	106,106,106,106	0
56	MG	DA	3175	1/1	0.91	0.28	75,75,75,75	0
56	MG	BA	1619	1/1	0.91	0.13	107,107,107,107	0
56	MG	CA	3036	1/1	0.91	0.20	203,203,203,203	0
56	MG	AA	1644	1/1	0.92	0.12	94,94,94,94	0
63	EDO	DA	3001	4/4	0.92	0.17	72,73,75,77	0
56	MG	CA	3095	1/1	0.92	0.10	81,81,81,81	0
56	MG	CA	3035	1/1	0.92	0.22	158,158,158,158	0
56	MG	CA	3098	1/1	0.92	0.11	110,110,110,110	0
56	MG	BA	1608	1/1	0.92	0.10	122,122,122,122	0
63	EDO	DA	3207	4/4	0.92	0.26	58,60,62,63	0
56	MG	CA	3100	1/1	0.92	0.17	110,110,110,110	0
56	MG	AA	1655	1/1	0.92	0.08	115,115,115,115	0
56	MG	BA	1634	1/1	0.92	0.13	116,116,116,116	0
56	MG	DA	3045	1/1	0.92	0.09	85,85,85,85	0
56	MG	DA	3140	1/1	0.92	0.15	57,57,57,57	0
56	MG	AA	1663	1/1	0.92	0.11	110,110,110,110	0
56	MG	BA	1637	1/1	0.92	0.26	93,93,93,93	0
56	MG	CA	3046	1/1	0.92	0.14	143,143,143,143	0
56	MG	DA	3121	1/1	0.92	0.26	91,91,91,91	0
56	MG	CA	3027	1/1	0.92	0.17	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3177	1/1	0.92	0.26	68,68,68,68	0
58	MPD	DA	3209	8/8	0.92	0.19	68,70,70,71	0
56	MG	AA	1627	1/1	0.92	0.44	99,99,99,99	0
56	MG	CA	3089	1/1	0.92	0.13	95,95,95,95	0
56	MG	CA	3029	1/1	0.92	0.22	177,177,177,177	0
56	MG	BA	1626	1/1	0.92	0.12	111,111,111,111	0
56	MG	CA	3017	1/1	0.92	0.06	106,106,106,106	0
56	MG	AA	1658	1/1	0.92	0.12	100,100,100,100	0
56	MG	CB	202	1/1	0.93	0.12	139,139,139,139	0
59	PUT	DA	3188	6/6	0.93	0.13	32,35,40,41	0
56	MG	CA	3069	1/1	0.93	0.09	115,115,115,115	0
56	MG	DA	3065	1/1	0.93	0.20	71,71,71,71	0
56	MG	BA	1601	1/1	0.93	0.09	95,95,95,95	0
56	MG	CA	3079	1/1	0.93	0.10	143,143,143,143	0
59	PUT	DA	3212	6/6	0.93	0.22	55,57,64,66	0
56	MG	CA	3030	1/1	0.93	0.08	124,124,124,124	0
56	MG	BA	1607	1/1	0.93	0.18	162,162,162,162	0
56	MG	DA	3142	1/1	0.93	0.25	79,79,79,79	0
56	MG	CA	3012	1/1	0.93	0.15	130,130,130,130	0
56	MG	DA	3156	1/1	0.93	0.29	74,74,74,74	0
56	MG	DA	3158	1/1	0.93	0.28	71,71,71,71	0
56	MG	CA	3074	1/1	0.94	0.16	206,206,206,206	0
56	MG	CA	3044	1/1	0.94	0.07	84,84,84,84	0
56	MG	CA	3102	1/1	0.94	0.13	114,114,114,114	0
56	MG	AA	1610	1/1	0.94	0.30	99,99,99,99	0
56	MG	DA	3007	1/1	0.94	0.09	112,112,112,112	0
64	PGE	DA	3216	10/10	0.94	0.21	62,64,65,65	0
56	MG	AA	1656	1/1	0.94	0.09	149,149,149,149	0
56	MG	CA	3153	1/1	0.94	0.19	90,90,90,90	0
58	MPD	AA	1676	8/8	0.94	0.20	97,100,100,102	0
56	MG	CA	3086	1/1	0.94	0.11	97,97,97,97	0
56	MG	DA	3081	1/1	0.94	0.11	94,94,94,94	0
56	MG	CA	3025	1/1	0.94	0.10	105,105,105,105	0
56	MG	CA	3041	1/1	0.94	0.08	71,71,71,71	0
56	MG	DA	3120	1/1	0.94	0.17	55,55,55,55	0
56	MG	DA	3230	1/1	0.94	0.15	45,45,45,45	0
56	MG	CA	3052	1/1	0.94	0.07	97,97,97,97	0
56	MG	AA	1649	1/1	0.95	0.09	77,77,77,77	0
56	MG	DA	3181	1/1	0.95	0.28	91,91,91,91	0
61	ZN	C5	101	1/1	0.95	0.07	148,148,148,148	0
56	MG	DB	205	1/1	0.95	0.09	49,49,49,49	0
56	MG	CA	3096	1/1	0.95	0.09	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3141	1/1	0.95	0.16	66,66,66,66	0
56	MG	AA	1633	1/1	0.95	0.14	101,101,101,101	0
56	MG	AA	1659	1/1	0.95	0.07	97,97,97,97	0
56	MG	CA	3015	1/1	0.95	0.21	83,83,83,83	0
56	MG	DA	3009	1/1	0.95	0.07	102,102,102,102	0
56	MG	DA	3146	1/1	0.95	0.09	72,72,72,72	0
56	MG	DA	3038	1/1	0.95	0.15	29,29,29,29	0
56	MG	BA	1610	1/1	0.95	0.09	109,109,109,109	0
56	MG	CA	3051	1/1	0.95	0.08	109,109,109,109	0
56	MG	AA	1632	1/1	0.95	0.08	124,124,124,124	0
56	MG	DA	3152	1/1	0.95	0.15	47,47,47,47	0
56	MG	BA	1613	1/1	0.95	0.09	78,78,78,78	0
56	MG	CA	3019	1/1	0.95	0.08	79,79,79,79	0
56	MG	AA	1639	1/1	0.95	0.07	132,132,132,132	0
56	MG	DA	3135	1/1	0.95	0.17	72,72,72,72	0
56	MG	BA	1616	1/1	0.95	0.13	149,149,149,149	0
63	EDO	DA	3197	4/4	0.96	0.11	68,68,69,69	0
56	MG	DA	3044	1/1	0.96	0.07	36,36,36,36	0
56	MG	DA	3227	1/1	0.96	0.06	45,45,45,45	0
56	MG	DA	3229	1/1	0.96	0.10	55,55,55,55	0
56	MG	AA	1651	1/1	0.96	0.06	70,70,70,70	0
56	MG	AA	1620	1/1	0.96	0.27	83,83,83,83	0
56	MG	BA	1631	1/1	0.96	0.06	71,71,71,71	0
56	MG	DA	3149	1/1	0.96	0.42	77,77,77,77	0
56	MG	AA	1635	1/1	0.96	0.07	100,100,100,100	0
59	PUT	DA	3002	6/6	0.96	0.15	45,52,54,55	0
64	PGE	DA	3186	10/10	0.96	0.09	39,46,49,50	0
56	MG	CA	3042	1/1	0.96	0.06	91,91,91,91	0
56	MG	CA	3066	1/1	0.96	0.07	125,125,125,125	0
56	MG	DA	3119	1/1	0.96	0.06	63,63,63,63	0
56	MG	CA	3043	1/1	0.96	0.08	101,101,101,101	0
65	SPD	DA	3187	10/10	0.96	0.14	38,40,48,50	0
56	MG	DA	3174	1/1	0.96	0.18	78,78,78,78	0
56	MG	DB	208	1/1	0.96	0.18	64,64,64,64	0
56	MG	BA	1620	1/1	0.96	0.07	97,97,97,97	0
56	MG	DA	3005	1/1	0.96	0.08	81,81,81,81	0
56	MG	CA	3011	1/1	0.96	0.12	117,117,117,117	0
56	MG	BA	1635	1/1	0.96	0.08	111,111,111,111	0
56	MG	DA	3013	1/1	0.96	0.09	71,71,71,71	0
56	MG	BA	1622	1/1	0.96	0.07	95,95,95,95	0
56	MG	DA	3029	1/1	0.97	0.08	61,61,61,61	0
56	MG	CA	3144	1/1	0.97	0.06	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3050	1/1	0.97	0.06	91,91,91,91	0
56	MG	DR	201	1/1	0.97	0.14	44,44,44,44	0
56	MG	AA	1640	1/1	0.97	0.07	62,62,62,62	0
56	MG	AA	1650	1/1	0.97	0.06	87,87,87,87	0
56	MG	CA	3114	1/1	0.97	0.22	62,62,62,62	0
56	MG	DA	3091	1/1	0.97	0.10	55,55,55,55	0
56	MG	DA	3099	1/1	0.97	0.06	78,78,78,78	0
56	MG	DA	3100	1/1	0.97	0.07	30,30,30,30	0
56	MG	CA	3053	1/1	0.97	0.17	108,108,108,108	0
56	MG	BA	1605	1/1	0.97	0.07	125,125,125,125	0
56	MG	DA	3137	1/1	0.97	0.13	47,47,47,47	0
56	MG	CA	3085	1/1	0.97	0.04	89,89,89,89	0
58	MPD	DS	203	8/8	0.97	0.17	37,40,44,47	0
56	MG	AA	1634	1/1	0.97	0.12	108,108,108,108	0
56	MG	DA	3160	1/1	0.97	0.08	72,72,72,72	0
56	MG	CA	3087	1/1	0.97	0.04	97,97,97,97	0
56	MG	CA	3070	1/1	0.97	0.05	112,112,112,112	0
56	MG	BA	1621	1/1	0.97	0.13	42,42,42,42	0
56	MG	DA	3016	1/1	0.97	0.08	44,44,44,44	0
56	MG	BA	1628	1/1	0.98	0.07	111,111,111,111	0
56	MG	AA	1653	1/1	0.98	0.05	75,75,75,75	0
56	MG	DA	3027	1/1	0.98	0.15	71,71,71,71	0
56	MG	AA	1643	1/1	0.98	0.06	78,78,78,78	0
56	MG	DA	3036	1/1	0.98	0.06	34,34,34,34	0
56	MG	AA	1638	1/1	0.98	0.05	103,103,103,103	0
56	MG	DA	3043	1/1	0.98	0.04	31,31,31,31	0
56	MG	DB	201	1/1	0.98	0.08	64,64,64,64	0
56	MG	CA	3045	1/1	0.98	0.07	93,93,93,93	0
56	MG	DA	3157	1/1	0.98	0.19	73,73,73,73	0
56	MG	DA	3053	1/1	0.98	0.05	78,78,78,78	0
56	MG	BA	1632	1/1	0.98	0.10	72,72,72,72	0
56	MG	AA	1652	1/1	0.98	0.20	57,57,57,57	0
56	MG	DA	3073	1/1	0.98	0.04	47,47,47,47	0
56	MG	DA	3080	1/1	0.98	0.07	109,109,109,109	0
56	MG	CA	3103	1/1	0.98	0.05	120,120,120,120	0
56	MG	DA	3083	1/1	0.98	0.04	69,69,69,69	0
56	MG	DA	3088	1/1	0.98	0.05	45,45,45,45	0
56	MG	BA	1645	1/1	0.98	0.07	98,98,98,98	0
61	ZN	D5	101	1/1	0.98	0.04	60,60,60,60	0
56	MG	DA	3094	1/1	0.98	0.10	35,35,35,35	0
56	MG	DA	3095	1/1	0.98	0.07	33,33,33,33	0
56	MG	DA	3096	1/1	0.98	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3097	1/1	0.98	0.07	45,45,45,45	0
56	MG	DA	3098	1/1	0.98	0.04	29,29,29,29	0
56	MG	BA	1602	1/1	0.98	0.06	100,100,100,100	0
56	MG	DA	3006	1/1	0.98	0.05	68,68,68,68	0
67	ACY	DA	3191	4/4	0.98	0.07	56,57,58,59	0
56	MG	DA	3107	1/1	0.98	0.11	47,47,47,47	0
56	MG	AA	1666	1/1	0.98	0.05	67,67,67,67	0
56	MG	DA	3114	1/1	0.98	0.12	62,62,62,62	0
56	MG	AA	1667	1/1	0.98	0.06	49,49,49,49	0
56	MG	DA	3086	1/1	0.99	0.04	39,39,39,39	0
56	MG	DA	3015	1/1	0.99	0.04	18,18,18,18	0
56	MG	DA	3090	1/1	0.99	0.05	26,26,26,26	0
56	MG	BA	1615	1/1	0.99	0.03	76,76,76,76	0
56	MG	DA	3017	1/1	0.99	0.04	56,56,56,56	0
56	MG	DA	3018	1/1	0.99	0.04	29,29,29,29	0
56	MG	DA	3020	1/1	0.99	0.22	33,33,33,33	0
56	MG	DA	3021	1/1	0.99	0.07	48,48,48,48	0
56	MG	DA	3022	1/1	0.99	0.05	43,43,43,43	0
56	MG	DA	3023	1/1	0.99	0.10	34,34,34,34	0
56	MG	AA	1646	1/1	0.99	0.04	65,65,65,65	0
56	MG	DA	3103	1/1	0.99	0.04	44,44,44,44	0
56	MG	DA	3104	1/1	0.99	0.06	42,42,42,42	0
56	MG	DA	3105	1/1	0.99	0.08	39,39,39,39	0
56	MG	DA	3106	1/1	0.99	0.09	31,31,31,31	0
56	MG	DB	202	1/1	0.99	0.04	29,29,29,29	0
56	MG	DA	3108	1/1	0.99	0.03	36,36,36,36	0
56	MG	DA	3111	1/1	0.99	0.04	32,32,32,32	0
56	MG	DA	3031	1/1	0.99	0.03	46,46,46,46	0
56	MG	DA	3032	1/1	0.99	0.04	42,42,42,42	0
56	MG	DA	3115	1/1	0.99	0.06	49,49,49,49	0
56	MG	DA	3116	1/1	0.99	0.07	28,28,28,28	0
56	MG	DB	204	1/1	0.99	0.03	56,56,56,56	0
56	MG	AA	1641	1/1	0.99	0.07	92,92,92,92	0
56	MG	DA	3039	1/1	0.99	0.01	20,20,20,20	0
56	MG	DA	3042	1/1	0.99	0.04	20,20,20,20	0
56	MG	AA	1662	1/1	0.99	0.09	110,110,110,110	0
56	MG	AA	1648	1/1	0.99	0.04	76,76,76,76	0
56	MG	AA	1631	1/1	0.99	0.03	56,56,56,56	0
56	MG	DA	3046	1/1	0.99	0.03	47,47,47,47	0
56	MG	DA	3228	1/1	0.99	0.03	53,53,53,53	0
56	MG	DA	3047	1/1	0.99	0.03	27,27,27,27	0
56	MG	DA	3048	1/1	0.99	0.04	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3049	1/1	0.99	0.06	33,33,33,33	0
56	MG	DA	3050	1/1	0.99	0.03	43,43,43,43	0
56	MG	BA	1611	1/1	0.99	0.05	66,66,66,66	0
56	MG	DA	3054	1/1	0.99	0.04	57,57,57,57	0
56	MG	DA	3055	1/1	0.99	0.06	49,49,49,49	0
56	MG	DA	3057	1/1	0.99	0.06	57,57,57,57	0
56	MG	AA	1629	1/1	0.99	0.06	83,83,83,83	0
56	MG	DD	302	1/1	0.99	0.03	48,48,48,48	0
56	MG	DA	3066	1/1	0.99	0.04	29,29,29,29	0
56	MG	DA	3067	1/1	0.99	0.08	55,55,55,55	0
56	MG	DA	3068	1/1	0.99	0.04	62,62,62,62	0
56	MG	DA	3069	1/1	0.99	0.05	44,44,44,44	0
56	MG	DA	3070	1/1	0.99	0.09	61,61,61,61	0
56	MG	DA	3071	1/1	0.99	0.03	91,91,91,91	0
56	MG	AA	1637	1/1	0.99	0.04	57,57,57,57	0
56	MG	DA	3074	1/1	0.99	0.02	33,33,33,33	0
56	MG	DA	3075	1/1	0.99	0.07	49,49,49,49	0
56	MG	DA	3076	1/1	0.99	0.06	38,38,38,38	0
56	MG	DA	3078	1/1	0.99	0.03	38,38,38,38	0
56	MG	DA	3079	1/1	0.99	0.07	63,63,63,63	0
56	MG	DA	3008	1/1	0.99	0.04	82,82,82,82	0
56	MG	DM	201	1/1	0.99	0.05	62,62,62,62	0
56	MG	DA	3082	1/1	0.99	0.05	55,55,55,55	0
56	MG	AA	1645	1/1	0.99	0.04	61,61,61,61	0
56	MG	DA	3084	1/1	0.99	0.03	57,57,57,57	0
56	MG	DA	3085	1/1	0.99	0.08	41,41,41,41	0
56	MG	DA	3019	1/1	1.00	0.02	43,43,43,43	0
56	MG	DA	3117	1/1	1.00	0.03	41,41,41,41	0
56	MG	DB	203	1/1	1.00	0.03	39,39,39,39	0
56	MG	DA	3051	1/1	1.00	0.02	17,17,17,17	0
56	MG	DA	3052	1/1	1.00	0.03	36,36,36,36	0
56	MG	DA	3033	1/1	1.00	0.04	26,26,26,26	0
56	MG	DA	3034	1/1	1.00	0.04	28,28,28,28	0
56	MG	DA	3035	1/1	1.00	0.03	24,24,24,24	0
56	MG	DA	3056	1/1	1.00	0.02	22,22,22,22	0
56	MG	DA	3014	1/1	1.00	0.04	19,19,19,19	0
56	MG	DA	3087	1/1	1.00	0.03	48,48,48,48	0
56	MG	DA	3058	1/1	1.00	0.07	31,31,31,31	0
56	MG	DA	3089	1/1	1.00	0.03	36,36,36,36	0
56	MG	DA	3059	1/1	1.00	0.07	37,37,37,37	0
56	MG	DA	3060	1/1	1.00	0.03	16,16,16,16	0
56	MG	DA	3092	1/1	1.00	0.03	31,31,31,31	0

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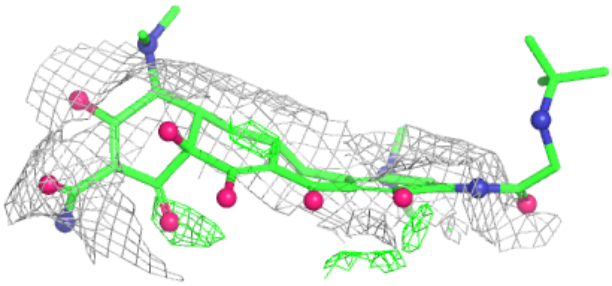
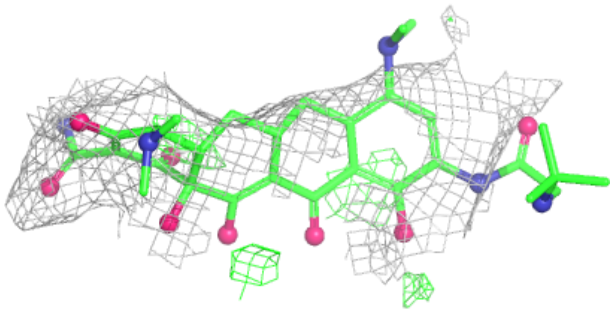
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3093	1/1	1.00	0.04	36,36,36,36	0
56	MG	DA	3061	1/1	1.00	0.03	19,19,19,19	0
56	MG	DA	3062	1/1	1.00	0.01	37,37,37,37	0
56	MG	DA	3037	1/1	1.00	0.08	31,31,31,31	0
56	MG	DA	3064	1/1	1.00	0.06	59,59,59,59	0
56	MG	AA	1668	1/1	1.00	0.09	54,54,54,54	0
56	MG	DA	3010	1/1	1.00	0.05	34,34,34,34	0
56	MG	DA	3040	1/1	1.00	0.05	26,26,26,26	0
56	MG	DA	3101	1/1	1.00	0.04	30,30,30,30	0
56	MG	DA	3102	1/1	1.00	0.05	56,56,56,56	0
56	MG	DA	3041	1/1	1.00	0.03	58,58,58,58	0
56	MG	DA	3024	1/1	1.00	0.06	32,32,32,32	0
56	MG	DA	3025	1/1	1.00	0.08	25,25,25,25	0
56	MG	DA	3026	1/1	1.00	0.02	40,40,40,40	0
56	MG	DA	3072	1/1	1.00	0.06	47,47,47,47	0
56	MG	DA	3011	1/1	1.00	0.09	28,28,28,28	0
56	MG	DA	3109	1/1	1.00	0.04	29,29,29,29	0
56	MG	DA	3110	1/1	1.00	0.02	19,19,19,19	0
56	MG	DA	3028	1/1	1.00	0.06	38,38,38,38	0
56	MG	DA	3012	1/1	1.00	0.03	29,29,29,29	0
56	MG	DA	3113	1/1	1.00	0.04	18,18,18,18	0
56	MG	DA	3030	1/1	1.00	0.04	25,25,25,25	0
56	MG	DA	3077	1/1	1.00	0.05	42,42,42,42	0

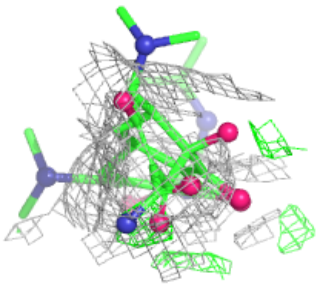
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around T1C BA 1643:

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

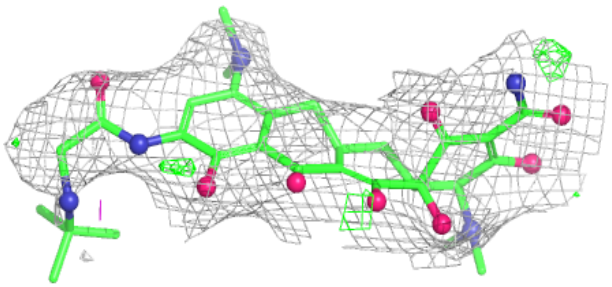


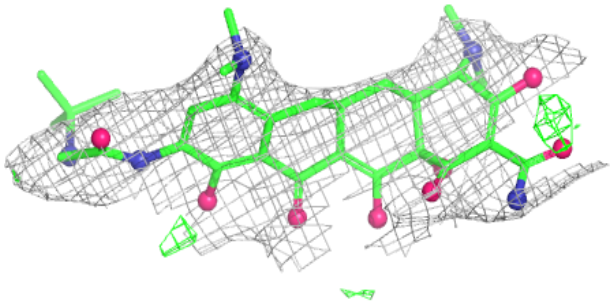


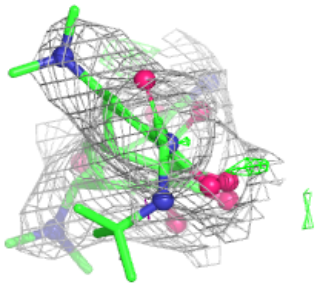


Electron density around T1C AA 1677:

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







6.5 Other polymers (i)

There are no such residues in this entry.