



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 11:24 PM EDT

PDB ID : 4YBB / pdb_00004ybb
Title : High-resolution structure of the Escherichia coli ribosome
Authors : Noeske, J.; Wasserman, M.R.; Terry, D.S.; Altman, R.B.; Blanchard, S.C.;
Cate, J.H.D.
Deposited on : 2015-02-18
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
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

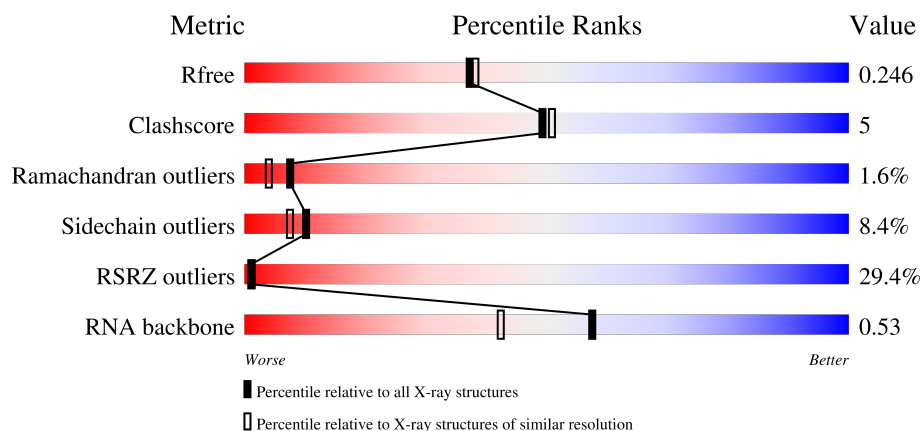
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)
RNA backbone	3983	1006 (2.42-1.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1534	6% 73% 22% 5%
1	BA	1534	6% 70% 24% 6%
2	AB	224	43% 80% 17% .
2	BB	224	61% 77% 21% .

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

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Mol	Chain	Length	Quality of chain
15	BO	88	 60% 61% 23% 15% .
16	AP	82	 17% 89% 7% .
16	BP	82	 91% 68% 24% 6% .
17	AQ	80	 20% 81% 18% .
17	BQ	80	 78% 46% 39% 14% .
18	AR	55	 22% 82% 18%
18	BR	55	 49% 65% 27% 5% .
19	AS	79	 46% 76% 22% ..
19	BS	79	 76% 66% 20% 10% .
20	AT	86	 24% 83% 17%
20	BT	86	 80% 63% 27% 8% ..
21	AU	56	 38% 77% 21% .
21	BU	56	 48% 79% 20% .
22	CA	2904	 15% 71% 23% 5%
23	CB	120	 82% 13% . .
23	DB	120	 88% 11% .
24	CC	271	 90% 70% 25% .
24	DC	271	 18% 89% 10% .
25	CD	209	 85% 78% 18% . .
26	CE	201	 85% 73% 21% 6%
26	DE	201	 2% 96% .
27	CF	177	 62% 68% 29% .
27	DF	177	 25% 82% 16% .
28	CG	176	 65% 76% 21% .
28	DG	176	 9% 88% 11% .

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Mol	Chain	Length	Quality of chain
29	CH	149	 67% 26% 7%
29	DH	149	 56% 23%
30	CJ	134	 72% 24%
30	DJ	134	 79% 23%
31	CK	142	 73% 18%
31	DK	142	 4% 91% 8%
32	CL	123	 72% 25% 5%
32	DL	123	 2% 82% 16%
33	CM	144	 88% 24% 7%
33	DM	144	 3% 85% 15%
34	CN	136	 81% 85% 11%
34	DN	136	 88% 10%
35	CO	125	 88% 67% 21% 6%
35	DO	125	 6% 86% 13%
36	CP	117	 56% 69% 26%
36	DP	117	 4% 91% 7%
37	CQ	114	 79% 81% 18%
37	DQ	114	 8% 89% 11%
38	CR	117	 78% 77% 21%
38	DR	117	 3% 89% 11%
39	CS	103	 83% 75% 21%
39	DS	103	 2% 87% 13%
40	CT	110	 90% 78% 17% 5%
40	DT	110	 95% 5%
41	CU	93	 89% 73% 17% 8%

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Mol	Chain	Length	Quality of chain
41	DU	93	
42	CV	102	
42	DV	102	
43	CW	94	
43	DW	94	
44	CX	76	
44	DX	76	
45	CY	77	
45	DY	77	
46	CZ	62	
46	DZ	62	
47	C0	58	
47	D0	58	
48	C1	56	
48	D1	56	
49	C2	51	
49	D2	51	
50	C3	46	
50	D3	46	
51	C4	64	
51	D4	64	
52	C5	38	
52	D5	38	
53	DA	2903	
54	DD	209	

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Mol	Chain	Length	Quality of chain
55	DI	135	84% 70%27% ..

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	DA	3137	-	-	-	X
57	PG4	DA	3193	-	-	X	-
57	PG4	DR	202	-	-	X	-
58	MPD	DN	201	-	-	X	-
59	PUT	DA	3223	-	-	X	-
61	PEG	D3	102	-	-	X	-
61	PEG	DP	201	-	-	X	-

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295060 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 RNA chain called 23S rRNA.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	2798	U	UNK	conflict	GB 731469900
CA	2800	A	UNK	conflict	GB 731469900

- Molecule 23 is a RNA chain called 5S rRNA.

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

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

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

- Molecule 30 is a protein called 50S ribosomal protein L11.

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

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

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

- Molecule 33 is a protein called 50S ribosomal protein L15.

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

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

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

- Molecule 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

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

- Molecule 42 is a protein called 50S ribosomal protein L24.

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

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

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

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	C0	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	D0	58	Total	C	N	O	S	0	2	0
			463	290	90	81	2			

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	DA	2897	Total	C	N	O	P	0	8	0
			62361	27827	11476	20154	2904			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	2798	U	UNK	conflict	GB 731469900
DA	2800	A	UNK	conflict	GB 731469900

- Molecule 54 is a protein called 50S ribosomal protein L3.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

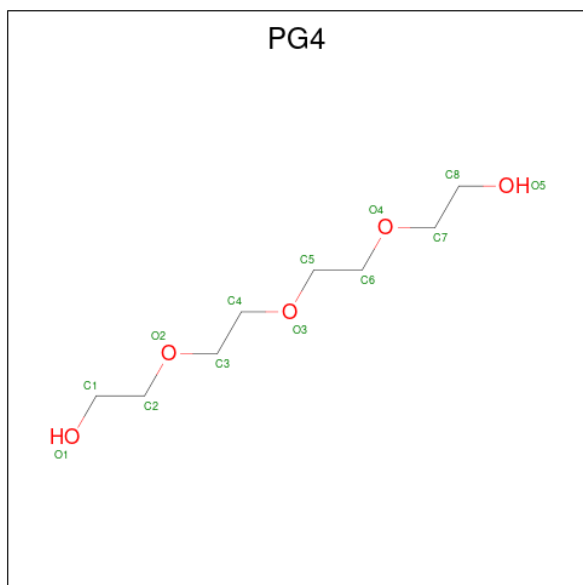
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	70	Total	Mg	0	0
			70	70		
56	BA	41	Total	Mg	0	0
			41	41		
56	CA	155	Total	Mg	0	0
			155	155		
56	CB	3	Total	Mg	0	0
			3	3		
56	C3	1	Total	Mg	0	0
			1	1		

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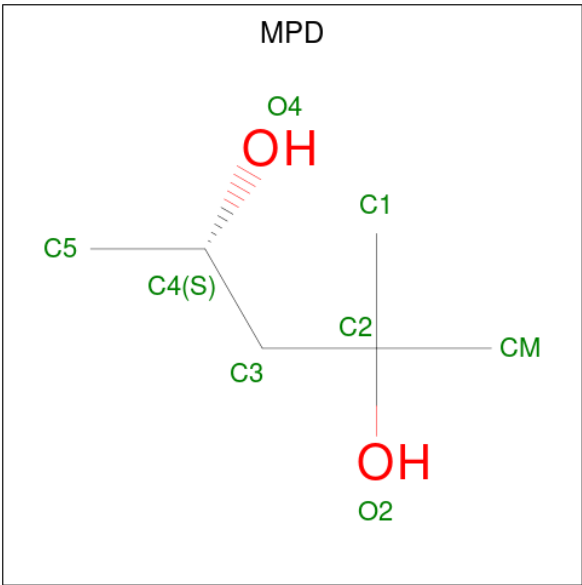
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DA	183	Total	Mg	0	0
			183	183		
56	DB	9	Total	Mg	0	0
			9	9		
56	DR	1	Total	Mg	0	0
			1	1		

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



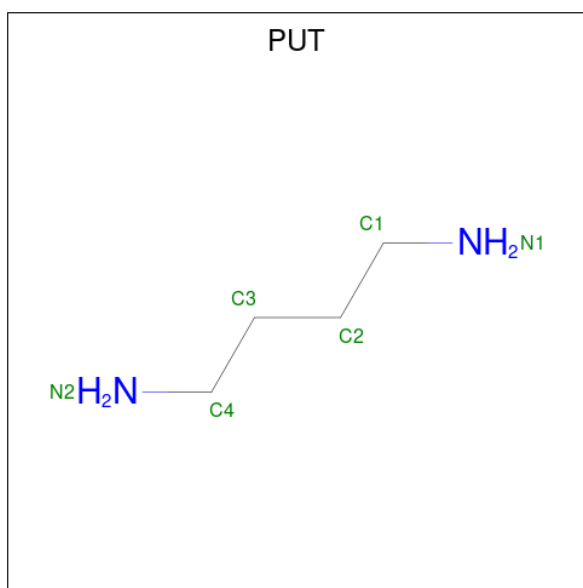
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			13	8	5		
57	BA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DQ	1	Total	C	O	0	0
			13	8	5		
57	DR	1	Total	C	O	0	0
			13	8	5		
57	DS	1	Total	C	O	0	0
			13	8	5		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AA	1	Total	C	O	0	0
			8	6	2		
58	AA	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		
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		

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



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

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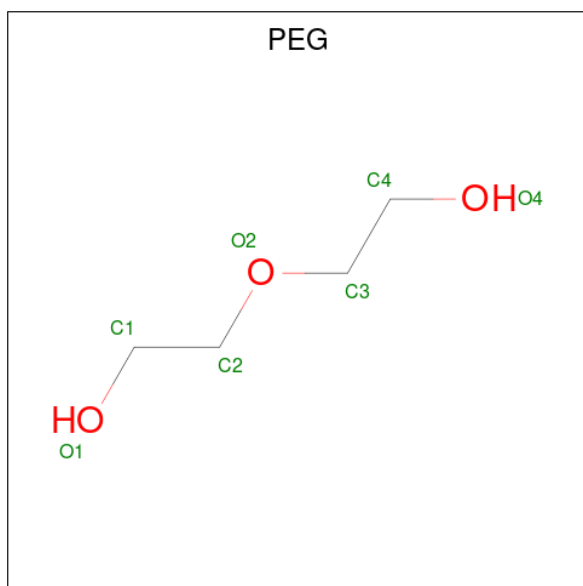
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DM	1	Total	C	N	0	0
			6	4	2		

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

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

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



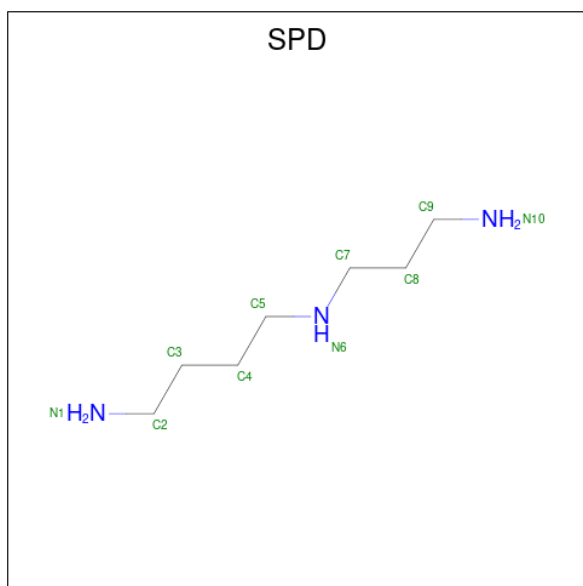
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 62 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



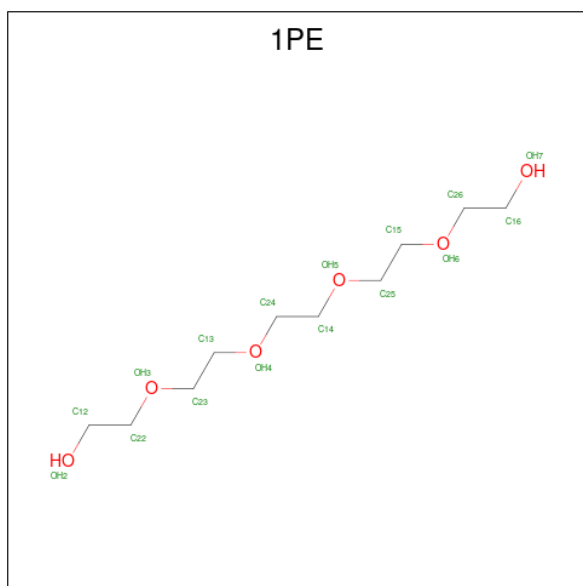
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	DA	1	Total C N 10 7 3	0	0
62	DA	1	Total C N 10 7 3	0	0
62	DA	1	Total C N 10 7 3	0	0

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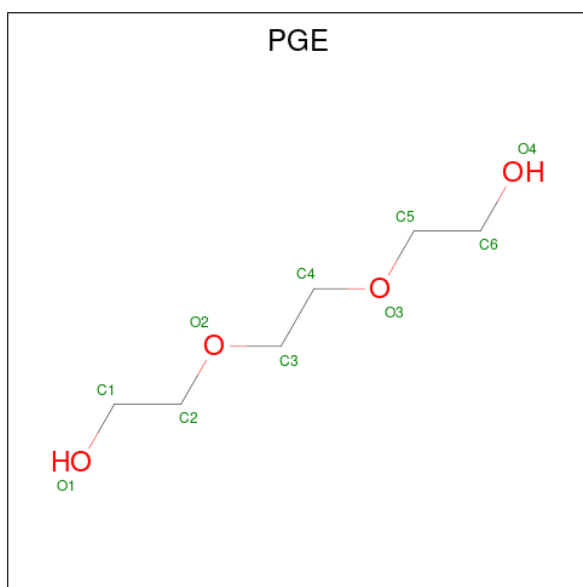
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	DA	1	Total	C	N	0	0
			10	7	3		

- Molecule 63 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



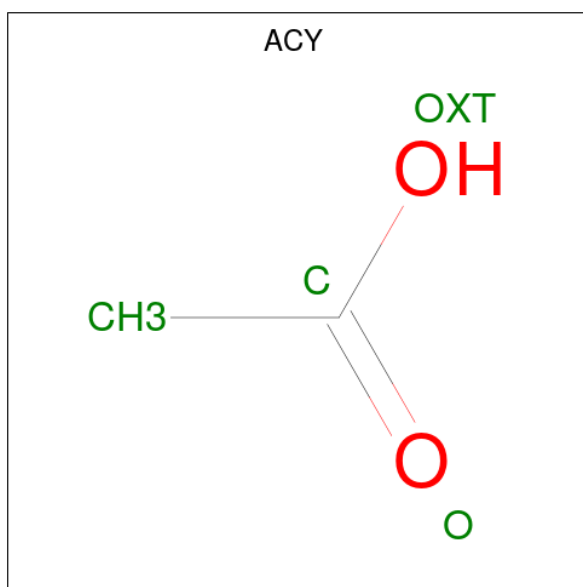
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	DA	1	Total	C	O	0	0
			16	10	6		
63	DA	1	Total	C	O	0	0
			16	10	6		

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



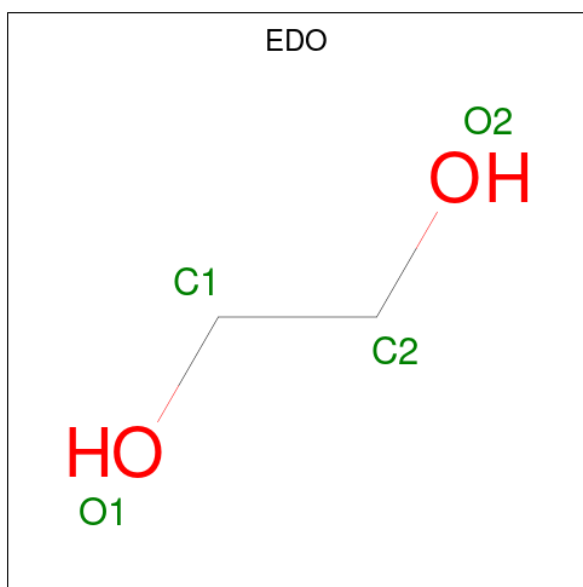
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DS	1	Total	C	O	0	0
			10	6	4		
64	DU	1	Total	C	O	0	0
			10	6	4		
64	D1	1	Total	C	O	0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

- Molecule 65 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 66 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



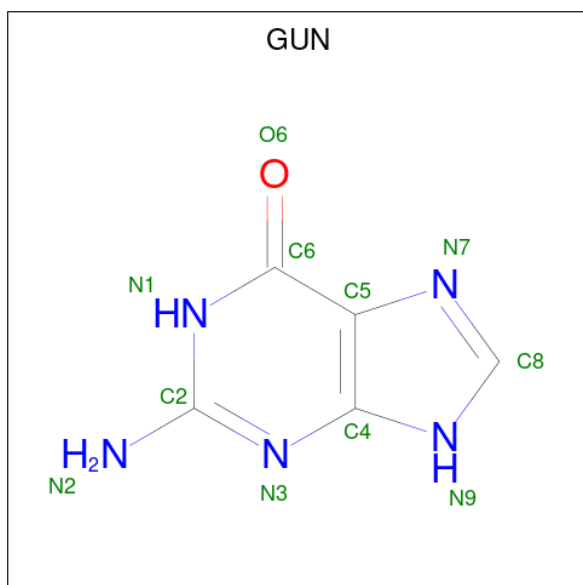
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		

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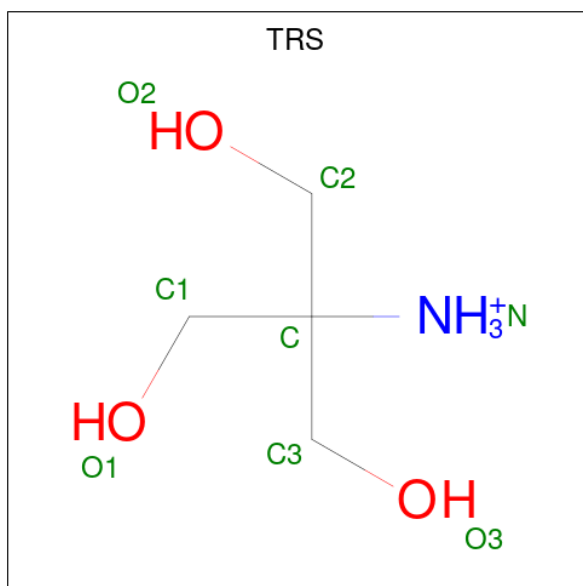
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DB	1	Total	C	O	0	0
			4	2	2		
66	DB	1	Total	C	O	0	0
			4	2	2		
66	DB	1	Total	C	O	0	0
			4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

- Molecule 67 is GUANINE (CCD ID: GUN) (formula: C₅H₅N₅O).



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

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



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

- Molecule 69 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AA	509	Total	O	0	0
			509	509		
69	AC	6	Total	O	0	0
			6	6		
69	AD	2	Total	O	0	0
			2	2		
69	AE	5	Total	O	0	0
			5	5		
69	AF	1	Total	O	0	0
			1	1		
69	AG	1	Total	O	0	0
			1	1		
69	AH	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AJ	2	Total 2	O 2	0	0
69	AK	6	Total 6	O 6	0	0
69	AL	10	Total 10	O 10	0	0
69	AM	4	Total 4	O 4	0	0
69	AN	6	Total 6	O 6	0	0
69	AO	2	Total 2	O 2	0	0
69	AP	2	Total 2	O 2	0	0
69	AS	1	Total 1	O 1	0	0
69	AT	2	Total 2	O 2	0	0
69	AU	2	Total 2	O 2	0	0
69	BA	286	Total 286	O 286	0	0
69	BD	12	Total 12	O 12	0	0
69	BE	1	Total 1	O 1	0	0
69	BF	2	Total 2	O 2	0	0
69	BL	5	Total 5	O 5	0	0
69	BN	3	Total 3	O 3	0	0
69	BO	1	Total 1	O 1	0	0
69	BP	3	Total 3	O 3	0	0
69	BT	5	Total 5	O 5	0	0
69	BU	2	Total 2	O 2	0	0
69	CA	692	Total 692	O 692	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	CB	13	Total 13	O 13	0	0
69	CC	8	Total 8	O 8	0	0
69	CD	6	Total 6	O 6	0	0
69	CE	6	Total 6	O 6	0	0
69	CK	1	Total 1	O 1	0	0
69	CL	1	Total 1	O 1	0	0
69	CM	5	Total 5	O 5	0	0
69	CO	1	Total 1	O 1	0	0
69	CS	1	Total 1	O 1	0	0
69	CU	2	Total 2	O 2	0	0
69	CV	2	Total 2	O 2	0	0
69	CW	1	Total 1	O 1	0	0
69	CY	1	Total 1	O 1	0	0
69	C3	2	Total 2	O 2	0	0
69	C4	1	Total 1	O 1	0	0
69	DA	4815	Total 4815	O 4815	0	0
69	DB	209	Total 209	O 209	0	0
69	DC	106	Total 106	O 106	0	0
69	DD	103	Total 103	O 103	0	0
69	DE	62	Total 62	O 62	0	0
69	DF	14	Total 14	O 14	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DG	6	Total 6	O 6	0	0
69	DH	2	Total 2	O 2	0	0
69	DK	59	Total 59	O 59	0	0
69	DL	45	Total 45	O 45	0	0
69	DM	67	Total 67	O 67	0	0
69	DN	74	Total 74	O 74	0	0
69	DO	42	Total 42	O 42	0	0
69	DP	37	Total 37	O 37	0	0
69	DQ	27	Total 27	O 27	0	0
69	DR	67	Total 67	O 67	0	0
69	DS	50	Total 50	O 50	0	0
69	DT	61	Total 61	O 61	0	0
69	DU	19	Total 19	O 19	0	0
69	DV	22	Total 22	O 22	0	0
69	DW	32	Total 32	O 32	0	0
69	DX	30	Total 30	O 30	0	0
69	DY	10	Total 10	O 10	0	0
69	DZ	8	Total 8	O 8	0	0
69	D0	25	Total 25	O 25	0	0
69	D1	47	Total 47	O 47	0	0
69	D2	9	Total 9	O 9	0	0

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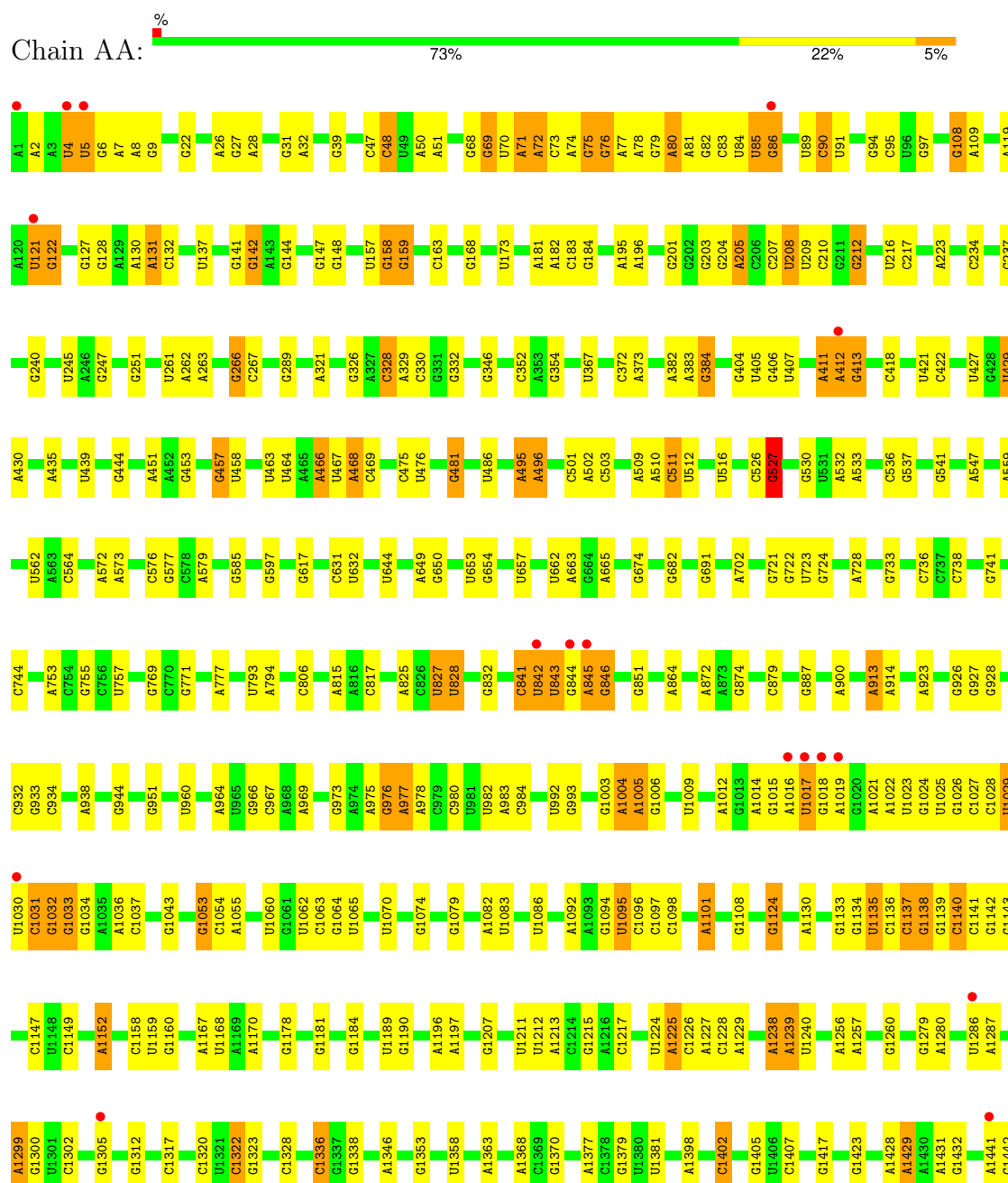
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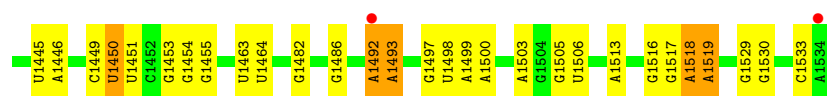
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	D3	25	Total 25	O 25	0	0
69	D4	38	Total 38	O 38	0	0
69	D5	14	Total 14	O 14	0	0

3 Residue-property plots

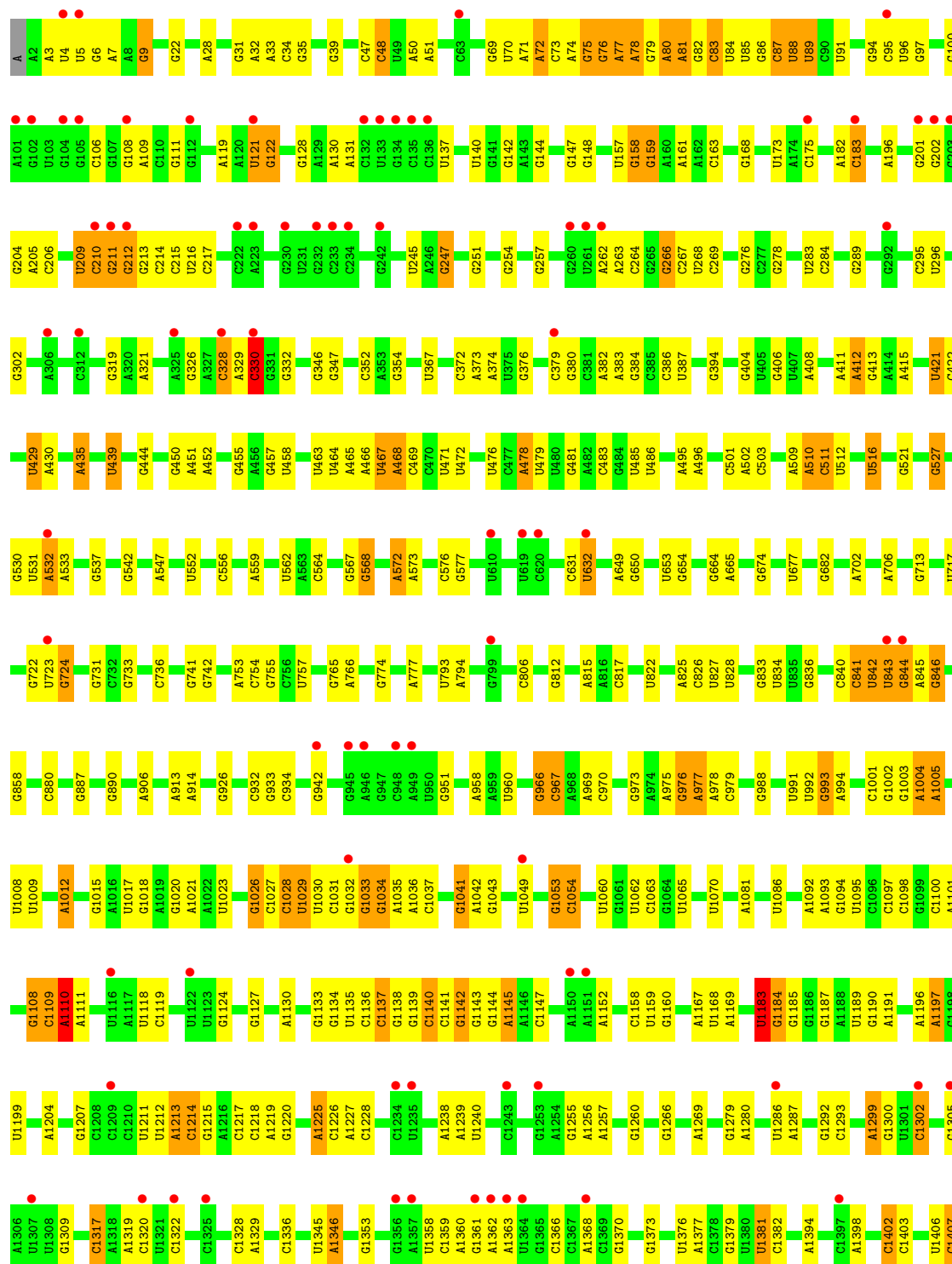
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

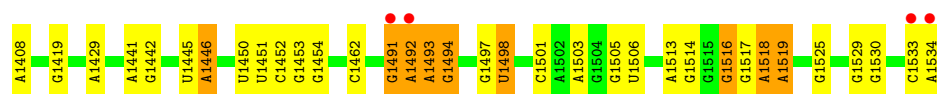
• Molecule 1: 16S rRNA



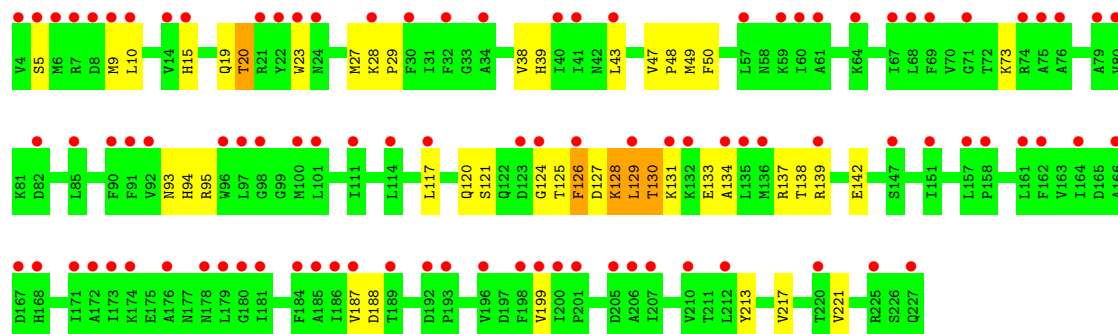
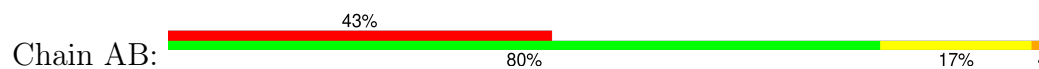


• Molecule 1: 16S rRNA

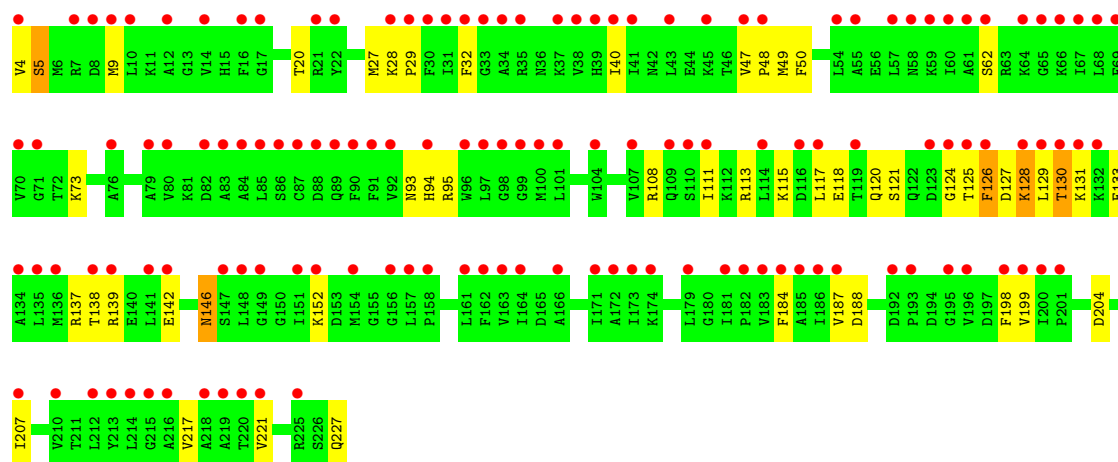
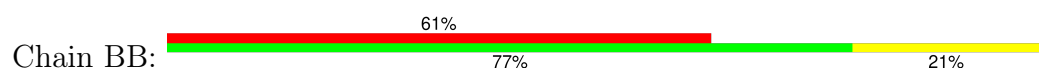




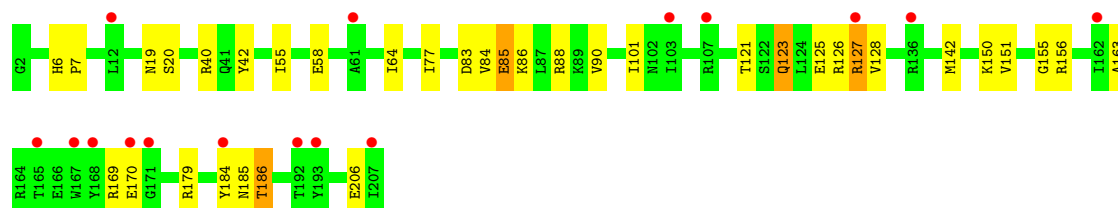
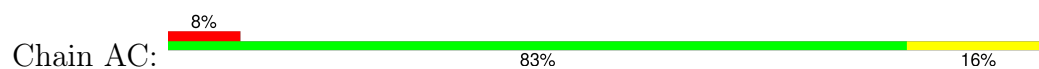
• Molecule 2: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S2

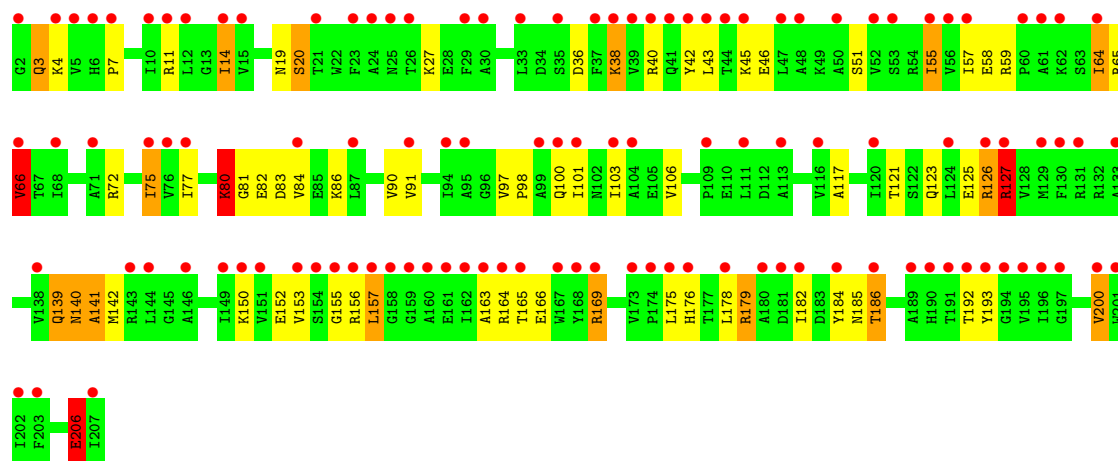


• Molecule 3: 30S ribosomal protein S3

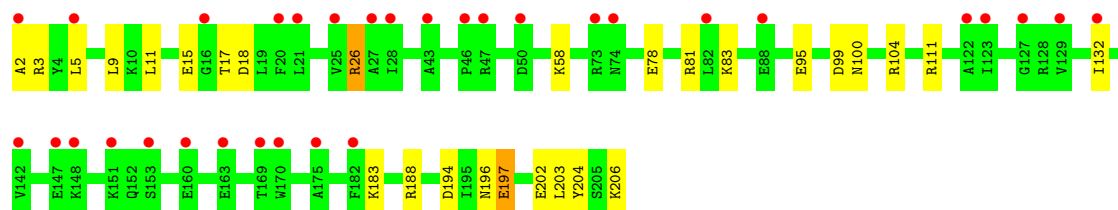
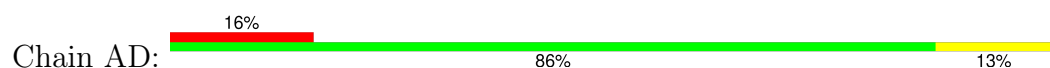


• Molecule 3: 30S ribosomal protein S3

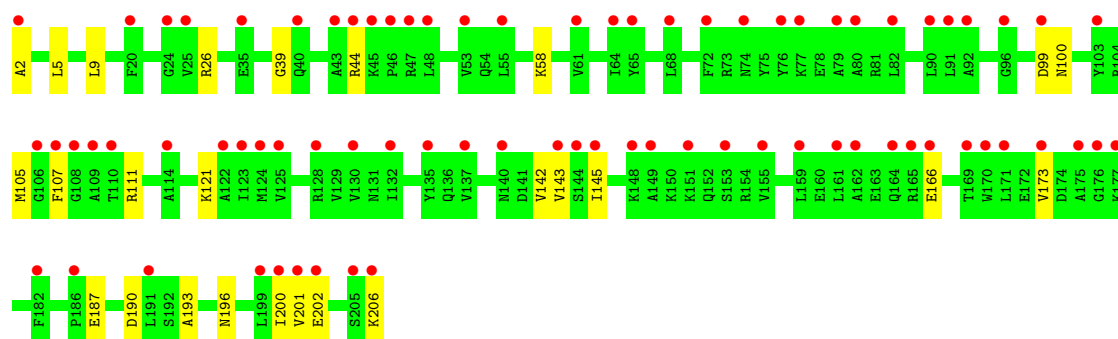
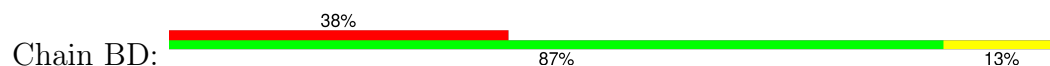




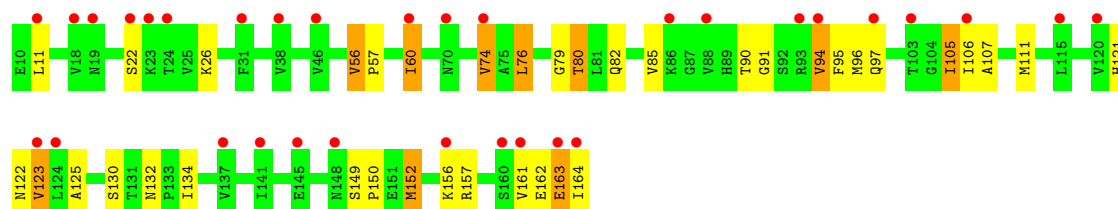
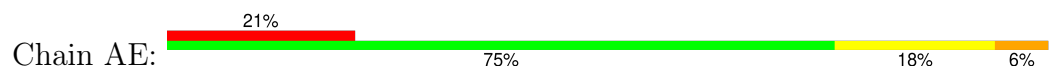
• Molecule 4: 30S ribosomal protein S4



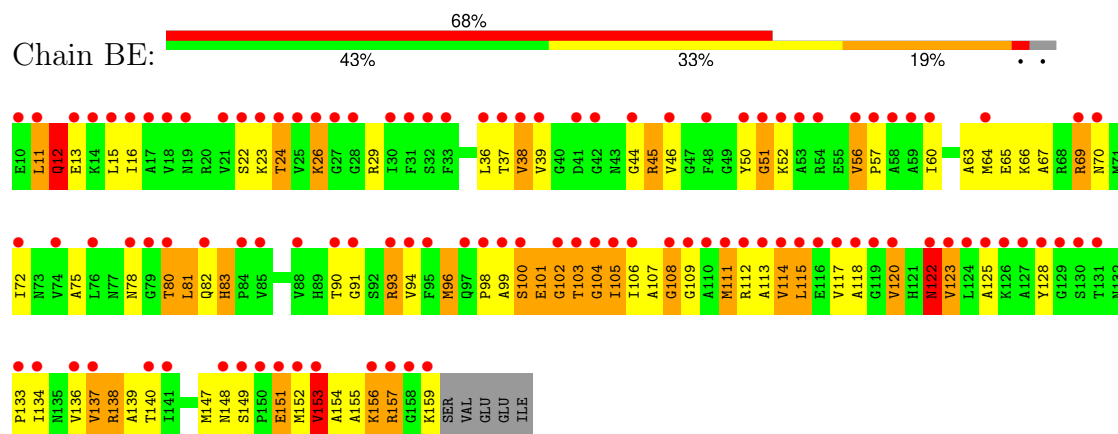
• Molecule 4: 30S ribosomal protein S4



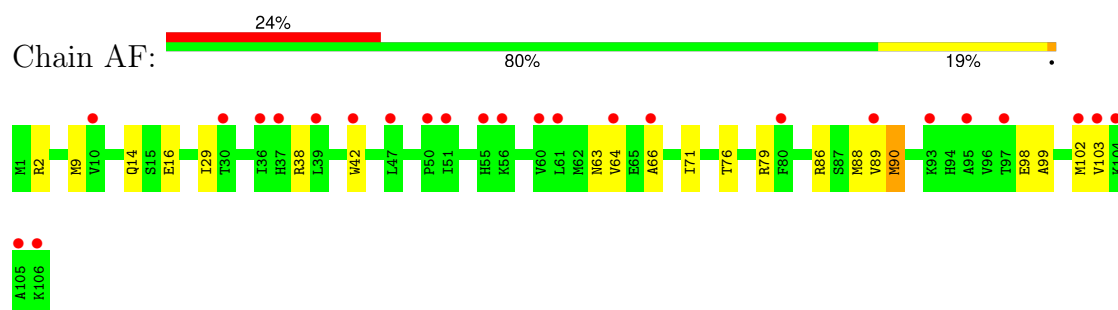
• Molecule 5: 30S ribosomal protein S5



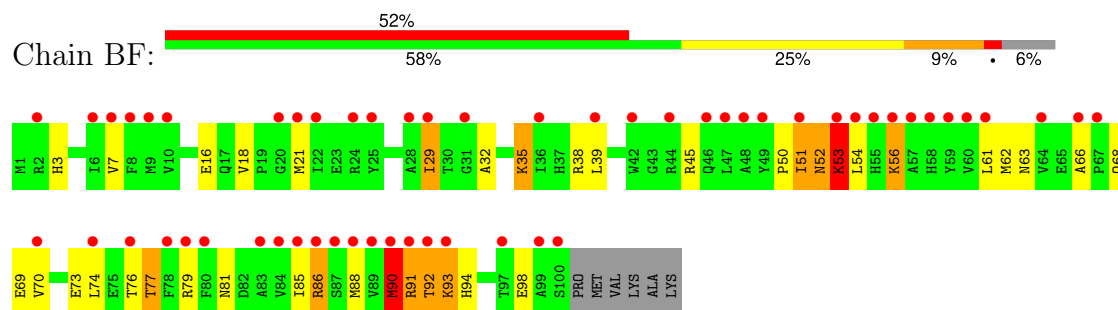
- Molecule 5: 30S ribosomal protein S5



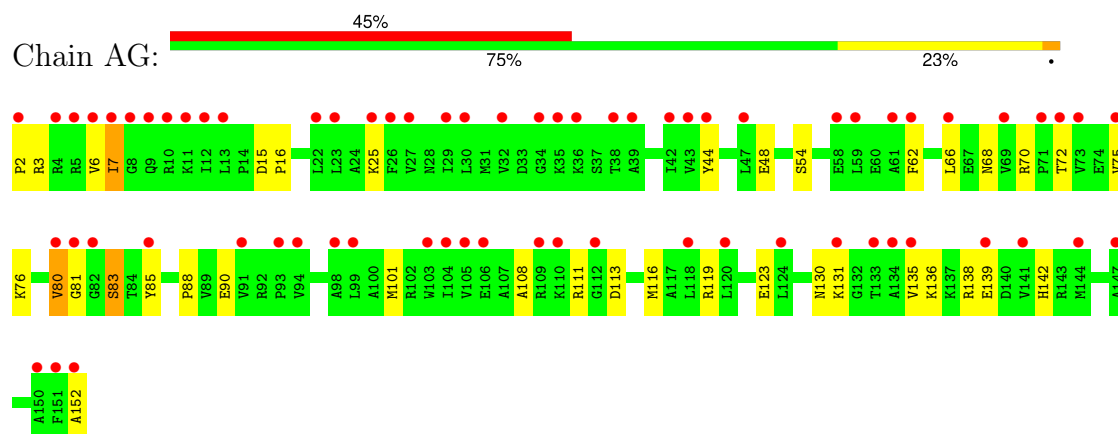
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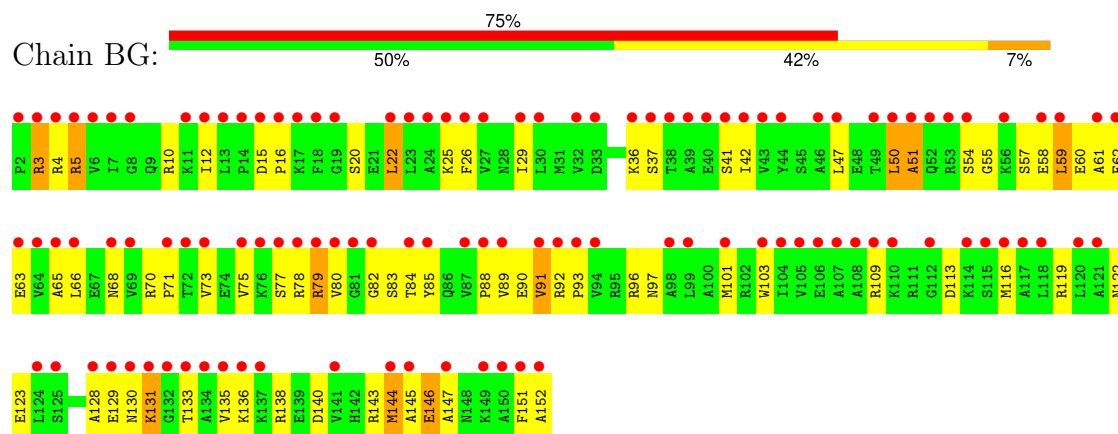
- Molecule 6: 30S ribosomal protein S6



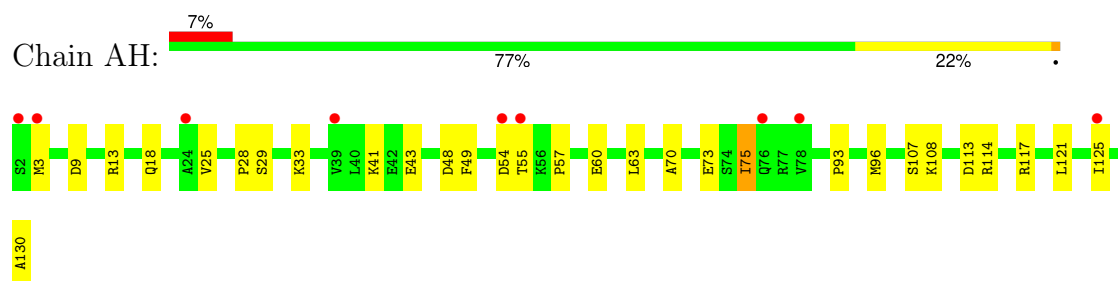
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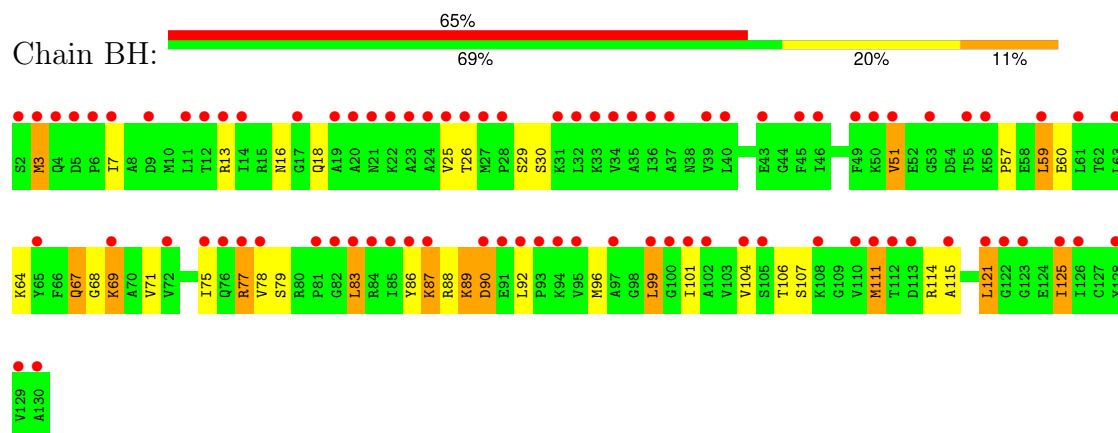
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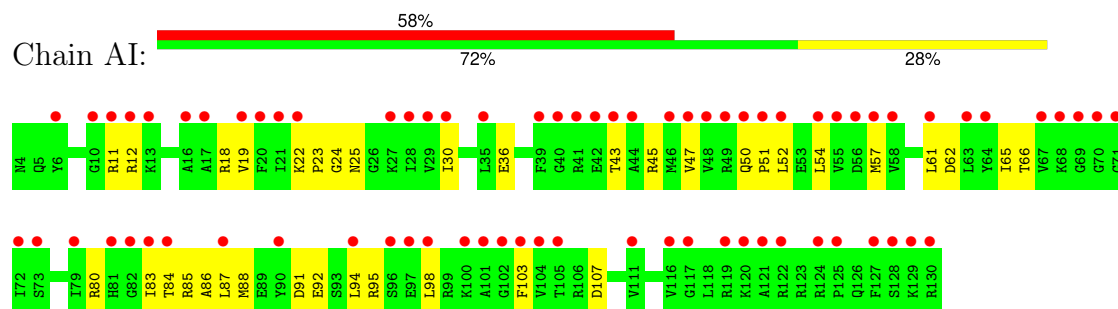
- Molecule 8: 30S ribosomal protein S8



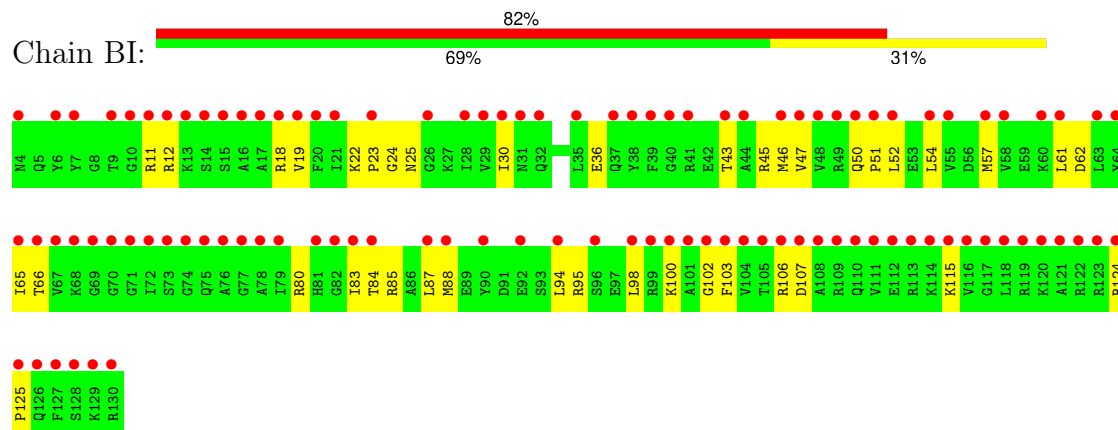
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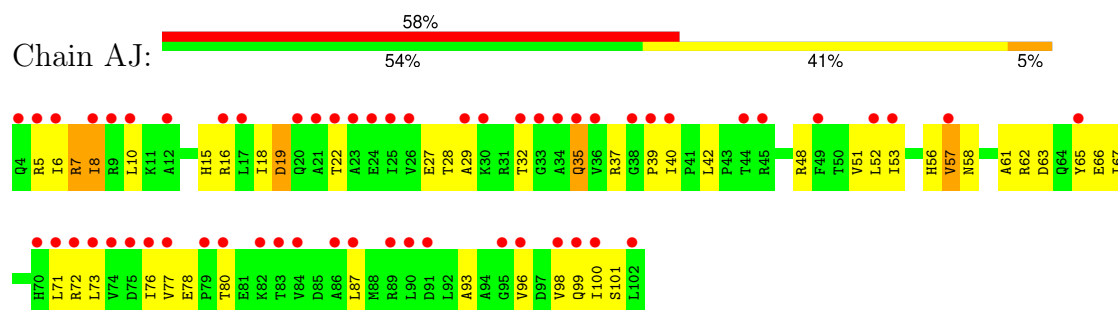
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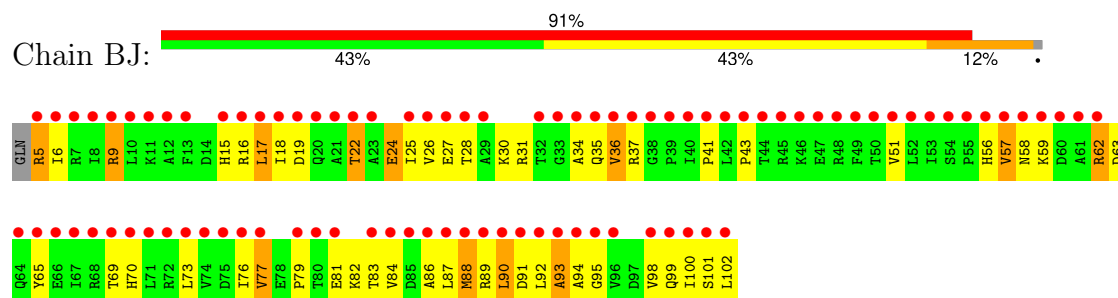
- Molecule 9: 30S ribosomal protein S9



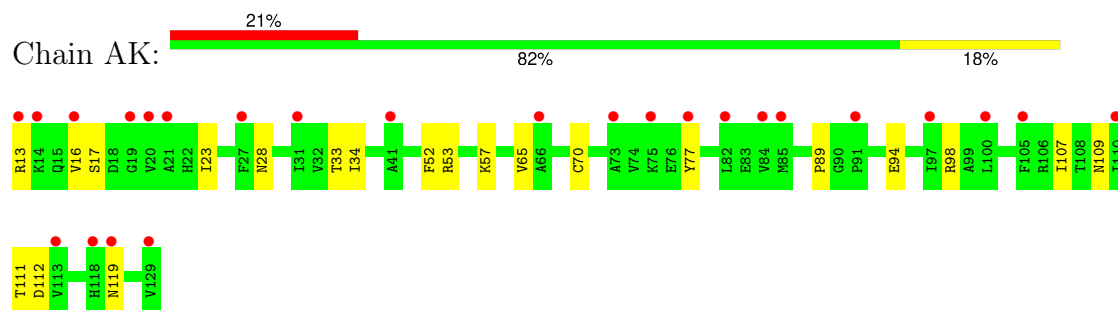
- Molecule 10: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S10

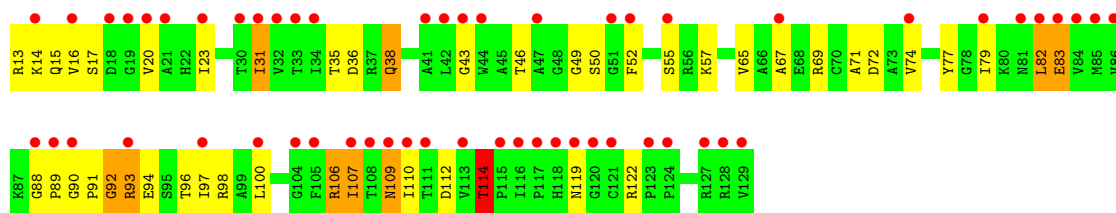


- Molecule 11: 30S ribosomal protein S11

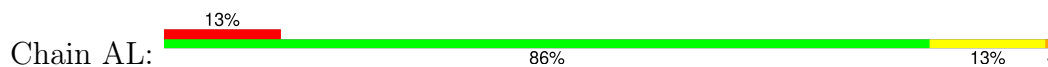


- Molecule 11: 30S ribosomal protein S11

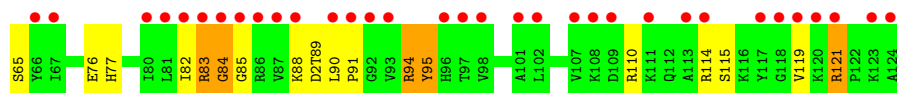
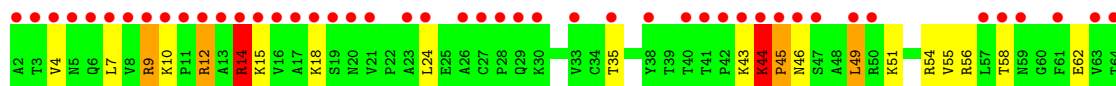




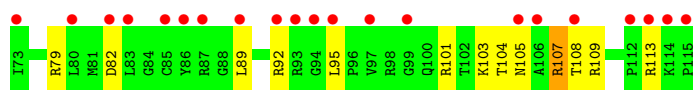
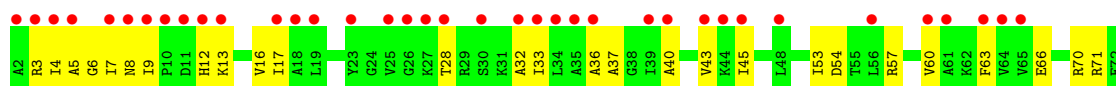
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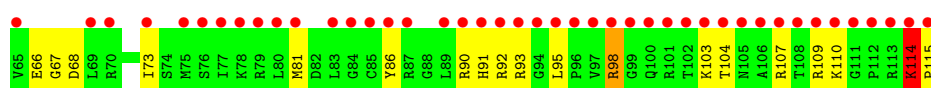
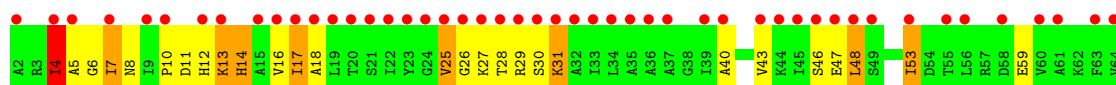
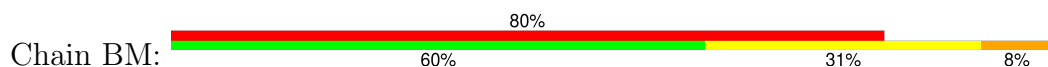
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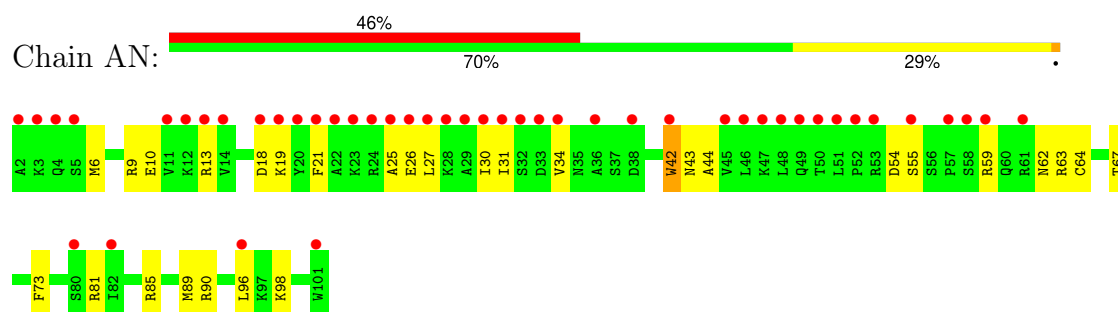
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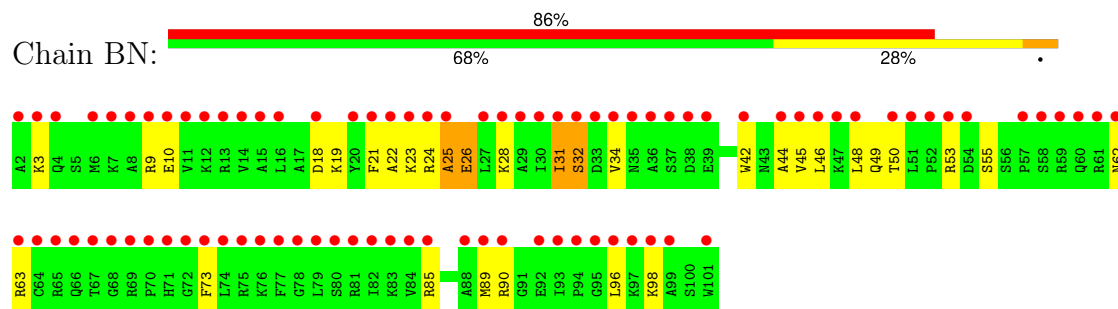
• Molecule 13: 30S ribosomal protein S13



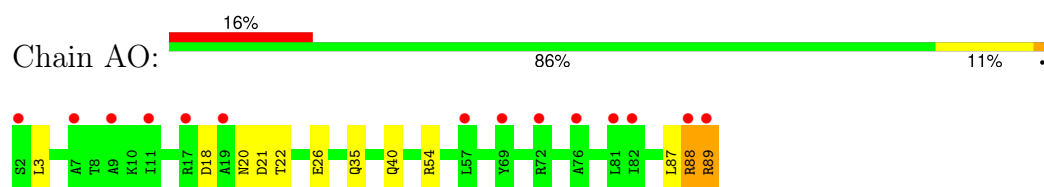
• Molecule 14: 30S ribosomal protein S14



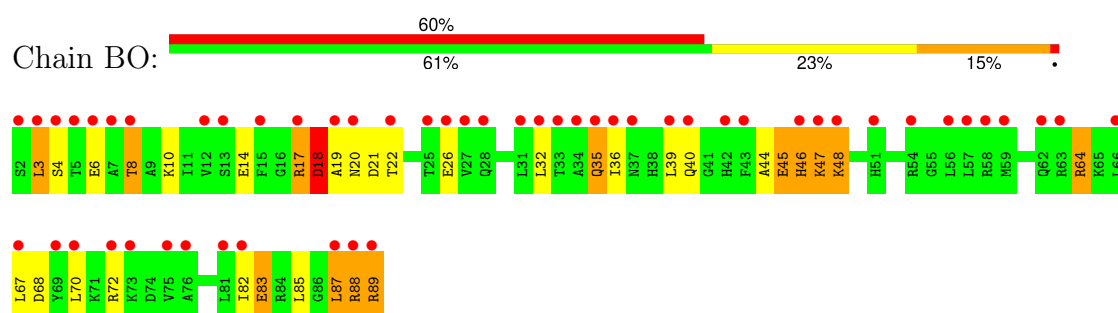
- Molecule 14: 30S ribosomal protein S14



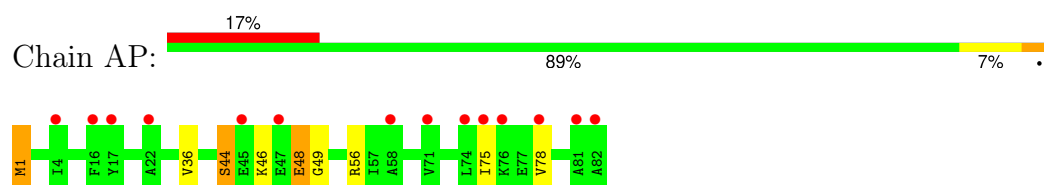
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

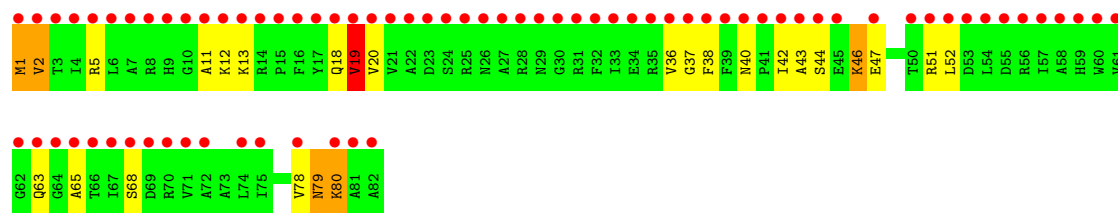


- Molecule 16: 30S ribosomal protein S16

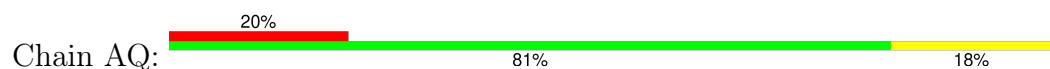


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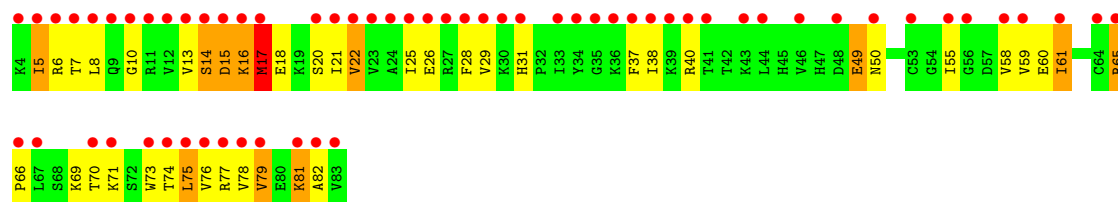
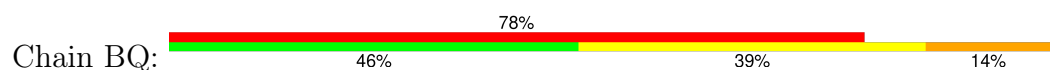




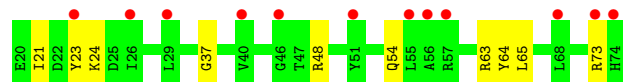
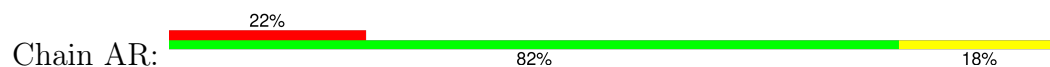
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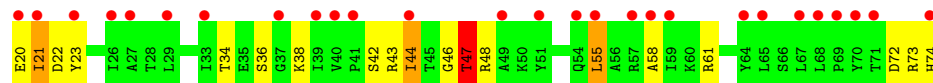
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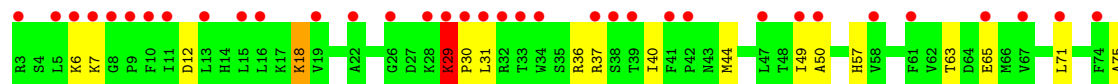
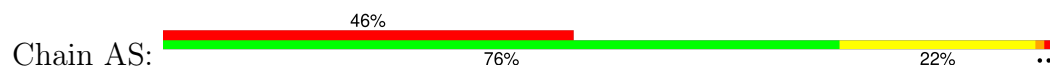
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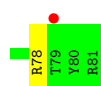


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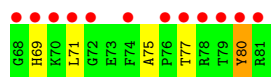
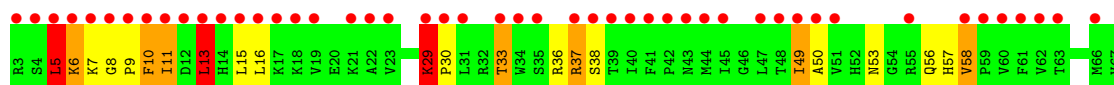
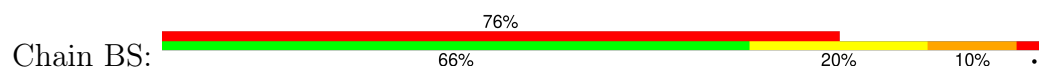


• Molecule 19: 30S ribosomal protein S19

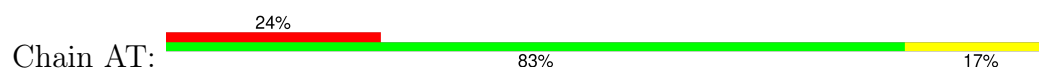




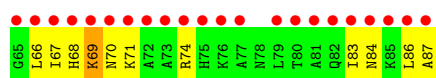
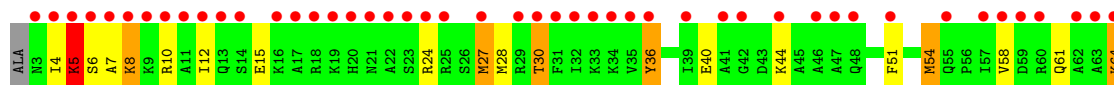
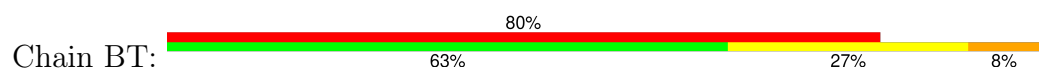
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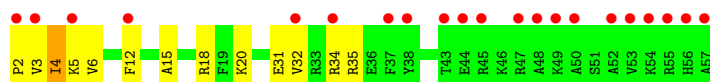
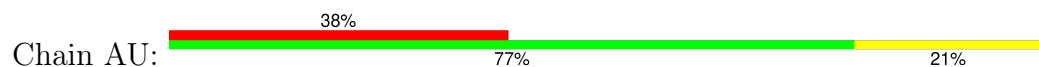
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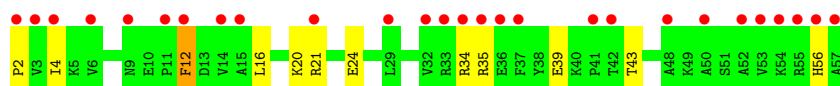
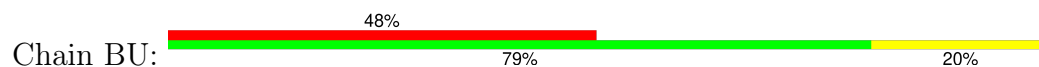
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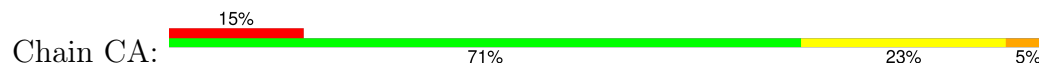
- Molecule 21: 30S ribosomal protein S21

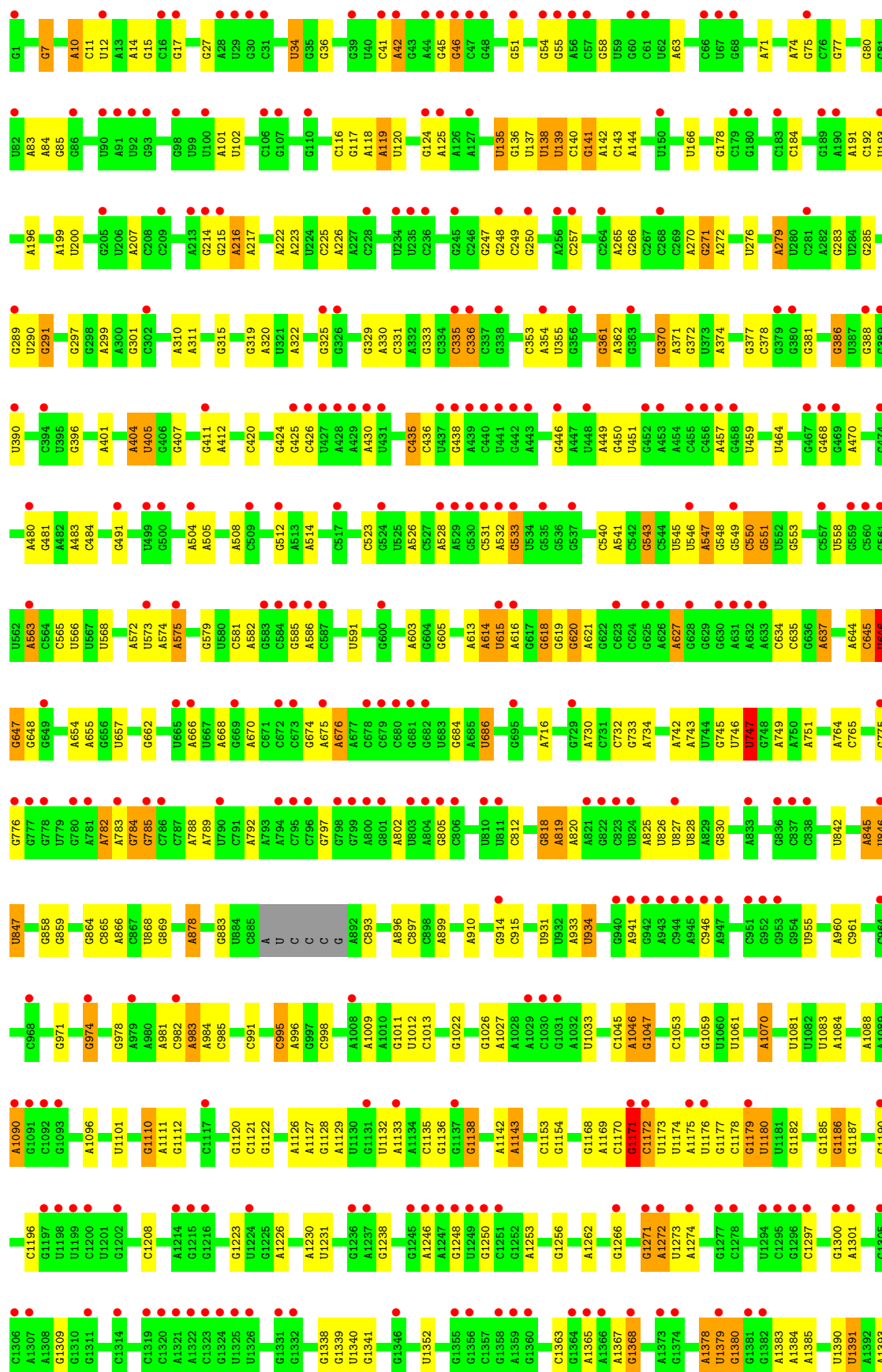


- Molecule 21: 30S ribosomal protein S21

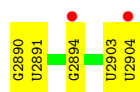


- Molecule 22: 23S rRNA



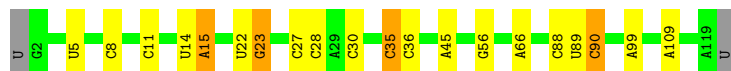


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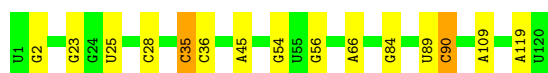
• Molecule 23: 5S rRNA

Chain CB: 82% 13% ..



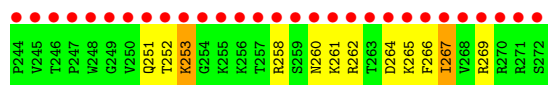
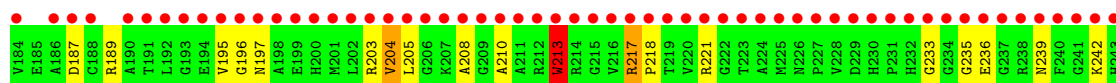
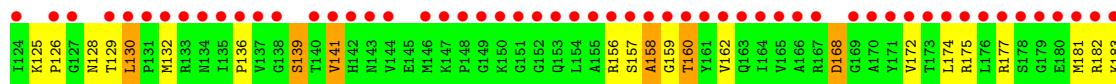
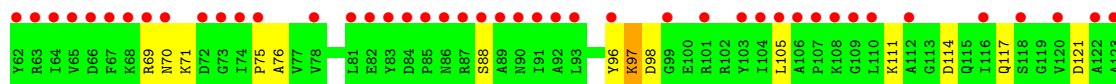
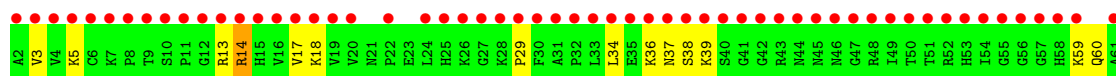
• Molecule 23: 5S rRNA

Chain DB: 88% 11% .



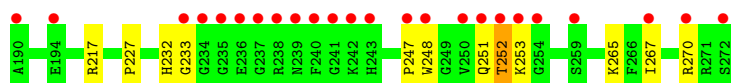
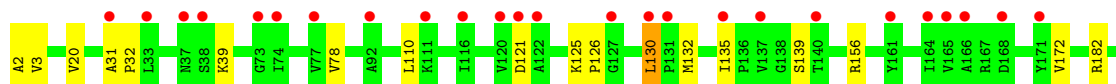
• Molecule 24: 50S ribosomal protein L2

Chain CC: 90% 70% 25% .

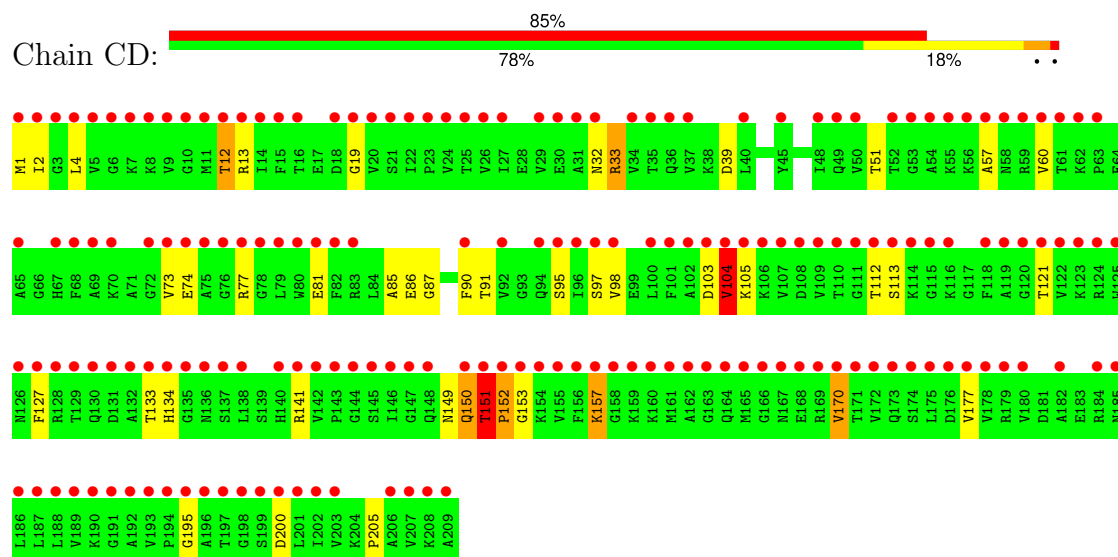


• Molecule 24: 50S ribosomal protein L2

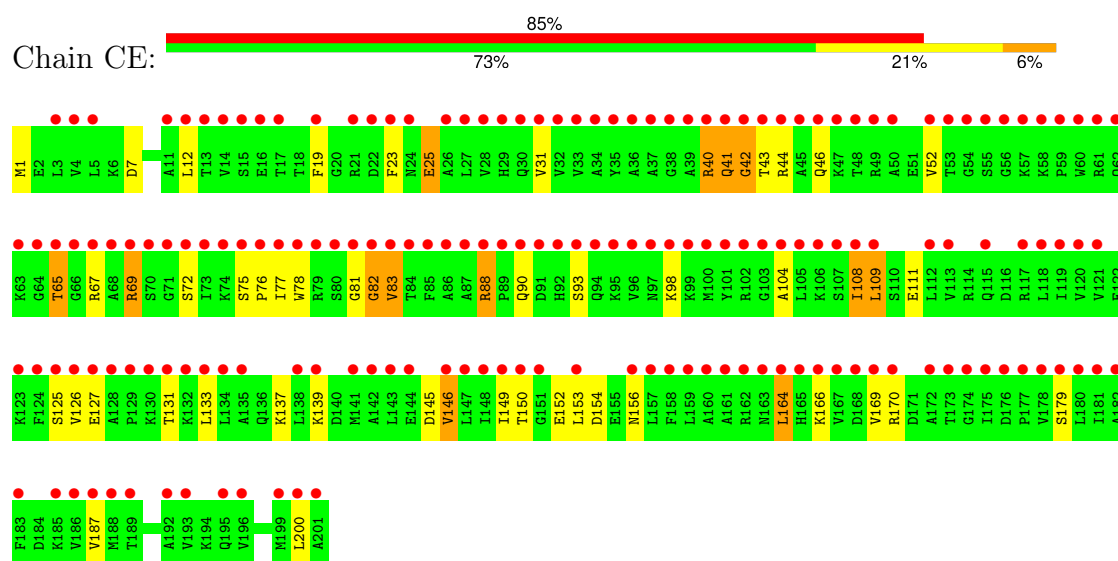
Chain DC: 18% 89% 10% .



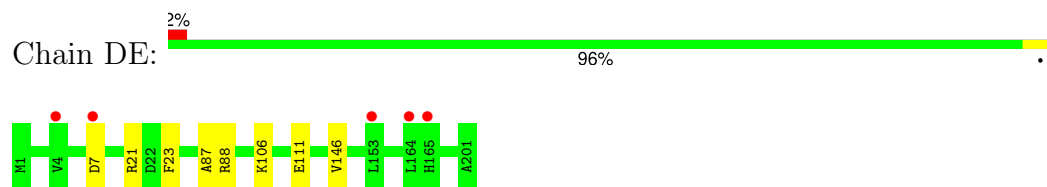
• Molecule 25: 50S ribosomal protein L3



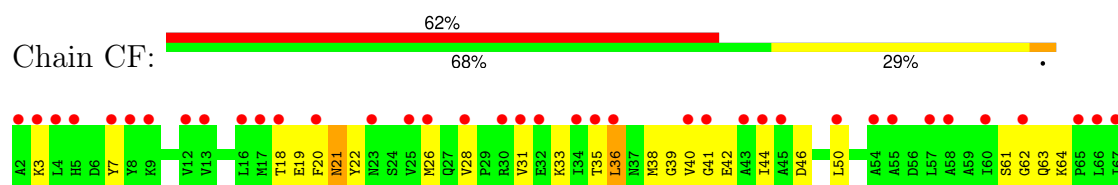
• Molecule 26: 50S ribosomal protein L4

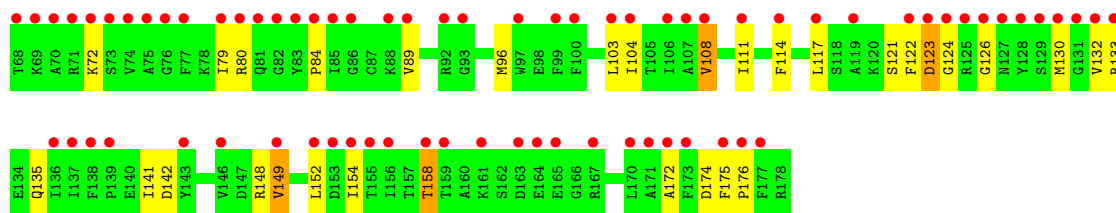


• Molecule 26: 50S ribosomal protein L4

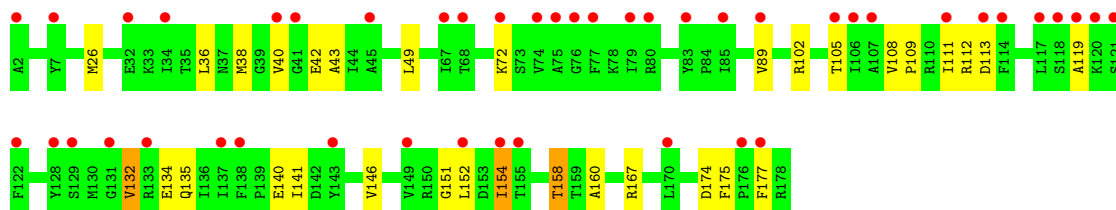
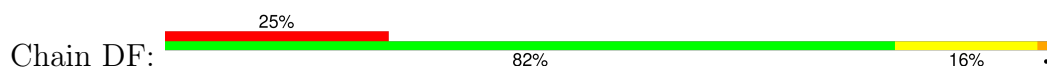


• Molecule 27: 50S ribosomal protein L5

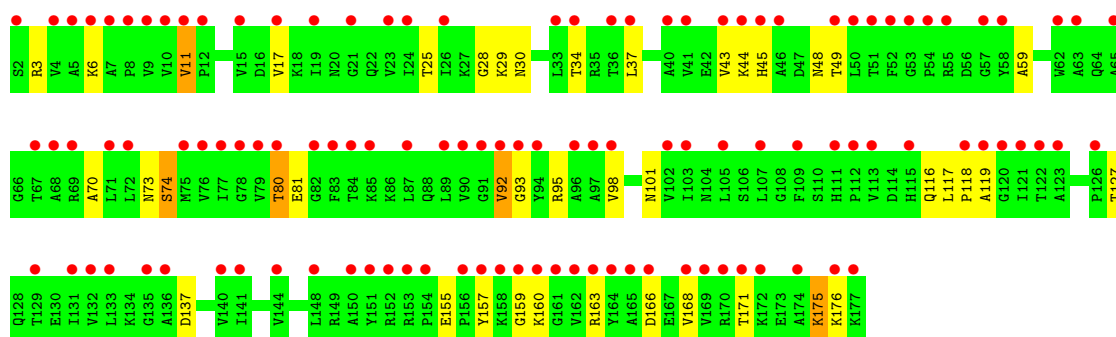
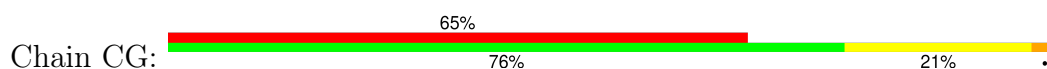




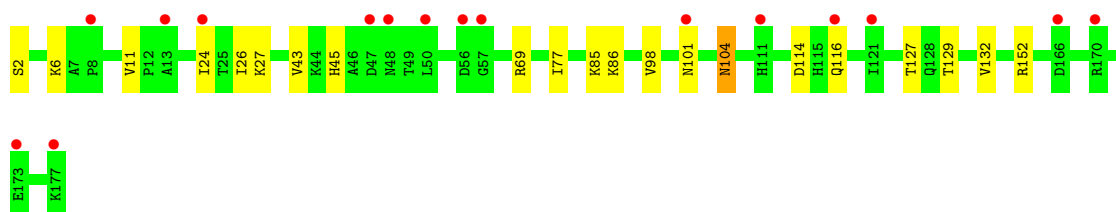
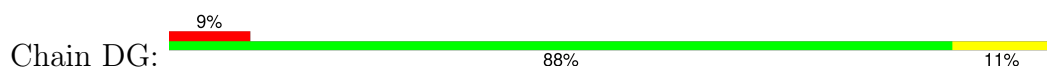
• Molecule 27: 50S ribosomal protein L5



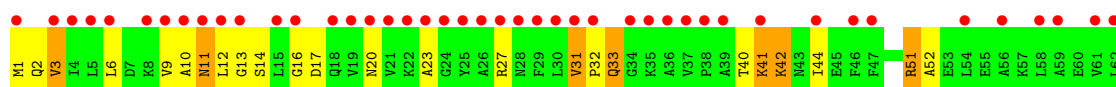
• Molecule 28: 50S ribosomal protein L6

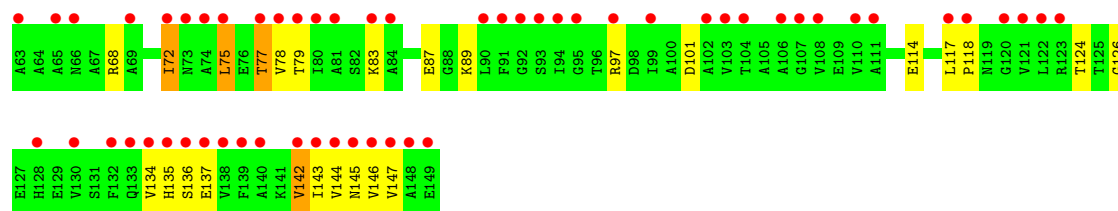


• Molecule 28: 50S ribosomal protein L6

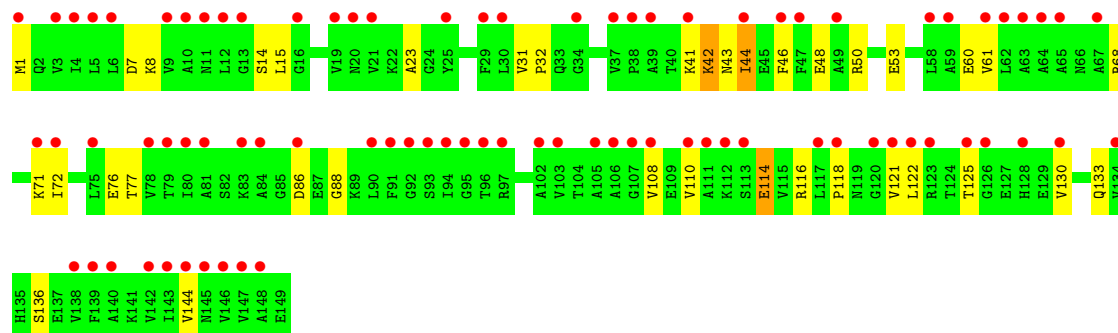
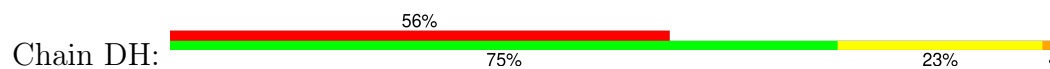


• Molecule 29: 50S ribosomal protein L9

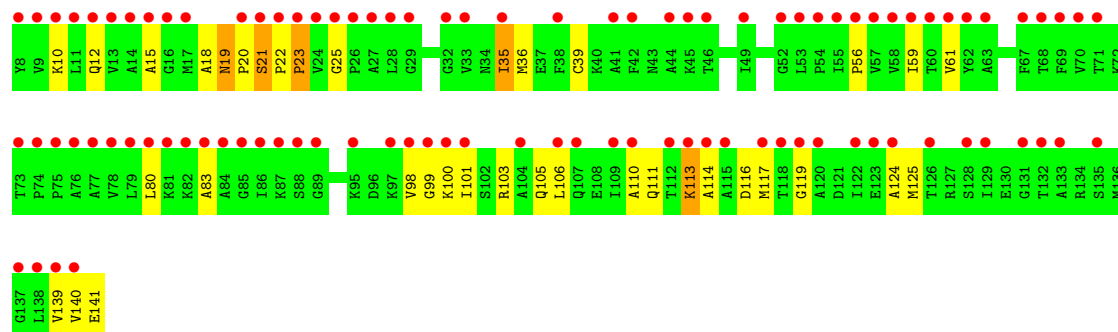
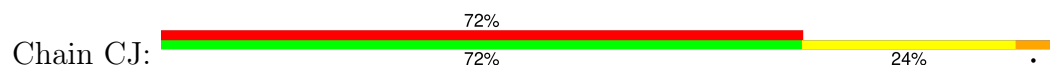




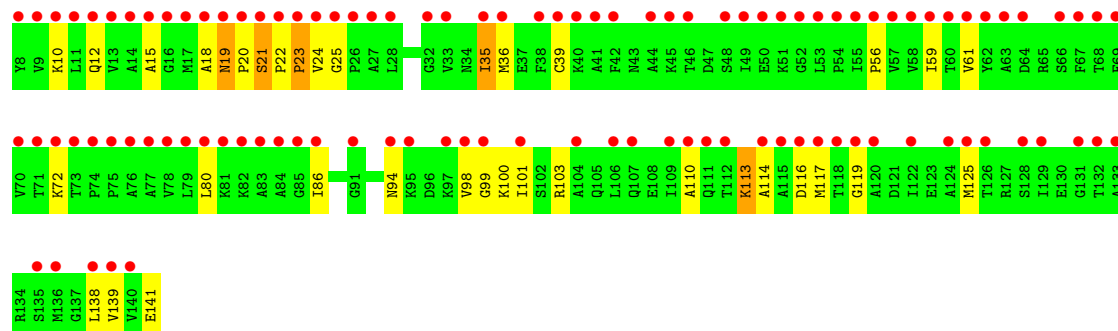
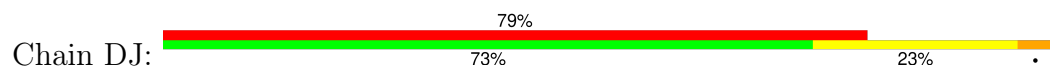
● Molecule 29: 50S ribosomal protein L9



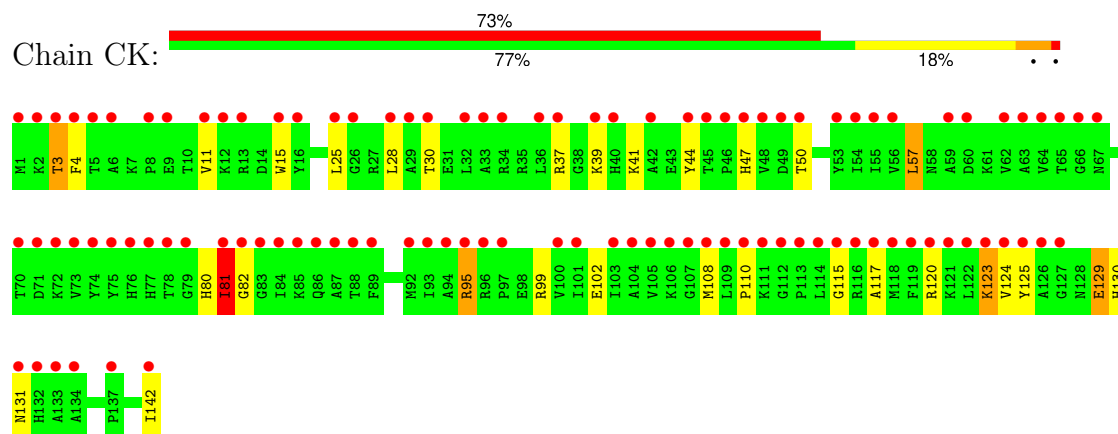
● Molecule 30: 50S ribosomal protein L11



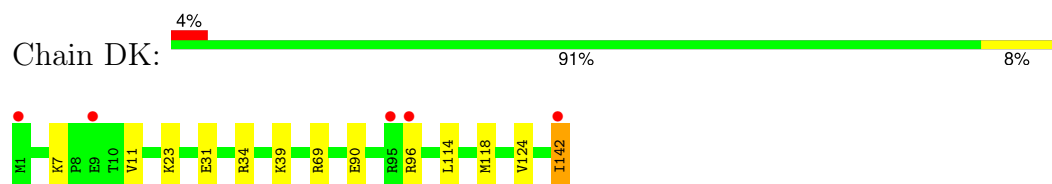
● Molecule 30: 50S ribosomal protein L11



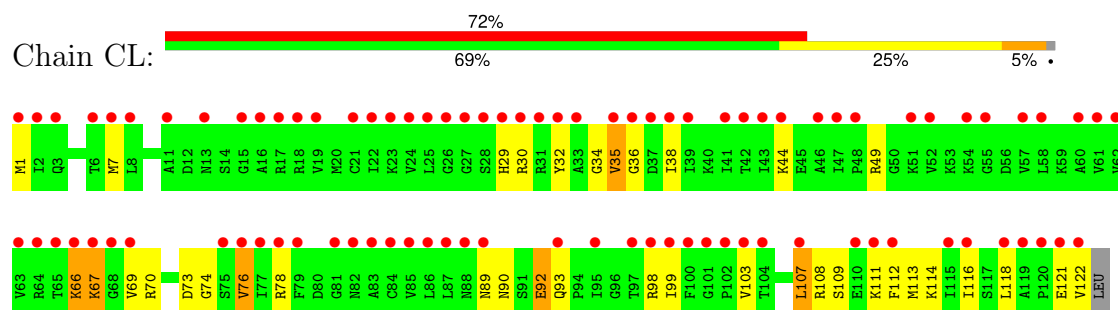
- Molecule 31: 50S ribosomal protein L13



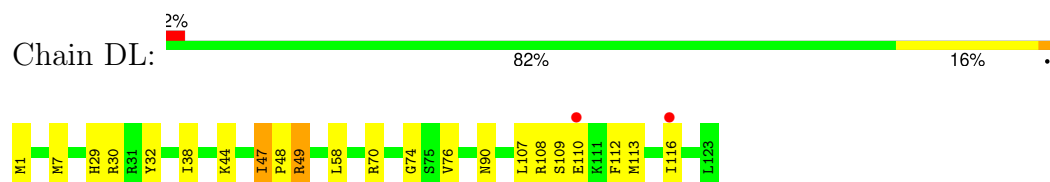
- Molecule 31: 50S ribosomal protein L13



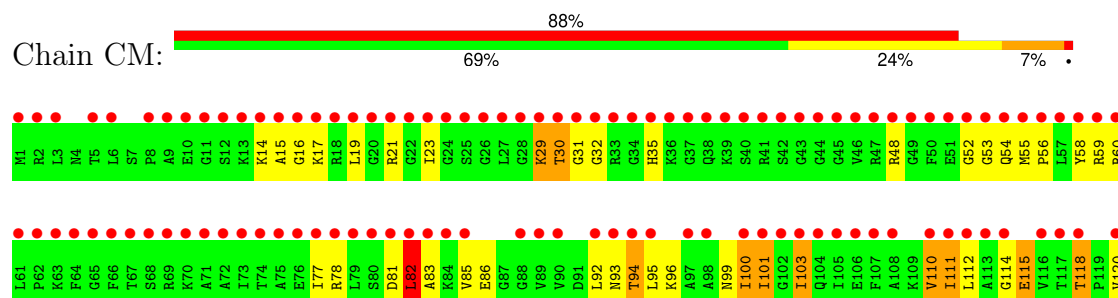
- Molecule 32: 50S ribosomal protein L14

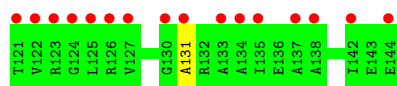


- Molecule 32: 50S ribosomal protein L14

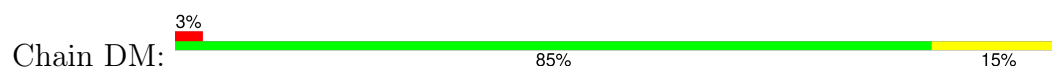


- Molecule 33: 50S ribosomal protein L15

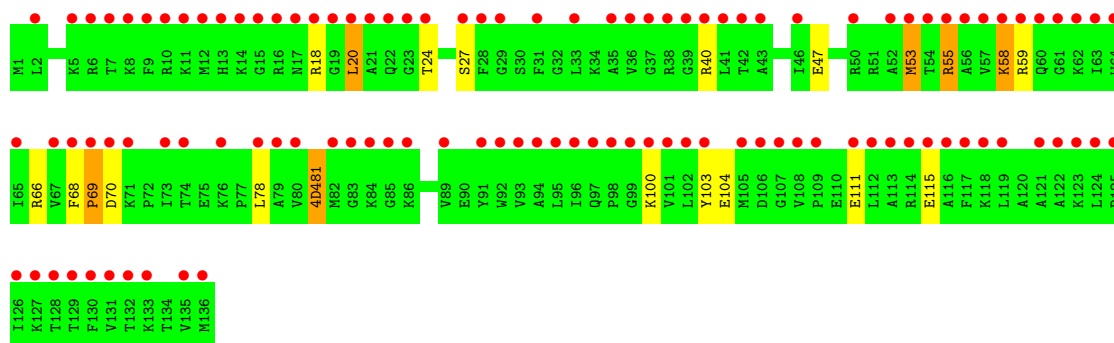
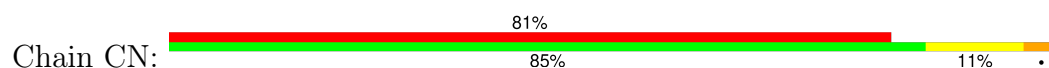




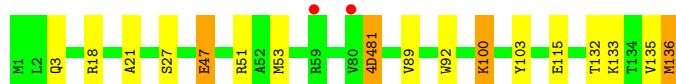
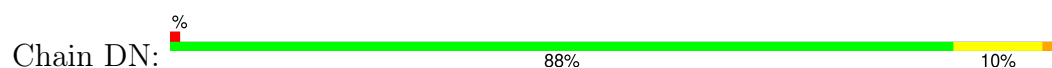
- Molecule 33: 50S ribosomal protein L15



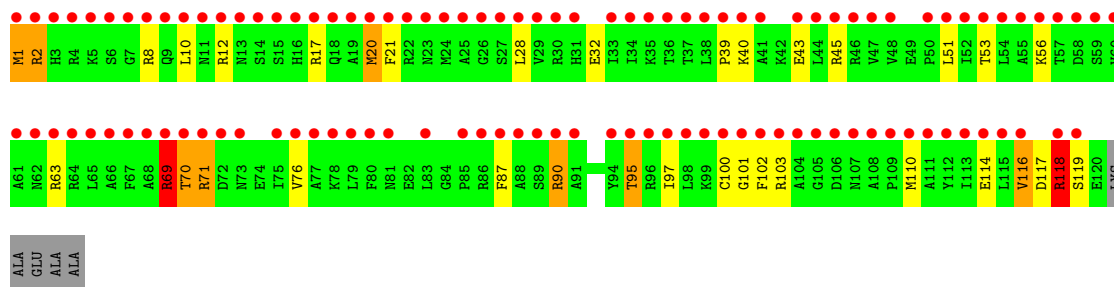
- Molecule 34: 50S ribosomal protein L16



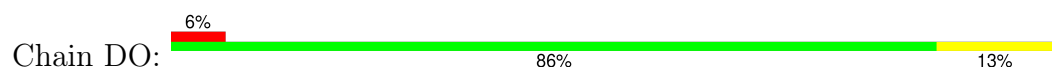
- Molecule 34: 50S ribosomal protein L16



- Molecule 35: 50S ribosomal protein L17

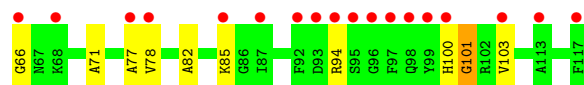
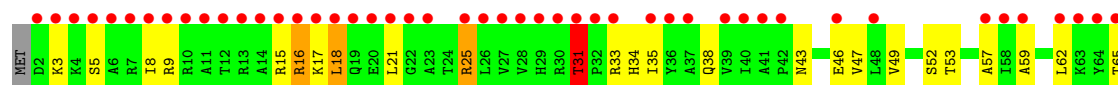


- Molecule 35: 50S ribosomal protein L17

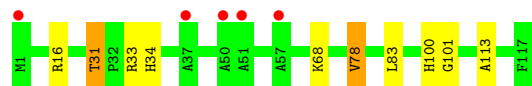




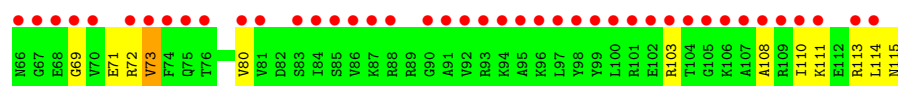
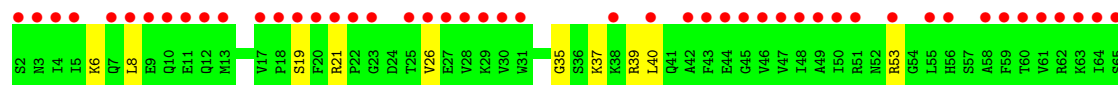
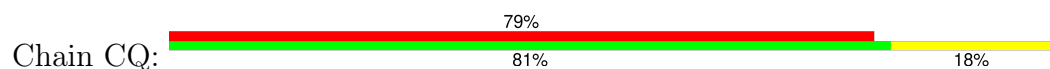
- Molecule 36: 50S ribosomal protein L18



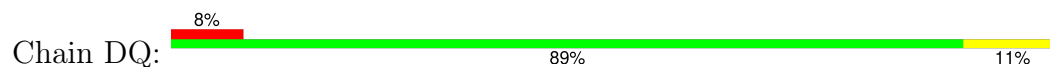
- Molecule 36: 50S ribosomal protein L18



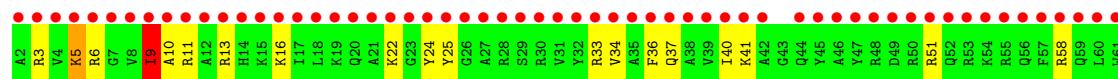
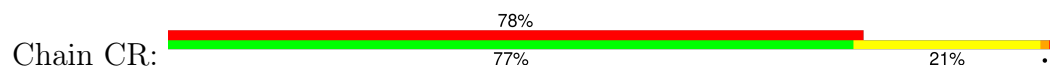
- Molecule 37: 50S ribosomal protein L19

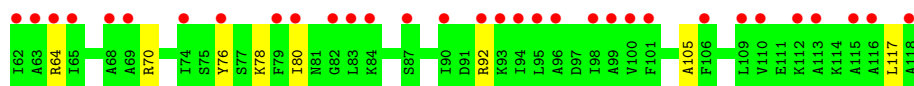


- Molecule 37: 50S ribosomal protein L19

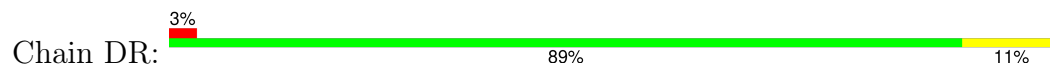


- Molecule 38: 50S ribosomal protein L20

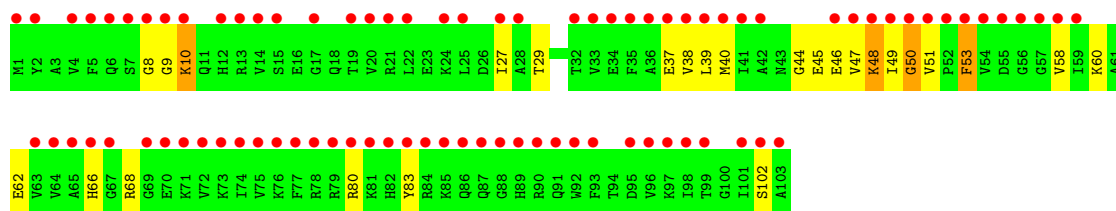
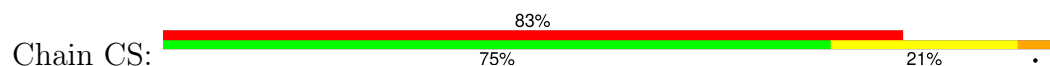




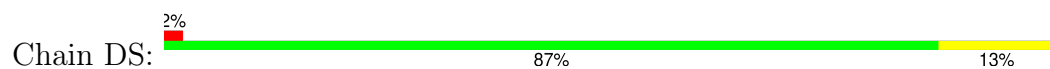
- Molecule 38: 50S ribosomal protein L20



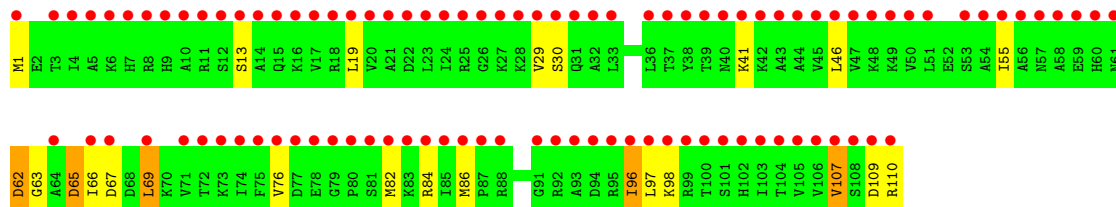
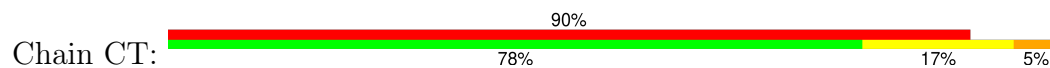
- Molecule 39: 50S ribosomal protein L21



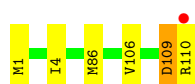
- Molecule 39: 50S ribosomal protein L21



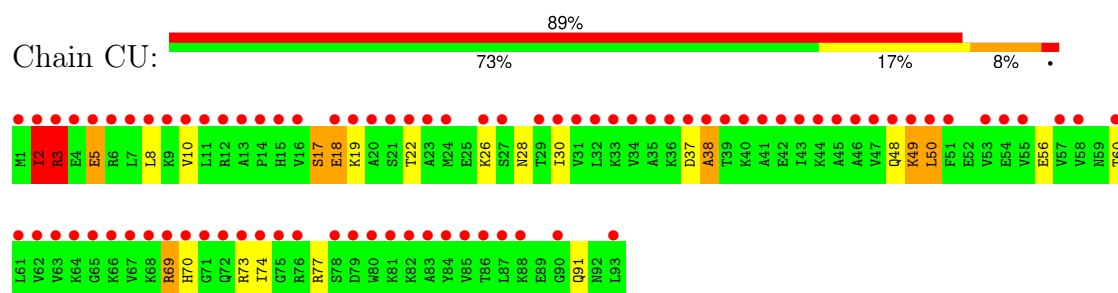
- Molecule 40: 50S ribosomal protein L22



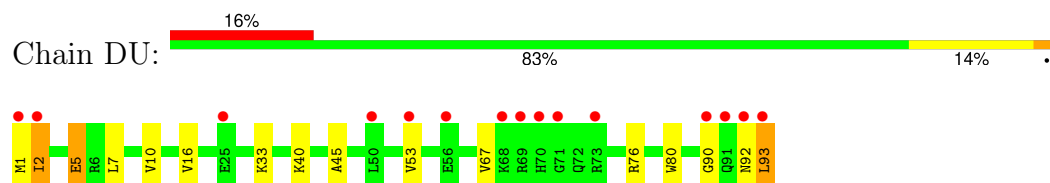
- Molecule 40: 50S ribosomal protein L22



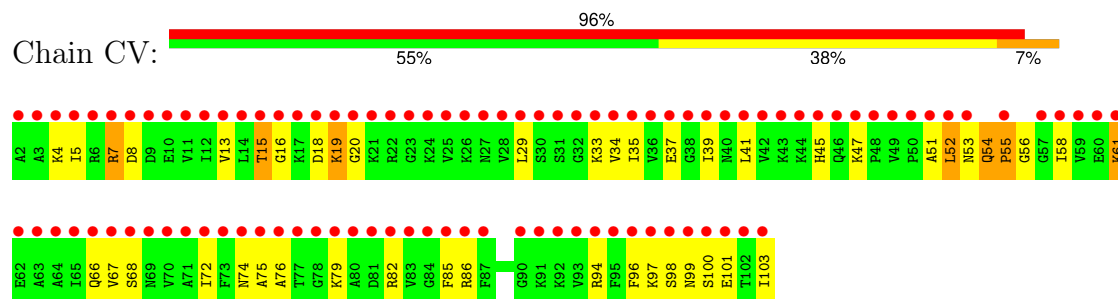
- Molecule 41: 50S ribosomal protein L23



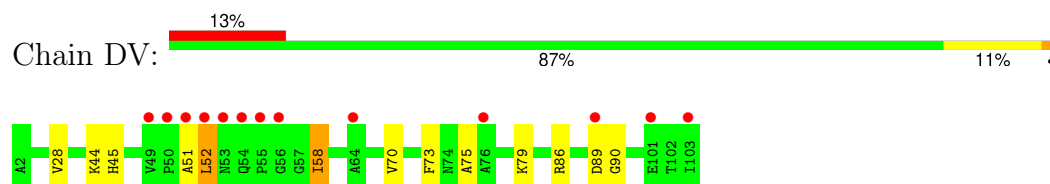
- Molecule 41: 50S ribosomal protein L23



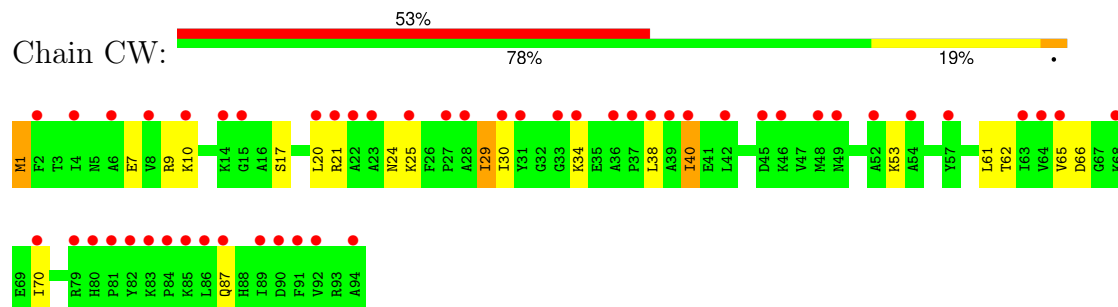
- Molecule 42: 50S ribosomal protein L24



- Molecule 42: 50S ribosomal protein L24



- Molecule 43: 50S ribosomal protein L25

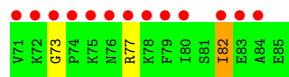
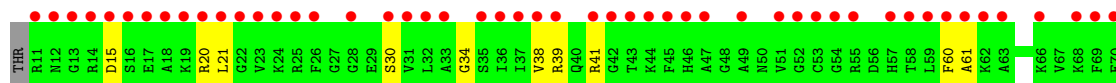
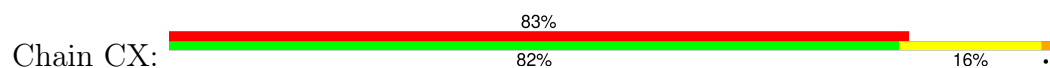


- Molecule 43: 50S ribosomal protein L25

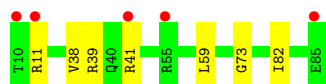




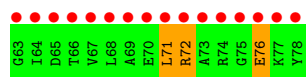
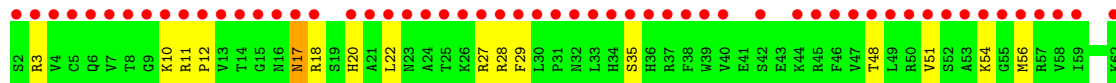
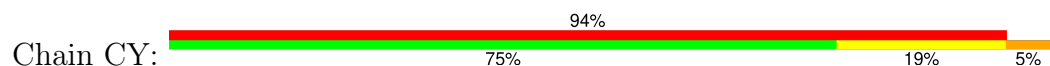
- Molecule 44: 50S ribosomal protein L27



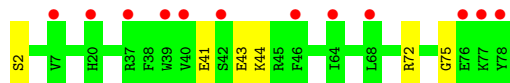
- Molecule 44: 50S ribosomal protein L27



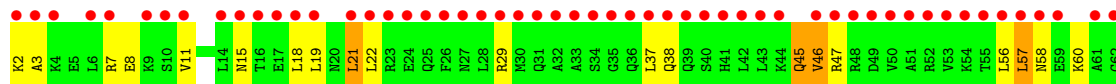
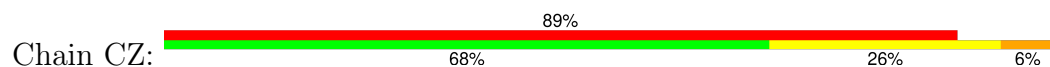
- Molecule 45: 50S ribosomal protein L28



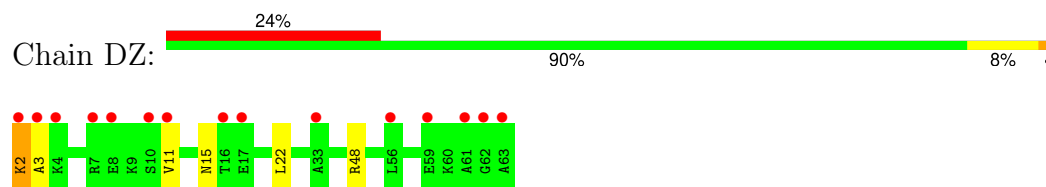
- Molecule 45: 50S ribosomal protein L28



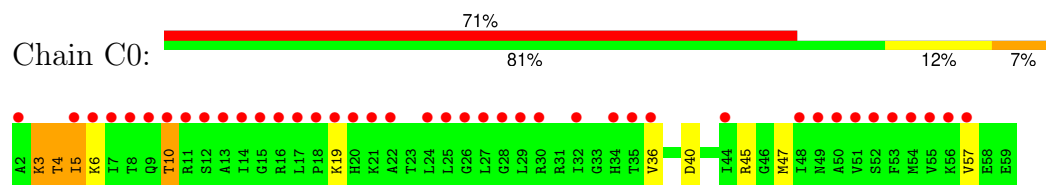
- Molecule 46: 50S ribosomal protein L29



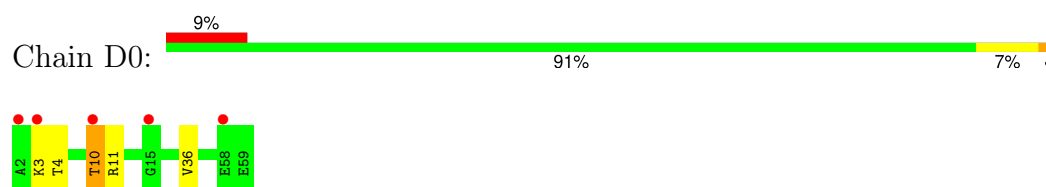
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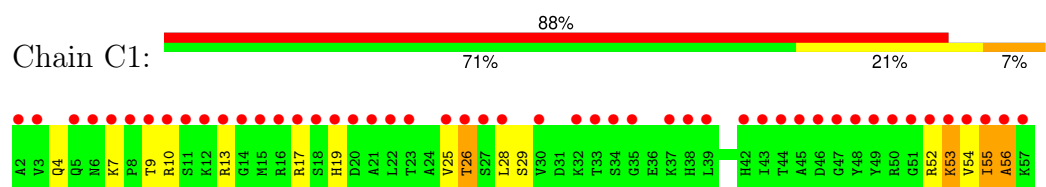
• Molecule 47: 50S ribosomal protein L30



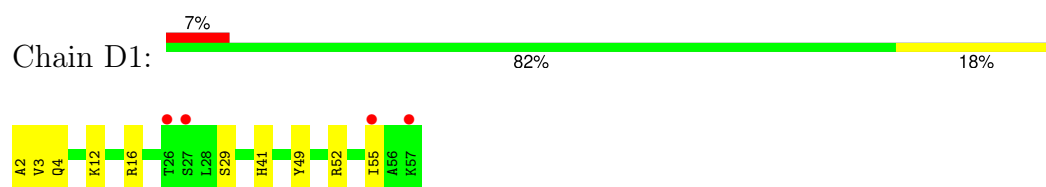
• Molecule 47: 50S ribosomal protein L30



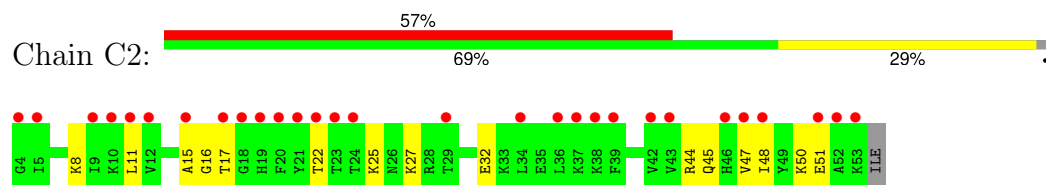
• Molecule 48: 50S ribosomal protein L32



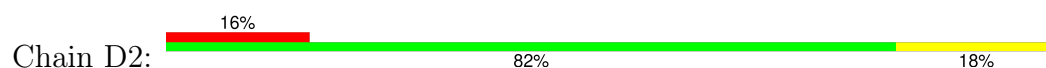
• Molecule 48: 50S ribosomal protein L32

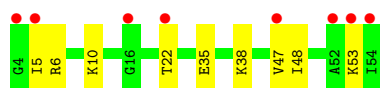


• Molecule 49: 50S ribosomal protein L33

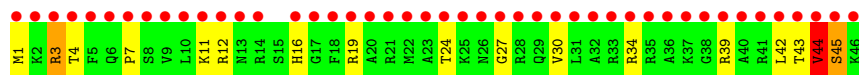


• Molecule 49: 50S ribosomal protein L33

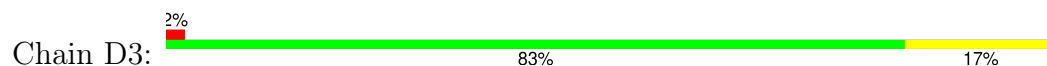




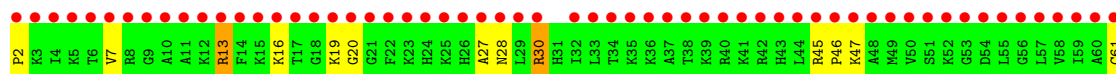
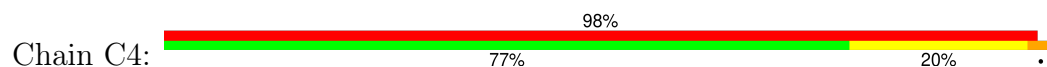
- Molecule 50: 50S ribosomal protein L34



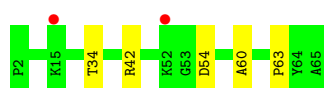
- Molecule 50: 50S ribosomal protein L34



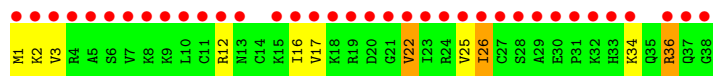
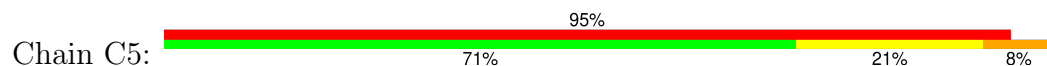
- Molecule 51: 50S ribosomal protein L35



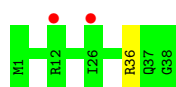
- Molecule 51: 50S ribosomal protein L35



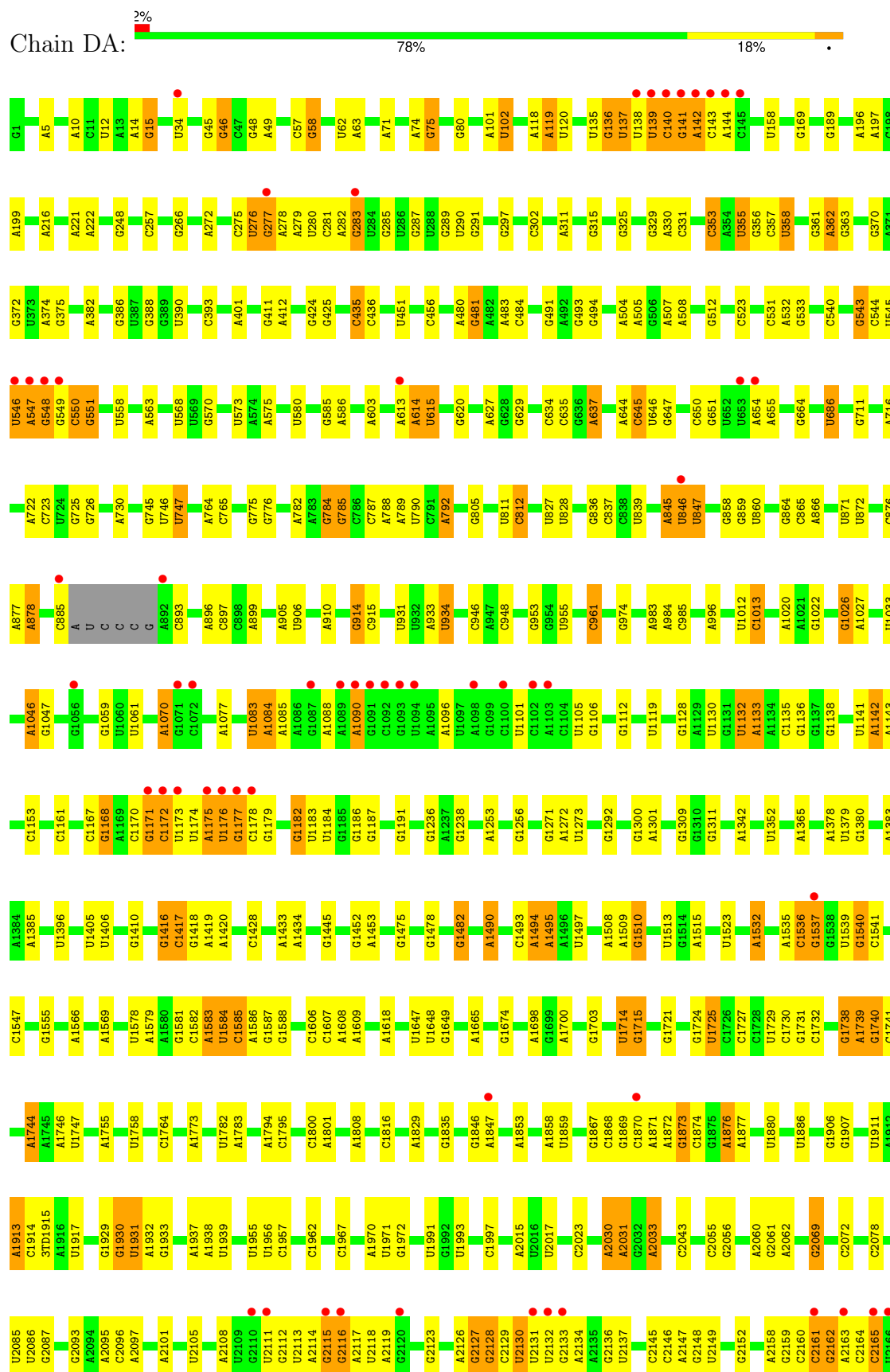
- Molecule 52: 50S ribosomal protein L36

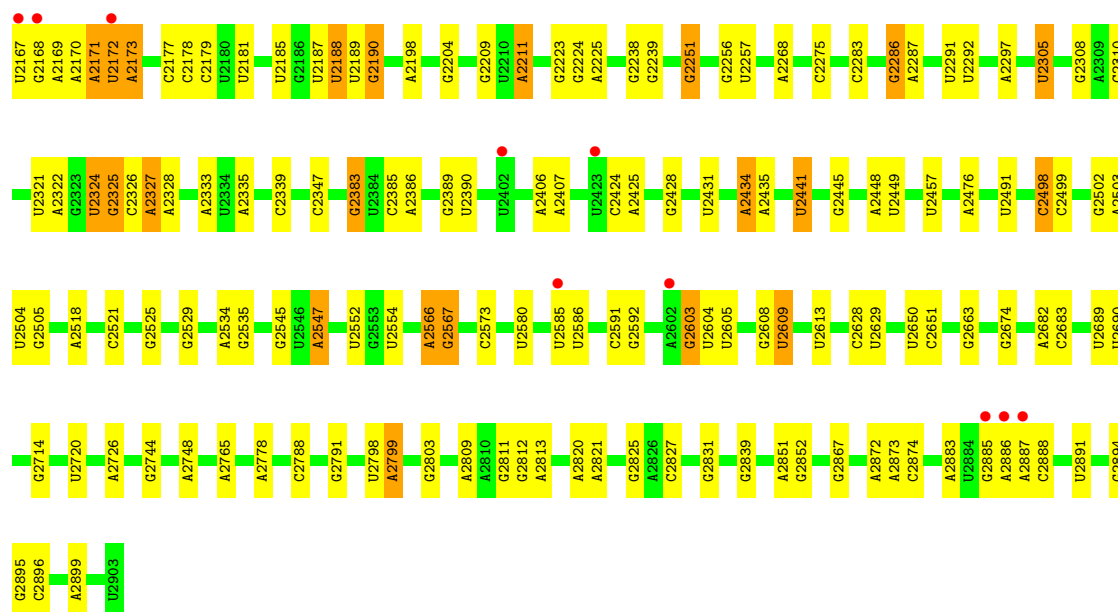


- Molecule 52: 50S ribosomal protein L36

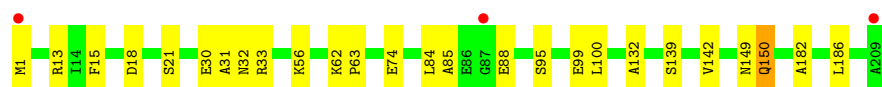
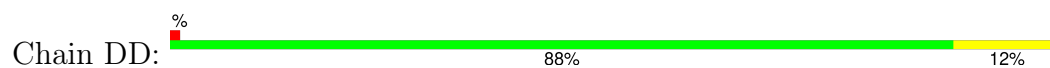


● Molecule 53: 23S rRNA

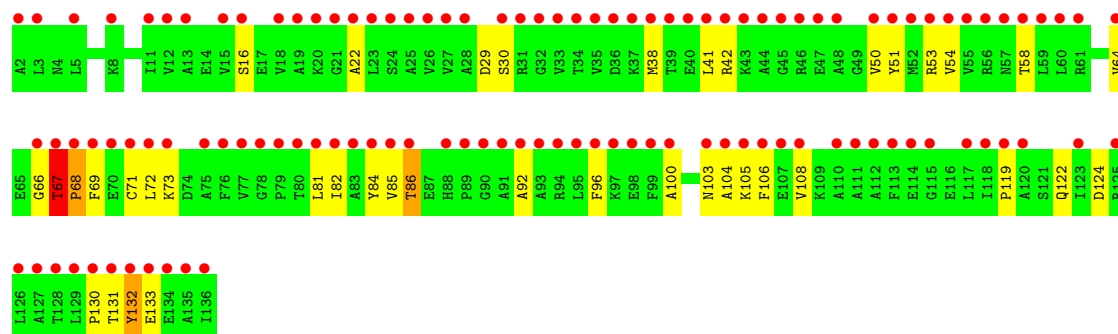
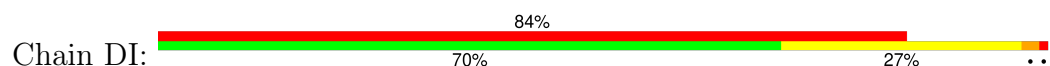




• Molecule 54: 50S ribosomal protein L3



• Molecule 55: 50S ribosomal protein L10



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.17Å 433.89Å 624.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.39 – 2.10 69.39 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.0 (69.39-2.10) 93.0 (69.39-2.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.218 , 0.234 0.235 , 0.246	Depositor DCC
R_{free} test set	10048 reflections (0.33%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	295060	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.32	0/36593	0.48	0/57081
1	BA	0.30	1/36568 (0.0%)	0.58	8/57042 (0.0%)
2	AB	0.48	0/1784	0.82	1/2403 (0.0%)
2	BB	0.48	0/1784	0.92	1/2403 (0.0%)
3	AC	0.47	0/1652	0.80	0/2225
3	BC	0.57	0/1652	1.12	10/2225 (0.4%)
4	AD	0.46	0/1665	0.76	0/2227
4	BD	0.54	0/1665	0.78	0/2227
5	AE	0.59	0/1157	0.88	2/1557 (0.1%)
5	BE	0.75	0/1118	1.49	16/1504 (1.1%)
6	AF	0.51	0/881	0.82	1/1189 (0.1%)
6	BF	0.65	0/835	1.18	4/1128 (0.4%)
7	AG	0.44	0/1196	0.78	0/1602
7	BG	0.56	0/1196	1.26	8/1602 (0.5%)
8	AH	0.55	0/989	0.84	0/1326
8	BH	0.54	0/989	1.12	6/1326 (0.5%)
9	AI	0.48	0/1034	0.84	0/1375
9	BI	0.42	0/1034	0.88	2/1375 (0.1%)
10	AJ	0.66	0/806	0.90	0/1089
10	BJ	0.90	0/797	0.92	2/1077 (0.2%)
11	AK	0.50	0/893	0.77	0/1205
11	BK	0.60	0/893	1.22	10/1205 (0.8%)
12	AL	0.59	0/960	0.79	0/1286
12	BL	0.64	0/960	1.16	8/1286 (0.6%)
13	AM	0.49	0/893	0.85	0/1193
13	BM	0.54	0/893	1.34	9/1193 (0.8%)
14	AN	0.54	0/817	0.86	1/1088 (0.1%)
14	BN	0.61	0/817	1.03	6/1088 (0.6%)
15	AO	0.51	0/722	0.71	0/964
15	BO	0.57	0/722	1.12	3/964 (0.3%)
16	AP	0.52	0/659	0.85	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BP	0.64	0/659	1.18	4/884 (0.5%)
17	AQ	0.55	0/658	0.83	1/881 (0.1%)
17	BQ	0.59	0/658	1.12	3/881 (0.3%)
18	AR	0.49	0/463	0.77	0/621
18	BR	0.63	0/463	1.28	2/621 (0.3%)
19	AS	0.47	0/653	0.82	2/877 (0.2%)
19	BS	0.53	0/653	1.22	6/877 (0.7%)
20	AT	0.52	0/676	0.83	0/895
20	BT	0.56	0/671	1.29	6/888 (0.7%)
21	AU	0.58	0/472	0.78	0/627
21	BU	0.53	0/472	0.80	0/627
22	CA	0.29	0/69165	0.57	17/107896 (0.0%)
23	CB	0.24	0/2828	0.49	0/4410
23	DB	0.44	0/2872	0.56	0/4478
24	CC	0.53	0/2122	1.03	9/2852 (0.3%)
24	DC	0.73	0/2122	0.91	2/2852 (0.1%)
25	CD	0.55	0/1586	1.00	2/2134 (0.1%)
26	CE	0.51	0/1571	1.04	5/2113 (0.2%)
26	DE	0.74	0/1571	0.86	1/2113 (0.0%)
27	CF	0.48	0/1435	1.10	5/1926 (0.3%)
27	DF	0.59	0/1435	0.86	0/1926
28	CG	0.52	0/1343	0.76	0/1816
28	DG	0.65	0/1343	0.87	0/1816
29	CH	0.48	0/1121	0.82	1/1515 (0.1%)
29	DH	0.51	0/1121	0.82	1/1515 (0.1%)
30	CJ	0.68	0/993	0.96	3/1341 (0.2%)
30	DJ	0.71	0/993	1.01	3/1341 (0.2%)
31	CK	0.46	0/1152	0.78	0/1551
31	DK	0.89	0/1152	0.93	0/1551
32	CL	0.48	0/947	0.93	1/1268 (0.1%)
32	DL	0.83	0/955	1.00	3/1279 (0.2%)
33	CM	0.56	0/1062	1.34	13/1413 (0.9%)
33	DM	0.81	0/1062	0.91	1/1413 (0.1%)
34	CN	0.43	0/1081	0.90	0/1443
34	DN	0.80	0/1092	0.90	2/1457 (0.1%)
35	CO	0.51	0/973	1.11	4/1301 (0.3%)
35	DO	0.90	0/1006	1.00	0/1345
36	CP	0.49	0/902	1.11	7/1209 (0.6%)
36	DP	0.64	0/910	0.85	1/1219 (0.1%)
37	CQ	0.47	0/929	0.97	2/1242 (0.2%)
37	DQ	0.79	0/929	0.85	0/1242
38	CR	0.51	1/960 (0.1%)	0.92	0/1278
38	DR	0.94	1/960 (0.1%)	0.93	1/1278 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	CS	0.48	0/829	1.05	6/1107 (0.5%)
39	DS	0.89	0/829	0.88	0/1107
40	CT	0.53	0/864	1.08	2/1156 (0.2%)
40	DT	0.94	0/864	0.90	0/1156
41	CU	0.53	0/745	1.20	6/994 (0.6%)
41	DU	0.76	0/745	0.97	1/994 (0.1%)
42	CV	0.56	0/788	1.19	2/1051 (0.2%)
42	DV	0.69	0/788	0.91	0/1051
43	CW	0.39	0/766	0.85	0/1025
43	DW	0.77	0/766	0.83	0/1025
44	CX	0.46	0/576	0.91	2/762 (0.3%)
44	DX	0.86	0/598	0.91	2/790 (0.3%)
45	CY	0.47	0/635	0.93	1/848 (0.1%)
45	DY	0.75	0/635	0.87	0/848
46	CZ	0.43	0/502	1.05	1/667 (0.1%)
46	DZ	0.61	0/502	0.84	0/667
47	C0	0.48	0/453	0.98	1/605 (0.2%)
47	D0	0.90	0/467	0.85	0/623
48	C1	0.52	0/450	1.03	2/599 (0.3%)
48	D1	0.87	0/450	0.92	0/599
49	C2	0.54	0/416	0.95	0/554
49	D2	0.71	0/421	0.86	0/561
50	C3	0.58	0/380	1.07	0/498
50	D3	0.85	0/380	0.99	0/498
51	C4	0.51	0/513	1.04	0/676
51	D4	0.78	0/513	0.86	0/676
52	C5	0.54	0/303	1.18	2/397 (0.5%)
52	D5	0.84	0/303	0.91	0/397
53	DA	0.56	0/69295	0.65	1/108100 (0.0%)
54	DD	0.92	1/1576 (0.1%)	0.97	3/2119 (0.1%)
55	DI	0.51	0/1037	0.90	1/1402 (0.1%)
All	All	0.48	4/309204 (0.0%)	0.71	239/462103 (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	BA	0	1
6	BF	0	1
24	DC	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	CD	0	1
30	CJ	0	1
30	DJ	0	1
32	CL	0	1
47	C0	0	1
47	D0	0	1
55	DI	0	1
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	CR	9	ILE	CA-CB	6.38	1.62	1.54
38	DR	42	ALA	CA-CB	-5.63	1.44	1.53
54	DD	132	ALA	CA-CB	-5.20	1.44	1.53
1	BA	1498	UR3	O3'-P	5.15	1.61	1.56

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	BE	104	GLY	N-CA-C	13.54	137.28	112.37
33	CM	101	ILE	N-CA-C	11.91	124.33	112.90
33	CM	52	GLY	N-CA-C	-11.27	94.98	112.45
41	CU	3	ARG	N-CA-C	-10.66	90.52	108.75
33	CM	103	ILE	N-CA-C	9.97	123.51	111.05
5	BE	153	VAL	N-CA-C	-9.96	98.63	111.09
5	BE	108	GLY	N-CA-C	9.96	125.59	112.25
7	BG	51	ALA	N-CA-C	-9.91	100.17	110.97
20	BT	8	LYS	N-CA-C	-9.76	100.64	111.28
5	BE	100	SER	N-CA-C	-9.74	98.11	110.19
55	DI	132	TYR	N-CA-C	9.31	121.03	111.07
24	CC	160	THR	N-CA-C	9.25	122.46	110.53
11	BK	50	SER	N-CA-C	-9.11	101.48	112.59
25	CD	151	THR	CA-C-N	-9.07	108.51	119.84
25	CD	151	THR	C-N-CA	-9.07	108.51	119.84
24	CC	13	ARG	N-CA-C	-9.03	102.40	113.41
30	DJ	116	ASP	N-CA-C	8.68	123.59	112.92
52	C5	22	VAL	N-CA-C	8.58	120.18	108.17
8	BH	90	ASP	N-CA-C	-8.56	102.83	113.28
7	BG	147	ALA	N-CA-C	-8.50	102.09	111.36
20	BT	83	ILE	N-CA-C	8.48	119.27	110.62
19	BS	69	HIS	N-CA-C	8.43	120.78	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	BF	92	THR	N-CA-C	8.29	128.46	110.80
18	BR	21	ILE	N-CA-C	-8.27	103.22	110.74
39	CS	51	VAL	CA-C-N	-8.13	111.38	119.76
39	CS	51	VAL	C-N-CA	-8.13	111.38	119.76
12	BL	85	GLY	N-CA-C	-8.11	93.95	113.18
8	BH	99	LEU	N-CA-C	-8.05	99.15	110.50
5	BE	139	ALA	N-CA-C	-7.98	102.17	112.23
6	BF	74	LEU	N-CA-C	-7.89	101.99	111.69
29	DH	121	VAL	N-CA-C	-7.86	104.71	112.17
35	CO	69	ARG	N-CA-C	-7.82	99.25	110.59
7	BG	54	SER	N-CA-C	-7.77	94.25	110.80
19	BS	8	GLY	CA-C-N	-7.77	110.13	119.84
19	BS	8	GLY	C-N-CA	-7.77	110.13	119.84
12	BL	14	ARG	CG-CD-NE	7.60	128.73	112.00
36	CP	31	THR	CA-C-N	-7.58	110.63	119.05
36	CP	31	THR	C-N-CA	-7.58	110.63	119.05
35	CO	100	CYS	N-CA-C	7.58	122.02	111.56
41	CU	2	ILE	N-CA-C	7.57	120.18	108.44
24	CC	158	ALA	N-CA-C	7.54	121.40	111.75
20	BT	69	LYS	N-CA-C	7.34	120.21	111.33
13	BM	109	ARG	N-CA-C	7.29	119.01	111.14
5	BE	56	VAL	CB-CA-C	-7.28	106.63	114.35
13	BM	17	ILE	CB-CA-C	-7.28	102.48	112.24
8	BH	68	GLY	N-CA-C	-7.27	95.95	113.18
5	BE	122	ASN	N-CA-C	7.26	124.92	114.39
5	BE	123	VAL	N-CA-C	7.25	124.41	109.34
1	BA	1110	A	O5'-C5'-C4'	7.21	122.31	111.50
33	CM	35	HIS	N-CA-C	7.20	120.26	108.52
37	CQ	21	ARG	N-CA-C	7.17	116.39	108.14
3	BC	206	GLU	N-CA-C	7.17	120.31	108.48
30	DJ	21	SER	CA-C-N	-7.00	113.17	120.38
30	DJ	21	SER	C-N-CA	-7.00	113.17	120.38
3	BC	64	ILE	N-CA-C	-6.99	98.10	108.45
5	BE	109	GLY	N-CA-C	-6.95	103.93	111.93
12	BL	44	LYS	CA-C-N	-6.92	111.19	119.84
12	BL	44	LYS	C-N-CA	-6.92	111.19	119.84
13	BM	95	LEU	CA-C-N	-6.89	112.87	119.76
13	BM	95	LEU	C-N-CA	-6.89	112.87	119.76
27	CF	108	VAL	CB-CA-C	-6.88	107.06	114.35
40	CT	46	LEU	N-CA-C	6.87	118.42	111.07
33	CM	101	ILE	CB-CA-C	-6.85	102.70	111.20
12	BL	84	GLY	N-CA-C	-6.81	105.48	111.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	CM	114	GLY	N-CA-C	6.81	126.88	112.17
22	CA	2225	A	C4'-C3'-O3'	6.78	119.58	109.40
24	CC	217	ARG	CA-C-N	6.77	126.81	119.90
24	CC	217	ARG	C-N-CA	6.77	126.81	119.90
19	AS	29	LYS	CA-C-N	-6.76	112.79	119.76
19	AS	29	LYS	C-N-CA	-6.76	112.79	119.76
3	BC	142	MET	N-CA-C	-6.72	103.42	111.69
3	BC	126	ARG	N-CA-C	6.71	120.69	112.23
39	CS	51	VAL	N-CA-C	-6.71	101.58	108.96
33	CM	15	ALA	N-CA-C	6.69	121.30	113.20
22	CA	2326	C	C4'-C3'-O3'	6.66	119.39	109.40
11	BK	72	ASP	N-CA-C	-6.66	100.61	110.46
11	BK	90	GLY	CA-C-N	6.65	126.34	119.56
11	BK	90	GLY	C-N-CA	6.65	126.34	119.56
30	CJ	116	ASP	N-CA-C	6.65	121.09	112.92
8	BH	67	GLN	N-CA-C	-6.62	96.71	110.80
22	CA	818	G	O3'-P-O5'	6.57	113.85	104.00
6	AF	66	ALA	N-CA-C	6.53	114.10	108.22
27	CF	28	VAL	CA-C-N	-6.50	113.08	119.78
27	CF	28	VAL	C-N-CA	-6.50	113.08	119.78
22	CA	2071	A	O3'-P-O5'	-6.44	94.33	104.00
20	BT	70	ASN	N-CA-C	6.42	118.28	111.28
14	AN	42	TRP	N-CA-C	6.41	118.27	111.28
1	BA	572	A	O3'-P-O5'	6.41	113.61	104.00
5	BE	123	VAL	CB-CA-C	-6.39	100.80	111.29
3	BC	106	VAL	N-CA-C	6.37	115.79	106.55
46	CZ	45	GLN	N-CA-C	-6.37	99.85	109.79
11	BK	90	GLY	N-CA-C	6.36	125.32	112.34
32	CL	89	ASN	N-CA-C	6.32	118.98	111.33
16	BP	19	VAL	N-CA-C	-6.31	101.42	109.30
17	BQ	15	ASP	N-CA-C	6.23	120.70	112.72
11	BK	114	THR	CA-C-N	-6.18	113.58	119.76
11	BK	114	THR	C-N-CA	-6.18	113.58	119.76
32	DL	110	GLU	N-CA-C	-6.17	104.56	111.28
10	BJ	86	ALA	N-CA-C	-6.15	105.60	113.23
41	DU	2	ILE	N-CA-C	6.12	116.44	107.75
22	CA	2326	C	P-O3'-C3'	6.08	129.33	120.20
45	CY	51	VAL	N-CA-C	6.08	117.23	108.48
14	BN	50	THR	N-CA-C	-6.07	105.36	112.89
30	CJ	21	SER	CA-C-N	-6.06	114.14	120.38
30	CJ	21	SER	C-N-CA	-6.06	114.14	120.38
22	CA	646	U	O3'-P-O5'	6.05	113.08	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BC	83	ASP	N-CA-C	6.02	117.84	111.28
1	BA	1142	G	O3'-P-O5'	6.00	113.00	104.00
10	BJ	91	ASP	N-CA-C	5.99	118.33	111.02
26	CE	65	THR	N-CA-C	-5.99	100.80	110.32
5	BE	80	THR	N-CA-C	5.96	118.02	109.14
24	CC	196	GLY	N-CA-C	5.95	127.29	113.18
33	CM	17	LYS	N-CA-C	5.95	118.89	110.50
6	BF	35	LYS	CA-CB-CG	5.95	126.00	114.10
33	CM	110	VAL	N-CA-C	5.95	119.41	111.44
52	C5	12	ARG	CG-CD-NE	-5.93	98.95	112.00
35	CO	102	PHE	N-CA-C	5.93	119.06	109.40
13	BM	98	ARG	N-CA-C	5.89	119.43	112.72
24	CC	213	TRP	CA-CB-CG	5.88	124.76	113.60
16	BP	11	ALA	N-CA-C	-5.87	100.03	108.60
5	BE	156	LYS	N-CA-C	-5.85	98.34	110.80
8	BH	51	VAL	N-CA-C	-5.84	99.94	108.11
44	DX	73	GLY	CA-C-N	5.80	125.90	119.87
44	DX	73	GLY	C-N-CA	5.80	125.90	119.87
11	BK	91	PRO	N-CA-C	5.77	121.34	113.84
17	AQ	81	LYS	N-CA-C	5.76	118.04	108.99
33	CM	118	THR	CA-C-N	-5.76	113.85	119.90
33	CM	118	THR	C-N-CA	-5.76	113.85	119.90
13	BM	30	SER	N-CA-C	-5.76	104.91	111.07
14	BN	31	ILE	N-CA-C	-5.71	104.79	110.62
22	CA	2425	A	C4'-C3'-O3'	5.71	117.97	109.40
53	DA	512	G	O4'-C1'-N9	5.70	116.75	108.20
38	DR	101	PHE	N-CA-C	5.70	120.24	113.28
20	BT	83	ILE	CB-CA-C	-5.70	104.44	112.14
19	BS	10	PHE	CA-CB-CG	-5.70	108.10	113.80
22	CA	1171	G	O5'-C5'-C4'	5.70	120.04	111.50
36	CP	8	ILE	N-CA-C	5.69	116.43	110.62
41	CU	74	ILE	N-CA-C	5.68	117.53	108.89
26	CE	40	ARG	N-CA-C	5.67	118.68	110.28
41	CU	3	ARG	CB-CA-C	5.66	120.88	109.68
7	BG	133	THR	N-CA-C	-5.65	105.20	111.36
8	BH	101	ILE	N-CA-C	5.65	118.28	108.90
33	DM	22	GLY	N-CA-C	5.65	119.17	112.33
6	BF	81	ASN	N-CA-C	5.64	118.36	109.96
22	CA	2585	U	C5'-C4'-O4'	-5.64	101.34	109.80
22	CA	2425	A	P-O3'-C3'	5.60	128.60	120.20
22	CA	2797	U	C5'-C4'-C3'	5.60	123.60	115.20
54	DD	142	VAL	CA-C-N	5.60	125.30	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DD	142	VAL	C-N-CA	5.60	125.30	119.64
40	CT	67	ASP	N-CA-C	5.59	118.14	111.71
24	DC	217	ARG	CA-C-N	5.59	125.60	119.90
24	DC	217	ARG	C-N-CA	5.59	125.60	119.90
26	DE	146	VAL	N-CA-C	5.58	115.72	108.35
54	DD	139	SER	N-CA-C	5.58	118.03	110.06
13	BM	86	TYR	N-CA-C	5.56	117.81	111.02
19	BS	13	LEU	N-CA-C	5.55	117.14	111.14
13	BM	25	VAL	CA-C-N	5.55	128.65	122.55
13	BM	25	VAL	C-N-CA	5.55	128.65	122.55
9	BI	100	LYS	N-CA-C	5.52	118.81	111.75
5	BE	118	ALA	N-CA-C	-5.51	105.43	111.82
22	CA	2250	G	O4'-C1'-N9	-5.51	99.94	108.20
20	BT	5	LYS	N-CA-C	-5.49	99.10	110.80
14	BN	24	ARG	N-CA-C	5.49	117.07	111.14
5	AE	123	VAL	N-CA-C	5.48	116.25	108.42
12	BL	94	ARG	CB-CG-CD	5.48	123.90	111.30
39	CS	44	GLY	N-CA-C	-5.48	106.15	112.50
18	BR	22	ASP	N-CA-C	5.47	118.38	109.24
22	CA	34	U	C5'-C4'-O4'	-5.45	100.93	109.10
3	BC	14	ILE	N-CA-C	5.44	120.66	109.34
44	CX	73	GLY	CA-C-N	5.44	125.53	119.87
44	CX	73	GLY	C-N-CA	5.44	125.53	119.87
24	CC	70	ASN	CB-CA-C	-5.43	102.22	111.02
26	CE	88	ARG	CA-CB-CG	5.43	124.95	114.10
22	CA	1171	G	C2'-C3'-O3'	-5.42	105.58	113.70
2	BB	128	LYS	N-CA-C	-5.42	99.90	108.73
5	BE	113	ALA	N-CA-C	5.41	117.17	111.28
39	CS	9	GLY	N-CA-C	-5.39	107.54	115.30
29	CH	13	GLY	N-CA-C	5.39	120.62	111.19
41	CU	3	ARG	CA-CB-CG	5.37	124.84	114.10
1	BA	89	U	O3'-P-O5'	-5.37	95.95	104.00
7	BG	151	PHE	N-CA-C	-5.37	106.60	112.72
5	AE	56	VAL	CB-CA-C	-5.34	108.69	114.35
12	BL	83	ARG	N-CA-C	5.33	121.33	114.56
17	BQ	49	GLU	N-CA-C	-5.33	102.73	110.24
36	CP	77	ALA	N-CA-C	5.32	117.08	111.28
1	BA	330	C	O4'-C1'-N1	5.32	116.47	108.50
19	BS	9	PRO	N-CA-C	-5.32	101.52	112.47
35	CO	101	GLY	N-CA-C	5.32	125.78	113.18
48	C1	54	VAL	N-CA-C	-5.29	102.16	109.46
16	BP	40	ASN	CA-C-N	5.28	126.31	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	BP	40	ASN	C-N-CA	5.28	126.31	120.45
47	C0	10	THR	N-CA-C	5.27	120.72	113.97
14	BN	25	ALA	N-CA-C	5.27	117.02	111.28
36	CP	101	GLY	CA-C-N	5.26	127.28	120.44
36	CP	101	GLY	C-N-CA	5.26	127.28	120.44
7	BG	144	MET	N-CA-C	-5.26	105.55	111.28
22	CA	1378	A	P-O3'-C3'	5.26	128.09	120.20
3	BC	57	ILE	N-CA-C	5.25	115.69	108.12
1	BA	412	A	O4'-C1'-N9	5.25	116.08	108.20
7	BG	50	LEU	N-CA-C	-5.25	105.64	111.36
22	CA	2225	A	P-O3'-C3'	5.24	128.06	120.20
36	DP	78	VAL	CB-CA-C	-5.22	105.09	112.14
1	BA	1183	U	C5'-C4'-C3'	-5.22	107.37	115.20
39	CS	50	GLY	N-CA-C	-5.22	100.81	113.18
11	BK	106	ARG	N-CA-C	-5.21	100.67	108.96
26	CE	40	ARG	CG-CD-NE	5.21	123.45	112.00
48	C1	53	LYS	N-CA-C	5.21	117.18	108.23
3	BC	66	VAL	N-CA-C	5.19	120.14	109.34
27	CF	142	ASP	N-CA-C	5.19	117.12	107.99
26	CE	146	VAL	N-CA-C	5.19	115.20	108.35
27	CF	114	PHE	N-CA-C	5.17	117.72	109.96
3	BC	100	GLN	N-CA-C	-5.16	101.34	109.50
17	BQ	5	ILE	N-CA-C	-5.16	104.43	110.05
2	AB	128	LYS	N-CA-C	-5.15	100.34	108.73
1	BA	1109	C	P-O3'-C3'	5.14	127.91	120.20
11	BK	71	ALA	N-CA-C	-5.14	106.84	113.01
41	CU	48	GLN	N-CA-C	5.14	116.96	111.36
33	CM	85	VAL	CB-CA-C	-5.14	105.33	111.85
15	BO	48	LYS	N-CA-C	-5.13	106.79	113.16
32	DL	47	ILE	CA-C-N	5.13	124.57	119.24
32	DL	47	ILE	C-N-CA	5.13	124.57	119.24
42	CV	54	GLN	CA-C-N	-5.12	113.43	119.84
42	CV	54	GLN	C-N-CA	-5.12	113.43	119.84
34	DN	3	GLN	CA-C-N	-5.12	114.48	119.76
34	DN	3	GLN	C-N-CA	-5.12	114.48	119.76
36	CP	62	LEU	N-CA-C	-5.12	101.05	109.40
15	BO	45	GLU	N-CA-C	-5.09	102.47	110.36
33	CM	54	GLN	N-CA-C	5.08	117.46	110.35
14	BN	25	ALA	CA-C-N	5.07	127.02	120.44
14	BN	25	ALA	C-N-CA	5.07	127.02	120.44
15	BO	44	ALA	N-CA-C	-5.05	105.66	111.07
9	BI	102	GLY	N-CA-C	-5.04	108.28	115.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CA	676	A	O3'-P-O5'	5.04	111.56	104.00
24	CC	38	SER	N-CA-C	5.04	116.95	108.73
12	BL	95	TYR	N-CA-C	5.02	116.82	109.24
5	BE	83	HIS	CA-C-N	-5.02	114.61	119.78
5	BE	83	HIS	C-N-CA	-5.02	114.61	119.78
7	BG	131	LYS	N-CA-C	5.01	118.60	112.03
37	CQ	69	GLY	N-CA-C	5.01	118.35	111.54

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BA	702	A	Sidechain
6	BF	90	MET	Peptide
47	C0	3	LYS	Peptide
25	CD	151	THR	Peptide
30	CJ	98	VAL	Peptide
32	CL	34	GLY	Peptide
47	D0	3[B]	LYS	Peptide
24	DC	232	HIS	Peptide
55	DI	67	THR	Peptide
30	DJ	98	VAL	Peptide

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	193	0
1	BA	32908	0	16580	237	0
2	AB	1753	0	1780	29	0
2	BB	1753	0	1780	30	0
3	AC	1625	0	1696	16	0
3	BC	1625	0	1696	36	0
4	AD	1643	0	1707	20	0
4	BD	1643	0	1707	17	0
5	AE	1144	0	1185	33	0
5	BE	1105	0	1148	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AF	862	0	864	16	0
6	BF	817	0	808	24	0
7	AG	1182	0	1238	24	0
7	BG	1182	0	1238	36	0
8	AH	979	0	1031	20	0
8	BH	979	0	1031	21	0
9	AI	1022	0	1070	29	0
9	BI	1022	0	1070	26	0
10	AJ	796	0	836	40	0
10	BJ	787	0	828	21	0
11	AK	877	0	887	14	0
11	BK	877	0	887	29	0
12	AL	957	0	1017	9	0
12	BL	957	0	1017	22	0
13	AM	884	0	941	33	0
13	BM	884	0	941	27	0
14	AN	805	0	844	30	0
14	BN	805	0	844	43	0
15	AO	714	0	734	8	0
15	BO	714	0	734	25	0
16	AP	649	0	666	6	0
16	BP	649	0	666	11	0
17	AQ	649	0	691	8	0
17	BQ	649	0	691	22	0
18	AR	456	0	478	9	0
18	BR	456	0	478	13	0
19	AS	638	0	665	16	0
19	BS	638	0	665	29	0
20	AT	670	0	719	14	0
20	BT	665	0	714	13	0
21	AU	465	0	491	9	0
21	BU	465	0	491	8	0
22	CA	62229	0	31319	415	0
23	CB	2529	0	1281	12	0
23	DB	2569	0	1301	10	0
24	CC	2083	0	2154	41	0
24	DC	2083	0	2154	18	0
25	CD	1565	0	1616	34	0
26	CE	1552	0	1619	28	0
26	DE	1552	0	1619	3	0
27	CF	1411	0	1444	22	0
27	DF	1411	0	1444	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	CG	1323	0	1371	9	0
28	DG	1323	0	1371	7	0
29	CH	1110	0	1148	15	0
29	DH	1110	0	1148	15	0
30	CJ	979	0	1028	27	0
30	DJ	979	0	1028	30	0
31	CK	1129	0	1162	17	0
31	DK	1129	0	1162	6	0
32	CL	938	0	1012	27	0
32	DL	946	0	1023	13	0
33	CM	1053	0	1129	33	0
33	DM	1053	0	1129	11	0
34	CN	1075	0	1155	9	0
34	DN	1092	0	1179	13	0
35	CO	960	0	1000	21	0
35	DO	993	0	1034	10	0
36	CP	892	0	923	15	0
36	DP	900	0	935	9	0
37	CQ	917	0	962	7	0
37	DQ	917	0	962	9	0
38	CR	947	0	1019	25	0
38	DR	947	0	1019	13	0
39	CS	816	0	839	10	0
39	DS	816	0	839	7	0
40	CT	857	0	922	8	0
40	DT	857	0	922	3	0
41	CU	739	0	807	19	0
41	DU	739	0	807	17	0
42	CV	780	0	831	27	0
42	DV	780	0	831	5	0
43	CW	753	0	780	8	0
43	DW	753	0	780	8	0
44	CX	569	0	581	7	0
44	DX	591	0	606	4	0
45	CY	625	0	652	11	0
45	DY	625	0	652	3	0
46	CZ	501	0	531	10	0
46	DZ	501	0	531	4	0
47	C0	449	0	488	3	0
47	D0	463	0	504	1	0
48	C1	444	0	458	12	0
48	D1	444	0	458	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	C2	409	0	440	7	0
49	D2	414	0	442	7	0
50	C3	377	0	418	14	0
50	D3	377	0	418	10	0
51	C4	504	0	572	10	0
51	D4	504	0	572	5	0
52	C5	302	0	340	8	0
52	D5	302	0	340	0	0
53	DA	62361	0	31381	309	0
54	DD	1576	0	1627	18	0
55	DI	1023	0	1052	24	0
56	AA	70	0	0	0	0
56	BA	41	0	0	0	0
56	C3	1	0	0	0	0
56	CA	155	0	0	0	0
56	CB	3	0	0	0	0
56	DA	183	0	0	0	0
56	DB	9	0	0	0	0
56	DR	1	0	0	0	0
57	AA	13	0	18	1	0
57	BA	13	0	18	2	0
57	DA	26	0	36	8	0
57	DQ	13	0	18	3	0
57	DR	13	0	18	10	0
57	DS	13	0	18	2	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	6	0
58	DS	8	0	14	0	0
58	DT	16	0	28	0	0
59	AA	24	0	48	1	0
59	DA	66	0	132	16	0
59	DM	6	0	12	0	0
60	AB	1	0	0	0	0
60	C5	1	0	0	0	0
60	D5	1	0	0	0	0
61	AL	7	0	10	0	0
61	D3	7	0	10	5	0
61	DA	42	0	60	3	0
61	DL	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DP	7	0	10	4	0
61	DQ	7	0	10	1	0
62	DA	40	0	76	7	0
63	DA	32	0	44	4	0
64	D1	10	0	14	0	0
64	D3	10	0	14	0	0
64	DA	50	0	70	3	0
64	DS	10	0	14	0	0
64	DU	10	0	14	1	0
65	DA	12	0	9	1	0
66	D0	4	0	6	0	0
66	D1	4	0	6	0	0
66	DA	24	0	36	11	0
66	DB	12	0	18	1	0
66	DR	4	0	6	0	0
67	DA	11	0	5	1	0
68	DA	8	0	12	0	0
69	AA	509	0	0	9	0
69	AC	6	0	0	0	0
69	AD	2	0	0	0	0
69	AE	5	0	0	0	0
69	AF	1	0	0	0	0
69	AG	1	0	0	0	0
69	AH	1	0	0	0	0
69	AJ	2	0	0	0	0
69	AK	6	0	0	0	0
69	AL	10	0	0	0	0
69	AM	4	0	0	0	0
69	AN	6	0	0	2	0
69	AO	2	0	0	0	0
69	AP	2	0	0	2	0
69	AS	1	0	0	0	0
69	AT	2	0	0	0	0
69	AU	2	0	0	0	0
69	BA	286	0	0	16	0
69	BD	12	0	0	0	0
69	BE	1	0	0	0	0
69	BF	2	0	0	0	0
69	BL	5	0	0	1	0
69	BN	3	0	0	0	0
69	BO	1	0	0	0	0
69	BP	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	BT	5	0	0	0	0
69	BU	2	0	0	0	0
69	C3	2	0	0	1	0
69	C4	1	0	0	0	0
69	CA	692	0	0	56	0
69	CB	13	0	0	1	0
69	CC	8	0	0	0	0
69	CD	6	0	0	0	0
69	CE	6	0	0	2	0
69	CK	1	0	0	0	0
69	CL	1	0	0	1	0
69	CM	5	0	0	0	0
69	CO	1	0	0	0	0
69	CS	1	0	0	0	0
69	CU	2	0	0	1	0
69	CV	2	0	0	0	0
69	CW	1	0	0	0	0
69	CY	1	0	0	0	0
69	D0	25	0	0	0	0
69	D1	47	0	0	3	0
69	D2	9	0	0	1	0
69	D3	25	0	0	0	0
69	D4	38	0	0	2	0
69	D5	14	0	0	0	0
69	DA	4815	0	0	46	0
69	DB	209	0	0	2	0
69	DC	106	0	0	2	0
69	DD	103	0	0	1	0
69	DE	62	0	0	0	0
69	DF	14	0	0	1	0
69	DG	6	0	0	0	0
69	DH	2	0	0	0	0
69	DK	59	0	0	1	0
69	DL	45	0	0	1	0
69	DM	67	0	0	0	0
69	DN	74	0	0	0	0
69	DO	42	0	0	1	0
69	DP	37	0	0	1	0
69	DQ	27	0	0	2	0
69	DR	67	0	0	1	0
69	DS	50	0	0	1	0
69	DT	61	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	DU	19	0	0	0	0
69	DV	22	0	0	0	0
69	DW	32	0	0	0	0
69	DX	30	0	0	2	0
69	DY	10	0	0	1	0
69	DZ	8	0	0	0	0
All	All	295060	0	194384	2516	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 5.

All (2516) 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)
14:BN:26:GLU:OE2	14:BN:26:GLU:N	1.97	0.96
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.44	0.94
14:AN:64:CYS:SG	69:AN:204:HOH:O	2.25	0.94
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.50	0.94
22:CA:1652:A:OP1	35:CO:8:ARG:NH2	2.04	0.90
14:BN:23:LYS:N	14:BN:26:GLU:OE1	2.04	0.90
22:CA:789:A:N1	69:CA:3287:HOH:O	2.06	0.89
1:AA:702:A:N6	53:DA:1846:G:O2'	2.05	0.89
53:DA:2885[B]:G:OP1	67:DA:3212:GUN:N2	2.06	0.89
11:AK:94:GLU:OE2	11:AK:98:ARG:NH2	2.06	0.89
5:BE:102:GLY:O	5:BE:104:GLY:N	2.05	0.88
6:BF:88:MET:SD	6:BF:90:MET:HE2	2.13	0.88
53:DA:2116:G:O6	53:DA:2171:A:N6	2.06	0.88
11:AK:13:ARG:NH2	11:AK:77:TYR:OH	2.07	0.88
1:AA:1130:A:OP1	9:AI:18:ARG:NH1	2.07	0.87
22:CA:878:A:N6	22:CA:899:A:O2'	2.07	0.86
22:CA:2429:G:OP2	69:CA:3861:HOH:O	1.91	0.86
14:BN:26:GLU:CD	14:BN:26:GLU:H	1.84	0.86
1:BA:140:U:O2	1:BA:183:C:N4	2.10	0.85
22:CA:2430:A:OP2	69:CA:3861:HOH:O	1.94	0.85
62:DA:3225:SPD:H52	62:DA:3225:SPD:H92	1.59	0.85
53:DA:1508:A:O2'	53:DA:1509:A:O4'	1.95	0.84
22:CA:459:U:O2'	41:CU:73:ARG:NH2	2.10	0.84
1:BA:978:A:OP2	1:BA:1362:A:N6	2.10	0.84
53:DA:141:G:OP2	53:DA:142:A:N6	2.11	0.84
22:CA:2579:C:OP1	69:CA:3871:HOH:O	1.96	0.83
53:DA:480:A:OP2	42:DV:44:LYS:NZ	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1147:C:O2	9:BI:18:ARG:NH2	2.14	0.81
26:CE:170:ARG:NH1	26:CE:179:SER:OG	2.13	0.81
13:BM:11:ASP:OD1	13:BM:12:HIS:N	2.14	0.81
20:AT:28:MET:HE1	20:AT:67:ILE:HD13	1.62	0.80
14:AN:67:THR:N	69:AN:204:HOH:O	2.15	0.80
22:CA:2210:U:O2	69:CA:3787:HOH:O	1.99	0.80
1:AA:127:G:O2'	17:AQ:6:ARG:NH1	2.15	0.79
22:CA:734:A:N3	69:CA:3705:HOH:O	2.14	0.79
53:DA:2224:G:OP1	24:DC:265:LYS:NZ	2.15	0.79
38:DR:19:LYS:HD3	57:DR:202:PG4:H22	1.64	0.79
22:CA:250:G:OP2	51:C4:13:ARG:NH1	2.14	0.79
4:AD:100:ASN:OD1	4:AD:111:ARG:NH1	2.16	0.79
24:CC:258:ARG:NH1	24:CC:264:ASP:OD1	2.16	0.78
22:CA:1154:G:OP2	38:CR:58:ARG:NH1	2.16	0.78
9:BI:12:ARG:NH2	9:BI:107:ASP:OD2	2.16	0.78
22:CA:2640:G:OP1	31:CK:95:ARG:NH1	2.17	0.78
38:DR:20:GLN:HG2	57:DR:202:PG4:H51	1.64	0.78
7:AG:68:ASN:O	7:AG:138:ARG:NH1	2.17	0.78
4:BD:100:ASN:OD1	4:BD:111:ARG:NH1	2.16	0.78
22:CA:1508:A:O2'	22:CA:1509:A:O4'	2.01	0.78
5:BE:151:GLU:O	5:BE:154:ALA:HB3	1.84	0.77
15:BO:18:ASP:OD1	15:BO:19:ALA:N	2.17	0.77
16:BP:1:MET:SD	16:BP:1:MET:N	2.53	0.77
53:DA:1236:G:N7	59:DA:3189:PUT:H41	2.00	0.77
1:AA:1147:C:O2	9:AI:18:ARG:NH2	2.18	0.76
1:BA:742:G:O6	69:BA:1865:HOH:O	2.03	0.76
1:BA:842:U:H3'	1:BA:843:U:C5'	2.16	0.76
63:DA:3203:1PE:H221	69:DA:3975:HOH:O	1.86	0.76
1:BA:1026:G:N1	1:BA:1035:A:N1	2.34	0.76
22:CA:2262:U:OP1	44:CX:41:ARG:NH2	2.19	0.76
25:CD:12:THR:OG1	25:CD:13:ARG:N	2.17	0.76
7:AG:111:ARG:NH1	7:AG:123:GLU:OE2	2.19	0.75
23:DB:90:C:OP2	69:DB:319:HOH:O	2.04	0.75
39:DS:37:GLU:O	69:DS:319:HOH:O	2.03	0.75
1:AA:1134:G:N2	1:AA:1140:C:N3	2.34	0.75
32:DL:113:MET:HE1	32:DL:116:ILE:HD11	1.69	0.75
22:CA:77:G:O2'	46:CZ:7:ARG:NH2	2.20	0.75
22:CA:2032:G:N7	69:CA:3866:HOH:O	2.20	0.74
53:DA:1311:G:N7	69:DA:6065:HOH:O	2.20	0.74
3:AC:40:ARG:NH1	3:AC:55:ILE:O	2.21	0.74
1:BA:836:G:N7	69:BA:1920:HOH:O	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1130:A:OP1	9:BI:18:ARG:NH1	2.21	0.74
16:BP:42:ILE:O	16:BP:44:SER:N	2.20	0.74
30:DJ:117:MET:HE2	30:DJ:117:MET:HA	1.67	0.73
1:BA:319:G:N7	69:BA:1722:HOH:O	2.20	0.73
13:AM:82:ASP:OD2	27:DF:112:ARG:NH2	2.20	0.73
22:CA:2134:A:N6	22:CA:2157:G:O2'	2.21	0.73
53:DA:2827:C:O2	66:DA:3198:EDO:H21	1.89	0.72
24:DC:251:GLN:NE2	69:DC:406:HOH:O	2.21	0.72
38:DR:19:LYS:HD3	57:DR:202:PG4:H41	1.71	0.72
1:BA:516:PSU:O2	69:BA:1970:HOH:O	2.07	0.72
22:CA:1588:G:N3	69:CA:3746:HOH:O	2.22	0.72
22:CA:1962:5MC:HM53	69:CA:3753:HOH:O	1.89	0.72
6:AF:102:MET:HE1	18:AR:24:LYS:HB3	1.72	0.71
1:BA:1109:C:H2'	1:BA:1110:A:H5''	1.72	0.71
16:BP:46:LYS:HD3	16:BP:47:GLU:H	1.54	0.71
22:CA:2685:G:OP1	32:CL:78:ARG:NH2	2.22	0.71
22:CA:820:A:N1	69:CA:3772:HOH:O	2.23	0.71
66:DA:3198:EDO:H12	64:DA:3204:PGE:H32	1.72	0.71
22:CA:732:C:OP2	69:CA:3273:HOH:O	2.09	0.71
1:BA:1279:G:OP1	10:BJ:9:ARG:NH2	2.24	0.71
8:BH:77:ARG:NE	8:BH:79:SER:O	2.24	0.71
53:DA:1027:A:N3	69:DA:6955:HOH:O	2.23	0.71
53:DA:2428:G:OP2	59:DA:3224:PUT:H11	1.89	0.71
9:AI:12:ARG:NH2	9:AI:107:ASP:OD2	2.24	0.70
1:BA:1204:A:OP2	69:BA:1817:HOH:O	2.09	0.70
12:BL:14:ARG:HA	12:BL:14:ARG:HH11	1.56	0.70
22:CA:568:U:H1'	22:CA:2030:6MZ:H9C1	1.73	0.70
22:CA:1825:U:OP2	69:CA:3822:HOH:O	2.09	0.70
41:DU:2:ILE:HG22	41:DU:7:LEU:HD21	1.73	0.70
30:DJ:113:LYS:O	30:DJ:117:MET:N	2.23	0.70
22:CA:1602:U:O4	69:CA:3603:HOH:O	2.08	0.70
1:BA:1266:G:N2	1:BA:1269:A:OP2	2.24	0.70
1:BA:1518:MA6:H103	1:BA:1519:MA6:C10	2.20	0.70
22:CA:616:A:OP2	69:CA:3263:HOH:O	2.08	0.70
22:CA:2495:G:N7	69:CA:3681:HOH:O	2.23	0.70
1:AA:1486:G:OP2	69:AA:1925:HOH:O	2.08	0.70
22:CA:978:G:N7	69:CA:3501:HOH:O	2.24	0.70
1:AA:1518:MA6:H103	1:AA:1519:MA6:C10	2.21	0.70
5:BE:66:LYS:O	5:BE:70:ASN:ND2	2.25	0.70
5:BE:83:HIS:CE1	8:BH:96:MET:HE3	2.27	0.70
19:BS:36:ARG:NH2	19:BS:75:ALA:O	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CA:581:C:OP2	38:CR:33:ARG:NE	2.25	0.69
22:CA:686:U:OP2	69:CA:3607:HOH:O	2.08	0.69
1:BA:9:G:H5'	5:BE:108:GLY:HA3	1.74	0.69
22:CA:2134:A:OP2	22:CA:2157:G:N2	2.24	0.69
22:CA:2268:A:OP1	69:CA:3440:HOH:O	2.09	0.69
21:AU:31:GLU:OE2	21:AU:34:ARG:NH2	2.25	0.69
1:BA:842:U:H3'	1:BA:843:U:H5'	1.74	0.69
57:DR:202:PG4:H62	69:DR:359:HOH:O	1.92	0.69
53:DA:568:U:H1'	53:DA:2030:6MZ:H9C1	1.74	0.69
1:AA:964:A:OP1	69:AA:2195:HOH:O	2.11	0.69
5:AE:94:VAL:HG22	5:AE:111:MET:HE3	1.74	0.69
24:CC:69:ARG:O	24:CC:189:ARG:NH2	2.26	0.69
30:CJ:113:LYS:O	30:CJ:117:MET:N	2.26	0.69
41:CU:3:ARG:NH2	41:CU:5:GLU:OE2	2.27	0.68
53:DA:2609:U:C5	66:DA:3194:EDO:H12	2.28	0.68
37:DQ:68:GLU:OE2	69:DQ:307:HOH:O	2.10	0.68
11:BK:94:GLU:OE2	11:BK:98:ARG:NH2	2.25	0.68
53:DA:1311:G:O2'	69:DA:6066:HOH:O	2.09	0.68
1:AA:845:A:O3'	18:AR:48:ARG:NH2	2.25	0.68
53:DA:1176:U:H2'	53:DA:1177:G:C8	2.27	0.68
53:DA:2428:G:N7	59:DA:3224:PUT:N1	2.42	0.68
53:DA:2072:C:OP1	69:DA:3838:HOH:O	2.11	0.68
53:DA:2310:C:OP1	69:DA:3597:HOH:O	2.12	0.68
5:BE:38:VAL:HG13	5:BE:117:VAL:HG21	1.75	0.68
22:CA:2720:U:OP1	37:CQ:53:ARG:NH2	2.26	0.68
53:DA:1167:C:OP2	69:DA:4751:HOH:O	2.12	0.68
30:DJ:113:LYS:HB3	30:DJ:117:MET:HE3	1.76	0.68
41:CU:5:GLU:HG3	46:CZ:22:LEU:HD13	1.75	0.68
23:DB:84:G:H21	66:DB:212:EDO:H11	1.59	0.68
29:DH:116:ARG:NH2	29:DH:133:GLN:OE1	2.27	0.68
1:BA:1376:U:O4	7:BG:10:ARG:NH1	2.27	0.67
32:CL:93:GLN:NE2	32:CL:111:LYS:O	2.27	0.67
22:CA:1998:A:OP2	25:CD:141:ARG:NH2	2.27	0.67
30:CJ:113:LYS:HB3	30:CJ:117:MET:HE3	1.76	0.67
1:AA:738:C:OP1	6:AF:2:ARG:NH2	2.27	0.67
1:AA:980:C:O3'	14:AN:13:ARG:NH2	2.27	0.67
53:DA:2720:U:OP1	37:DQ:53:ARG:NH2	2.28	0.67
22:CA:1187:G:N7	69:CA:3493:HOH:O	2.27	0.67
43:DW:4:ILE:HG13	43:DW:50:MET:HE1	1.77	0.67
5:BE:101:GLU:O	5:BE:103:THR:N	2.28	0.67
41:CU:28:ASN:ND2	41:CU:91:GLN:OE1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CA:591:U:H1'	51:C4:2:PRO:HD2	1.77	0.67
50:D3:32:ALA:CB	61:D3:102:PEG:H12	2.25	0.67
1:AA:453:G:N7	59:AA:1673:PUT:H42	2.10	0.67
13:AM:4:ILE:O	13:AM:6:GLY:N	2.28	0.67
1:BA:1360:A:N7	69:BA:1815:HOH:O	2.28	0.67
1:BA:439:U:H4'	4:BD:121:LYS:HD2	1.77	0.66
22:CA:1250:G:OP2	33:CM:21:ARG:NH2	2.28	0.66
1:AA:412:A:H1'	1:AA:413:G:H5'	1.75	0.66
1:AA:806:C:H4'	57:AA:1670:PG4:H11	1.76	0.66
32:CL:108:ARG:HD3	32:CL:113:MET:HE1	1.76	0.66
53:DA:2799:A:N7	69:DA:5142:HOH:O	2.28	0.66
3:AC:19:ASN:ND2	14:AN:90:ARG:O	2.28	0.66
6:BF:18:VAL:HA	6:BF:21:MET:HE3	1.76	0.66
7:AG:138:ARG:NH2	7:AG:139:GLU:OE2	2.29	0.66
53:DA:846:U:O2'	53:DA:847:U:OP2	2.11	0.66
32:CL:7:MET:HE1	32:CL:44:LYS:HG3	1.78	0.66
1:AA:536:C:OP1	69:AA:1765:HOH:O	2.13	0.66
12:BL:49:LEU:O	69:BL:203:HOH:O	2.13	0.66
13:AM:4:ILE:O	13:AM:7:ILE:N	2.26	0.66
1:BA:1197:A:OP1	69:BA:1934:HOH:O	2.12	0.66
22:CA:733:G:OP1	69:CA:3711:HOH:O	2.14	0.66
22:CA:1385:A:O2'	22:CA:1396:U:O2	2.12	0.66
22:CA:2127:G:O2'	22:CA:2173:A:N3	2.29	0.66
28:DG:101:ASN:ND2	28:DG:116:GLN:OE1	2.28	0.66
1:AA:1486:G:OP1	69:AA:1920:HOH:O	2.13	0.66
22:CA:998:C:OP2	38:CR:58:ARG:NH2	2.28	0.66
22:CA:1378:A:O2'	22:CA:1380:G:N7	2.23	0.66
32:CL:38:ILE:O	69:CL:201:HOH:O	2.14	0.66
9:BI:22:LYS:O	9:BI:62:ASP:N	2.29	0.65
22:CA:1823:G:N7	69:CA:3872:HOH:O	2.29	0.65
35:CO:69:ARG:O	35:CO:71:ARG:N	2.29	0.65
22:CA:1417:C:OP1	69:CA:3746:HOH:O	2.13	0.65
1:BA:1033:G:N2	1:BA:1034:G:N3	2.45	0.65
53:DA:788:A:OP1	59:DA:3223:PUT:H42	1.97	0.65
53:DA:2127:G:O2'	53:DA:2128:G:O4'	2.13	0.65
3:AC:179:ARG:NH1	3:AC:206:GLU:OE1	2.29	0.65
22:CA:450:G:O6	69:CA:3238:HOH:O	2.11	0.65
25:CD:151:THR:O	25:CD:153:GLY:N	2.25	0.65
1:AA:7:A:N6	5:AE:97:GLN:OE1	2.30	0.65
1:BA:450:G:O5'	69:BA:1918:HOH:O	2.14	0.65
1:BA:1361:G:N2	1:BA:1362:A:N7	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DA:2017:U:O4	66:DA:3209:EDO:H22	1.97	0.65
1:AA:263:A:OP2	20:AT:74:ARG:NH1	2.29	0.65
22:CA:85:G:OP1	42:CV:7:ARG:N	2.28	0.65
50:C3:11:LYS:NZ	69:C3:201:HOH:O	2.29	0.65
1:AA:771:G:N7	69:AA:1798:HOH:O	2.30	0.65
1:BA:1028:C:O2'	1:BA:1029:U:O5'	2.13	0.65
28:DG:104:ASN:ND2	28:DG:114:ASP:OD1	2.30	0.65
1:BA:880:C:OP1	12:BL:9:ARG:NH2	2.30	0.65
1:BA:1220:G:OP1	19:BS:37:ARG:NH2	2.30	0.65
26:CE:125:SER:O	26:CE:137:LYS:NZ	2.29	0.65
64:DA:3218:PGE:O4	69:DA:7614:HOH:O	2.14	0.65
62:DA:3225:SPD:H92	62:DA:3225:SPD:C5	2.27	0.65
1:AA:8:A:C6	4:AD:206:LYS:HB3	2.32	0.64
5:BE:104:GLY:HA3	5:BE:122:ASN:HA	1.79	0.64
22:CA:528:A:OP1	69:CA:3840:HOH:O	2.15	0.64
23:CB:5:U:O2'	23:CB:27:C:O2	2.16	0.64
53:DA:812:C:O2'	38:DR:13:ARG:NH1	2.30	0.64
44:DX:39:ARG:NH1	69:DX:124:HOH:O	2.30	0.64
11:AK:119:ASN:OD1	21:AU:35:ARG:NH1	2.31	0.64
2:BB:120:GLN:O	2:BB:125:THR:N	2.30	0.64
9:BI:84:THR:HG21	9:BI:103:PHE:HB3	1.79	0.64
22:CA:2430:A:OP1	69:CA:3859:HOH:O	2.15	0.64
53:DA:2209:G:N3	69:DA:5103:HOH:O	2.30	0.64
9:AI:22:LYS:O	9:AI:62:ASP:N	2.29	0.64
25:CD:85:ALA:O	25:CD:87:GLY:N	2.28	0.64
26:CE:76:PRO:HA	26:CE:82:GLY:HA2	1.80	0.64
30:CJ:117:MET:HA	30:CJ:117:MET:HE2	1.80	0.64
30:DJ:100:LYS:CB	30:DJ:141:GLU:HB2	2.27	0.64
53:DA:2033:A:H5'	69:DA:4744:HOH:O	1.97	0.64
8:AH:54:ASP:OD1	8:AH:55:THR:N	2.30	0.64
30:CJ:100:LYS:CB	30:CJ:141:GLU:HB2	2.28	0.64
53:DA:139:U:O4	41:DU:2:ILE:HG13	1.98	0.64
1:BA:415:A:O2'	53:DA:2152:G:N2	2.30	0.63
43:DW:4:ILE:CG1	43:DW:50:MET:HE1	2.28	0.63
14:AN:89:MET:HE1	14:AN:98:LYS:HD2	1.79	0.63
5:BE:154:ALA:C	5:BE:156:LYS:H	2.07	0.63
53:DA:2127:G:O2'	53:DA:2128:G:O5'	2.15	0.63
1:AA:845:A:O2'	18:AR:48:ARG:NH2	2.31	0.63
7:BG:25:LYS:CB	7:BG:101:MET:HE1	2.27	0.63
3:BC:139:GLN:O	3:BC:141:ALA:N	2.31	0.63
53:DA:136:G:H1	53:DA:143:C:N4	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1183:U:O2'	1:BA:1185:G:OP2	2.16	0.63
1:AA:928:G:O2'	1:AA:1533:C:OP1	2.16	0.63
19:AS:36:ARG:NH2	19:AS:75:ALA:O	2.32	0.63
47:C0:40:ASP:OD1	47:C0:45:ARG:NH1	2.32	0.63
38:DR:20:GLN:HG3	57:DR:202:PG4:H42	1.80	0.63
5:BE:154:ALA:HA	5:BE:157:ARG:HB3	1.81	0.63
1:BA:1328:C:H5''	13:BM:28:THR:HG21	1.80	0.63
42:CV:74:ASN:O	42:CV:76:ALA:N	2.31	0.63
53:DA:1061:U:OP2	30:DJ:10:LYS:NZ	2.31	0.63
1:AA:405:U:OP2	4:AD:3:ARG:NH1	2.32	0.63
37:CQ:113:ARG:O	37:CQ:115:ASN:N	2.31	0.63
20:AT:28:MET:HE3	20:AT:58:VAL:HG12	1.80	0.62
1:BA:263:A:OP1	20:BT:74:ARG:NH1	2.31	0.62
22:CA:2031:A:C6	22:CA:2498:OMC:H1'	2.34	0.62
23:DB:54:G:H21	27:DF:26:MET:HE3	1.65	0.62
22:CA:528:A:C2	22:CA:2043:C:H4'	2.34	0.62
1:BA:1187:G:H5'	9:BI:115:LYS:HE3	1.82	0.62
14:BN:89:MET:HE1	14:BN:98:LYS:HD2	1.82	0.62
19:BS:29:LYS:HB3	19:BS:30:PRO:HD2	1.82	0.62
22:CA:2498:OMC:HM22	22:CA:2499:C:H5'	1.82	0.62
26:CE:23:PHE:CD1	26:CE:111:GLU:HG3	2.35	0.62
46:CZ:45:GLN:O	46:CZ:47:ARG:N	2.28	0.62
30:DJ:100:LYS:HB2	30:DJ:141:GLU:HB2	1.82	0.62
34:CN:53:MET:HE1	34:CN:103:TYR:CG	2.35	0.62
27:CF:7:TYR:OH	27:CF:172:ALA:O	2.17	0.62
53:DA:878:A:N6	53:DA:899:A:O2'	2.32	0.62
2:BB:133:GLU:OE2	2:BB:137:ARG:NH1	2.33	0.62
4:BD:202:GLU:OE2	5:BE:112:ARG:NH1	2.33	0.62
28:CG:159:GLY:O	28:CG:163:ARG:NH1	2.33	0.62
30:CJ:110:ALA:O	30:CJ:114:ALA:N	2.33	0.62
7:BG:25:LYS:HB3	7:BG:101:MET:HE1	1.81	0.61
22:CA:297:G:H5''	42:CV:85:PHE:HB2	1.81	0.61
1:BA:465:A:H2'	1:BA:466:A:C8	2.34	0.61
28:CG:11:VAL:O	28:CG:48:ASN:ND2	2.33	0.61
25:CD:103:ASP:O	25:CD:105:LYS:N	2.29	0.61
33:CM:93:ASN:OD1	33:CM:94:THR:N	2.32	0.61
5:AE:79:GLY:O	5:AE:121:HIS:N	2.28	0.61
14:BN:21:PHE:C	14:BN:26:GLU:OE1	2.44	0.61
35:CO:20:MET:HE1	35:CO:40:LYS:HD3	1.82	0.61
1:AA:1225:A:H2'	1:AA:1226:C:C5	2.35	0.61
5:AE:85:VAL:HG13	5:AE:96:MET:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DA:1186:G:OP1	69:DA:3652:HOH:O	2.16	0.61
1:AA:411:A:OP2	4:AD:26:ARG:NH2	2.33	0.61
24:CC:136:PRO:O	24:CC:139:SER:OG	2.17	0.61
27:CF:61:SER:O	27:CF:63:GLN:N	2.34	0.61
30:DJ:110:ALA:O	30:DJ:114:ALA:N	2.34	0.61
53:DA:456:C:OP1	69:DA:4875:HOH:O	2.16	0.61
1:BA:531:U:H4'	1:BA:532:A:H4'	1.83	0.61
22:CA:2307:G:H4'	22:CA:2308:G:O5'	2.01	0.61
22:CA:1059:G:H4'	30:CJ:117:MET:HE1	1.83	0.60
2:AB:120:GLN:O	2:AB:125:THR:N	2.34	0.60
1:BA:1492:A:OP2	1:BA:1493:A:N6	2.35	0.60
10:BJ:65:TYR:HB2	14:BN:96:LEU:HD11	1.83	0.60
41:CU:3:ARG:HG2	41:CU:3:ARG:HH11	1.66	0.60
53:DA:545:U:H2'	53:DA:546:U:O3'	2.01	0.60
55:DI:131:THR:OG1	55:DI:133:GLU:O	2.19	0.60
1:AA:8:A:N6	4:AD:202:GLU:O	2.34	0.60
13:AM:3:ARG:O	13:AM:57:ARG:NH2	2.33	0.60
5:BE:151:GLU:HG3	5:BE:152:MET:HE2	1.83	0.60
11:BK:92:GLY:O	11:BK:94:GLU:N	2.32	0.60
42:CV:74:ASN:C	42:CV:76:ALA:H	2.10	0.60
7:AG:90:GLU:N	7:AG:90:GLU:OE2	2.34	0.60
25:CD:1:MET:HE3	25:CD:205:PRO:CG	2.31	0.60
53:DA:1013:C:OP2	69:DA:5610:HOH:O	2.16	0.60
53:DA:1172:C:N4	53:DA:1173:U:O2	2.35	0.60
9:AI:95:ARG:O	9:AI:98:LEU:N	2.35	0.60
5:BE:111:MET:HG3	5:BE:140:THR:HG21	1.82	0.60
50:D3:22:MET:HE2	50:D3:31:LEU:CD1	2.31	0.60
17:AQ:60:GLU:OE1	17:AQ:77:ARG:NE	2.33	0.60
22:CA:2171:A:O2'	22:CA:2173:A:OP1	2.19	0.60
4:BD:99:ASP:OD1	4:BD:100:ASN:N	2.35	0.60
35:DO:114:GLU:OE2	35:DO:118:ARG:NH2	2.33	0.60
10:AJ:63:ASP:HB3	10:AJ:65:TYR:CE1	2.36	0.60
20:BT:67:ILE:HG13	20:BT:71:LYS:HD3	1.84	0.60
38:CR:9:ILE:C	38:CR:9:ILE:HD12	2.27	0.60
53:DA:2609:U:C6	66:DA:3194:EDO:H12	2.36	0.60
12:AL:110:ARG:NH1	12:AL:112:GLN:O	2.34	0.60
1:AA:844:G:H2'	1:AA:844:G:N3	2.16	0.60
9:AI:88:MET:SD	9:AI:95:ARG:HG2	2.42	0.60
1:BA:846:G:OP1	18:BR:48:ARG:NH2	2.33	0.60
22:CA:2131:U:H5'	22:CA:2132:U:H5''	1.84	0.60
35:CO:1:MET:HE2	35:CO:1:MET:H1	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:CP:17:LYS:HE2	36:CP:17:LYS:HA	1.84	0.60
52:C5:26:ILE:H	52:C5:26:ILE:HD13	1.66	0.60
14:AN:31:ILE:HA	14:AN:34:VAL:HG23	1.84	0.59
1:BA:537:G:OP1	12:BL:110:ARG:NH2	2.34	0.59
25:CD:1:MET:HE3	25:CD:205:PRO:HG3	1.83	0.59
45:DY:72:ARG:O	45:DY:75:GLY:N	2.28	0.59
1:AA:1178:G:N2	1:AA:1181:G:OP2	2.34	0.59
15:BO:64:ARG:NH1	15:BO:68:ASP:OD1	2.35	0.59
22:CA:605:G:N3	22:CA:657:U:O2'	2.34	0.59
1:AA:427:U:O2'	1:AA:541:G:OP1	2.21	0.59
1:AA:1228:C:P	13:AM:107:ARG:HH22	2.26	0.59
5:AE:161:VAL:HG12	5:AE:162:GLU:H	1.67	0.59
11:AK:112:ASP:HB3	21:AU:2:PRO:HG2	1.83	0.59
1:BA:1060:U:OP1	14:BN:85:ARG:NH2	2.36	0.59
5:BE:45:ARG:HA	5:BE:72:ILE:O	2.01	0.59
23:CB:30:C:OP1	36:CP:3:LYS:NZ	2.35	0.59
25:CD:149:ASN:OD1	25:CD:150:GLN:N	2.35	0.59
53:DA:297:G:OP2	69:DA:7999:HOH:O	2.16	0.59
53:DA:558:U:OP2	69:DA:5211:HOH:O	2.15	0.59
1:BA:476:U:O4	69:BA:1912:HOH:O	2.17	0.59
16:BP:78:VAL:O	16:BP:79:ASN:HB2	2.01	0.59
22:CA:207:A:OP2	69:CA:3827:HOH:O	2.16	0.59
53:DA:141:G:H2'	53:DA:142:A:C2	2.37	0.59
1:BA:1492:A:H2'	22:CA:1913:A:C6	2.38	0.59
22:CA:1368:G:N7	69:CA:3533:HOH:O	2.31	0.59
55:DI:132:TYR:N	55:DI:133:GLU:HB2	2.16	0.59
8:BH:3:MET:N	8:BH:3:MET:SD	2.75	0.59
22:CA:826:U:O2'	33:CM:53:GLY:HA3	2.03	0.59
29:DH:1:MET:HE3	29:DH:23:ALA:HA	1.85	0.59
36:DP:68:LYS:HB3	61:DP:201:PEG:H22	1.84	0.59
5:BE:157:ARG:O	5:BE:159:LYS:N	2.34	0.59
17:BQ:17:MET:HE3	17:BQ:20:SER:O	2.03	0.59
1:AA:80:A:C2	1:AA:90:C:N3	2.71	0.59
22:CA:1534:U:O2'	22:CA:1537:G:O6	2.20	0.59
53:DA:1171:G:C4	53:DA:1172:C:N4	2.71	0.59
53:DA:711:G:OP1	69:DA:5064:HOH:O	2.16	0.58
53:DA:787:C:OP1	59:DA:3223:PUT:N1	2.36	0.58
53:DA:2683:C:O2	32:DL:70:ARG:NH2	2.30	0.58
1:AA:825:A:O2'	8:AH:13:ARG:NH1	2.37	0.58
1:BA:1493:A:OP2	1:BA:1493:A:C8	2.56	0.58
7:BG:68:ASN:O	7:BG:138:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DH:41:LYS:HA	29:DH:44:ILE:HG23	1.84	0.58
12:AL:43:LYS:HE2	12:AL:89:D2T:H7	1.85	0.58
3:BC:126:ARG:O	3:BC:127:ARG:HB2	2.03	0.58
53:DA:1119:U:OP2	69:DA:5002:HOH:O	2.16	0.58
47:D0:10:THR:HG22	47:D0:11:ARG:HG3	1.85	0.58
1:BA:736:C:H5'	6:BF:88:MET:HE2	1.85	0.58
22:CA:646:U:C5'	22:CA:647:G:H5''	2.33	0.58
27:CF:122:PHE:O	27:CF:124:GLY:N	2.35	0.58
53:DA:1292:G:N3	69:DA:6760:HOH:O	2.31	0.58
23:DB:23:G:O6	69:DB:304:HOH:O	2.17	0.58
4:AD:78:GLU:OE2	4:AD:81:ARG:NH2	2.36	0.58
19:AS:29:LYS:HB3	19:AS:30:PRO:HD2	1.85	0.58
8:BH:64:LYS:HB3	8:BH:71:VAL:HG21	1.86	0.58
9:BI:88:MET:SD	9:BI:95:ARG:HG2	2.44	0.58
13:BM:4:ILE:O	13:BM:6:GLY:N	2.36	0.58
3:AC:142:MET:HE2	3:AC:170:GLU:HG3	1.85	0.58
1:BA:521:G:OP1	69:BA:1874:HOH:O	2.17	0.58
5:BE:100:SER:O	5:BE:122:ASN:ND2	2.37	0.58
15:BO:17:ARG:N	15:BO:17:ARG:HD3	2.19	0.58
53:DA:15:G:OP2	69:DA:5595:HOH:O	2.16	0.58
53:DA:2886[B]:A:N3	53:DA:2886[B]:A:H2'	2.17	0.58
51:D4:63:PRO:O	69:D4:128:HOH:O	2.17	0.58
22:CA:666:A:H4'	33:CM:48:ARG:HD2	1.86	0.58
22:CA:784:G:H5'	22:CA:785:G:OP1	2.04	0.58
26:CE:41:GLN:O	26:CE:43:THR:N	2.30	0.58
8:AH:113:ASP:OD1	8:AH:117:ARG:NH2	2.37	0.58
1:BA:991:U:H4'	1:BA:992:U:H5''	1.86	0.58
2:BB:126:PHE:C	2:BB:128:LYS:H	2.10	0.58
5:BE:156:LYS:HD2	8:BH:71:VAL:HG13	1.85	0.58
53:DA:2674:G:H4'	32:DL:30:ARG:HD2	1.85	0.58
10:AJ:48:ARG:NH1	10:AJ:66:GLU:OE1	2.37	0.58
53:DA:2275:C:C6	57:DA:3193:PG4:H41	2.38	0.58
53:DA:2831:G:OP1	54:DD:56:LYS:NZ	2.36	0.58
53:DA:2872:A:N7	69:DA:4918:HOH:O	2.32	0.58
5:AE:85:VAL:CG1	5:AE:96:MET:HE3	2.35	0.57
7:BG:92:ARG:HB3	7:BG:93:PRO:HD2	1.86	0.57
53:DA:948:C:O2'	63:DA:3203:1PE:H241	2.04	0.57
53:DA:1171:G:H2'	53:DA:1172:C:C4	2.39	0.57
27:DF:158:THR:HG22	27:DF:160:ALA:H	1.69	0.57
55:DI:103:ASN:O	55:DI:105:LYS:N	2.37	0.57
37:DQ:31:TRP:CD1	57:DQ:202:PG4:H31	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:691:G:O6	11:AK:57:LYS:NZ	2.33	0.57
1:BA:1329:A:H5''	13:BM:26:GLY:H	1.69	0.57
53:DA:1171:G:H2'	53:DA:1172:C:C5	2.39	0.57
53:DA:1665:A:OP1	69:DA:4215:HOH:O	2.17	0.57
14:AN:21:PHE:HA	14:AN:25:ALA:HB3	1.85	0.57
1:BA:825:A:O2'	8:BH:13:ARG:NH1	2.37	0.57
22:CA:1779:U:H5	22:CA:1784:A:N7	2.02	0.57
53:DA:1698:A:OP2	59:DA:3213:PUT:H22	2.05	0.57
8:AH:96:MET:HE3	8:AH:130:ALA:CB	2.34	0.57
22:CA:396:G:H1'	45:CY:29:PHE:HB3	1.84	0.57
22:CA:1143:A:OP2	69:CA:3517:HOH:O	2.17	0.57
33:CM:29:LYS:O	33:CM:31:GLY:N	2.37	0.57
54:DD:149:ASN:OD1	54:DD:150[B]:MEQ:N	2.36	0.57
13:BM:81:MET:O	13:BM:92:ARG:NH2	2.37	0.57
22:CA:1754:A:N1	22:CA:2716:C:O2'	2.35	0.57
30:CJ:100:LYS:HA	30:CJ:139:VAL:O	2.04	0.57
32:CL:1:MET:HE3	32:CL:32:TYR:CZ	2.39	0.57
32:CL:107:LEU:O	32:CL:109:SER:N	2.37	0.57
53:DA:2286:G:OP2	49:D2:6:ARG:NH2	2.37	0.57
1:BA:100:G:OP2	69:BA:1869:HOH:O	2.17	0.57
35:CO:45:ARG:HG2	35:CO:95:THR:HG21	1.86	0.57
53:DA:136:G:C2	53:DA:144:A:C2	2.92	0.57
28:DG:127:THR:HG22	28:DG:129:THR:H	1.70	0.57
1:AA:207:C:N4	1:AA:212:G:O6	2.37	0.57
1:AA:1060:U:OP1	14:AN:85:ARG:NH2	2.37	0.57
2:AB:27:MET:HE2	2:AB:188:ASP:O	2.04	0.57
18:AR:37:GLY:O	18:AR:63:ARG:NH2	2.35	0.57
25:CD:151:THR:HG22	25:CD:152:PRO:N	2.19	0.57
1:BA:1109:C:C2'	1:BA:1110:A:H5''	2.35	0.57
6:BF:51:ILE:C	6:BF:53:LYS:H	2.12	0.57
14:BN:49:GLN:NE2	19:BS:10:PHE:CE2	2.73	0.57
53:DA:585:G:N7	38:DR:6:ARG:NH1	2.48	0.57
5:BE:101:GLU:O	5:BE:102:GLY:C	2.48	0.57
12:BL:7:LEU:HD22	12:BL:12:ARG:HD2	1.87	0.57
22:CA:2550:G:O6	22:CA:2551:C:N4	2.38	0.57
53:DA:142:A:H2'	53:DA:143:C:C6	2.40	0.57
53:DA:1172:C:C4	53:DA:1173:U:H1'	2.39	0.57
53:DA:2257:U:O2	57:DA:3193:PG4:H71	2.04	0.57
53:DA:2434:A:N7	69:DA:6970:HOH:O	2.32	0.57
53:DA:2441:U:O2'	62:DA:3225:SPD:H91	2.04	0.57
3:AC:126:ARG:O	3:AC:127:ARG:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:DU:1:MET:HE2	41:DU:1:MET:N	2.20	0.56
1:BA:483:C:O2	16:BP:13:LYS:NZ	2.38	0.56
1:AA:617:G:O2'	69:AA:1936:HOH:O	2.18	0.56
2:AB:126:PHE:C	2:AB:128:LYS:H	2.13	0.56
1:BA:1317:C:H2'	14:BN:49:GLN:HE21	1.70	0.56
53:DA:357:C:H2'	53:DA:358:U:C6	2.41	0.56
53:DA:1020:A:C2	53:DA:1141:U:C2	2.93	0.56
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.70	0.56
46:CZ:7:ARG:HG2	46:CZ:56:LEU:HD13	1.87	0.56
1:AA:261:U:OP2	20:AT:74:ARG:NH2	2.38	0.56
22:CA:2004:G:OP2	69:CA:3658:HOH:O	2.18	0.56
48:D1:16:ARG:O	69:D1:208:HOH:O	2.17	0.56
1:AA:203:G:N2	1:AA:204:G:O6	2.39	0.56
13:BM:93:ARG:NH2	19:BS:80:TYR:OH	2.39	0.56
36:CP:33:ARG:O	36:CP:34:HIS:HB2	2.05	0.56
53:DA:544:C:H3'	53:DA:545:U:C2	2.41	0.56
53:DA:1478:G:H1	53:DA:1513:U:H3	1.54	0.56
11:BK:119:ASN:OD1	21:BU:35:ARG:NH1	2.36	0.56
22:CA:2469:A:O2'	34:CN:55:ARG:NH2	2.35	0.56
62:DA:3225:SPD:H82	69:DA:5539:HOH:O	2.06	0.56
6:AF:88:MET:SD	6:AF:90:MET:HE2	2.46	0.56
1:BA:276:G:OP1	17:BQ:14:SER:OG	2.21	0.56
22:CA:192:C:O2'	22:CA:802:A:N3	2.34	0.56
45:DY:41:GLU:N	69:DY:102:HOH:O	2.39	0.56
1:BA:840:C:C5	1:BA:842:U:H5'	2.41	0.56
3:BC:179:ARG:HD2	3:BC:206:GLU:HB2	1.88	0.56
6:BF:3:HIS:HB2	6:BF:92:THR:HG23	1.87	0.56
24:CC:260:ASN:O	24:CC:262:ARG:N	2.39	0.56
26:CE:52:VAL:HG21	26:CE:81:GLY:CA	2.35	0.56
30:CJ:100:LYS:HB2	30:CJ:141:GLU:HB2	1.88	0.56
53:DA:788:A:H3'	59:DA:3223:PUT:H41	1.88	0.56
1:AA:1135:U:N3	1:AA:1137:C:O2	2.40	0.56
1:BA:81:A:N7	1:BA:83:C:N4	2.54	0.56
1:BA:1189:U:OP1	14:BN:98:LYS:NZ	2.39	0.56
1:BA:404:G:N7	4:BD:2:ALA:HB3	2.21	0.55
22:CA:139:U:HO2'	22:CA:141:G:H1	1.51	0.55
24:CC:158:ALA:HB1	24:CC:197:ASN:HB3	1.87	0.55
30:DJ:19:ASN:HA	30:DJ:39:CYS:SG	2.46	0.55
22:CA:526:A:OP1	69:CA:3842:HOH:O	2.18	0.55
22:CA:614:A:O2'	22:CA:615:U:OP2	2.25	0.55
53:DA:1059:G:H4'	30:DJ:117:MET:HE1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:DS:21:ARG:HH21	57:DS:202:PG4:H71	1.71	0.55
48:D1:12:LYS:NZ	69:D1:240:HOH:O	2.38	0.55
9:AI:84:THR:HG21	9:AI:103:PHE:HB3	1.87	0.55
1:BA:451:A:H2'	69:BA:1918:HOH:O	2.06	0.55
18:BR:42:SER:O	18:BR:46:GLY:N	2.40	0.55
36:CP:52:SER:OG	36:CP:53:THR:N	2.39	0.55
10:AJ:7:ARG:HG2	10:AJ:101:SER:HB2	1.87	0.55
5:BE:26:LYS:HA	5:BE:26:LYS:HE3	1.87	0.55
8:BH:88:ARG:O	8:BH:89:LYS:HB3	2.06	0.55
30:DJ:100:LYS:HA	30:DJ:139:VAL:O	2.06	0.55
9:AI:85:ARG:HA	9:AI:88:MET:HE3	1.88	0.55
26:CE:41:GLN:C	26:CE:43:THR:H	2.15	0.55
39:CS:49:ILE:HG22	39:CS:53:PHE:C	2.31	0.55
46:CZ:11:VAL:O	46:CZ:15:ASN:ND2	2.39	0.55
7:BG:90:GLU:N	7:BG:90:GLU:OE1	2.40	0.55
22:CA:370:G:N7	69:CA:3474:HOH:O	2.33	0.55
23:DB:2:G:C2	23:DB:119:A:C2	2.95	0.55
54:DD:149:ASN:OD1	54:DD:150[A]:MEQ:N	2.36	0.55
1:BA:1366:C:O2'	10:BJ:62:ARG:NH2	2.38	0.55
7:BG:37:SER:O	7:BG:41:SER:OG	2.24	0.55
22:CA:1993:U:H4'	25:CD:133:THR:HG22	1.88	0.55
22:CA:2359:C:O2	33:CM:60:ARG:NH2	2.39	0.55
1:AA:842:U:H3'	1:AA:843:U:C5'	2.37	0.55
1:AA:976:G:OP2	1:AA:1358:U:O2'	2.25	0.55
6:AF:16:GLU:HG2	4:BD:193:ALA:HA	1.87	0.55
1:BA:394:G:OP2	69:BA:1887:HOH:O	2.18	0.55
32:CL:70:ARG:NH1	32:CL:74:GLY:O	2.40	0.55
35:CO:56:LYS:NZ	35:CO:87:PHE:O	2.39	0.55
53:DA:1847:A:P	53:DA:1847:A:H8	2.30	0.55
1:BA:6:G:O6	5:BE:100:SER:N	2.22	0.55
22:CA:1170:C:H2'	22:CA:1171:G:H8	1.72	0.55
22:CA:2507:C:OP1	69:CA:3600:HOH:O	2.18	0.55
28:CG:70:ALA:O	28:CG:74:SER:OG	2.25	0.55
53:DA:282:A:H2'	53:DA:283:G:C8	2.42	0.55
53:DA:2031:A:C6	53:DA:2498:OMC:H1'	2.42	0.55
30:DJ:119:GLY:O	30:DJ:125:MET:HE3	2.06	0.55
32:DL:107:LEU:O	32:DL:109:SER:N	2.40	0.55
7:BG:16:PRO:HB3	9:BI:43:THR:HG23	1.88	0.54
22:CA:301:G:OP2	42:CV:82:ARG:NH1	2.40	0.54
22:CA:1394:U:H4'	22:CA:1603:A:H4'	1.89	0.54
33:CM:111:ILE:HG22	33:CM:112:LEU:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DA:189:G:N7	66:DA:3197:EDO:H21	2.22	0.54
53:DA:1171:G:N3	53:DA:1179:G:N2	2.56	0.54
1:AA:1217:C:P	14:AN:9:ARG:HH21	2.29	0.54
1:AA:1226:C:N4	13:AM:103:LYS:HE3	2.22	0.54
13:AM:6:GLY:CA	13:AM:66:GLU:HG3	2.37	0.54
7:BG:113:ASP:OD2	7:BG:122:ASN:ND2	2.40	0.54
22:CA:1941:C:OP2	69:CA:3788:HOH:O	2.18	0.54
22:CA:2334:U:O4	36:CP:16:ARG:NH2	2.40	0.54
22:CA:2360:G:H1'	33:CM:60:ARG:HD3	1.88	0.54
26:CE:98:LYS:NZ	69:CE:303:HOH:O	2.40	0.54
49:C2:25:LYS:NZ	49:C2:32:GLU:O	2.36	0.54
33:DM:85:VAL:HB	33:DM:94:THR:CG2	2.37	0.54
13:AM:95:LEU:C	13:AM:109:ARG:HG2	2.32	0.54
29:CH:79:THR:HA	29:CH:145:ASN:HB2	1.88	0.54
50:C3:44:VAL:HG13	50:C3:45:SER:H	1.72	0.54
14:BN:53:ARG:HH22	19:BS:37:ARG:NH2	2.06	0.54
22:CA:550:C:H2'	22:CA:551:G:H5''	1.90	0.54
53:DA:142:A:C5	53:DA:143:C:C4	2.95	0.54
55:DI:22:ALA:HA	55:DI:86:THR:HA	1.88	0.54
1:BA:1134:G:N2	1:BA:1140:C:N3	2.56	0.54
22:CA:585:G:N7	38:CR:6:ARG:NH1	2.50	0.54
3:AC:7:PRO:HG2	3:AC:184:TYR:CG	2.42	0.54
22:CA:430:A:N7	69:CA:3729:HOH:O	2.34	0.54
40:CT:84:ARG:HB2	40:CT:96:ILE:HG12	1.88	0.54
41:CU:69:ARG:NH1	41:CU:69:ARG:HB3	2.23	0.54
53:DA:953:G:OP2	34:DN:18[B]:ARG:NH1	2.41	0.54
10:AJ:40:ILE:CG1	10:AJ:73:LEU:HB3	2.37	0.54
8:BH:106:THR:HG21	8:BH:121:LEU:HD13	1.89	0.54
22:CA:139:U:O2'	22:CA:141:G:N1	2.36	0.54
53:DA:2297:A:H5''	53:DA:2297:A:C8	2.42	0.54
42:DV:45:HIS:CD2	42:DV:58:ILE:HD13	2.43	0.54
1:AA:1189:U:OP1	14:AN:98:LYS:NZ	2.38	0.54
27:DF:119:ALA:O	27:DF:167:ARG:NH1	2.41	0.54
1:AA:407:U:OP1	4:AD:3:ARG:NH2	2.40	0.54
15:BO:89:ARG:NH1	22:CA:716:A:OP1	2.41	0.54
22:CA:2189:U:H2'	22:CA:2190:G:H5'	1.90	0.54
11:AK:16:VAL:HG23	11:AK:17:SER:H	1.72	0.54
1:BA:1217:C:OP2	14:BN:9:ARG:NH2	2.33	0.54
23:CB:90:C:H6	23:CB:90:C:H5''	1.72	0.54
53:DA:550:C:H2'	53:DA:551:G:H5''	1.89	0.54
36:DP:68:LYS:HE3	61:DP:201:PEG:H41	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:D3:29:GLN:HG2	61:D3:102:PEG:H21	1.91	0.54
10:AJ:65:TYR:HB3	14:AN:96:LEU:HD11	1.90	0.53
1:BA:1144:G:N2	1:BA:1145:A:C2	2.76	0.53
12:BL:65:SER:HB2	12:BL:82:ILE:HD11	1.89	0.53
22:CA:582:A:N7	69:CA:3262:HOH:O	2.34	0.53
22:CA:1170:C:H2'	22:CA:1171:G:C8	2.42	0.53
53:DA:551:G:H5'	53:DA:551:G:H8	1.73	0.53
53:DA:2172:U:H4'	53:DA:2173:A:H5'	1.90	0.53
34:DN:89:VAL:CG1	58:DN:201:MPD:HM3	2.38	0.53
1:AA:951:G:OP2	13:AM:101:ARG:NH2	2.41	0.53
13:AM:79:ARG:NH1	27:DF:113:ASP:OD1	2.41	0.53
1:BA:196:A:OP1	20:BT:64:LYS:NZ	2.40	0.53
22:CA:184:C:O2'	22:CA:217:A:N3	2.35	0.53
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.90	0.53
1:AA:843:U:OP1	1:AA:846:G:N2	2.42	0.53
13:AM:8:ASN:OD1	13:AM:9:ILE:N	2.42	0.53
11:BK:83:GLU:OE2	11:BK:109:ASN:ND2	2.41	0.53
22:CA:1993:U:H4'	25:CD:133:THR:CG2	2.38	0.53
23:CB:35:C:C2'	23:CB:36:C:H5'	2.38	0.53
48:C1:55:ILE:HG22	48:C1:56:ALA:N	2.23	0.53
53:DA:2383:G:O6	69:DA:4990:HOH:O	2.18	0.53
1:BA:35:G:N3	12:BL:115:SER:OG	2.42	0.53
1:BA:72:A:C6	1:BA:73:C:N3	2.76	0.53
6:BF:50:PRO:CD	18:BR:74:HIS:HB3	2.39	0.53
17:BQ:60:GLU:OE2	17:BQ:77:ARG:NH1	2.42	0.53
22:CA:2127:G:N2	22:CA:2161:C:O2	2.40	0.53
1:BA:374:A:H5''	1:BA:452:A:N1	2.23	0.53
53:DA:142:A:H1'	41:DU:1:MET:HE1	1.89	0.53
53:DA:142:A:O2'	53:DA:143:C:O4'	2.25	0.53
10:AJ:40:ILE:HG12	10:AJ:73:LEU:HB3	1.89	0.53
1:BA:774:G:H21	57:BA:1642:PG4:H52	1.74	0.53
22:CA:528:A:C2	22:CA:2042:A:H2'	2.43	0.53
22:CA:1419:A:O2'	22:CA:1421:G:N7	2.32	0.53
27:DF:112:ARG:NH1	27:DF:134:GLU:OE2	2.41	0.53
1:AA:404:G:N7	4:AD:2:ALA:HB3	2.23	0.53
5:AE:149:SER:HB3	5:AE:152:MET:CG	2.39	0.53
14:BN:25:ALA:HA	14:BN:28:LYS:HG2	1.90	0.53
1:AA:526:C:C2'	1:AA:527:G7M:H5'	2.39	0.53
14:BN:28:LYS:O	14:BN:31:ILE:HG22	2.09	0.53
19:BS:10:PHE:CD2	19:BS:11:ILE:N	2.77	0.53
53:DA:45:G:H5''	53:DA:46:G:H5'	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1379:G:N7	7:AG:2:PRO:HB2	2.24	0.53
22:CA:1363:C:O2'	22:CA:1809:A:N3	2.40	0.53
26:CE:152:GLU:O	26:CE:154:ASP:N	2.42	0.53
29:DH:68:ARG:NH2	29:DH:114:GLU:OE1	2.42	0.53
35:CO:1:MET:HE2	35:CO:1:MET:N	2.24	0.53
22:CA:45:G:H5''	22:CA:46:G:H5'	1.92	0.52
53:DA:1046:A:H4'	55:DI:58:THR:HG21	1.91	0.52
38:DR:58:ARG:HA	38:DR:61:TRP:CE3	2.44	0.52
1:AA:938:A:H5'	7:AG:76:LYS:NZ	2.23	0.52
1:AA:1124:G:H5'	10:AJ:37:ARG:HH11	1.73	0.52
2:AB:49:MET:HE1	2:AB:199:VAL:HG13	1.91	0.52
15:AO:20:ASN:O	15:AO:22:THR:N	2.41	0.52
1:BA:264:C:O2'	17:BQ:66:PRO:O	2.26	0.52
7:BG:109:ARG:O	7:BG:119:ARG:NH2	2.42	0.52
7:BG:130:ASN:HA	7:BG:135:VAL:HG11	1.91	0.52
20:BT:44:LYS:HD3	20:BT:87:ALA:HA	1.90	0.52
22:CA:223:A:N1	22:CA:407:G:O2'	2.41	0.52
22:CA:2526:G:O2'	52:C5:1:MET:HB3	2.09	0.52
38:CR:105:ALA:HB1	39:CS:40:MET:HE1	1.91	0.52
46:CZ:7:ARG:O	46:CZ:60:LYS:NZ	2.42	0.52
53:DA:550:C:C2'	53:DA:551:G:H5''	2.39	0.52
1:BA:216:U:H5''	1:BA:464:U:H4'	1.91	0.52
22:CA:1808:A:O2'	45:CY:3:ARG:NH1	2.42	0.52
30:CJ:100:LYS:HB3	30:CJ:141:GLU:HB2	1.89	0.52
53:DA:141:G:H3'	53:DA:142:A:C5	2.44	0.52
53:DA:1170:C:H2'	53:DA:1171:G:C8	2.44	0.52
34:DN:89:VAL:HG12	58:DN:201:MPD:HM3	1.90	0.52
1:AA:1032:G:H2'	1:AA:1033:G:H4'	1.90	0.52
1:BA:87:C:H2'	1:BA:88:U:C6	2.43	0.52
11:BK:112:ASP:HB3	21:BU:2:PRO:HG2	1.90	0.52
22:CA:797:G:N7	69:CA:3296:HOH:O	2.34	0.52
22:CA:1869:G:H3'	22:CA:1870:C:H5'	1.92	0.52
30:CJ:119:GLY:O	30:CJ:125:MET:HE3	2.09	0.52
41:CU:60:THR:O	69:CU:102:HOH:O	2.19	0.52
52:C5:22:VAL:HG11	52:C5:36:ARG:HG3	1.90	0.52
53:DA:543:G:H5''	53:DA:543:G:H8	1.74	0.52
53:DA:1536:C:H4'	53:DA:1537:G:H5''	1.91	0.52
1:AA:418:C:N4	69:AA:1753:HOH:O	2.43	0.52
13:AM:12:HIS:HA	13:AM:45:ILE:CG1	2.39	0.52
22:CA:1789:A:OP2	24:CC:221:ARG:NH1	2.41	0.52
33:CM:29:LYS:O	33:CM:30:THR:OG1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:CU:49:LYS:HD3	41:CU:49:LYS:N	2.24	0.52
53:DA:1105:U:H2'	53:DA:1106:G:H8	1.75	0.52
1:AA:537:G:OP1	12:AL:110:ARG:NH2	2.43	0.52
7:BG:15:ASP:HB2	7:BG:20:SER:H	1.75	0.52
7:BG:83:SER:HB3	7:BG:85:TYR:CZ	2.45	0.52
22:CA:1011:G:OP2	38:CR:70:ARG:NH1	2.42	0.52
7:BG:88:PRO:HD2	7:BG:152:ALA:HA	1.91	0.52
22:CA:842:U:O4	69:CA:3496:HOH:O	2.18	0.52
22:CA:1138:G:N3	31:CK:108:MET:HE2	2.25	0.52
32:CL:108:ARG:CD	32:CL:113:MET:HE1	2.39	0.52
33:CM:29:LYS:C	33:CM:31:GLY:H	2.17	0.52
52:C5:1:MET:HE1	52:C5:36:ARG:HB2	1.90	0.52
53:DA:1869:G:C2	53:DA:1873:G:C6	2.98	0.52
53:DA:2256:G:N2	57:DA:3193:PG4:H61	2.25	0.52
63:DA:3185:1PE:H222	69:DA:6271:HOH:O	2.09	0.52
31:DK:96:ARG:NH2	69:DK:319:HOH:O	2.24	0.52
9:AI:85:ARG:HA	9:AI:88:MET:CE	2.39	0.52
13:AM:12:HIS:ND1	13:AM:45:ILE:HG13	2.24	0.52
1:BA:374:A:H5''	1:BA:452:A:C2	2.44	0.52
3:BC:40:ARG:HG2	3:BC:55:ILE:HG12	1.90	0.52
5:BE:114:VAL:HG22	5:BE:115:LEU:HD13	1.92	0.52
7:BG:59:LEU:HD23	7:BG:59:LEU:H	1.75	0.52
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.74	0.52
11:BK:88:GLY:H	11:BK:114:THR:HG22	1.74	0.52
22:CA:388:G:N7	22:CA:390:U:H2'	2.25	0.52
53:DA:1433:A:O2'	53:DA:1434:A:H5'	2.10	0.52
53:DA:2256:G:H21	57:DA:3193:PG4:H31	1.75	0.52
58:DN:201:MPD:HM2	58:DN:201:MPD:O4	2.08	0.52
1:AA:1428:A:H2'	1:AA:1429:A:O4'	2.10	0.52
15:AO:26:GLU:OE1	15:AO:26:GLU:N	2.35	0.52
1:BA:79:G:H2'	1:BA:80:A:O4'	2.10	0.52
5:BE:154:ALA:O	5:BE:157:ARG:N	2.43	0.52
22:CA:1915:3TD:H2'	22:CA:1916:A:O4'	2.10	0.52
24:CC:252:THR:HG22	24:CC:253:LYS:H	1.73	0.52
32:CL:121:GLU:HG2	32:CL:122:VAL:HG23	1.91	0.52
35:CO:2:ARG:O	35:CO:2:ARG:HD3	2.10	0.52
53:DA:278:A:C2	53:DA:362:A:C8	2.98	0.52
1:AA:412:A:H1'	1:AA:413:G:C5'	2.39	0.52
1:AA:1060:U:H4'	10:AJ:53:ILE:HG23	1.91	0.52
17:BQ:14:SER:HB3	17:BQ:22:VAL:HG13	1.92	0.52
22:CA:1582:C:N4	22:CA:1583:A:C6	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CK:99:ARG:NH1	31:CK:102:GLU:OE1	2.43	0.52
42:CV:61:LYS:HA	42:CV:61:LYS:HE3	1.92	0.52
53:DA:62:U:O4'	58:DA:3205:MPD:H31	2.10	0.52
50:D3:32:ALA:HB2	61:D3:102:PEG:H12	1.91	0.52
8:AH:48:ASP:OD1	8:AH:49:PHE:N	2.38	0.51
1:BA:1309:G:OP2	13:BM:98:ARG:NE	2.39	0.51
5:BE:104:GLY:HA3	5:BE:122:ASN:CA	2.40	0.51
14:BN:18:ASP:OD1	14:BN:19:LYS:N	2.43	0.51
24:CC:260:ASN:C	24:CC:262:ARG:H	2.18	0.51
27:CF:108:VAL:HG11	27:CF:176:PRO:HG2	1.92	0.51
27:CF:108:VAL:HG13	27:CF:111:ILE:HD12	1.92	0.51
53:DA:614:A:O2'	53:DA:615:U:OP2	2.26	0.51
41:DU:33:LYS:HG3	41:DU:80:TRP:CE3	2.45	0.51
1:AA:157:U:C2'	1:AA:158:G:H5'	2.40	0.51
1:AA:181:A:N6	1:AA:195:A:OP2	2.43	0.51
14:AN:42:TRP:HD1	14:AN:44:ALA:N	2.09	0.51
1:BA:531:U:H4'	1:BA:532:A:C5'	2.40	0.51
3:BC:72:ARG:HB3	3:BC:75:ILE:CG2	2.40	0.51
3:BC:80:LYS:HA	3:BC:80:LYS:HE3	1.92	0.51
22:CA:818:G:O2'	22:CA:819:A:O4'	2.27	0.51
22:CA:1367:A:OP1	69:CA:3534:HOH:O	2.19	0.51
22:CA:1847:A:HO2'	22:CA:1848:A:H8	1.55	0.51
22:CA:2081:U:OP1	45:CY:17:ASN:ND2	2.41	0.51
24:CC:111:LYS:NZ	24:CC:114:ASP:OD1	2.41	0.51
53:DA:1418:G:H2'	53:DA:1579:A:N6	2.26	0.51
53:DA:2324:U:H3'	53:DA:2325:G:C5'	2.40	0.51
53:DA:2603:G:OP2	69:DA:4829:HOH:O	2.19	0.51
1:BA:1226:C:N4	13:BM:103:LYS:HE3	2.25	0.51
1:BA:1406:U:H2'	1:BA:1407:5MC:H5'	1.91	0.51
3:BC:117:ALA:HB2	3:BC:200:VAL:CG1	2.40	0.51
5:BE:93:ARG:HG3	5:BE:128:TYR:HB2	1.93	0.51
22:CA:1937:A:H1'	22:CA:1939:5MU:H72	1.93	0.51
22:CA:2550:G:C6	22:CA:2551:C:C4	2.97	0.51
53:DA:2251:OMG:OP1	34:DN:81[A]:4D4:NH2	2.34	0.51
41:DU:80:TRP:HB3	64:DU:101:PGE:H32	1.92	0.51
1:AA:216:U:H2'	1:AA:217:C:C6	2.46	0.51
1:AA:741:G:OP1	15:AO:35:GLN:NE2	2.43	0.51
3:BC:42:TYR:CZ	3:BC:90:VAL:HG21	2.46	0.51
22:CA:381:G:OP1	45:CY:18:ARG:NH2	2.37	0.51
22:CA:1792:G:H5'	24:CC:204:VAL:HG23	1.93	0.51
22:CA:2611:C:OP2	69:CA:3871:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:DA:3193:PG4:H12	69:DA:6907:HOH:O	2.10	0.51
1:BA:31:G:O2'	1:BA:48:C:N4	2.43	0.51
1:BA:467:U:H3'	1:BA:468:A:H5''	1.93	0.51
22:CA:2264:C:N4	44:CX:15:ASP:OD2	2.43	0.51
24:CC:210:ALA:HA	24:CC:213:TRP:CE2	2.45	0.51
58:DA:3211:MPD:O4	58:DA:3211:MPD:O2	2.28	0.51
1:AA:121:U:H5''	1:AA:122:G:OP2	2.11	0.51
1:AA:1016:A:N3	1:AA:1016:A:H2'	2.26	0.51
1:AA:1449:C:C2'	1:AA:1450:U:H5'	2.40	0.51
7:AG:88:PRO:HG2	7:AG:152:ALA:HB2	1.93	0.51
10:AJ:15:HIS:CE1	10:AJ:16:ARG:HD3	2.46	0.51
13:AM:12:HIS:HA	13:AM:45:ILE:HG12	1.93	0.51
22:CA:2306:C:N4	27:CF:39:GLY:O	2.44	0.51
45:CY:10:LYS:HE3	45:CY:54:LYS:HD3	1.93	0.51
48:C1:53:LYS:HE3	48:C1:56:ALA:HA	1.93	0.51
53:DA:287:G:H1	53:DA:353:C:H42	1.58	0.51
53:DA:784:G:H5'	53:DA:785:G:OP1	2.10	0.51
53:DA:789:A:OP1	59:DA:3223:PUT:H11	2.10	0.51
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.92	0.51
5:BE:133:PRO:O	5:BE:137:VAL:HG12	2.10	0.51
22:CA:1172:C:H2'	22:CA:1173:U:O4'	2.10	0.51
42:CV:18:ASP:O	42:CV:20:GLY:N	2.44	0.51
47:C0:5:ILE:HG13	47:C0:6:LYS:N	2.25	0.51
27:DF:102:ARG:NH1	69:DF:206:HOH:O	2.43	0.51
1:AA:411:A:P	4:AD:26:ARG:HH22	2.33	0.51
1:AA:1299:A:H2'	1:AA:1299:A:N3	2.26	0.51
1:BA:966:2MG:H2'	1:BA:967:5MC:C6	2.45	0.51
14:BN:22:ALA:C	14:BN:26:GLU:OE1	2.53	0.51
22:CA:2286:G:H4'	22:CA:2287:A:O5'	2.11	0.51
24:DC:78:VAL:HG21	24:DC:110:LEU:HD21	1.93	0.51
41:DU:1:MET:HE2	41:DU:1:MET:H1	1.76	0.51
1:AA:722:G:H3'	1:AA:722:G:N3	2.25	0.51
10:AJ:6:ILE:HG13	10:AJ:76:ILE:HB	1.91	0.51
14:AN:27:LEU:O	14:AN:31:ILE:HG12	2.11	0.51
16:AP:56:ARG:NH1	69:AP:102:HOH:O	2.43	0.51
19:AS:29:LYS:HB3	19:AS:30:PRO:CD	2.41	0.51
3:BC:55:ILE:CD1	3:BC:66:VAL:HG13	2.41	0.51
15:BO:45:GLU:HG2	15:BO:46:HIS:H	1.75	0.51
35:CO:90:ARG:CZ	35:CO:116:VAL:HG11	2.41	0.51
48:C1:55:ILE:HG22	48:C1:56:ALA:H	1.75	0.51
53:DA:1171:G:C2	53:DA:1179:G:C2	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:DB:35:C:H2'	23:DB:36:C:H5'	1.92	0.51
2:AB:117:LEU:HA	2:AB:120:GLN:HG2	1.93	0.50
7:BG:25:LYS:HB2	7:BG:101:MET:HE1	1.92	0.50
14:BN:23:LYS:C	14:BN:26:GLU:OE2	2.54	0.50
22:CA:138:U:OP2	22:CA:139:U:H5'	2.10	0.50
24:CC:235:GLY:HA3	24:CC:239:ASN:HB2	1.92	0.50
26:CE:81:GLY:N	69:CE:301:HOH:O	2.44	0.50
54:DD:1:MET:HE2	54:DD:100:LEU:CD1	2.41	0.50
1:BA:257:G:O6	69:BA:1714:HOH:O	2.19	0.50
1:BA:1406:U:C2'	1:BA:1407:5MC:H5'	2.42	0.50
2:BB:9:MET:CE	2:BB:50:PHE:HD2	2.24	0.50
5:BE:105:ILE:HG23	5:BE:105:ILE:O	2.11	0.50
6:BF:50:PRO:HD3	18:BR:74:HIS:HB3	1.93	0.50
22:CA:579:G:O2'	22:CA:2019:A:OP1	2.29	0.50
22:CA:2496:C:OP2	34:CN:81:4D4:H8	2.10	0.50
16:AP:46:LYS:NZ	69:AP:101:HOH:O	2.44	0.50
22:CA:646:U:H5'	22:CA:647:G:H5''	1.92	0.50
32:CL:1:MET:HB2	32:CL:67:LYS:HG3	1.93	0.50
53:DA:1913:A:OP1	53:DA:1913:A:H4'	2.12	0.50
4:AD:99:ASP:OD1	4:AD:100:ASN:N	2.45	0.50
1:BA:202:G:HO2'	1:BA:468:A:H8	1.59	0.50
1:BA:991:U:H4'	1:BA:992:U:C5'	2.41	0.50
1:BA:1462:C:O2'	37:CQ:111:LYS:NZ	2.44	0.50
4:BD:201:VAL:HG11	5:BE:103:THR:HB	1.92	0.50
15:BO:67:LEU:HD22	15:BO:88:ARG:HH22	1.77	0.50
22:CA:981:A:OP2	22:CA:982:C:N4	2.40	0.50
24:CC:17:VAL:HB	24:CC:204:VAL:HG13	1.93	0.50
53:DA:2116:G:N7	53:DA:2165:C:N4	2.57	0.50
41:DU:1:MET:HE2	41:DU:1:MET:CA	2.41	0.50
1:AA:841:C:C5	1:AA:843:U:H5'	2.47	0.50
8:AH:18:GLN:CG	8:AH:70:ALA:HB1	2.42	0.50
13:AM:16:VAL:HG12	13:AM:17:ILE:HD12	1.93	0.50
7:BG:57:SER:OG	7:BG:58:GLU:N	2.44	0.50
9:BI:85:ARG:HA	9:BI:88:MET:HE3	1.94	0.50
10:BJ:81:GLU:HA	10:BJ:84:VAL:HG12	1.92	0.50
13:BM:10:PRO:HB2	13:BM:18:ALA:HB1	1.94	0.50
22:CA:1665:A:H5''	32:CL:66:LYS:HG2	1.92	0.50
53:DA:1090:A:N1	53:DA:1101:U:O2	2.45	0.50
54:DD:18:ASP:HB2	57:DQ:202:PG4:H82	1.93	0.50
2:AB:130:THR:O	2:AB:131:LYS:HB2	2.10	0.50
1:BA:1183:U:O2'	1:BA:1184:G:O5'	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BG:51:ALA:O	7:BG:55:GLY:N	2.36	0.50
22:CA:971:G:OP2	22:CA:974:G:N2	2.44	0.50
22:CA:1390:U:H2'	22:CA:1391:U:H5'	1.94	0.50
69:CA:3823:HOH:O	47:C0:47:MET:HE2	2.10	0.50
24:CC:132:MET:HE3	24:CC:172:VAL:HG21	1.93	0.50
30:CJ:19:ASN:N	30:CJ:20:PRO:HD2	2.26	0.50
38:CR:22:LYS:HE2	38:CR:22:LYS:HA	1.93	0.50
53:DA:2325:G:C6	53:DA:2326:C:N4	2.79	0.50
53:DA:2887[B]:A:H2'	53:DA:2888[B]:C:O4'	2.11	0.50
66:DA:3210:EDO:H21	38:DR:16:LYS:HG3	1.94	0.50
29:DH:7:ASP:OD1	29:DH:8:LYS:N	2.44	0.50
31:DK:23:LYS:HE2	31:DK:142:ILE:OXT	2.12	0.50
1:AA:204:G:C3'	1:AA:205:A:H5''	2.42	0.50
1:BA:147:G:N2	1:BA:175:C:O2	2.45	0.50
2:BB:130:THR:O	2:BB:131:LYS:HB2	2.11	0.50
6:BF:52:ASN:O	6:BF:53:LYS:HB2	2.12	0.50
22:CA:662:G:O3'	33:CM:16:GLY:HA2	2.11	0.50
22:CA:1422:G:N2	22:CA:1577:C:HI1'	2.27	0.50
25:CD:112:THR:O	25:CD:195:GLY:HA2	2.12	0.50
38:CR:9:ILE:HD12	38:CR:10:ALA:N	2.27	0.50
53:DA:664:G:OP2	69:DA:5108:HOH:O	2.19	0.50
53:DA:1172:C:C5	53:DA:1173:U:N1	2.80	0.50
53:DA:1758:U:OP2	69:DA:4561:HOH:O	2.19	0.50
30:DJ:100:LYS:HB3	30:DJ:141:GLU:HB2	1.93	0.50
33:DM:79:LEU:HD11	33:DM:112:LEU:HD12	1.94	0.50
35:DO:1:MET:N	69:DO:241:HOH:O	2.44	0.50
50:D3:12:ARG:HG2	50:D3:12:ARG:HH21	1.77	0.50
20:BT:27:MET:HG3	20:BT:28:MET:N	2.27	0.50
40:CT:1:MET:HE2	40:CT:62:ASP:OD2	2.12	0.50
53:DA:1420:A:C8	53:DA:2211:A:N6	2.80	0.50
32:DL:70:ARG:NH1	32:DL:74:GLY:O	2.45	0.50
1:AA:109:A:C6	1:AA:326:G:C6	3.00	0.50
3:BC:3:GLN:OE1	3:BC:3:GLN:N	2.45	0.50
5:BE:102:GLY:C	5:BE:104:GLY:N	2.70	0.50
17:BQ:14:SER:OG	17:BQ:17:MET:HE1	2.12	0.50
22:CA:1515:A:HO2'	22:CA:1556:C:HO2'	1.60	0.50
32:CL:78:ARG:NH1	37:CQ:71:GLU:OE2	2.45	0.50
24:DC:132:MET:HE3	24:DC:172:VAL:HG21	1.94	0.50
16:AP:1:MET:SD	16:AP:1:MET:N	2.64	0.49
1:BA:1491:G:C6	1:BA:1492:A:C6	3.00	0.49
42:CV:7:ARG:NH2	42:CV:8:ASP:OD1	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DA:1583:A:O2'	53:DA:1584:U:O5'	2.30	0.49
32:DL:70:ARG:HD3	32:DL:76:VAL:HG22	1.93	0.49
1:BA:1373:G:H5''	7:BG:36:LYS:HB2	1.93	0.49
22:CA:335:C:O2'	22:CA:336:C:OP1	2.25	0.49
41:CU:5:GLU:CG	46:CZ:22:LEU:HD13	2.42	0.49
53:DA:2813:A:H2	53:DA:2887[B]:A:N1	2.10	0.49
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	1.95	0.49
1:AA:1016:A:N1	1:AA:1017:U:O2'	2.44	0.49
10:AJ:76:ILE:CD1	10:AJ:87:LEU:HD11	2.42	0.49
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.93	0.49
1:BA:674:G:N2	1:BA:717:U:O2	2.45	0.49
22:CA:1262:A:C2	48:C1:7:LYS:HD2	2.47	0.49
45:CY:11:ARG:HG2	45:CY:12:PRO:HD2	1.94	0.49
1:AA:457:G:N2	1:AA:476:U:O2	2.45	0.49
20:AT:44:LYS:HG3	20:AT:45:ALA:N	2.27	0.49
3:BC:7:PRO:O	3:BC:11:ARG:HG3	2.12	0.49
8:BH:59:LEU:HD12	8:BH:60:GLU:N	2.26	0.49
8:BH:86:TYR:C	8:BH:87:LYS:HD2	2.37	0.49
15:BO:45:GLU:O	15:BO:47:LYS:N	2.44	0.49
17:BQ:81:LYS:HD3	17:BQ:81:LYS:N	2.27	0.49
22:CA:1340:U:C5	22:CA:1603:A:C8	3.00	0.49
30:CJ:18:ALA:C	30:CJ:20:PRO:HD2	2.38	0.49
32:CL:99:ILE:HD13	32:CL:118:LEU:HB2	1.94	0.49
28:DG:2:SER:OG	28:DG:6:LYS:NZ	2.44	0.49
33:DM:91:ASP:H	33:DM:94:THR:HB	1.78	0.49
1:AA:1005:A:H3'	1:AA:1006:G:C8	2.48	0.49
5:AE:156:LYS:NZ	8:AH:73:GLU:OE1	2.45	0.49
6:AF:29:ILE:HD13	6:AF:64:VAL:HG11	1.93	0.49
9:AI:52:LEU:HD13	9:AI:57:MET:HE2	1.94	0.49
1:BA:842:U:N3	1:BA:844:G:H5'	2.27	0.49
11:BK:43:GLY:HA3	11:BK:74:VAL:HG12	1.95	0.49
22:CA:2130:U:O2'	22:CA:2133:G:O2'	2.31	0.49
35:CO:28:LEU:O	35:CO:32:GLU:N	2.40	0.49
29:DH:41:LYS:HA	29:DH:44:ILE:CG2	2.42	0.49
41:DU:2:ILE:HG21	41:DU:45:ALA:HB1	1.94	0.49
1:AA:147:G:H2'	1:AA:148:G:C8	2.47	0.49
1:BA:79:G:N2	1:BA:91:U:N3	2.59	0.49
1:BA:842:U:C2	1:BA:844:G:H5'	2.48	0.49
12:BL:82:ILE:HG12	12:BL:95:TYR:HB3	1.93	0.49
22:CA:550:C:C2'	22:CA:551:G:H5''	2.42	0.49
36:CP:49:VAL:HG21	36:CP:82:ALA:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DP:31:THR:HG22	36:DP:34:HIS:H	1.77	0.49
12:BL:121:ARG:HG2	12:BL:121:ARG:HH11	1.77	0.49
40:CT:96:ILE:H	40:CT:96:ILE:HD13	1.77	0.49
53:DA:2886[A]:A:C5	53:DA:2887[A]:A:N7	2.81	0.49
1:AA:184:G:O2'	20:AT:69:LYS:NZ	2.36	0.49
8:AH:9:ASP:OD1	8:AH:13:ARG:HD2	2.12	0.49
10:AJ:53:ILE:HG13	14:AN:85:ARG:CZ	2.42	0.49
1:BA:842:U:H3'	1:BA:843:U:H5''	1.95	0.49
1:BA:1381:U:C5	1:BA:1382:C:C5	3.01	0.49
2:BB:120:GLN:HG3	2:BB:121:SER:N	2.28	0.49
6:BF:39:LEU:HD13	6:BF:62:MET:HG3	1.93	0.49
22:CA:374:A:C2	22:CA:401:A:C4	3.01	0.49
27:CF:135:GLN:OE1	27:CF:135:GLN:N	2.46	0.49
53:DA:933:A:H5'	53:DA:934:U:OP2	2.12	0.49
53:DA:1083:U:H4'	55:DI:42:ARG:NH1	2.28	0.49
53:DA:1724:G:C2'	53:DA:1725:U:H5'	2.42	0.49
30:DJ:18:ALA:C	30:DJ:20:PRO:HD2	2.37	0.49
61:DQ:201:PEG:H22	69:DQ:313:HOH:O	2.12	0.49
1:AA:71:A:O2'	1:AA:72:A:OP2	2.27	0.49
1:AA:526:C:H2'	1:AA:527:G7M:H5'	1.93	0.49
1:BA:664:G:H22	1:BA:741:G:H1	1.61	0.49
1:BA:976:G:OP2	1:BA:1358:U:O2'	2.30	0.49
11:BK:67:ALA:HB2	11:BK:96:THR:HG23	1.94	0.49
22:CA:982:C:H5''	22:CA:983:A:OP1	2.13	0.49
36:CP:31:THR:HG22	36:CP:33:ARG:N	2.28	0.49
53:DA:374:A:C2	53:DA:401:A:C4	3.01	0.49
38:DR:20:GLN:CG	57:DR:202:PG4:H42	2.43	0.49
6:AF:86:ARG:NH1	18:AR:64:TYR:O	2.46	0.49
19:BS:15:LEU:HD13	19:BS:33:THR:HG21	1.95	0.49
22:CA:1680:U:O2'	22:CA:1763:G:N7	2.44	0.49
22:CA:2055:C:H5'	22:CA:2056:G:OP1	2.13	0.49
26:CE:127:GLU:O	26:CE:156:ASN:ND2	2.46	0.49
53:DA:644:A:H2'	53:DA:645:C:O4'	2.12	0.49
54:DD:13:ARG:NH1	69:DD:479:HOH:O	2.41	0.49
1:AA:1238:A:H5'	1:AA:1336:C:H41	1.77	0.48
5:AE:56:VAL:N	5:AE:57:PRO:HD2	2.28	0.48
6:AF:76:THR:O	6:AF:79:ARG:N	2.44	0.48
1:BA:958:A:N6	19:BS:77:THR:O	2.46	0.48
1:BA:1516:2MG:N2	1:BA:1519:MA6:OP2	2.43	0.48
22:CA:627:A:OP1	33:CM:78:ARG:NH1	2.39	0.48
31:CK:81:ILE:HG12	31:CK:82:GLY:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:C4:62:LEU:HB3	51:C4:65:ALA:HB2	1.95	0.48
53:DA:1026:G:H2'	53:DA:1027:A:C8	2.48	0.48
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.48	0.48
1:BA:754:C:OP1	15:BO:72:ARG:NH2	2.47	0.48
1:BA:933:G:N7	7:BG:3:ARG:NH2	2.62	0.48
5:BE:106:ILE:O	5:BE:106:ILE:HG13	2.13	0.48
7:BG:79:ARG:HA	7:BG:83:SER:O	2.13	0.48
11:BK:16:VAL:HG13	11:BK:17:SER:N	2.29	0.48
11:BK:16:VAL:HG13	11:BK:17:SER:H	1.78	0.48
11:BK:107:ILE:HD11	11:BK:110:ILE:HG12	1.95	0.48
13:BM:31:LYS:HA	13:BM:31:LYS:HE3	1.93	0.48
14:BN:10:GLU:HG3	14:BN:63:ARG:HD2	1.95	0.48
14:BN:32:SER:HA	14:BN:42:TRP:CZ2	2.48	0.48
15:BO:4:SER:O	15:BO:8:THR:HG23	2.13	0.48
15:BO:18:ASP:OD1	15:BO:20:ASN:N	2.28	0.48
22:CA:377:G:C6	22:CA:378:C:C4	3.00	0.48
53:DA:580:U:O3'	38:DR:31:VAL:HG13	2.13	0.48
24:DC:130:LEU:CD1	24:DC:135:ILE:HG13	2.43	0.48
32:DL:7:MET:HE1	32:DL:44:LYS:HG3	1.95	0.48
1:AA:131:A:H2'	1:AA:132:C:C6	2.49	0.48
2:AB:15:HIS:HB3	2:AB:43:LEU:HD11	1.95	0.48
2:AB:120:GLN:HG3	2:AB:121:SER:N	2.29	0.48
1:BA:380:G:N2	1:BA:383:A:OP2	2.45	0.48
1:BA:890:G:O2'	1:BA:906:A:N6	2.47	0.48
6:BF:73:GLU:O	6:BF:77:THR:OG1	2.31	0.48
18:BR:34:THR:HG22	18:BR:38:LYS:HB2	1.95	0.48
19:BS:11:ILE:HB	19:BS:38:SER:HB3	1.95	0.48
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.94	0.48
22:CA:1309:G:H4'	50:C3:7:PRO:HB2	1.95	0.48
29:CH:75:LEU:O	29:CH:77:THR:N	2.44	0.48
32:CL:35:VAL:HG22	32:CL:69:VAL:HG12	1.94	0.48
33:CM:82:LEU:HD23	33:CM:83:ALA:N	2.28	0.48
51:C4:45:ARG:N	51:C4:46:PRO:HD2	2.29	0.48
53:DA:1172:C:C5	53:DA:1173:U:C2	3.02	0.48
1:AA:383:A:C5	1:AA:384:G:H1'	2.49	0.48
1:AA:429:U:H5'	4:AD:9:LEU:HD12	1.95	0.48
1:BA:841:C:H5'	1:BA:842:U:OP2	2.13	0.48
1:BA:1302:C:C5	13:BM:17:ILE:HD11	2.49	0.48
3:BC:45:LYS:HG3	3:BC:46:GLU:N	2.28	0.48
12:BL:56:ARG:HG3	12:BL:62:GLU:HB2	1.95	0.48
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CA:618:G:O6	69:CA:3267:HOH:O	2.19	0.48
22:CA:991:C:H5'	22:CA:1186:G:H5'	1.95	0.48
22:CA:1638:C:O2	22:CA:2698:U:O2'	2.24	0.48
24:CC:160:THR:HG22	24:CC:177:ARG:HG2	1.94	0.48
59:DA:3214:PUT:H32	69:DA:8098:HOH:O	2.14	0.48
32:DL:1:MET:HE3	32:DL:32:TYR:CZ	2.49	0.48
41:DU:1:MET:HE2	41:DU:1:MET:HA	1.94	0.48
14:AN:10:GLU:HG3	14:AN:63:ARG:HD2	1.96	0.48
8:BH:29:SER:HB3	8:BH:57:PRO:HB2	1.95	0.48
22:CA:1616:A:O2'	69:CA:3372:HOH:O	2.20	0.48
22:CA:2599:G:N7	24:CC:236:GLU:HB2	2.28	0.48
22:CA:2604:U:O2	69:CA:3811:HOH:O	2.16	0.48
29:DH:42:LYS:HG2	29:DH:43:ASN:N	2.28	0.48
1:AA:900:A:OP2	69:AA:2151:HOH:O	2.20	0.48
1:AA:973:G:H1'	10:AJ:56:HIS:HD2	1.78	0.48
1:AA:1137:C:H1'	1:AA:1138:G:N2	2.28	0.48
13:AM:40:ALA:HB3	13:AM:43:VAL:CG2	2.43	0.48
5:BE:81:LEU:CD1	5:BE:120:VAL:HG11	2.43	0.48
5:BE:81:LEU:O	5:BE:98:PRO:HB3	2.13	0.48
12:BL:14:ARG:HH11	12:BL:14:ARG:CA	2.26	0.48
19:BS:10:PHE:CG	19:BS:11:ILE:N	2.82	0.48
36:CP:43:ASN:ND2	36:CP:46:GLU:OE1	2.42	0.48
43:CW:38:LEU:HG	43:CW:40:ILE:HD13	1.95	0.48
53:DA:2086:U:H2'	53:DA:2087:G:C8	2.49	0.48
23:DB:90:C:H5''	23:DB:90:C:H6	1.77	0.48
32:DL:113:MET:CE	32:DL:116:ILE:HD11	2.41	0.48
2:AB:133:GLU:OE2	2:AB:137:ARG:NH1	2.39	0.48
8:AH:96:MET:HE3	8:AH:130:ALA:HB1	1.96	0.48
1:BA:376:G:H5''	16:BP:5:ARG:HB2	1.96	0.48
14:BN:31:ILE:HA	14:BN:34:VAL:HG23	1.94	0.48
14:BN:45:VAL:HG12	19:BS:10:PHE:HE1	1.79	0.48
27:CF:42:GLU:OE1	27:CF:148:ARG:NH2	2.47	0.48
39:CS:39:LEU:O	39:CS:49:ILE:HG23	2.14	0.48
34:DN:47:GLU:OE2	34:DN:51:ARG:NE	2.46	0.48
1:AA:736:C:H5'	6:AF:88:MET:HE2	1.94	0.48
1:AA:1016:A:C2	1:AA:1017:U:H4'	2.48	0.48
10:AJ:53:ILE:CG2	10:AJ:61:ALA:HB1	2.44	0.48
1:BA:510:A:C5'	1:BA:511:C:P	3.01	0.48
22:CA:1714:U:H5''	22:CA:1715:G:H5'	1.95	0.48
28:CG:80:THR:CG2	28:CG:81:GLU:N	2.77	0.48
53:DA:837:C:N4	69:DA:6883:HOH:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DN:53:MET:HE1	34:DN:103:TYR:CG	2.48	0.48
1:AA:1003:G:N2	1:AA:1004:A:O2'	2.46	0.48
13:AM:107:ARG:HH21	13:AM:113:ARG:HB3	1.79	0.48
1:BA:159:G:N2	1:BA:161:A:H3'	2.29	0.48
6:BF:86:ARG:HH11	6:BF:86:ARG:CG	2.27	0.48
10:BJ:17:LEU:HD11	10:BJ:94:ALA:HB3	1.95	0.48
22:CA:1339:G:N2	22:CA:1603:A:N3	2.62	0.48
27:CF:38:MET:HG2	27:CF:152:LEU:HB3	1.96	0.48
53:DA:137:U:H2'	53:DA:140:C:C1'	2.44	0.48
53:DA:1342:A:OP1	41:DU:40:LYS:NZ	2.40	0.48
27:DF:40:VAL:HG11	27:DF:43:ALA:HB2	1.95	0.48
55:DI:66:GLY:O	55:DI:67:THR:CB	2.62	0.48
4:AD:17:THR:HG22	4:AD:18:ASP:N	2.29	0.48
1:BA:1492:A:N7	1:BA:1493:A:C2	2.82	0.48
19:BS:29:LYS:CB	19:BS:30:PRO:HD2	2.44	0.48
22:CA:563:A:N3	38:CR:37:GLN:NE2	2.61	0.48
22:CA:2020:A:H5'	48:C1:9:THR:CG2	2.44	0.48
42:CV:54:GLN:N	42:CV:55:PRO:HD3	2.28	0.48
53:DA:2251:OMG:HM23	53:DA:2251:OMG:H1'	1.67	0.48
30:DJ:21:SER:HB3	30:DJ:22:PRO:HD3	1.96	0.48
1:BA:121:U:H5''	1:BA:122:G:OP2	2.14	0.47
1:BA:205:A:N1	1:BA:206:C:N4	2.62	0.47
14:BN:42:TRP:CE2	14:BN:44:ALA:HB3	2.49	0.47
22:CA:17:G:H4'	38:CR:25:TYR:CE2	2.48	0.47
22:CA:1338:G:O2'	22:CA:1393:A:N1	2.37	0.47
22:CA:1339:G:OP1	41:CU:17:SER:OG	2.30	0.47
22:CA:1497:U:OP2	22:CA:1498:C:N4	2.46	0.47
27:CF:20:PHE:HB2	27:CF:22:TYR:CE1	2.49	0.47
29:CH:51:ARG:HG3	29:CH:52:ALA:N	2.28	0.47
35:CO:20:MET:HE1	35:CO:40:LYS:CD	2.43	0.47
38:CR:78:LYS:HE2	38:CR:117:LEU:HD21	1.95	0.47
42:CV:74:ASN:O	42:CV:74:ASN:ND2	2.44	0.47
53:DA:811:U:H2'	33:DM:21:ARG:HA	1.96	0.47
53:DA:1105:U:H2'	53:DA:1106:G:C8	2.49	0.47
53:DA:2305:U:C2	27:DF:151:GLY:HA3	2.48	0.47
53:DA:2609:U:H5	66:DA:3194:EDO:H12	1.74	0.47
58:DA:3205:MPD:C5	58:DA:3205:MPD:HM2	2.44	0.47
1:AA:1429:A:O2'	53:DA:1703:G:O3'	2.32	0.47
10:AJ:8:ILE:HA	10:AJ:99:GLN:O	2.14	0.47
22:CA:514:A:N3	22:CA:581:C:O2'	2.41	0.47
25:CD:151:THR:C	25:CD:153:GLY:N	2.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:CM:55:MET:HE1	33:CM:59:ARG:HH21	1.77	0.47
53:DA:1738:G:HO2'	53:DA:1739:A:H8	1.61	0.47
53:DA:2291:U:H2'	53:DA:2292:U:C6	2.49	0.47
53:DA:2813:A:H2	53:DA:2887[B]:A:C6	2.31	0.47
1:AA:913:A:OP1	12:AL:88:LYS:NZ	2.47	0.47
11:AK:16:VAL:HG23	11:AK:17:SER:N	2.28	0.47
22:CA:223:A:O2'	22:CA:420:C:O2	2.30	0.47
22:CA:249:C:H5'	22:CA:2394:C:O2'	2.13	0.47
22:CA:2200:C:O2	22:CA:2226:C:N4	2.47	0.47
31:CK:37:ARG:NH2	31:CK:44:TYR:OH	2.47	0.47
40:CT:82:MET:HE3	40:CT:98:LYS:HB2	1.96	0.47
53:DA:545:U:H3'	53:DA:546:U:H4'	1.95	0.47
30:DJ:22:PRO:HB2	30:DJ:23:PRO:HD3	1.96	0.47
1:AA:159:G:H8	1:AA:159:G:H5''	1.79	0.47
1:AA:196:A:OP1	20:AT:64:LYS:NZ	2.47	0.47
10:AJ:51:VAL:HB	14:AN:81:ARG:HB2	1.96	0.47
14:AN:42:TRP:CD1	14:AN:43:ASN:N	2.83	0.47
1:BA:552:U:O2'	12:BL:83:ARG:O	2.29	0.47
5:BE:26:LYS:HE3	5:BE:26:LYS:CA	2.44	0.47
5:BE:81:LEU:HB3	5:BE:147:MET:SD	2.54	0.47
5:BE:154:ALA:C	5:BE:156:LYS:N	2.73	0.47
22:CA:118:A:N3	22:CA:178:G:H1'	2.29	0.47
26:CE:52:VAL:HG21	26:CE:81:GLY:HA2	1.95	0.47
42:CV:13:VAL:HG21	42:CV:39:ILE:CG2	2.44	0.47
45:CY:72:ARG:HB2	45:CY:72:ARG:CZ	2.45	0.47
53:DA:1847:A:H8	53:DA:1847:A:O5'	1.98	0.47
53:DA:2162:G:H5''	53:DA:2171:A:H2'	1.95	0.47
53:DA:2534:A:H2'	53:DA:2535:G:O5'	2.14	0.47
1:AA:26:A:H2'	1:AA:27:G:H5'	1.95	0.47
7:AG:25:LYS:CB	7:AG:101:MET:HE1	2.44	0.47
9:AI:23:PRO:HA	9:AI:61:LEU:HA	1.95	0.47
13:AM:33:ILE:HD11	13:AM:63:PHE:CE1	2.50	0.47
1:BA:411:A:P	4:BD:26:ARG:HH12	2.38	0.47
1:BA:455:G:C2	1:BA:478:A:C2	3.02	0.47
22:CA:558:U:H1'	31:CK:47:HIS:HB3	1.96	0.47
22:CA:2167:U:O2'	22:CA:2169:A:N7	2.44	0.47
53:DA:1378:A:O2'	53:DA:1380:G:N7	2.47	0.47
53:DA:1582:C:C4	53:DA:1583:A:C2	3.02	0.47
53:DA:1971:U:OP2	53:DA:1971:U:H4'	2.14	0.47
23:DB:28:C:OP1	36:DP:31:THR:HG21	2.15	0.47
29:DH:43:ASN:O	29:DH:46:PHE:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DI:68:PRO:HD2	55:DI:69:PHE:CE2	2.49	0.47
2:AB:27:MET:HE1	2:AB:187:VAL:O	2.13	0.47
20:AT:28:MET:HE1	20:AT:67:ILE:CD1	2.41	0.47
9:BI:36:GLU:HA	9:BI:45:ARG:HE	1.79	0.47
22:CA:647:G:N2	22:CA:2350:C:O3'	2.48	0.47
22:CA:820:A:N6	69:CA:3772:HOH:O	2.43	0.47
22:CA:1178:C:C2	22:CA:1179:G:N7	2.82	0.47
39:CS:8:GLY:O	39:CS:10:LYS:NZ	2.39	0.47
53:DA:289:G:H2'	53:DA:290:U:O4'	2.14	0.47
53:DA:871:U:H2'	53:DA:872:U:C6	2.50	0.47
59:DA:3222:PUT:H41	59:DA:3222:PUT:H11	1.47	0.47
24:DC:125:LYS:HB2	24:DC:126:PRO:HD2	1.96	0.47
1:AA:207:C:H2'	1:AA:208:U:C2	2.49	0.47
1:AA:944:G:N1	1:AA:1338:G:OP2	2.41	0.47
1:AA:1228:C:P	13:AM:107:ARG:NH2	2.88	0.47
2:AB:20:THR:HG22	2:AB:39:HIS:CE1	2.50	0.47
5:AE:80:THR:OG1	5:AE:122:ASN:O	2.32	0.47
6:AF:14:GLN:NE2	4:BD:166:GLU:OE1	2.48	0.47
15:AO:89:ARG:NH1	53:DA:716:A:P	2.88	0.47
15:AO:89:ARG:NH1	53:DA:716:A:OP1	2.48	0.47
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.95	0.47
1:BA:765:G:C6	1:BA:812:G:C4	3.02	0.47
7:BG:4:ARG:HG3	7:BG:5:ARG:N	2.29	0.47
7:BG:42:ILE:HG21	7:BG:116:MET:HG3	1.96	0.47
13:BM:93:ARG:NH2	19:BS:80:TYR:CE1	2.82	0.47
22:CA:621:A:OP2	33:CM:99:ASN:ND2	2.45	0.47
22:CA:818:G:H2'	22:CA:819:A:H5''	1.97	0.47
22:CA:2019:A:H4'	38:CR:34:VAL:HG21	1.96	0.47
22:CA:2379:G:H4'	36:CP:21:LEU:HD11	1.97	0.47
22:CA:2674:G:H4'	32:CL:30:ARG:HD2	1.97	0.47
23:CB:23:G:O6	69:CB:304:HOH:O	2.19	0.47
29:CH:68:ARG:NH1	29:CH:114:GLU:OE1	2.48	0.47
35:CO:8:ARG:HB3	35:CO:10:LEU:HG	1.95	0.47
36:CP:34:HIS:N	36:CP:65:THR:O	2.47	0.47
53:DA:281:C:H2'	53:DA:282:A:C8	2.50	0.47
53:DA:493:G:H2'	53:DA:494:G:O4'	2.14	0.47
53:DA:1171:G:N3	53:DA:1179:G:C2	2.83	0.47
53:DA:1171:G:H3'	53:DA:1172:C:C5	2.50	0.47
53:DA:1475:G:H5'	69:DA:4930:HOH:O	2.14	0.47
53:DA:1714:U:H5''	53:DA:1715:G:H5'	1.97	0.47
53:DA:2498:OMC:HM22	53:DA:2499:C:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:DA:3222:PUT:H42	69:DL:343:HOH:O	2.13	0.47
30:DJ:19:ASN:N	30:DJ:20:PRO:HD2	2.29	0.47
5:AE:162:GLU:HG3	5:AE:163:GLU:N	2.28	0.47
8:AH:108:LYS:HG3	8:AH:121:LEU:HD11	1.97	0.47
9:AI:19:VAL:HG13	9:AI:65:ILE:HG22	1.97	0.47
10:AJ:7:ARG:CG	10:AJ:101:SER:HB2	2.44	0.47
1:BA:1394:A:C5	1:BA:1501:C:H4'	2.49	0.47
2:BB:217:VAL:O	2:BB:221:VAL:HG23	2.15	0.47
3:BC:7:PRO:HG2	3:BC:184:TYR:CG	2.50	0.47
4:BD:107:PHE:CG	4:BD:145:ILE:HD11	2.50	0.47
13:BM:14:HIS:HB2	13:BM:17:ILE:HD12	1.97	0.47
22:CA:1070:A:N7	22:CA:1096:A:O2'	2.46	0.47
22:CA:1246:A:O2'	26:CE:40:ARG:NH2	2.47	0.47
22:CA:1581:G:C6	22:CA:1582:C:C4	3.03	0.47
29:CH:72:ILE:HG23	29:CH:142:VAL:HG22	1.97	0.47
41:CU:8:LEU:O	46:CZ:29:ARG:NH1	2.46	0.47
42:CV:39:ILE:HG22	42:CV:39:ILE:O	2.14	0.47
49:C2:11:LEU:HA	49:C2:50:LYS:O	2.15	0.47
53:DA:1133:A:N3	59:DA:3214:PUT:H22	2.30	0.47
53:DA:1309:G:H4'	50:D3:7:PRO:HB2	1.96	0.47
55:DI:29:ASP:OD1	55:DI:30:SER:N	2.48	0.47
30:DJ:12:GLN:HA	30:DJ:56:PRO:HA	1.97	0.47
30:DJ:113:LYS:O	30:DJ:117:MET:HG2	2.15	0.47
33:DM:57:LEU:HD22	51:D4:54:ASP:HB3	1.97	0.47
1:AA:76:G:H2'	1:AA:76:G:N3	2.29	0.47
7:AG:130:ASN:HA	7:AG:135:VAL:HG11	1.96	0.47
5:BE:136:VAL:O	5:BE:138:ARG:N	2.47	0.47
11:BK:49:GLY:O	11:BK:69:ARG:NH2	2.48	0.47
11:BK:97:ILE:HD11	21:BU:16:LEU:HG	1.96	0.47
13:BM:8:ASN:O	13:BM:10:PRO:HD2	2.15	0.47
17:BQ:10:GLY:HA3	17:BQ:25:ILE:HD13	1.97	0.47
22:CA:574:A:H4'	22:CA:575:A:C5'	2.45	0.47
22:CA:668:A:H2'	22:CA:670:A:H62	1.80	0.47
33:CM:77:ILE:HG23	33:CM:100:ILE:HD11	1.96	0.47
35:CO:103:ARG:HD3	35:CO:110:MET:HE2	1.97	0.47
43:CW:1:MET:HE2	43:CW:1:MET:HA	1.95	0.47
53:DA:1555:G:OP1	59:DA:3220:PUT:H41	2.13	0.47
1:AA:75:G:C2	1:AA:76:G:H1'	2.50	0.47
1:AA:451:A:H61	1:AA:481:G:H5'	1.80	0.47
2:AB:129:LEU:HD22	2:AB:134:ALA:HB2	1.97	0.47
3:AC:185:ASN:OD1	3:AC:186:THR:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AS:44:MET:HE2	19:AS:49:ILE:HD13	1.97	0.47
1:BA:1053:G:N7	1:BA:1199:U:H3'	2.30	0.47
1:BA:1345:U:H4'	1:BA:1346:A:H5'	1.97	0.47
1:BA:1376:U:H2'	1:BA:1377:A:C8	2.50	0.47
2:BB:117:LEU:HA	2:BB:120:GLN:HG2	1.97	0.47
3:BC:19:ASN:ND2	14:BN:90:ARG:O	2.47	0.47
12:BL:14:ARG:NH1	12:BL:15:LYS:H	2.13	0.47
13:BM:114:LYS:CB	13:BM:115:PRO:HD3	2.45	0.47
22:CA:135:U:H3	22:CA:144:A:H61	1.61	0.47
22:CA:545:U:H2'	22:CA:547:A:H5'	1.96	0.47
22:CA:751:A:C6	22:CA:789:A:C6	3.03	0.47
22:CA:1061:U:OP2	30:CJ:10:LYS:NZ	2.48	0.47
29:CH:135:HIS:CG	29:CH:136:SER:H	2.32	0.47
32:CL:38:ILE:HD11	32:CL:112:PHE:CZ	2.50	0.47
53:DA:137:U:H5''	53:DA:140:C:C4	2.50	0.47
53:DA:435:C:H2'	53:DA:436:C:H5'	1.96	0.47
28:DG:86:LYS:HG2	28:DG:132:VAL:HG22	1.97	0.47
38:DR:19:LYS:CD	57:DR:202:PG4:H41	2.43	0.47
1:AA:109:A:H2'	1:AA:326:G:N2	2.31	0.46
1:AA:1464:U:P	37:DQ:109:ARG:HH12	2.38	0.46
5:AE:94:VAL:HG22	5:AE:111:MET:CE	2.44	0.46
2:BB:28:LYS:N	2:BB:29:PRO:CD	2.78	0.46
3:BC:185:ASN:OD1	3:BC:186:THR:N	2.47	0.46
14:BN:32:SER:HB2	14:BN:42:TRP:NE1	2.30	0.46
22:CA:1081:U:H4'	30:CJ:124:ALA:HB1	1.96	0.46
22:CA:1585:C:C2'	22:CA:1586:A:H5'	2.45	0.46
22:CA:1869:G:H3'	22:CA:1870:C:C5'	2.45	0.46
42:CV:4:LYS:O	42:CV:94:ARG:NH2	2.42	0.46
53:DA:137:U:C6	53:DA:140:C:H1'	2.51	0.46
51:D4:42:ARG:NH2	69:D4:113:HOH:O	2.48	0.46
1:AA:1229:A:OP2	13:AM:113:ARG:NH1	2.48	0.46
8:AH:3:MET:SD	8:AH:3:MET:N	2.73	0.46
10:AJ:35:GLN:HG3	10:AJ:78:GLU:HG2	1.98	0.46
14:AN:21:PHE:HA	14:AN:25:ALA:CB	2.45	0.46
19:AS:7:LYS:H	19:AS:7:LYS:HD2	1.79	0.46
7:BG:50:LEU:CD1	7:BG:61:ALA:HB1	2.45	0.46
14:BN:42:TRP:NE1	14:BN:44:ALA:HB3	2.30	0.46
15:BO:20:ASN:O	15:BO:22:THR:N	2.46	0.46
27:CF:122:PHE:C	27:CF:124:GLY:H	2.23	0.46
53:DA:545:U:H6	53:DA:548:G:P	2.38	0.46
53:DA:1700:A:N1	69:DA:6711:HOH:O	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:DC:227:PRO:HA	24:DC:233:GLY:HA2	1.96	0.46
30:DJ:20:PRO:HB2	30:DJ:23:PRO:HD2	1.97	0.46
37:DQ:112:GLU:HG2	37:DQ:114:LEU:HG	1.96	0.46
41:DU:92:ASN:O	41:DU:93:LEU:HB2	2.16	0.46
7:AG:62:PHE:HE2	7:AG:66:LEU:HD22	1.81	0.46
10:AJ:42:LEU:HB2	10:AJ:71:LEU:HB3	1.96	0.46
1:BA:677:U:H3	1:BA:713:G:H22	1.62	0.46
5:BE:11:LEU:HG	5:BE:12:GLN:N	2.30	0.46
10:BJ:5:ARG:HB3	10:BJ:77:VAL:HG13	1.97	0.46
11:BK:14:LYS:O	11:BK:15:GLN:HB3	2.16	0.46
11:BK:98:ARG:HA	21:BU:12:PHE:CZ	2.51	0.46
19:BS:30:PRO:HB2	19:BS:50:ALA:HB2	1.97	0.46
29:CH:31:VAL:HB	29:CH:32:PRO:HD3	1.97	0.46
30:CJ:19:ASN:HA	30:CJ:39:CYS:SG	2.55	0.46
53:DA:1161:C:O2'	39:DS:8:GLY:HA2	2.14	0.46
66:DA:3198:EDO:H12	64:DA:3204:PGE:C3	2.42	0.46
42:DV:73:PHE:CE2	42:DV:75:ALA:HA	2.51	0.46
48:D1:2:ALA:N	69:D1:204:HOH:O	2.48	0.46
1:AA:468:A:C8	1:AA:469:C:C6	3.03	0.46
1:AA:1018:G:N3	1:AA:1018:G:H2'	2.30	0.46
10:AJ:22:THR:CG2	10:AJ:39:PRO:HB3	2.46	0.46
1:BA:502:A:H2'	1:BA:503:C:O4'	2.15	0.46
22:CA:846:U:O2'	22:CA:847:U:P	2.74	0.46
22:CA:2271:G:O6	69:CA:3441:HOH:O	2.21	0.46
22:CA:2790:U:H4'	22:CA:2791:G:OP1	2.15	0.46
24:CC:233:GLY:H	24:CC:242:LYS:HE3	1.81	0.46
40:CT:62:ASP:N	40:CT:62:ASP:OD1	2.49	0.46
53:DA:483:A:H2'	53:DA:484:C:H5'	1.96	0.46
53:DA:961:C:H5'	63:DA:3203:1PE:H222	1.98	0.46
53:DA:2256:G:N3	57:DA:3193:PG4:H31	2.29	0.46
54:DD:99:GLU:HG2	54:DD:182:ALA:HB2	1.98	0.46
49:D2:22:THR:OG1	51:D4:34:THR:OG1	2.26	0.46
1:AA:1152:A:H5''	10:AJ:15:HIS:HB2	1.97	0.46
1:AA:1492:A:H4'	12:AL:44:LYS:HE2	1.97	0.46
9:AI:19:VAL:HG11	9:AI:83:ILE:HA	1.98	0.46
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.97	0.46
13:AM:54:ASP:HA	13:AM:57:ARG:HD2	1.98	0.46
1:BA:1299:A:H2'	1:BA:1299:A:N3	2.31	0.46
6:BF:76:THR:O	6:BF:79:ARG:N	2.47	0.46
16:BP:79:ASN:O	16:BP:80:LYS:HG3	2.15	0.46
22:CA:747:5MU:O2	22:CA:2014:A:H1'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CA:1808:A:N1	45:CY:28:ARG:HD2	2.31	0.46
25:CD:121:THR:HB	25:CD:127:PHE:CD2	2.51	0.46
50:C3:43:THR:OG1	50:C3:44:VAL:N	2.48	0.46
55:DI:54:VAL:HG22	55:DI:81:LEU:HD13	1.96	0.46
1:AA:1134:G:H2'	1:AA:1135:U:C6	2.51	0.46
13:BM:93:ARG:NH2	19:BS:80:TYR:HE1	2.13	0.46
22:CA:1820:U:C4	24:CC:159:GLY:HA3	2.50	0.46
22:CA:1853:A:N6	22:CA:1888:G:O2'	2.48	0.46
23:CB:8:C:O3'	36:CP:25:ARG:NH1	2.48	0.46
24:CC:117:GLN:N	24:CC:128:ASN:OD1	2.48	0.46
24:CC:217:ARG:HB3	24:CC:218:PRO:HD2	1.97	0.46
25:CD:113:SER:HB3	25:CD:170:VAL:HG21	1.98	0.46
29:CH:1:MET:SD	29:CH:27:ARG:NH1	2.89	0.46
32:CL:76:VAL:HG22	37:CQ:73:VAL:HG23	1.97	0.46
53:DA:845:A:H5'	53:DA:846:U:OP2	2.15	0.46
34:DN:21:ALA:HB1	34:DN:100:LYS:HG3	1.98	0.46
3:AC:123:GLN:HG2	3:AC:128:VAL:HG21	1.97	0.46
7:AG:83:SER:HB2	7:AG:85:TYR:CE2	2.51	0.46
10:AJ:15:HIS:CG	10:AJ:16:ARG:N	2.84	0.46
5:BE:81:LEU:HD12	5:BE:120:VAL:HG11	1.97	0.46
7:BG:16:PRO:HB2	9:BI:46:MET:SD	2.56	0.46
14:BN:45:VAL:HG12	19:BS:10:PHE:CE1	2.50	0.46
22:CA:1127:A:N7	22:CA:2488:G:O2'	2.47	0.46
42:CV:51:ALA:O	42:CV:52:LEU:HB2	2.16	0.46
50:C3:30:VAL:O	50:C3:34:ARG:HG3	2.15	0.46
55:DI:82:ILE:HD12	55:DI:84:TYR:CE2	2.51	0.46
2:AB:126:PHE:CG	2:AB:127:ASP:N	2.84	0.46
14:AN:21:PHE:HB2	14:AN:55:SER:O	2.16	0.46
20:AT:44:LYS:HB3	20:AT:87:ALA:HB3	1.98	0.46
1:BA:532:A:N3	1:BA:532:A:H2'	2.30	0.46
1:BA:1004:A:C2	1:BA:1026:G:C2	3.04	0.46
5:BE:56:VAL:N	5:BE:57:PRO:HD2	2.31	0.46
12:BL:43:LYS:HD2	12:BL:91:PRO:HG3	1.97	0.46
22:CA:533:G:H5'	38:CR:24:TYR:CE1	2.51	0.46
22:CA:1274:A:N3	22:CA:1297:C:HI'	2.30	0.46
22:CA:1783:A:H5'	22:CA:2608:G:H4'	1.97	0.46
25:CD:97:SER:OG	25:CD:98:VAL:N	2.49	0.46
25:CD:149:ASN:O	25:CD:151:THR:O	2.33	0.46
27:CF:40:VAL:HG11	27:CF:50:LEU:HD13	1.98	0.46
42:CV:13:VAL:HG21	42:CV:39:ILE:HG23	1.98	0.46
53:DA:139:U:O2'	53:DA:141:G:N1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DA:1585:C:H2'	53:DA:1586:A:O4'	2.15	0.46
24:DC:31:ALA:HB3	24:DC:32:PRO:HD3	1.97	0.46
35:DO:29:VAL:O	35:DO:78:LYS:NZ	2.45	0.46
5:AE:94:VAL:HG13	5:AE:111:MET:HE1	1.98	0.46
1:BA:510:A:H5''	1:BA:511:C:OP2	2.16	0.46
2:BB:62:SER:HB2	2:BB:227:GLN:HG3	1.97	0.46
5:BE:154:ALA:O	5:BE:156:LYS:N	2.36	0.46
15:BO:89:ARG:HH12	22:CA:716:A:P	2.39	0.46
18:BR:34:THR:CG2	18:BR:38:LYS:HB2	2.45	0.46
22:CA:749:A:H4'	22:CA:1271:G:N3	2.30	0.46
22:CA:1794:A:H2'	22:CA:1795:C:C6	2.51	0.46
22:CA:1982:U:OP1	69:CA:3704:HOH:O	2.21	0.46
50:C3:3:ARG:NE	50:C3:3:ARG:HA	2.31	0.46
55:DI:50:VAL:HG22	55:DI:85:VAL:HG13	1.98	0.46
1:AA:872:A:C8	1:AA:874:G:C8	3.04	0.46
14:AN:18:ASP:OD1	14:AN:19:LYS:N	2.49	0.46
1:BA:1108:G:H5''	3:BC:176:HIS:CE1	2.51	0.46
4:BD:187:GLU:N	4:BD:190:ASP:OD2	2.41	0.46
7:BG:130:ASN:O	7:BG:130:ASN:ND2	2.48	0.46
9:BI:23:PRO:HA	9:BI:61:LEU:HA	1.98	0.46
9:BI:85:ARG:HA	9:BI:88:MET:CE	2.46	0.46
11:BK:112:ASP:OD1	11:BK:114:THR:HG23	2.16	0.46
15:BO:26:GLU:OE1	15:BO:26:GLU:N	2.44	0.46
22:CA:1170:C:N4	22:CA:1171:G:O6	2.49	0.46
30:CJ:22:PRO:HB2	30:CJ:23:PRO:HD3	1.98	0.46
32:CL:103:VAL:O	32:CL:122:VAL:HB	2.16	0.46
33:CM:94:THR:CG2	33:CM:95:LEU:N	2.79	0.46
39:CS:48:LYS:H	39:CS:48:LYS:HE2	1.81	0.46
44:CX:21:LEU:HA	44:CX:39:ARG:HB2	1.98	0.46
26:DE:23:PHE:CD1	26:DE:111:GLU:HG3	2.50	0.46
55:DI:132:TYR:HB3	55:DI:133:GLU:HG2	1.98	0.46
30:DJ:35:ILE:CG2	30:DJ:36:MET:N	2.79	0.46
34:DN:92:TRP:HE1	58:DN:201:MPD:HM1	1.81	0.46
46:DZ:11:VAL:O	46:DZ:15:ASN:ND2	2.49	0.46
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.47	0.45
6:AF:42:TRP:CH2	6:AF:102:MET:HE3	2.51	0.45
8:AH:28:PRO:O	8:AH:33:LYS:NZ	2.38	0.45
10:AJ:6:ILE:CG1	10:AJ:76:ILE:HB	2.46	0.45
11:AK:111:THR:HG23	21:AU:3:VAL:HG22	1.98	0.45
1:BA:157:U:C2'	1:BA:158:G:H5'	2.46	0.45
1:BA:1110:A:H5'	1:BA:1110:A:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1119:C:OP2	9:BI:11:ARG:NH1	2.48	0.45
3:BC:64:ILE:HD13	3:BC:91:VAL:CG1	2.46	0.45
9:BI:19:VAL:HG11	9:BI:83:ILE:HA	1.98	0.45
11:BK:13:ARG:HG3	11:BK:77:TYR:HE1	1.80	0.45
20:BT:36:TYR:C	20:BT:36:TYR:CD1	2.93	0.45
22:CA:483:A:H2'	22:CA:484:C:H5'	1.98	0.45
24:CC:125:LYS:HB2	24:CC:126:PRO:HD2	1.98	0.45
26:CE:145:ASP:HA	26:CE:166:LYS:HB3	1.98	0.45
51:C4:27:ALA:O	51:C4:28:ASN:HB2	2.16	0.45
37:DQ:2:SER:O	37:DQ:6:LYS:HB2	2.16	0.45
38:DR:105:ALA:HB1	39:DS:40:MET:HE1	1.98	0.45
39:DS:41:ILE:HD13	39:DS:103:ALA:HA	1.97	0.45
1:BA:1093:A:OP1	7:BG:4:ARG:NH2	2.48	0.45
13:BM:13:LYS:O	13:BM:14:HIS:CG	2.70	0.45
14:BN:42:TRP:CD1	14:BN:45:VAL:HG23	2.51	0.45
22:CA:2544:G:H5'	22:CA:2645:G:C2	2.50	0.45
22:CA:2722:G:H2'	22:CA:2723:C:C6	2.51	0.45
23:CB:11:C:O2'	23:CB:15:A:N6	2.48	0.45
49:C2:15:ALA:C	49:C2:17:THR:H	2.24	0.45
53:DA:142:A:C5	53:DA:143:C:N4	2.84	0.45
53:DA:2224:G:P	24:DC:265:LYS:NZ	2.89	0.45
54:DD:149:ASN:CG	54:DD:150[A]:MEQ:H	2.23	0.45
30:DJ:86:ILE:HD13	30:DJ:138:LEU:HD21	1.97	0.45
1:AA:1170:A:H5'	2:AB:139:ARG:NH2	2.30	0.45
2:AB:10:LEU:HD12	2:AB:15:HIS:ND1	2.31	0.45
3:AC:150:LYS:HB3	3:AC:169:ARG:CG	2.46	0.45
7:AG:44:TYR:O	7:AG:48:GLU:N	2.40	0.45
1:BA:840:C:H2'	1:BA:841:C:C5'	2.46	0.45
1:BA:1003:G:H21	1:BA:1005:A:H5'	1.81	0.45
10:BJ:92:LEU:O	10:BJ:93:ALA:HB2	2.16	0.45
20:BT:5:LYS:HD3	20:BT:7:ALA:H	1.80	0.45
21:BU:21:ARG:HA	21:BU:24:GLU:HB3	1.98	0.45
22:CA:846:U:H1'	22:CA:847:U:C5	2.51	0.45
22:CA:1724:G:C2'	22:CA:1725:U:H5'	2.47	0.45
22:CA:2133:G:H2'	22:CA:2157:G:H22	1.82	0.45
22:CA:2261:C:C2	22:CA:2280:G:N2	2.84	0.45
23:CB:14:U:H3'	23:CB:15:A:H5'	1.98	0.45
26:CE:23:PHE:CE2	26:CE:25:GLU:HG2	2.51	0.45
41:CU:2:ILE:HG12	41:CU:3:ARG:N	2.32	0.45
53:DA:846:U:O2'	53:DA:847:U:P	2.74	0.45
53:DA:2189:U:H2'	53:DA:2190:G:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DA:2321:U:H5'	53:DA:2322:A:OP2	2.16	0.45
66:DA:3210:EDO:O1	57:DR:202:PG4:H32	2.16	0.45
27:DF:140:GLU:OE1	27:DF:140:GLU:N	2.49	0.45
37:DQ:4:ILE:H	37:DQ:4:ILE:HD12	1.82	0.45
1:AA:657:U:O2	15:AO:22:THR:HG23	2.16	0.45
1:AA:1423:G:OP1	32:DL:49:ARG:NH2	2.49	0.45
5:AE:82:GLN:CD	5:AE:150:PRO:HD3	2.41	0.45
1:BA:833:G:C6	1:BA:834:U:C4	3.04	0.45
1:BA:1097:C:H4'	2:BB:139:ARG:HH21	1.81	0.45
16:BP:2:VAL:HG13	16:BP:65:ALA:HA	1.98	0.45
17:BQ:61:ILE:HG13	17:BQ:73:TRP:HE3	1.82	0.45
22:CA:637:A:P	33:CM:112:LEU:HB3	2.56	0.45
22:CA:1047:G:N2	22:CA:1110:G:O2'	2.50	0.45
22:CA:2024:G:C4	22:CA:2040:G:N2	2.84	0.45
53:DA:2886[A]:A:H2'	53:DA:2887[A]:A:H8	1.81	0.45
58:DA:3205:MPD:HM2	58:DA:3205:MPD:H52	1.98	0.45
24:DC:2:ALA:N	24:DC:20:VAL:O	2.49	0.45
55:DI:132:TYR:H	55:DI:133:GLU:HB2	1.82	0.45
1:AA:1312:G:C5'	19:AS:6:LYS:HE2	2.47	0.45
1:BA:77:A:H2'	1:BA:78:A:C8	2.52	0.45
1:BA:501:C:OP1	12:BL:114:ARG:NH2	2.50	0.45
1:BA:736:C:C5'	6:BF:88:MET:HE2	2.46	0.45
1:BA:1041:G:H2'	1:BA:1042:A:C8	2.51	0.45
13:BM:48:LEU:HD22	13:BM:53:ILE:HG12	1.99	0.45
22:CA:27:G:C2	22:CA:512:G:N3	2.85	0.45
22:CA:644:A:H2'	22:CA:645:C:O4'	2.16	0.45
22:CA:1906:G:C8	22:CA:1929:G:H2'	2.52	0.45
22:CA:2807:U:C4	22:CA:2808:G:N7	2.84	0.45
24:CC:210:ALA:HA	24:CC:213:TRP:NE1	2.32	0.45
53:DA:1171:G:C4	53:DA:1179:G:N2	2.84	0.45
53:DA:1539:U:H2'	53:DA:1540:G:H8	1.80	0.45
53:DA:1853:A:N1	53:DA:2087:G:HI'	2.31	0.45
55:DI:85:VAL:HG22	55:DI:92:ALA:HB2	1.98	0.45
55:DI:119:PRO:HG2	55:DI:122:GLN:HB2	1.98	0.45
44:DX:39:ARG:HD3	69:DX:101:HOH:O	2.16	0.45
1:AA:405:U:O4	4:AD:2:ALA:N	2.50	0.45
7:AG:16:PRO:HB3	9:AI:43:THR:HG23	1.98	0.45
1:BA:96:U:O2'	1:BA:97:G:H5'	2.17	0.45
1:BA:464:U:N3	1:BA:467:U:OP2	2.37	0.45
1:BA:542:G:H5'	4:BD:39:GLY:HA3	1.98	0.45
1:BA:1309:G:HI'	13:BM:73:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BE:134:ILE:HD12	5:BE:134:ILE:H	1.82	0.45
7:BG:26:PHE:CD2	7:BG:62:PHE:HE2	2.35	0.45
14:BN:23:LYS:O	14:BN:26:GLU:OE2	2.35	0.45
16:BP:46:LYS:HD3	16:BP:47:GLU:N	2.26	0.45
22:CA:2636:C:H4'	25:CD:81:GLU:CD	2.41	0.45
23:CB:28:C:P	36:CP:31:THR:HG21	2.57	0.45
53:DA:1846:G:H2'	53:DA:1847:A:C8	2.52	0.45
54:DD:85:ALA:H	54:DD:88:GLU:HG3	1.82	0.45
32:DL:47:ILE:HB	32:DL:48:PRO:HD2	1.98	0.45
33:DM:81:ASP:HB3	33:DM:100:ILE:HD13	1.98	0.45
43:DW:50:MET:HE2	43:DW:56:PHE:CE1	2.52	0.45
1:AA:5:U:H3'	1:AA:5:U:H6	1.81	0.45
1:AA:1031:C:O2'	1:AA:1032:G:OP2	2.26	0.45
1:AA:1079:G:H5'	5:AE:134:ILE:CD1	2.46	0.45
1:AA:1097:C:H4'	2:AB:139:ARG:HH21	1.81	0.45
10:AJ:67:ILE:HG13	14:AN:96:LEU:HD13	1.99	0.45
21:AU:6:VAL:HG22	21:AU:15:ALA:HB1	1.99	0.45
1:BA:247:G:C6	1:BA:278:G:C2	3.05	0.45
1:BA:1402:4OC:HM22	1:BA:1403:C:H5'	1.98	0.45
5:BE:153:VAL:O	5:BE:156:LYS:HB2	2.17	0.45
22:CA:2114:A:N6	22:CA:2119:A:N7	2.65	0.45
29:CH:41:LYS:HA	29:CH:44:ILE:HD13	1.99	0.45
39:CS:27:ILE:O	39:CS:66:HIS:NE2	2.49	0.45
40:CT:29:VAL:CG1	40:CT:55:ILE:HD11	2.46	0.45
42:CV:45:HIS:HD2	42:CV:58:ILE:HG23	1.82	0.45
53:DA:48:G:N2	53:DA:49:A:N1	2.64	0.45
53:DA:836:G:OP1	69:DA:8111:HOH:O	2.21	0.45
5:AE:161:VAL:O	5:AE:164:ILE:N	2.47	0.45
5:BE:148:ASN:ND2	5:BE:153:VAL:HG12	2.31	0.45
6:BF:91:ARG:HG3	6:BF:93:LYS:NZ	2.32	0.45
8:BH:7:ILE:HB	8:BH:77:ARG:NH1	2.32	0.45
22:CA:457:A:N1	22:CA:470:A:H5''	2.31	0.45
53:DA:1746:A:H2'	53:DA:1747:U:C6	2.52	0.45
53:DA:2256:G:H21	57:DA:3193:PG4:C3	2.29	0.45
35:DO:73:ASN:HA	35:DO:76:VAL:HG13	1.99	0.45
5:AE:94:VAL:CG2	5:AE:111:MET:HE3	2.44	0.45
8:AH:25:VAL:HG22	8:AH:63:LEU:HD21	1.99	0.45
10:AJ:5:ARG:HG2	10:AJ:77:VAL:HA	1.99	0.45
1:BA:842:U:O5'	1:BA:842:U:H6	2.00	0.45
2:BB:124:GLY:O	2:BB:125:THR:HG22	2.16	0.45
7:BG:50:LEU:HD13	7:BG:61:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BK:23:ILE:HD11	11:BK:93:ARG:HA	1.98	0.45
14:BN:49:GLN:CD	19:BS:10:PHE:CZ	2.95	0.45
42:CV:5:ILE:HD12	42:CV:67:VAL:HG12	1.98	0.45
35:DO:38:LEU:HB3	35:DO:39:PRO:HD3	1.98	0.45
36:DP:31:THR:HG22	36:DP:33:ARG:H	1.81	0.45
1:AA:7:A:O2'	5:AE:106:ILE:HD11	2.16	0.45
1:AA:31:G:O2'	1:AA:48:C:N4	2.50	0.45
7:AG:111:ARG:O	7:AG:119:ARG:NH2	2.48	0.45
1:BA:731:G:H5'	1:BA:766:A:H4'	1.98	0.45
16:BP:38:PHE:CE2	16:BP:51:ARG:HB3	2.52	0.45
22:CA:17:G:H4'	38:CR:25:TYR:HE2	1.81	0.45
22:CA:193:U:H5	69:CA:3617:HOH:O	1.99	0.45
22:CA:1250:G:C5'	38:CR:6:ARG:HD3	2.47	0.45
22:CA:1509:A:O2'	22:CA:1510:G:OP2	2.32	0.45
22:CA:2046:G:H1'	48:C1:19:HIS:CD2	2.52	0.45
22:CA:2291:U:H2'	22:CA:2292:U:C6	2.52	0.45
22:CA:2303:G:H1'	27:CF:123:ASP:HB3	1.99	0.45
22:CA:2572:A:C8	25:CD:150:GLN:HB3	2.52	0.45
22:CA:2584:U:H2'	22:CA:2585:U:H5'	1.99	0.45
27:CF:40:VAL:HG13	27:CF:41:GLY:N	2.32	0.45
51:C4:7:VAL:HB	51:C4:61:CYS:HB3	1.99	0.45
53:DA:1932:A:H2'	53:DA:1933:G:O4'	2.17	0.45
62:DA:3225:SPD:C5	62:DA:3225:SPD:C9	2.94	0.45
34:DN:132:THR:HG22	34:DN:133:LYS:N	2.32	0.45
1:AA:1029:U:O2'	1:AA:1032:G:N1	2.49	0.44
4:AD:58:LYS:HD2	4:AD:204:TYR:OH	2.16	0.44
6:AF:102:MET:CE	18:AR:24:LYS:HB3	2.45	0.44
10:AJ:52:LEU:HD23	10:AJ:62:ARG:HD3	1.97	0.44
1:BA:722:G:N3	1:BA:722:G:H3'	2.32	0.44
5:BE:50:TYR:O	5:BE:63:ALA:HB2	2.17	0.44
6:BF:32:ALA:HB2	6:BF:70:VAL:HG11	1.99	0.44
10:BJ:15:HIS:HB3	10:BJ:70:HIS:NE2	2.31	0.44
22:CA:1248:G:C2	38:CR:3:ARG:HD2	2.52	0.44
25:CD:133:THR:HG23	25:CD:134:HIS:N	2.32	0.44
38:CR:58:ARG:HG3	38:CR:92:ARG:HD2	1.98	0.44
41:CU:37:ASP:CG	41:CU:38:ALA:H	2.24	0.44
43:CW:29:ILE:HG12	43:CW:30:ILE:N	2.31	0.44
50:C3:44:VAL:HG22	50:C3:45:SER:N	2.32	0.44
53:DA:629:G:H4'	53:DA:650:C:O2	2.17	0.44
53:DA:1587:G:O2'	53:DA:1588:G:H5'	2.17	0.44
53:DA:2078:C:OP1	69:DA:6791:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DI:103:ASN:C	55:DI:105:LYS:H	2.24	0.44
34:DN:136:MET:HE3	43:DW:57:TYR:CD1	2.52	0.44
2:AB:121:SER:HA	2:AB:126:PHE:CE2	2.53	0.44
2:AB:217:VAL:O	2:AB:221:VAL:HG23	2.17	0.44
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	2.00	0.44
5:AE:74:VAL:HG22	5:AE:76:LEU:HD23	1.99	0.44
5:AE:105:ILE:HG23	5:AE:123:VAL:HG23	2.00	0.44
2:BB:94:HIS:O	2:BB:95:ARG:C	2.60	0.44
5:BE:157:ARG:C	5:BE:159:LYS:N	2.75	0.44
6:BF:3:HIS:CD2	6:BF:94:HIS:HA	2.52	0.44
7:BG:79:ARG:HG2	7:BG:84:THR:HA	1.99	0.44
22:CA:543:G:H8	22:CA:543:G:H5''	1.82	0.44
22:CA:2502:G:C5'	22:CA:2503:2MA:H5''	2.47	0.44
24:CC:37:ASN:HB3	24:CC:60:GLN:O	2.17	0.44
24:CC:141:VAL:O	24:CC:162:VAL:N	2.43	0.44
35:CO:114:GLU:HB2	35:CO:118:ARG:HD2	1.99	0.44
41:CU:17:SER:O	41:CU:19:LYS:N	2.38	0.44
50:C3:12:ARG:HG2	50:C3:12:ARG:HH21	1.82	0.44
53:DA:57:C:H2'	53:DA:58:G:O4'	2.18	0.44
53:DA:1070:A:N7	53:DA:1096:A:O2'	2.47	0.44
27:DF:132:VAL:HG22	27:DF:152:LEU:HB3	2.00	0.44
41:DU:53:VAL:HG11	41:DU:92:ASN:HB3	1.99	0.44
49:D2:47:VAL:CG1	49:D2:48:ILE:N	2.80	0.44
1:AA:158:G:H2'	1:AA:159:G:H5''	1.99	0.44
6:AF:90:MET:HE1	18:AR:23:TYR:CZ	2.52	0.44
17:AQ:8:LEU:HD13	17:AQ:25:ILE:HG13	1.99	0.44
20:AT:27:MET:CE	20:AT:57:ILE:HG12	2.48	0.44
1:BA:977:A:O2'	1:BA:979:C:OP2	2.34	0.44
3:BC:153:VAL:HG23	3:BC:157:LEU:HD21	1.99	0.44
5:BE:107:ALA:HB2	5:BE:125:ALA:HB3	1.99	0.44
17:BQ:65:ARG:H	17:BQ:65:ARG:HD2	1.83	0.44
22:CA:225:C:H2'	22:CA:226:A:O4'	2.17	0.44
22:CA:247:G:H4'	22:CA:386:G:C5	2.52	0.44
22:CA:320:A:H4'	22:CA:322:A:N7	2.33	0.44
22:CA:449:A:OP2	69:CA:3239:HOH:O	2.20	0.44
22:CA:1581:G:C5	22:CA:1582:C:C5	3.05	0.44
22:CA:2133:G:N2	22:CA:2158:A:C6	2.86	0.44
22:CA:2619:C:OP1	25:CD:157:LYS:NZ	2.44	0.44
33:CM:81:ASP:O	33:CM:83:ALA:N	2.50	0.44
33:CM:100:ILE:HG12	33:CM:101:ILE:HG23	2.00	0.44
53:DA:481:G:C4	53:DA:507:A:C2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DA:2813:A:H2	53:DA:2887[B]:A:N6	2.16	0.44
61:DA:3201:PEG:H32	69:DA:3916:HOH:O	2.17	0.44
54:DD:13:ARG:HD3	54:DD:21:SER:OG	2.17	0.44
29:DH:116:ARG:NH2	29:DH:133:GLN:HB3	2.32	0.44
35:DO:116:VAL:HG12	35:DO:117:ASP:N	2.32	0.44
1:AA:1031:C:H4'	1:AA:1032:G:O5'	2.17	0.44
2:AB:28:LYS:N	2:AB:29:PRO:CD	2.81	0.44
3:AC:42:TYR:CZ	3:AC:90:VAL:HG21	2.52	0.44
11:AK:34:ILE:HG12	11:AK:70:CYS:SG	2.58	0.44
19:AS:29:LYS:CB	19:AS:30:PRO:HD2	2.46	0.44
2:BB:49:MET:HE1	2:BB:199:VAL:HG13	1.99	0.44
5:BE:37:THR:HG21	5:BE:64:MET:HE2	1.99	0.44
5:BE:101:GLU:C	5:BE:101:GLU:CD	2.86	0.44
9:BI:50:GLN:N	9:BI:51:PRO:HD2	2.33	0.44
20:BT:51:PHE:HA	20:BT:54:MET:HG2	1.98	0.44
22:CA:299:A:N3	22:CA:319:G:O2'	2.45	0.44
29:CH:40:THR:C	29:CH:42:LYS:H	2.25	0.44
33:CM:96:LYS:HD3	33:CM:103:ILE:HA	2.00	0.44
53:DA:1867:G:O2'	53:DA:1868:C:H5'	2.17	0.44
53:DA:2386:A:N3	44:DX:41[A]:ARG:HG3	2.32	0.44
41:DU:67:VAL:HG22	41:DU:76:ARG:HG3	1.99	0.44
1:AA:495:A:C2	1:AA:496:A:C6	3.05	0.44
10:AJ:10:LEU:CD2	10:AJ:98:VAL:HG12	2.48	0.44
1:BA:216:U:H2'	1:BA:217:C:C6	2.53	0.44
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	1.97	0.44
1:BA:977:A:H2'	1:BA:978:A:H5''	2.00	0.44
1:BA:1169:A:O2'	2:BB:139:ARG:NH2	2.50	0.44
1:BA:1219:A:OP1	14:BN:53:ARG:HD2	2.18	0.44
2:BB:146:ASN:OD1	2:BB:146:ASN:N	2.50	0.44
5:BE:24:THR:HA	5:BE:29:ARG:HA	1.99	0.44
22:CA:674:G:H1'	26:CE:69:ARG:CD	2.48	0.44
22:CA:1450:G:O6	22:CA:1451:C:N4	2.51	0.44
22:CA:1887:C:OP2	69:CA:3696:HOH:O	2.21	0.44
22:CA:2349:G:OP1	51:C4:45:ARG:NH2	2.44	0.44
24:CC:71:LYS:NZ	24:CC:98:ASP:OD2	2.51	0.44
53:DA:280:U:H2'	53:DA:281:C:C6	2.53	0.44
53:DA:2628:C:H5''	59:DA:3195:PUT:H32	1.99	0.44
30:DJ:20:PRO:HB2	30:DJ:23:PRO:CG	2.47	0.44
36:DP:68:LYS:CE	61:DP:201:PEG:H41	2.47	0.44
3:AC:156:ARG:H	3:AC:163:ALA:HA	1.83	0.44
9:AI:36:GLU:HA	9:AI:45:ARG:HE	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AN:30:ILE:O	14:AN:34:VAL:HG23	2.17	0.44
1:BA:1026:G:O6	1:BA:1035:A:N6	2.50	0.44
1:BA:1525:G:OP1	11:BK:122:ARG:NH2	2.50	0.44
3:BC:65:ARG:O	3:BC:66:VAL:O	2.34	0.44
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	2.00	0.44
11:BK:13:ARG:NH1	11:BK:77:TYR:OH	2.51	0.44
14:BN:28:LYS:HZ1	14:BN:48:LEU:HA	1.82	0.44
20:BT:67:ILE:CG1	20:BT:71:LYS:HD3	2.47	0.44
22:CA:2680:U:O2'	22:CA:2681:C:P	2.76	0.44
23:CB:22:U:H2'	23:CB:23:G:C8	2.52	0.44
30:CJ:35:ILE:CG2	30:CJ:36:MET:N	2.81	0.44
53:DA:2327:A:H2'	53:DA:2328:A:C8	2.52	0.44
53:DA:2812:G:H2'	53:DA:2813:A:O4'	2.18	0.44
43:DW:2:PHE:HB3	43:DW:50:MET:HE3	1.99	0.44
1:AA:843:U:H3	2:BB:115:LYS:HD3	1.82	0.44
5:AE:132:ASN:OD1	5:AE:134:ILE:HG22	2.18	0.44
12:AL:110:ARG:HB2	12:AL:119:VAL:HG21	1.98	0.44
13:AM:66:GLU:OE1	13:AM:70:ARG:NH2	2.48	0.44
1:BA:1225:A:H2'	1:BA:1226:C:C5	2.52	0.44
3:BC:40:ARG:HG2	3:BC:55:ILE:CG1	2.48	0.44
5:BE:90:THR:HG22	5:BE:91:GLY:N	2.33	0.44
18:BR:34:THR:HG23	18:BR:36:SER:H	1.82	0.44
53:DA:1783:A:H5'	53:DA:2608:G:H4'	1.99	0.44
33:DM:77:ILE:HD11	33:DM:101:ILE:CG2	2.48	0.44
42:DV:89:ASP:CG	42:DV:90:GLY:H	2.26	0.44
1:AA:85:U:H6	1:AA:86:G:N1	2.15	0.44
1:AA:1322:C:P	19:AS:78:ARG:HH22	2.40	0.44
1:AA:1463:U:H2'	1:AA:1464:U:C6	2.53	0.44
3:AC:6:HIS:CG	14:AN:89:MET:HB3	2.52	0.44
7:AG:25:LYS:HB3	7:AG:101:MET:HE1	1.99	0.44
10:AJ:29:ALA:HA	10:AJ:32:THR:HG22	2.00	0.44
17:AQ:49:GLU:O	17:AQ:50:ASN:HB2	2.18	0.44
6:BF:53:LYS:HA	6:BF:53:LYS:NZ	2.33	0.44
22:CA:12:U:O2	22:CA:12:U:H2'	2.18	0.44
22:CA:118:A:C8	22:CA:119:A:C8	3.06	0.44
22:CA:2307:G:N2	22:CA:2312:U:C4	2.86	0.44
22:CA:2582:G:C2	22:CA:2583:G:C8	3.06	0.44
27:CF:103:LEU:O	27:CF:108:VAL:HG23	2.17	0.44
53:DA:1416:G:C4	53:DA:1417:C:C5	3.06	0.44
53:DA:1721:G:H1'	53:DA:1739:A:N6	2.33	0.44
27:DF:158:THR:CG2	27:DF:160:ALA:H	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:237:G:OP1	17:AQ:42:THR:OG1	2.30	0.44
7:AG:72:THR:HG22	7:AG:142:HIS:NE2	2.33	0.44
20:AT:44:LYS:HG3	20:AT:45:ALA:H	1.83	0.44
1:BA:263:A:P	20:BT:74:ARG:NH1	2.91	0.44
1:BA:1217:C:P	14:BN:9:ARG:HH21	2.38	0.44
1:BA:1450:U:O2'	1:BA:1451:U:H2'	2.17	0.44
3:BC:38:LYS:HD3	3:BC:38:LYS:N	2.33	0.44
13:BM:40:ALA:HB3	13:BM:43:VAL:HG13	2.00	0.44
13:BM:46:SER:O	13:BM:47:GLU:HB3	2.18	0.44
14:BN:46:LEU:HD22	19:BS:13:LEU:HD23	2.00	0.44
22:CA:396:G:C1'	45:CY:29:PHE:HB3	2.47	0.44
22:CA:2683:C:H4'	25:CD:13:ARG:NH1	2.33	0.44
24:CC:182:ARG:NH2	24:CC:183:LYS:O	2.51	0.44
53:DA:1494:A:C2	53:DA:1495:A:C4	3.05	0.44
53:DA:2813:A:H2	53:DA:2887[B]:A:H61	1.63	0.44
29:DH:31:VAL:HB	29:DH:32:PRO:HD3	2.00	0.44
30:DJ:80:LEU:CD2	30:DJ:101:ILE:HD13	2.48	0.44
38:DR:20:GLN:HG3	57:DR:202:PG4:H31	1.98	0.44
43:DW:50:MET:HE2	43:DW:56:PHE:HE1	1.83	0.44
2:AB:213:TYR:O	2:AB:217:VAL:HG23	2.18	0.43
3:AC:83:ASP:HA	3:AC:86:LYS:HG2	1.99	0.43
4:AD:188:ARG:NH2	4:AD:197:GLU:OE2	2.48	0.43
10:AJ:28:THR:O	10:AJ:32:THR:HG22	2.18	0.43
13:AM:4:ILE:CG2	13:AM:60:VAL:HG11	2.48	0.43
17:AQ:7:THR:HG21	17:AQ:60:GLU:CG	2.48	0.43
1:BA:724:G:OP2	1:BA:833:G:O2'	2.29	0.43
6:BF:91:ARG:CG	6:BF:93:LYS:NZ	2.80	0.43
22:CA:468:G:N7	50:C3:39:ARG:NH2	2.63	0.43
22:CA:1090:A:N1	22:CA:1101:U:O2	2.51	0.43
22:CA:2030:6MZ:H9C2	69:CA:3585:HOH:O	2.17	0.43
27:CF:33:LYS:HA	27:CF:96:MET:SD	2.58	0.43
27:CF:44:ILE:HG21	27:CF:79:ILE:HG22	2.00	0.43
36:CP:31:THR:HG22	36:CP:33:ARG:H	1.83	0.43
52:C5:1:MET:HB3	52:C5:34:LYS:HE2	2.00	0.43
53:DA:1490:A:N6	69:DA:5107:HOH:O	2.36	0.43
53:DA:1539:U:C2	53:DA:1540:G:C8	3.06	0.43
53:DA:2223:G:O3'	24:DC:265:LYS:NZ	2.51	0.43
24:DC:130:LEU:HD11	24:DC:135:ILE:CG1	2.47	0.43
24:DC:156:ARG:NH2	69:DC:393:HOH:O	2.49	0.43
36:DP:100:HIS:CG	36:DP:101:GLY:N	2.86	0.43
41:DU:5:GLU:HG2	46:DZ:22:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1014:A:OP1	19:AS:18:LYS:NZ	2.51	0.43
8:AH:41:LYS:HD2	8:AH:48:ASP:HA	2.00	0.43
1:BA:83:C:O2'	1:BA:86:G:O6	2.36	0.43
1:BA:993:G:O2'	1:BA:994:A:N7	2.50	0.43
1:BA:1127:G:H1	1:BA:1145:A:H61	1.65	0.43
12:BL:45:PRO:HD2	12:BL:46:ASN:H	1.84	0.43
22:CA:2627:G:O2'	22:CA:2781:A:N1	2.41	0.43
27:CF:126:GLY:O	27:CF:158:THR:HG21	2.17	0.43
48:C1:25:VAL:HG13	48:C1:26:THR:N	2.33	0.43
53:DA:5:A:C2	53:DA:2899:A:C2	3.06	0.43
53:DA:1187:G:H5''	39:DS:83:TYR:CE1	2.53	0.43
53:DA:2161:C:H4'	53:DA:2173:A:P	2.58	0.43
1:AA:464:U:C2	1:AA:466:A:H5''	2.53	0.43
2:AB:49:MET:HE1	2:AB:199:VAL:CG1	2.48	0.43
8:AH:93:PRO:HG3	8:AH:125:ILE:HD13	2.00	0.43
14:AN:21:PHE:CD1	14:AN:55:SER:HB3	2.52	0.43
1:BA:268:U:H2'	1:BA:269:C:C6	2.53	0.43
1:BA:1359:C:O2'	1:BA:1361:G:N7	2.52	0.43
2:BB:4:VAL:HG12	2:BB:5:SER:N	2.33	0.43
5:BE:36:LEU:HD21	5:BE:137:VAL:HG11	2.00	0.43
8:BH:67:GLN:C	8:BH:69:LYS:H	2.25	0.43
10:BJ:19:ASP:HA	10:BJ:22:THR:HB	2.00	0.43
16:BP:19:VAL:HG12	16:BP:37:GLY:C	2.43	0.43
22:CA:1509:A:N3	22:CA:1510:G:C8	2.86	0.43
22:CA:2578:G:OP1	69:CA:3833:HOH:O	2.21	0.43
29:CH:126:GLY:O	29:CH:146:VAL:N	2.48	0.43
43:CW:21:ARG:NH2	43:CW:87:GLN:O	2.47	0.43
59:DA:3195:PUT:H21	69:DA:5561:HOH:O	2.18	0.43
27:DF:135:GLN:N	27:DF:135:GLN:OE1	2.48	0.43
30:DJ:99:GLY:O	30:DJ:139:VAL:HG22	2.17	0.43
61:DP:201:PEG:H22	61:DP:201:PEG:H42	1.54	0.43
39:DS:93:PHE:HB3	57:DS:202:PG4:H51	1.99	0.43
1:AA:75:G:C4	1:AA:76:G:C8	3.06	0.43
2:AB:9:MET:CE	2:AB:50:PHE:HD2	2.31	0.43
5:AE:95:PHE:CZ	5:AE:97:GLN:HG3	2.54	0.43
1:BA:532:A:H61	3:BC:193:TYR:HD2	1.66	0.43
2:BB:32:PHE:N	2:BB:40:ILE:O	2.52	0.43
2:BB:121:SER:HA	2:BB:126:PHE:CE2	2.53	0.43
2:BB:126:PHE:CG	2:BB:127:ASP:N	2.86	0.43
11:BK:106:ARG:HG2	11:BK:106:ARG:HH11	1.84	0.43
12:BL:51:LYS:HD2	12:BL:51:LYS:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BN:62:ASN:HB3	14:BN:73:PHE:CD2	2.53	0.43
17:BQ:69:LYS:O	17:BQ:71:LYS:N	2.51	0.43
19:BS:49:ILE:HD13	19:BS:71:LEU:HD22	1.98	0.43
22:CA:125:A:OP2	50:C3:19:ARG:NH2	2.44	0.43
22:CA:572:A:OP2	39:CS:80:ARG:NH2	2.39	0.43
22:CA:666:A:C5'	33:CM:48:ARG:HD2	2.48	0.43
22:CA:1045:C:H4'	22:CA:1046:A:H5'	2.00	0.43
22:CA:1185:G:H5''	22:CA:1186:G:OP2	2.17	0.43
22:CA:1435:G:O2'	22:CA:1436:G:H5'	2.19	0.43
22:CA:2161:C:O2'	22:CA:2173:A:OP2	2.36	0.43
22:CA:2469:A:HO2'	34:CN:55:ARG:HH21	1.63	0.43
22:CA:2751:G:C2	28:CG:3:ARG:NH1	2.87	0.43
49:C2:44:ARG:C	49:C2:45:GLN:HG2	2.44	0.43
53:DA:388:G:N7	53:DA:390:U:H2'	2.33	0.43
53:DA:2886[A]:A:C6	53:DA:2887[A]:A:C5	3.06	0.43
1:BA:302:G:N3	1:BA:556:C:H4'	2.34	0.43
1:BA:1408:A:C2	1:BA:1494:G:C4	3.07	0.43
22:CA:782:A:H5'	22:CA:783:A:C2	2.53	0.43
22:CA:868:U:C4	22:CA:869:G:N7	2.86	0.43
22:CA:2889:C:N4	22:CA:2890:G:C6	2.87	0.43
31:CK:57:LEU:HD23	31:CK:129:GLU:HA	2.00	0.43
35:CO:20:MET:HG3	35:CO:21:PHE:N	2.32	0.43
42:CV:16:GLY:C	42:CV:18:ASP:H	2.26	0.43
50:C3:24:THR:HG23	50:C3:27:GLY:H	1.83	0.43
53:DA:1183:U:H2'	53:DA:1184:U:C6	2.54	0.43
53:DA:1847:A:P	53:DA:1847:A:C8	3.10	0.43
53:DA:2788:C:O2'	53:DA:2809:A:N3	2.45	0.43
54:DD:33:ARG:NH2	54:DD:74:GLU:O	2.51	0.43
49:D2:35:GLU:OE2	49:D2:48:ILE:HD11	2.18	0.43
5:AE:90:THR:HG22	5:AE:91:GLY:N	2.34	0.43
7:AG:108:ALA:HB3	7:AG:116:MET:HE1	2.01	0.43
9:AI:24:GLY:H	9:AI:61:LEU:HA	1.84	0.43
10:AJ:56:HIS:O	10:AJ:57:VAL:HG12	2.19	0.43
1:BA:81:A:C2	1:BA:89:U:O2	2.72	0.43
1:BA:844:G:H3'	1:BA:844:G:N3	2.33	0.43
5:BE:44:GLY:O	5:BE:45:ARG:O	2.35	0.43
8:BH:29:SER:OG	8:BH:30:SER:N	2.51	0.43
10:BJ:6:ILE:HB	10:BJ:76:ILE:O	2.19	0.43
11:BK:98:ARG:HG2	21:BU:12:PHE:HZ	1.83	0.43
22:CA:55:G:C2	22:CA:116:C:C2	3.06	0.43
22:CA:2086:U:H2'	22:CA:2087:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CA:2716:C:O2'	22:CA:2717:C:H5'	2.19	0.43
29:CH:23:ALA:O	29:CH:27:ARG:N	2.49	0.43
31:CK:4:PHE:O	38:CR:64:ARG:NH2	2.49	0.43
53:DA:141:G:H3'	53:DA:142:A:C4	2.54	0.43
53:DA:876:C:H2'	53:DA:877:A:O4'	2.19	0.43
53:DA:1385:A:O2'	53:DA:1396:U:O2	2.33	0.43
53:DA:1540:G:H2'	53:DA:1541:C:C6	2.54	0.43
59:DA:3195:PUT:H41	69:DA:5231:HOH:O	2.17	0.43
55:DI:64:VAL:HG13	55:DI:69:PHE:C	2.43	0.43
55:DI:64:VAL:HG13	55:DI:69:PHE:HB2	2.01	0.43
1:AA:475:C:H2'	1:AA:476:U:O4'	2.19	0.43
1:AA:502:A:H2'	1:AA:503:C:O4'	2.18	0.43
8:AH:75:ILE:O	8:AH:75:ILE:HG23	2.19	0.43
1:BA:429:U:H5'	4:BD:9:LEU:HD12	2.00	0.43
1:BA:1190:G:H5'	3:BC:176:HIS:NE2	2.33	0.43
1:BA:1191:A:H5''	3:BC:4:LYS:HE3	2.01	0.43
5:BE:75:ALA:O	5:BE:82:GLN:NE2	2.52	0.43
13:BM:8:ASN:C	13:BM:10:PRO:HD2	2.43	0.43
13:BM:66:GLU:C	13:BM:68:ASP:H	2.26	0.43
14:BN:49:GLN:OE1	19:BS:10:PHE:CZ	2.72	0.43
17:BQ:28:PHE:HD2	17:BQ:37:PHE:HB3	1.82	0.43
17:BQ:49:GLU:O	17:BQ:50:ASN:HB2	2.19	0.43
22:CA:1871:A:O2'	22:CA:1872:A:C8	2.72	0.43
22:CA:1973:G:C6	22:CA:1974:C:C4	3.07	0.43
22:CA:2840:C:H5''	35:CO:53:THR:OG1	2.18	0.43
23:CB:35:C:H2'	23:CB:36:C:H5'	2.00	0.43
27:CF:50:LEU:CD2	27:CF:84:PRO:HB2	2.49	0.43
30:CJ:21:SER:HB3	30:CJ:22:PRO:HD3	1.99	0.43
45:CY:71:LEU:HD13	45:CY:76:GLU:HB3	1.99	0.43
53:DA:570:G:H2'	53:DA:2030:6MZ:N7	2.34	0.43
53:DA:914:G:C8	53:DA:914:G:H3'	2.53	0.43
53:DA:2116:G:C6	53:DA:2171:A:N6	2.84	0.43
28:DG:69:ARG:C	28:DG:69:ARG:HD3	2.44	0.43
30:DJ:56:PRO:HG2	30:DJ:72:LYS:HB2	2.01	0.43
48:D1:3:VAL:HG22	48:D1:4:GLN:N	2.34	0.43
1:AA:1464:U:OP2	37:DQ:109:ARG:NH1	2.52	0.43
11:AK:107:ILE:HG13	21:AU:12:PHE:CE2	2.54	0.43
13:AM:107:ARG:HG2	13:AM:107:ARG:HH11	1.83	0.43
1:BA:86:G:H1'	1:BA:87:C:C6	2.54	0.43
1:BA:386:C:C4	1:BA:387:U:C5	3.06	0.43
1:BA:451:A:N1	69:BA:1879:HOH:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1144:G:H5''	1:BA:1145:A:OP2	2.19	0.43
5:BE:16:ILE:HD12	5:BE:16:ILE:N	2.34	0.43
12:BL:14:ARG:NH1	12:BL:15:LYS:HE2	2.33	0.43
22:CA:36:G:N3	22:CA:450:G:O2'	2.51	0.43
22:CA:335:C:HO2'	22:CA:336:C:P	2.41	0.43
22:CA:619:G:OP2	22:CA:620:G:N2	2.49	0.43
22:CA:1390:U:C2'	22:CA:1391:U:H5'	2.49	0.43
22:CA:2419:U:H5''	49:C2:22:THR:HG21	2.01	0.43
24:CC:182:ARG:NH2	24:CC:266:PHE:HB3	2.34	0.43
25:CD:33:ARG:NH2	25:CD:74:GLU:O	2.52	0.43
30:CJ:80:LEU:CD2	30:CJ:101:ILE:HD13	2.49	0.43
53:DA:637:A:N1	53:DA:651:G:O2'	2.49	0.43
53:DA:1539:U:H2'	53:DA:1540:G:C8	2.54	0.43
53:DA:1930:G:O2'	53:DA:1931:U:OP2	2.37	0.43
29:DH:71:LYS:HB3	29:DH:108:VAL:HG22	2.00	0.43
31:DK:69:ARG:O	31:DK:90:GLU:HB2	2.19	0.43
1:AA:141:G:H2'	1:AA:142:G:H5''	2.01	0.43
5:AE:11:LEU:C	5:AE:11:LEU:HD12	2.44	0.43
7:AG:80:VAL:HG12	7:AG:81:GLY:N	2.34	0.43
7:AG:135:VAL:HG23	7:AG:136:LYS:N	2.33	0.43
9:AI:50:GLN:N	9:AI:51:PRO:HD2	2.34	0.43
9:AI:91:ASP:O	9:AI:92:GLU:CB	2.67	0.43
1:BA:209:U:H4'	1:BA:210:C:OP2	2.19	0.43
1:BA:1498:UR3:O4'	1:BA:1519:MA6:H2	2.19	0.43
3:BC:20:SER:OG	3:BC:36:ASP:OD2	2.36	0.43
7:BG:71:PRO:HG3	7:BG:103:TRP:CH2	2.54	0.43
10:BJ:26:VAL:HG13	10:BJ:36:VAL:HG11	2.01	0.43
17:BQ:74:THR:HG22	17:BQ:75:LEU:N	2.34	0.43
18:BR:72:ASP:O	18:BR:73:ARG:HD2	2.19	0.43
22:CA:10:A:C2	22:CA:2800:A:C4	3.07	0.43
22:CA:1179:G:C5	22:CA:1180:U:H1'	2.52	0.43
24:CC:97:LYS:HD3	24:CC:97:LYS:N	2.34	0.43
30:CJ:83:ALA:O	30:CJ:105:GLN:NE2	2.51	0.43
34:CN:66:ARG:NH1	34:CN:104:GLU:OE1	2.52	0.43
46:CZ:21:LEU:CD1	46:CZ:46:VAL:HG13	2.49	0.43
53:DA:1433:A:C2'	53:DA:1434:A:H5'	2.48	0.43
53:DA:2895:G:H2'	53:DA:2896:C:C6	2.54	0.43
30:DJ:20:PRO:HB2	30:DJ:23:PRO:HG2	2.00	0.43
31:DK:114:LEU:HG	31:DK:118:MET:HE3	2.01	0.43
1:AA:1152:A:H5''	10:AJ:15:HIS:CD2	2.54	0.43
1:AA:1328:C:H5''	13:AM:28:THR:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:19:GLN:HA	2:AB:38:VAL:HA	2.01	0.43
2:AB:129:LEU:O	2:AB:130:THR:CB	2.67	0.43
4:AD:95:GLU:OE2	4:AD:104:ARG:CZ	2.67	0.43
5:AE:94:VAL:HG13	5:AE:111:MET:CE	2.49	0.43
5:AE:157:ARG:HD2	8:AH:43:GLU:O	2.19	0.43
9:AI:24:GLY:N	9:AI:61:LEU:HA	2.34	0.43
10:AJ:22:THR:HG21	10:AJ:39:PRO:CB	2.49	0.43
13:AM:89:LEU:HD23	13:AM:92:ARG:HH21	1.84	0.43
1:BA:214:C:C4	1:BA:215:C:C5	3.07	0.43
5:BE:83:HIS:NE2	8:BH:96:MET:HE3	2.34	0.43
22:CA:51:G:N3	22:CA:119:A:C2	2.86	0.43
22:CA:319:G:C4	22:CA:333:G:N2	2.87	0.43
22:CA:825:A:H2'	22:CA:826:U:O4'	2.18	0.43
22:CA:1027:A:N7	22:CA:1126:A:C2	2.86	0.43
22:CA:2478:A:OP2	52:C5:2:LYS:NZ	2.51	0.43
22:CA:2502:G:H5''	22:CA:2503:2MA:H5''	2.01	0.43
22:CA:2632:A:C2	22:CA:2787:C:C2	3.07	0.43
23:CB:35:C:O2'	23:CB:36:C:H5'	2.19	0.43
30:CJ:111:GLN:O	30:CJ:114:ALA:HB3	2.19	0.43
31:CK:120:ARG:O	31:CK:123:LYS:NZ	2.49	0.43
33:CM:56:PRO:HB2	33:CM:58:TYR:CE1	2.54	0.43
53:DA:864:G:C6	53:DA:865:C:N4	2.87	0.43
53:DA:1141:U:H4'	53:DA:1142:A:O4'	2.19	0.43
30:DJ:114:ALA:CB	30:DJ:125:MET:SD	3.07	0.43
50:D3:29:GLN:HG2	61:D3:102:PEG:H32	2.01	0.43
1:AA:501:C:OP1	12:AL:114:ARG:NH2	2.52	0.42
1:AA:1492:A:H2'	1:AA:1493:A:O4'	2.18	0.42
10:AJ:53:ILE:HG22	10:AJ:61:ALA:O	2.18	0.42
10:BJ:5:ARG:HH21	10:BJ:79:PRO:HG3	1.85	0.42
17:BQ:15:ASP:HA	17:BQ:21:ILE:HD12	2.00	0.42
17:BQ:31:HIS:HB2	17:BQ:38:ILE:CD1	2.49	0.42
22:CA:166:U:OP2	69:CA:3785:HOH:O	2.22	0.42
22:CA:446:G:OP1	38:CR:5:LYS:NZ	2.52	0.42
22:CA:1790:C:O2'	24:CC:208:ALA:HB2	2.18	0.42
22:CA:2304:G:O2'	27:CF:130:MET:O	2.37	0.42
24:CC:17:VAL:HB	24:CC:204:VAL:CG1	2.49	0.42
51:C4:16:LYS:HE2	51:C4:20:GLY:HA2	2.01	0.42
52:C5:16:ILE:HD13	52:C5:25:VAL:HG22	2.01	0.42
53:DA:2566:A:H4'	53:DA:2567:G:H5''	2.01	0.42
54:DD:84:LEU:HD22	54:DD:88:GLU:HB3	2.00	0.42
27:DF:42:GLU:HG2	27:DF:49:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:DP:83:LEU:HD11	36:DP:113:ALA:O	2.19	0.42
2:AB:47:VAL:N	2:AB:48:PRO:HD2	2.35	0.42
1:BA:295:C:C4	1:BA:296:U:C4	3.07	0.42
1:BA:757:U:OP1	1:BA:822:U:O2'	2.36	0.42
4:BD:105:MET:SD	4:BD:143:VAL:HG13	2.59	0.42
14:BN:32:SER:HB2	14:BN:42:TRP:HE1	1.84	0.42
15:BO:88:ARG:C	15:BO:89:ARG:HG3	2.44	0.42
22:CA:1009:A:N3	22:CA:1153:C:O2'	2.44	0.42
22:CA:1338:G:H5''	41:CU:17:SER:HB2	2.00	0.42
22:CA:1509:A:O2'	22:CA:1510:G:P	2.76	0.42
22:CA:1936:A:H2	22:CA:1943:U:H3	1.61	0.42
22:CA:2032:G:N3	25:CD:150:GLN:HG2	2.33	0.42
22:CA:2056:G:C2	22:CA:2057:G:C8	3.07	0.42
22:CA:2307:G:H22	22:CA:2311:A:H2'	1.84	0.42
24:CC:121:ASP:N	24:CC:121:ASP:OD1	2.51	0.42
26:CE:75:SER:OG	26:CE:77:ILE:HG12	2.18	0.42
43:CW:1:MET:HA	43:CW:1:MET:CE	2.49	0.42
53:DA:1740:G:H2'	53:DA:1741:C:O4'	2.20	0.42
24:DC:251:GLN:C	24:DC:252:THR:O	2.62	0.42
1:AA:157:U:H2'	1:AA:158:G:H5'	2.01	0.42
1:AA:1405:G:O4'	1:AA:1519:MA6:H4'	2.20	0.42
10:AJ:93:ALA:HB3	10:AJ:96:VAL:HG23	2.01	0.42
13:AM:32:ALA:O	13:AM:36:ALA:N	2.47	0.42
1:BA:973:G:H1'	10:BJ:56:HIS:HD2	1.84	0.42
19:BS:29:LYS:HB3	19:BS:30:PRO:CD	2.49	0.42
22:CA:124:G:C5	50:C3:19:ARG:NH1	2.87	0.42
22:CA:191:A:H2'	22:CA:192:C:C6	2.54	0.42
22:CA:846:U:H1'	22:CA:847:U:H5	1.84	0.42
22:CA:1341:G:OP1	22:CA:1397:U:N3	2.47	0.42
22:CA:2531:A:H5'	28:CG:157:TYR:CZ	2.54	0.42
22:CA:2788:C:H2'	22:CA:2789:C:C6	2.55	0.42
26:CE:77:ILE:HG13	26:CE:78:TRP:HE3	1.84	0.42
26:CE:169:VAL:C	26:CE:170:ARG:HG2	2.42	0.42
29:CH:31:VAL:C	29:CH:33:GLN:H	2.27	0.42
41:CU:69:ARG:NE	41:CU:69:ARG:O	2.52	0.42
48:C1:13:ARG:HD2	48:C1:17:ARG:NH2	2.35	0.42
53:DA:914:G:C8	53:DA:914:G:C3'	3.02	0.42
27:DF:141:ILE:HG23	27:DF:146:VAL:CG1	2.50	0.42
50:D3:33:ARG:HG2	61:D3:102:PEG:H42	2.01	0.42
1:AA:1082:A:H2'	1:AA:1083:U:O4'	2.20	0.42
8:AH:29:SER:HB3	8:AH:57:PRO:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AJ:65:TYR:CB	14:AN:96:LEU:HD11	2.50	0.42
1:BA:213:G:N7	1:BA:214:C:C4	2.87	0.42
1:BA:1319:A:OP2	19:BS:5:LEU:CD1	2.68	0.42
1:BA:1361:G:H2'	1:BA:1362:A:H5'	2.01	0.42
6:BF:38:ARG:NH1	6:BF:61:LEU:HD21	2.34	0.42
9:BI:52:LEU:HD13	9:BI:57:MET:HE2	2.00	0.42
11:BK:82:LEU:CD2	11:BK:82:LEU:N	2.83	0.42
13:BM:12:HIS:O	13:BM:13:LYS:HG3	2.19	0.42
20:BT:27:MET:O	20:BT:30:THR:OG1	2.31	0.42
22:CA:270:A:OP1	22:CA:271:G:H2'	2.20	0.42
22:CA:290:U:C2	22:CA:291:G:C8	3.07	0.42
22:CA:634:C:H2'	22:CA:635:C:C6	2.55	0.42
22:CA:830:G:C4	22:CA:2448:A:C5	3.08	0.42
22:CA:1867:G:O2'	22:CA:1868:C:H5'	2.19	0.42
22:CA:1867:G:O6	22:CA:1875:G:N2	2.52	0.42
30:CJ:12:GLN:HA	30:CJ:56:PRO:HA	2.02	0.42
53:DA:158:U:H1'	53:DA:169:G:N2	2.33	0.42
53:DA:1172:C:N4	53:DA:1173:U:C2	2.87	0.42
53:DA:1609:A:N6	69:DA:5835:HOH:O	2.52	0.42
35:DO:32:GLU:CD	35:DO:86:ARG:HH22	2.28	0.42
41:DU:1:MET:H1	41:DU:1:MET:CE	2.33	0.42
1:AA:1074:G:O2'	1:AA:1101:A:N1	2.50	0.42
1:AA:1431:A:C6	1:AA:1432:G:C6	3.08	0.42
2:AB:124:GLY:O	2:AB:125:THR:HG22	2.19	0.42
4:AD:11:LEU:O	4:AD:15:GLU:HG2	2.20	0.42
4:AD:58:LYS:HD3	4:AD:203:LEU:HD23	2.00	0.42
1:BA:109:A:H2'	1:BA:326:G:N2	2.35	0.42
1:BA:511:C:H5'	4:BD:44:ARG:NH1	2.35	0.42
2:BB:27:MET:CE	2:BB:187:VAL:HG12	2.50	0.42
3:BC:150:LYS:HB2	3:BC:169:ARG:CG	2.49	0.42
10:BJ:24:GLU:C	10:BJ:26:VAL:N	2.77	0.42
11:BK:20:VAL:N	11:BK:35:THR:O	2.52	0.42
13:BM:7:ILE:C	13:BM:7:ILE:HD12	2.45	0.42
18:BR:20:GLU:HA	18:BR:55:LEU:HD13	2.01	0.42
22:CA:41:C:H2'	22:CA:42:A:O4'	2.20	0.42
22:CA:845:A:H3'	22:CA:845:A:N3	2.35	0.42
22:CA:1434:A:O2'	22:CA:1435:G:O4'	2.28	0.42
22:CA:1938:A:OP2	69:CA:3666:HOH:O	2.21	0.42
22:CA:1969:A:O2'	22:CA:1972:G:N3	2.45	0.42
22:CA:2143:C:H2'	22:CA:2144:G:O4'	2.20	0.42
22:CA:2234:G:C6	22:CA:2235:G:N7	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CA:2547:A:H4'	32:CL:29:HIS:NE2	2.35	0.42
24:CC:129:THR:C	24:CC:130:LEU:HD23	2.43	0.42
33:CM:77:ILE:O	33:CM:110:VAL:O	2.37	0.42
53:DA:137:U:C6	53:DA:140:C:C6	3.06	0.42
53:DA:686:U:H2'	53:DA:788:A:N1	2.34	0.42
29:DH:72:ILE:HD11	29:DH:110:VAL:HG21	2.00	0.42
30:DJ:86:ILE:CD1	30:DJ:138:LEU:HD21	2.49	0.42
35:DO:96:ARG:HD2	35:DO:114:GLU:OE1	2.19	0.42
41:DU:1:MET:C	41:DU:2:ILE:HG23	2.44	0.42
1:AA:585:G:N3	1:AA:879:C:H4'	2.34	0.42
12:AL:49:LEU:O	12:AL:51:LYS:NZ	2.48	0.42
13:AM:103:LYS:HG2	13:AM:104:THR:HG23	2.01	0.42
3:BC:51:SER:OG	3:BC:72:ARG:NH1	2.52	0.42
3:BC:97:VAL:HB	3:BC:98:PRO:HD2	2.02	0.42
9:BI:80:ARG:O	9:BI:84:THR:HG23	2.19	0.42
11:BK:17:SER:HA	11:BK:79:ILE:HA	2.00	0.42
11:BK:97:ILE:HD11	21:BU:16:LEU:CG	2.50	0.42
14:BN:31:ILE:HG23	14:BN:42:TRP:CH2	2.55	0.42
22:CA:1120:G:C6	22:CA:1121:C:C4	3.07	0.42
22:CA:1196:C:H1'	22:CA:1226:A:C4	2.54	0.42
22:CA:1604:C:O2'	22:CA:1610:A:N1	2.48	0.42
22:CA:1638:C:H4'	22:CA:2710:C:O2	2.20	0.42
22:CA:2020:A:H5'	48:C1:9:THR:HG21	2.02	0.42
22:CA:2636:C:H2'	22:CA:2637:U:C6	2.54	0.42
22:CA:2824:C:C4	22:CA:2825:G:C5	3.08	0.42
24:CC:168:ASP:OD1	24:CC:168:ASP:N	2.53	0.42
31:CK:110:PRO:O	31:CK:115:GLY:HA3	2.19	0.42
32:CL:108:ARG:HH12	37:CQ:35:GLY:N	2.17	0.42
34:CN:68:PHE:O	34:CN:69:PRO:C	2.62	0.42
41:CU:3:ARG:CZ	41:CU:5:GLU:HB2	2.49	0.42
42:CV:34:VAL:HG13	42:CV:67:VAL:HG22	2.02	0.42
53:DA:382:A:C2	53:DA:393:C:C2	3.07	0.42
53:DA:1405:U:H2'	53:DA:1406:U:C6	2.54	0.42
53:DA:1482:G:H1'	53:DA:1509:A:H61	1.83	0.42
23:DB:35:C:C2'	23:DB:36:C:H5'	2.50	0.42
30:DJ:18:ALA:O	30:DJ:19:ASN:CB	2.67	0.42
40:DT:110:ARG:OXT	40:DT:110:ARG:CG	2.66	0.42
1:AA:1064:G:H1'	1:AA:1190:G:N2	2.35	0.42
1:BA:147:G:H2'	1:BA:148:G:C8	2.54	0.42
1:BA:1100:C:OP2	2:BB:95:ARG:HD3	2.20	0.42
3:BC:206:GLU:CD	3:BC:206:GLU:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:58:LYS:HA	4:BD:200:ILE:HG12	2.01	0.42
5:BE:96:MET:CE	5:BE:115:LEU:HD11	2.50	0.42
22:CA:289:G:H2'	22:CA:290:U:O4'	2.19	0.42
22:CA:526:A:N6	22:CA:2626:C:H4'	2.34	0.42
22:CA:1914:C:C2'	22:CA:1915:3TD:H5'A	2.50	0.42
22:CA:2189:U:H2'	22:CA:2190:G:C5'	2.49	0.42
22:CA:2273:A:H2'	22:CA:2274:A:C8	2.54	0.42
22:CA:2360:G:C1'	33:CM:60:ARG:HD3	2.49	0.42
22:CA:2550:G:C5	22:CA:2551:C:C5	3.07	0.42
28:CG:101:ASN:OD1	28:CG:116:GLN:NE2	2.49	0.42
39:CS:37:GLU:HB3	39:CS:53:PHE:CE1	2.54	0.42
41:CU:2:ILE:CG1	41:CU:3:ARG:N	2.83	0.42
53:DA:136:G:N1	53:DA:143:C:N4	2.65	0.42
53:DA:483:A:C2'	53:DA:484:C:H5'	2.50	0.42
53:DA:1715:G:N2	53:DA:1744:A:OP2	2.40	0.42
53:DA:1868:C:H2'	53:DA:1869:G:O4'	2.19	0.42
53:DA:2839:G:O2'	35:DO:49:GLU:OE1	2.33	0.42
54:DD:30:GLU:O	54:DD:31:ALA:C	2.61	0.42
31:DK:7:LYS:O	31:DK:11:VAL:HG23	2.19	0.42
1:AA:2:A:O2'	4:AD:83:LYS:NZ	2.43	0.42
10:AJ:5:ARG:HH21	10:AJ:77:VAL:HG22	1.85	0.42
12:AL:74:LEU:HD21	12:AL:104:CYS:SG	2.60	0.42
20:AT:27:MET:HE1	20:AT:57:ILE:CG1	2.49	0.42
1:BA:632:U:H2'	1:BA:632:U:O2	2.20	0.42
1:BA:1118:U:H5''	9:BI:106:ARG:HG3	2.02	0.42
5:BE:65:GLU:OE1	5:BE:69:ARG:NH2	2.50	0.42
5:BE:115:LEU:HB3	5:BE:120:VAL:HG23	2.00	0.42
7:BG:22:LEU:HA	7:BG:25:LYS:HE2	2.01	0.42
7:BG:145:ALA:O	7:BG:146:GLU:CG	2.68	0.42
8:BH:78:VAL:HG11	8:BH:125:ILE:HD11	2.01	0.42
15:BO:32:LEU:O	15:BO:36:ILE:HG13	2.20	0.42
19:BS:10:PHE:CD2	19:BS:10:PHE:C	2.97	0.42
22:CA:933:A:H5'	22:CA:934:U:OP2	2.20	0.42
22:CA:995:C:N3	31:CK:3:THR:N	2.67	0.42
22:CA:1262:A:H2	48:C1:7:LYS:HD2	1.84	0.42
22:CA:1384:A:O2'	22:CA:1404:C:O2	2.37	0.42
22:CA:2232:C:P	45:CY:27:ARG:HH12	2.42	0.42
24:CC:76:ALA:HB2	24:CC:96:TYR:CD1	2.55	0.42
32:CL:98:ARG:C	32:CL:99:ILE:HD12	2.44	0.42
40:CT:69:LEU:HB3	40:CT:107:VAL:HG22	2.00	0.42
46:CZ:11:VAL:HG13	46:CZ:57:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DA:277:G:O2'	53:DA:278:A:OP2	2.37	0.42
53:DA:792:A:N3	53:DA:2072:C:O2'	2.43	0.42
53:DA:1132:U:H3'	53:DA:1133:A:H5''	2.02	0.42
53:DA:1532:A:H5''	53:DA:1532:A:H8	1.85	0.42
53:DA:1956:U:H2'	53:DA:1957:C:H5'	2.01	0.42
1:AA:923:A:OP1	5:AE:26:LYS:HG2	2.20	0.42
1:AA:1377:A:N3	7:AG:2:PRO:HG3	2.35	0.42
2:AB:94:HIS:O	2:AB:95:ARG:C	2.62	0.42
9:AI:19:VAL:HA	9:AI:65:ILE:HG22	2.02	0.42
9:AI:30:ILE:HA	9:AI:65:ILE:HG13	2.02	0.42
1:BA:408:A:C2	1:BA:435:A:C2	3.08	0.42
3:BC:164:ARG:NH1	3:BC:166:GLU:OE1	2.53	0.42
11:BK:31:ILE:HB	11:BK:46:THR:HG22	2.02	0.42
22:CA:435:C:H2'	22:CA:436:C:H5'	2.00	0.42
22:CA:551:G:H5'	22:CA:551:G:H8	1.84	0.42
22:CA:675:A:C6	22:CA:676:A:C6	3.08	0.42
22:CA:820:A:C6	69:CA:3772:HOH:O	2.72	0.42
22:CA:1352:U:OP2	69:CA:3353:HOH:O	2.22	0.42
22:CA:1992:G:N2	22:CA:1996:C:O2'	2.53	0.42
22:CA:2127:G:N3	22:CA:2162:G:N7	2.68	0.42
24:CC:252:THR:O	24:CC:253:LYS:C	2.62	0.42
30:CJ:99:GLY:O	30:CJ:139:VAL:HG22	2.20	0.42
42:CV:86:ARG:HH12	42:CV:100:SER:HB3	1.85	0.42
42:CV:96:PHE:CE1	42:CV:103:ILE:HG13	2.54	0.42
53:DA:2095:A:H2'	53:DA:2096:C:O4'	2.20	0.42
48:D1:41:HIS:HA	48:D1:49:TYR:OH	2.20	0.42
5:AE:107:ALA:HB2	5:AE:125:ALA:HB3	2.02	0.42
11:AK:28:ASN:O	11:AK:57:LYS:HD3	2.20	0.42
13:AM:12:HIS:HA	13:AM:45:ILE:HG13	2.02	0.42
13:AM:33:ILE:O	13:AM:37:ALA:N	2.46	0.42
1:BA:1049:U:H2'	14:BN:3:LYS:HE3	2.00	0.42
1:BA:1137:C:H1'	1:BA:1138:G:N2	2.35	0.42
3:BC:155:GLY:O	3:BC:157:LEU:N	2.53	0.42
3:BC:178:LEU:H	3:BC:178:LEU:HD22	1.85	0.42
9:BI:24:GLY:N	9:BI:61:LEU:HA	2.35	0.42
10:BJ:35:GLN:HG3	10:BJ:36:VAL:N	2.35	0.42
22:CA:335:C:O2'	22:CA:336:C:P	2.77	0.42
22:CA:335:C:H5''	42:CV:82:ARG:HD3	2.01	0.42
22:CA:1272:A:C5	22:CA:1618:6MZ:H1'	2.54	0.42
22:CA:1637:A:H5'	22:CA:1760:C:O2'	2.20	0.42
24:CC:75:PRO:HB2	24:CC:97:LYS:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:CE:1:MET:HE2	26:CE:19:PHE:HB2	2.02	0.42
26:CE:42:GLY:HA3	26:CE:90:GLN:O	2.19	0.42
49:C2:48:ILE:H	49:C2:48:ILE:HD12	1.84	0.42
53:DA:141:G:H2'	53:DA:142:A:N3	2.33	0.42
53:DA:860:U:OP1	62:DA:3187:SPD:H92	2.20	0.42
53:DA:2188:U:H2'	53:DA:2189:U:O4'	2.19	0.42
24:DC:247:PRO:HD2	24:DC:248:TRP:CE3	2.54	0.42
40:DT:1:MET:N	40:DT:109:ASP:OD1	2.49	0.42
44:DX:38:VAL:HG12	44:DX:59:LEU:HB2	2.02	0.42
1:AA:933:G:O6	7:AG:3:ARG:NH1	2.49	0.41
1:AA:1152:A:H5'	10:AJ:72:ARG:HH22	1.85	0.41
4:AD:95:GLU:OE2	4:AD:104:ARG:NH1	2.53	0.41
1:BA:1001:C:H2'	1:BA:1002:G:H8	1.84	0.41
1:BA:1213:A:O2'	1:BA:1214:C:H5''	2.19	0.41
1:BA:1317:C:C2'	14:BN:49:GLN:HE21	2.33	0.41
15:BO:46:HIS:C	15:BO:48:LYS:H	2.28	0.41
18:BR:43:ARG:HG2	18:BR:44:ILE:H	1.85	0.41
22:CA:214:G:HO2'	22:CA:216:A:HO2'	1.58	0.41
22:CA:2586:U:H2'	22:CA:2587:A:O4'	2.20	0.41
22:CA:2615:U:C2	48:C1:4:GLN:HA	2.55	0.41
31:CK:125:TYR:CE2	31:CK:130:HIS:HA	2.55	0.41
32:CL:35:VAL:HG12	32:CL:36:GLY:N	2.35	0.41
40:CT:84:ARG:HB2	40:CT:96:ILE:CD1	2.50	0.41
43:CW:24:ASN:O	43:CW:24:ASN:ND2	2.53	0.41
52:C5:17:VAL:CG1	52:C5:26:ILE:HD12	2.50	0.41
53:DA:75:G:H4'	46:DZ:48:ARG:NH2	2.35	0.41
53:DA:1175:A:N3	53:DA:1175:A:H2'	2.35	0.41
53:DA:1876:A:H2'	53:DA:1877:A:O4'	2.20	0.41
58:DA:3190:MPD:H52	58:DA:3190:MPD:C1	2.50	0.41
54:DD:186:LEU:HD21	37:DQ:4:ILE:HG21	2.01	0.41
40:DT:4:ILE:HG12	40:DT:106:VAL:HG22	2.02	0.41
46:DZ:2:LYS:O	46:DZ:3:ALA:HB3	2.20	0.41
1:AA:457:G:O6	1:AA:475:C:N4	2.45	0.41
1:AA:744:C:O2'	1:AA:851:G:N2	2.48	0.41
1:AA:1402:4OC:HM42	1:AA:1500:A:H61	1.85	0.41
7:AG:6:VAL:HG12	7:AG:7:ILE:N	2.35	0.41
10:AJ:35:GLN:HB2	10:AJ:77:VAL:HB	2.01	0.41
19:AS:63:THR:HG22	19:AS:65:GLU:H	1.84	0.41
20:AT:29:ARG:O	20:AT:33:LYS:HG3	2.20	0.41
1:BA:374:A:OP1	1:BA:452:A:N1	2.53	0.41
15:BO:45:GLU:HG2	15:BO:46:HIS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:BQ:16:LYS:O	17:BQ:17:MET:SD	2.78	0.41
18:BR:46:GLY:O	18:BR:47:THR:O	2.38	0.41
21:BU:39:GLU:HG2	21:BU:43:THR:HB	2.02	0.41
22:CA:674:G:H1'	26:CE:69:ARG:NE	2.34	0.41
22:CA:684:G:OP1	50:C3:16:HIS:ND1	2.44	0.41
22:CA:818:G:C2'	22:CA:819:A:H5''	2.51	0.41
22:CA:2445:2MG:HM21	22:CA:2449:U:O4	2.20	0.41
26:CE:83:VAL:O	26:CE:83:VAL:HG12	2.20	0.41
32:CL:92:GLU:O	32:CL:93:GLN:HB2	2.19	0.41
53:DA:523:C:H4'	53:DA:540:C:O2	2.20	0.41
53:DA:1084:A:C6	53:DA:1085:A:C6	3.08	0.41
53:DA:2114:A:OP2	53:DA:2115:G:C6	2.73	0.41
53:DA:2129:C:N4	53:DA:2130:U:O4	2.54	0.41
53:DA:2547:A:H4'	32:DL:29:HIS:NE2	2.35	0.41
24:DC:130:LEU:HD11	24:DC:135:ILE:HG13	2.02	0.41
31:DK:31:GLU:HG3	31:DK:142:ILE:HG13	2.03	0.41
50:D3:22:MET:HE2	50:D3:31:LEU:HD12	2.02	0.41
1:AA:68:G:C5	1:AA:69:G:H1'	2.55	0.41
1:AA:736:C:C5'	6:AF:88:MET:HE2	2.51	0.41
1:AA:757:U:O2'	1:AA:879:C:O2	2.34	0.41
6:AF:99:ALA:HB1	6:AF:103:VAL:HB	2.01	0.41
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	2.02	0.41
13:AM:107:ARG:NH2	13:AM:113:ARG:HB3	2.35	0.41
1:BA:532:A:N6	3:BC:193:TYR:HB3	2.36	0.41
2:BB:184:PHE:CE2	2:BB:198:PHE:CD1	3.08	0.41
5:BE:99:ALA:C	5:BE:100:SER:O	2.58	0.41
8:BH:83:LEU:C	8:BH:83:LEU:HD22	2.46	0.41
8:BH:111:MET:HB2	8:BH:115:ALA:HB3	2.02	0.41
14:BN:53:ARG:NH2	19:BS:37:ARG:NH2	2.68	0.41
19:BS:53:ASN:ND2	19:BS:56:GLN:O	2.53	0.41
22:CA:250:G:P	51:C4:13:ARG:HH12	2.41	0.41
22:CA:279:A:H61	22:CA:361:G:H1'	1.85	0.41
22:CA:2747:G:O6	22:CA:2755:C:H5''	2.20	0.41
25:CD:1:MET:HE3	25:CD:205:PRO:HG2	2.01	0.41
25:CD:104:VAL:O	25:CD:105:LYS:HB3	2.20	0.41
26:CE:7:ASP:N	26:CE:7:ASP:OD1	2.53	0.41
30:CJ:106:LEU:HD11	30:CJ:140:VAL:HG11	2.02	0.41
31:CK:80:HIS:HB3	31:CK:81:ILE:HG22	2.02	0.41
33:CM:111:ILE:CG2	33:CM:112:LEU:N	2.83	0.41
34:CN:69:PRO:O	34:CN:70:ASP:HB3	2.19	0.41
35:CO:12:ARG:O	35:CO:17:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:CQ:103:ARG:HB3	37:CQ:108:ALA:HB2	2.02	0.41
43:CW:21:ARG:HA	43:CW:25:LYS:O	2.19	0.41
53:DA:846:U:HO2'	53:DA:847:U:P	2.40	0.41
53:DA:1494:A:HO2'	53:DA:1495:A:P	2.44	0.41
53:DA:2521:C:C2	53:DA:2545:G:N2	2.88	0.41
53:DA:2886[B]:A:H3'	53:DA:2887[B]:A:C5'	2.51	0.41
24:DC:267:ILE:HD13	24:DC:270:ARG:HH11	1.85	0.41
54:DD:13:ARG:HD2	54:DD:15:PHE:CZ	2.55	0.41
27:DF:175:PHE:HD2	27:DF:177:PHE:CZ	2.38	0.41
55:DI:51:TYR:OH	55:DI:53:ARG:NH1	2.53	0.41
42:DV:51:ALA:O	42:DV:52:LEU:CB	2.68	0.41
1:AA:674:G:H3'	69:AA:1910:HOH:O	2.20	0.41
1:AA:842:U:H3'	1:AA:843:U:H4'	2.02	0.41
1:AA:982:U:H5''	14:AN:6:MET:HE2	2.01	0.41
1:AA:1417:G:C6	1:AA:1482:G:C6	3.08	0.41
14:AN:54:ASP:OD1	14:AN:59:ARG:NE	2.47	0.41
1:BA:33:A:H2'	1:BA:34:C:C6	2.55	0.41
1:BA:254:G:H4'	17:BQ:20:SER:HB2	2.01	0.41
1:BA:421:U:H3'	1:BA:421:U:H6	1.85	0.41
1:BA:451:A:H5''	69:BP:101:HOH:O	2.21	0.41
1:BA:1012:A:N1	1:BA:1018:G:O6	2.53	0.41
4:BD:105:MET:SD	4:BD:143:VAL:CG1	3.09	0.41
15:BO:40:GLN:HA	15:BO:40:GLN:NE2	2.36	0.41
22:CA:1248:G:C5	38:CR:3:ARG:HB2	2.56	0.41
22:CA:1583:A:H1'	22:CA:1585:C:N4	2.36	0.41
22:CA:1599:U:C4	22:CA:1600:C:N4	2.89	0.41
25:CD:77:ARG:NH2	25:CD:200:ASP:OD1	2.44	0.41
33:CM:95:LEU:HD22	33:CM:100:ILE:HD13	2.03	0.41
42:CV:52:LEU:HD23	42:CV:52:LEU:HA	1.92	0.41
44:CX:61:ALA:CB	44:CX:82:ILE:HD12	2.50	0.41
53:DA:275:C:H3'	53:DA:276:U:H5''	2.02	0.41
53:DA:547:A:C8	53:DA:547:A:H3'	2.54	0.41
53:DA:1794:A:H2'	53:DA:1795:C:C6	2.55	0.41
53:DA:2886[A]:A:C4	53:DA:2887[A]:A:C8	3.09	0.41
28:DG:24:ILE:HD11	28:DG:43:VAL:HG11	2.02	0.41
34:DN:92:TRP:NE1	58:DN:201:MPD:HM1	2.36	0.41
14:AN:62:ASN:HB3	14:AN:73:PHE:CD2	2.56	0.41
19:AS:40:ILE:HD11	19:AS:71:LEU:HD23	2.03	0.41
1:BA:209:U:H2'	1:BA:209:U:O2	2.20	0.41
1:BA:296:U:O2'	1:BA:556:C:O2	2.34	0.41
5:BE:156:LYS:O	5:BE:159:LYS:NZ	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BJ:57:VAL:HG13	10:BJ:58:ASN:N	2.35	0.41
12:BL:84:GLY:HA2	12:BL:95:TYR:HA	2.02	0.41
20:BT:6:SER:C	20:BT:8:LYS:H	2.28	0.41
22:CA:11:C:H2'	22:CA:12:U:H5'	2.02	0.41
22:CA:1609:A:O2'	22:CA:1610:A:H5'	2.21	0.41
29:CH:11:ASN:OD1	29:CH:11:ASN:N	2.53	0.41
36:CP:15:ARG:HA	36:CP:18:LEU:HD22	2.01	0.41
42:CV:82:ARG:HB2	42:CV:97:LYS:HG3	2.02	0.41
53:DA:141:G:C2'	53:DA:142:A:C4	3.04	0.41
53:DA:435:C:C2'	53:DA:436:C:H5'	2.50	0.41
53:DA:1153:C:OP2	69:DA:3826:HOH:O	2.20	0.41
65:DA:3202:ACY:H1	69:DA:7057:HOH:O	2.21	0.41
26:DE:87:ALA:O	26:DE:88:ARG:HD3	2.21	0.41
29:DH:133:GLN:HE21	29:DH:136:SER:HA	1.84	0.41
55:DI:96:PHE:O	55:DI:100:ALA:N	2.53	0.41
33:DM:1:MET:O	33:DM:2:ARG:HD2	2.20	0.41
36:DP:16:ARG:NH2	69:DP:314:HOH:O	2.42	0.41
49:D2:38:LYS:NZ	69:D2:102:HOH:O	2.46	0.41
49:D2:47:VAL:HG12	49:D2:48:ILE:N	2.35	0.41
1:AA:510:A:H5''	1:AA:511:C:P	2.61	0.41
11:AK:109:ASN:ND2	21:AU:5:LYS:HB3	2.36	0.41
14:AN:54:ASP:HA	14:AN:59:ARG:HD3	2.02	0.41
16:AP:75:ILE:HA	16:AP:78:VAL:HG12	2.01	0.41
1:BA:471:U:H2'	1:BA:472:U:C6	2.56	0.41
1:BA:567:G:H2'	1:BA:568:G:O4'	2.19	0.41
1:BA:977:A:C2'	1:BA:978:A:H5''	2.51	0.41
1:BA:1255:G:C6	1:BA:1279:G:C8	3.08	0.41
2:BB:113:ARG:CZ	2:BB:117:LEU:HD21	2.50	0.41
5:BE:133:PRO:HA	5:BE:136:VAL:HG12	2.02	0.41
8:BH:96:MET:HB3	8:BH:99:LEU:HB2	2.03	0.41
15:BO:82:ILE:HG13	15:BO:83:GLU:N	2.35	0.41
19:BS:58:VAL:HG11	19:BS:75:ALA:HA	2.02	0.41
22:CA:404:A:H1'	22:CA:405:U:OP2	2.21	0.41
22:CA:864:G:C6	22:CA:865:C:N4	2.89	0.41
22:CA:1434:A:H2'	22:CA:1435:G:H8	1.85	0.41
22:CA:1833:C:C4	22:CA:1834:U:C4	3.09	0.41
22:CA:2394:C:OP2	51:C4:30:ARG:HD3	2.21	0.41
25:CD:1:MET:HB3	25:CD:205:PRO:HG2	2.01	0.41
42:CV:33:LYS:HE2	42:CV:66:GLN:NE2	2.35	0.41
53:DA:1020:A:N6	69:DA:6936:HOH:O	2.48	0.41
53:DA:1869:G:N1	53:DA:1873:G:C6	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DA:2591:C:H2'	53:DA:2592:G:C8	2.55	0.41
57:DA:3217:PG4:H32	57:DA:3217:PG4:H51	1.58	0.41
27:DF:108:VAL:HG13	27:DF:111:ILE:HD12	2.03	0.41
27:DF:108:VAL:N	27:DF:109:PRO:CD	2.84	0.41
34:DN:136:MET:HE3	43:DW:57:TYR:HD1	1.85	0.41
50:D3:22:MET:HE2	50:D3:31:LEU:HD13	2.00	0.41
1:AA:579:A:O2'	15:AO:54:ARG:NH1	2.53	0.41
1:AA:597:G:C2	1:AA:644:U:C2	3.09	0.41
1:AA:1224:U:H3'	1:AA:1225:A:H5'	2.03	0.41
5:AE:57:PRO:HA	5:AE:60:ILE:CG1	2.51	0.41
9:AI:54:LEU:HD12	9:AI:54:LEU:N	2.36	0.41
1:BA:1361:G:H2'	1:BA:1362:A:C5'	2.51	0.41
2:BB:47:VAL:N	2:BB:48:PRO:HD2	2.35	0.41
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	2.03	0.41
22:CA:7:G:H4'	31:CK:15:TRP:CH2	2.56	0.41
22:CA:42:A:C2	22:CA:438:G:C2	3.09	0.41
22:CA:1914:C:C2	22:CA:1915:3TD:N1	2.89	0.41
22:CA:2251:OMG:HM23	22:CA:2251:OMG:H1'	1.59	0.41
22:CA:2445:2MG:HM23	22:CA:2446:G:H1'	2.02	0.41
24:CC:175:ARG:NH1	24:CC:181:MET:HE1	2.35	0.41
24:CC:267:ILE:N	24:CC:267:ILE:CD1	2.83	0.41
31:CK:117:ALA:HA	31:CK:120:ARG:HD2	2.02	0.41
33:CM:23:ILE:H	33:CM:23:ILE:HD12	1.86	0.41
34:CN:58:LYS:N	34:CN:58:LYS:HD3	2.35	0.41
41:CU:50:LEU:HD13	41:CU:50:LEU:N	2.36	0.41
50:C3:44:VAL:O	50:C3:45:SER:CB	2.69	0.41
53:DA:1509:A:O2'	53:DA:1510:G:P	2.79	0.41
55:DI:72:LEU:O	55:DI:73:LYS:C	2.62	0.41
1:AA:328:C:O2	1:AA:328:C:H2'	2.21	0.41
1:AA:1079:G:H5'	5:AE:134:ILE:HD13	2.03	0.41
1:AA:1149:C:OP2	9:AI:11:ARG:NH2	2.54	0.41
1:AA:1449:C:C2	1:AA:1455:G:C2	3.08	0.41
9:AI:80:ARG:O	9:AI:84:THR:HG23	2.20	0.41
11:AK:52:PHE:O	11:AK:53:ARG:HD2	2.21	0.41
19:AS:6:LYS:HD3	19:AS:6:LYS:HA	1.88	0.41
21:AU:4:ILE:HG23	21:AU:18:ARG:NH1	2.36	0.41
5:BE:50:TYR:O	5:BE:51:GLY:O	2.38	0.41
5:BE:115:LEU:CA	5:BE:120:VAL:HG23	2.50	0.41
9:BI:30:ILE:HA	9:BI:65:ILE:HG13	2.02	0.41
13:BM:103:LYS:HG2	13:BM:104:THR:HG23	2.02	0.41
22:CA:54:G:C6	22:CA:117:G:N2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CA:742:A:H2'	22:CA:743:A:C8	2.55	0.41
22:CA:2796:U:H3	22:CA:2799:A:N6	2.19	0.41
25:CD:57:ALA:O	25:CD:60:VAL:HG12	2.21	0.41
26:CE:46:GLN:CB	26:CE:83:VAL:HG11	2.51	0.41
35:CO:43:GLU:OE1	35:CO:43:GLU:HA	2.21	0.41
35:CO:116:VAL:HG12	35:CO:117:ASP:N	2.35	0.41
42:CV:16:GLY:O	42:CV:18:ASP:N	2.49	0.41
53:DA:102:U:O2	53:DA:102:U:H2'	2.20	0.41
53:DA:1178:C:C2'	53:DA:1179:G:H5'	2.51	0.41
53:DA:1416:G:HO2'	53:DA:1417:C:P	2.43	0.41
53:DA:1417:C:H2'	53:DA:1418:G:O4'	2.20	0.41
53:DA:2015:A:H1'	61:DA:3227:PEG:H42	2.03	0.41
53:DA:2162:G:OP1	53:DA:2171:A:H2'	2.20	0.41
54:DD:62:LYS:N	54:DD:63:PRO:CD	2.83	0.41
27:DF:38:MET:HE3	27:DF:152:LEU:HD12	2.02	0.41
29:DH:130:VAL:HG21	29:DH:144:VAL:HG21	2.02	0.41
43:DW:2:PHE:CD1	43:DW:50:MET:HE3	2.56	0.41
1:AA:108:G:C5'	1:AA:108:G:N3	2.84	0.41
1:AA:864:A:H4'	5:AE:90:THR:HG23	2.03	0.41
1:AA:1095:U:H2'	1:AA:1096:C:C6	2.56	0.41
1:AA:1312:G:H5'	19:AS:6:LYS:CE	2.51	0.41
5:AE:162:GLU:HG2	8:AH:114:ARG:NH2	2.36	0.41
7:AG:131:LYS:HA	7:AG:135:VAL:HG21	2.02	0.41
9:AI:50:GLN:C	9:AI:52:LEU:N	2.79	0.41
13:AM:6:GLY:HA2	13:AM:66:GLU:HG3	2.01	0.41
16:AP:44:SER:C	16:AP:46:LYS:H	2.29	0.41
16:AP:48:GLU:HG2	16:AP:49:GLY:H	1.85	0.41
19:AS:12:ASP:OD1	19:AS:37:ARG:NH2	2.54	0.41
19:AS:31:LEU:HD12	19:AS:31:LEU:N	2.36	0.41
1:BA:205:A:C2	1:BA:206:C:C5	3.08	0.41
1:BA:211:G:N2	1:BA:212:G:H1'	2.36	0.41
1:BA:502:A:OP1	12:BL:115:SER:HB3	2.21	0.41
1:BA:826:C:O2	8:BH:16:ASN:ND2	2.54	0.41
1:BA:951:G:N3	1:BA:970:C:O2'	2.50	0.41
1:BA:1062:U:H2'	1:BA:1063:C:C6	2.56	0.41
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.51	0.41
5:BE:13:GLU:CB	5:BE:39:VAL:HG12	2.51	0.41
6:BF:29:ILE:HG23	6:BF:66:ALA:HB2	2.03	0.41
6:BF:53:LYS:HA	6:BF:53:LYS:HZ2	1.86	0.41
7:BG:65:ALA:HA	7:BG:128:ALA:HA	2.03	0.41
10:BJ:18:ILE:HD12	10:BJ:70:HIS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BJ:87:LEU:HD13	10:BJ:88:MET:N	2.35	0.41
12:BL:76:GLU:O	12:BL:77:HIS:HB2	2.21	0.41
12:BL:110:ARG:HB2	12:BL:119:VAL:HG21	2.03	0.41
14:BN:23:LYS:N	14:BN:26:GLU:CD	2.74	0.41
15:BO:3:LEU:HD13	15:BO:35:GLN:HE21	1.86	0.41
15:BO:17:ARG:HD3	15:BO:17:ARG:H	1.83	0.41
15:BO:46:HIS:O	15:BO:48:LYS:N	2.48	0.41
15:BO:87:LEU:O	15:BO:88:ARG:CB	2.69	0.41
17:BQ:6:ARG:CZ	17:BQ:6:ARG:HB3	2.51	0.41
22:CA:464:U:C6	22:CA:788:A:C2	3.09	0.41
22:CA:676:A:H2	22:CA:2069:G7M:N3	2.19	0.41
22:CA:1187:G:H5''	39:CS:83:TYR:CE2	2.56	0.41
22:CA:1379:U:H4'	22:CA:1380:G:OP1	2.21	0.41
22:CA:1693:U:O2'	24:CC:14:ARG:NH2	2.54	0.41
22:CA:1847:A:O2'	22:CA:1848:A:H8	2.03	0.41
22:CA:2032:G:C2	25:CD:150:GLN:HG2	2.56	0.41
22:CA:2053:G:N2	22:CA:2054:A:H1'	2.36	0.41
22:CA:2061:G:H5''	22:CA:2503:2MA:CM2	2.50	0.41
22:CA:2271:G:H5''	44:CX:20:ARG:HE	1.86	0.41
22:CA:2360:G:O4'	33:CM:60:ARG:NH2	2.50	0.41
22:CA:2396:G:C2	22:CA:2421:G:C2	3.09	0.41
22:CA:2550:G:C6	22:CA:2551:C:N4	2.89	0.41
22:CA:2650:U:O2'	22:CA:2651:C:H5'	2.21	0.41
26:CE:108:ILE:HG13	26:CE:109:LEU:N	2.36	0.41
27:CF:36:LEU:N	27:CF:36:LEU:HD13	2.35	0.41
28:CG:175:LYS:HG2	28:CG:176:LYS:H	1.85	0.41
31:CK:41:LYS:NZ	31:CK:50:THR:O	2.50	0.41
32:CL:109:SER:C	32:CL:111:LYS:H	2.29	0.41
32:CL:113:MET:SD	32:CL:116:ILE:HD11	2.61	0.41
53:DA:118:A:C8	53:DA:119:A:C8	3.09	0.41
53:DA:355:U:H2'	53:DA:356:G:C8	2.56	0.41
53:DA:722:A:H2'	53:DA:723:C:O4'	2.20	0.41
53:DA:1077:A:H4'	30:DJ:94:ASN:HB2	2.03	0.41
53:DA:1607:C:OP1	69:DA:5123:HOH:O	2.22	0.41
55:DI:132:TYR:CD2	55:DI:132:TYR:C	2.98	0.41
58:DN:201:MPD:O4	58:DN:201:MPD:CM	2.69	0.41
49:D2:10:LYS:HE3	49:D2:53:LYS:O	2.21	0.41
1:AA:4:U:C2'	1:AA:5:U:OP2	2.69	0.41
1:AA:263:A:P	20:AT:74:ARG:HH11	2.43	0.41
2:AB:23:TRP:HB3	2:AB:39:HIS:CD2	2.56	0.41
3:AC:85:GLU:HB2	3:AC:88:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AF:9:MET:HE1	18:AR:65:LEU:HA	2.03	0.41
15:AO:87:LEU:O	15:AO:88:ARG:CB	2.68	0.41
1:BA:106:C:O2	1:BA:379:C:H4'	2.21	0.41
1:BA:1513:A:H2'	1:BA:1514:G:C8	2.56	0.41
2:BB:138:THR:O	2:BB:142:GLU:N	2.44	0.41
5:BE:39:VAL:HG22	5:BE:67:ALA:HB1	2.02	0.41
7:BG:131:LYS:O	7:BG:131:LYS:HG3	2.19	0.41
9:BI:54:LEU:HD12	9:BI:54:LEU:N	2.36	0.41
22:CA:981:A:N1	22:CA:2027:G:O2'	2.47	0.41
22:CA:1223:G:P	39:CS:68:ARG:HH12	2.43	0.41
22:CA:1248:G:C4	38:CR:3:ARG:HD2	2.56	0.41
22:CA:2011:U:H2'	22:CA:2012:G:O4'	2.21	0.41
22:CA:2547:A:C2	22:CA:2562:U:C2	3.09	0.41
26:CE:131:THR:HB	26:CE:164:LEU:HD22	2.02	0.41
30:CJ:20:PRO:HB2	30:CJ:23:PRO:HD2	2.03	0.41
30:CJ:113:LYS:O	30:CJ:117:MET:HG2	2.21	0.41
38:CR:76:TYR:CZ	38:CR:80:ILE:HG13	2.56	0.41
53:DA:374:A:H2'	53:DA:375:G:H5'	2.03	0.41
33:DM:48:ARG:HD2	51:D4:60:ALA:O	2.20	0.41
33:DM:78:ARG:HG2	33:DM:113:ALA:HB3	2.03	0.41
1:AA:108:G:N3	1:AA:108:G:H5'	2.36	0.40
1:AA:501:C:H2'	1:AA:502:A:C8	2.55	0.40
1:AA:827:U:H5''	1:AA:828:U:OP2	2.21	0.40
8:AH:18:GLN:HG3	8:AH:70:ALA:CB	2.52	0.40
9:AI:30:ILE:HB	9:AI:65:ILE:HD11	2.03	0.40
1:BA:75:G:C6	1:BA:76:G:C5	3.09	0.40
1:BA:1004:A:C6	1:BA:1005:A:C6	3.09	0.40
1:BA:1053:G:P	1:BA:1054:C:H3'	2.61	0.40
1:BA:1218:C:H2'	1:BA:1219:A:C8	2.55	0.40
2:BB:108:ARG:HA	2:BB:111:ILE:HG12	2.03	0.40
2:BB:118:GLU:OE2	2:BB:152:LYS:NZ	2.37	0.40
6:BF:92:THR:HG22	6:BF:93:LYS:N	2.35	0.40
8:BH:89:LYS:HA	8:BH:92:LEU:HG	2.03	0.40
9:BI:95:ARG:O	9:BI:98:LEU:N	2.54	0.40
10:BJ:27:GLU:HA	10:BJ:30:LYS:HE2	2.03	0.40
13:BM:13:LYS:O	13:BM:14:HIS:ND1	2.55	0.40
14:BN:21:PHE:HB2	14:BN:55:SER:O	2.21	0.40
17:BQ:58:VAL:HB	17:BQ:79:VAL:O	2.21	0.40
20:BT:61:GLN:HA	20:BT:61:GLN:OE1	2.21	0.40
22:CA:565:C:H2'	22:CA:566:U:O4'	2.21	0.40
22:CA:1857:G:O2'	22:CA:1884:G:N2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CA:2796:U:H3	22:CA:2799:A:H61	1.68	0.40
24:CC:29:PRO:HG2	24:CC:34:LEU:HD11	2.03	0.40
25:CD:2:ILE:HD13	25:CD:90:PHE:CZ	2.56	0.40
28:CG:93:GLY:HA2	28:CG:95:ARG:HH12	1.86	0.40
53:DA:1182:G:H2'	53:DA:1183:U:O4'	2.22	0.40
53:DA:1445:G:N2	53:DA:1547:C:C2	2.89	0.40
53:DA:2389:G:H5''	53:DA:2390:U:O4'	2.21	0.40
66:DA:3210:EDO:O1	57:DR:202:PG4:C3	2.69	0.40
23:DB:90:C:H5'	34:DN:18[A]:ARG:HG2	2.02	0.40
33:DM:89:VAL:O	33:DM:94:THR:HG21	2.20	0.40
1:AA:841:C:C6	1:AA:843:U:H5'	2.55	0.40
1:BA:148:G:N3	1:BA:1446:A:H2	2.19	0.40
1:BA:328:C:H2'	1:BA:328:C:O2	2.21	0.40
1:BA:450:G:P	69:BA:1918:HOH:O	2.77	0.40
1:BA:806:C:O4'	57:BA:1642:PG4:H72	2.21	0.40
2:BB:188:ASP:HB2	2:BB:204:ASP:CG	2.46	0.40
17:BQ:8:LEU:HD13	17:BQ:73:TRP:CZ3	2.56	0.40
22:CA:541:A:C2	22:CA:553:G:C2	3.09	0.40
22:CA:1468:U:H2'	22:CA:1522:A:N6	2.36	0.40
24:CC:132:MET:CE	24:CC:172:VAL:HG21	2.51	0.40
30:CJ:101:ILE:O	30:CJ:141:GLU:N	2.54	0.40
33:CM:82:LEU:HG	33:CM:120:VAL:HG21	2.03	0.40
36:CP:35:ILE:HG21	36:CP:71:ALA:HA	2.03	0.40
53:DA:2650:U:O2'	53:DA:2651:C:H5'	2.21	0.40
62:DA:3183:SPD:H42	69:DA:6984:HOH:O	2.20	0.40
26:DE:21:ARG:HD3	26:DE:106:LYS:HB3	2.03	0.40
1:AA:579:A:H5'	1:AA:728:A:H1'	2.02	0.40
1:AA:983:A:H5''	1:AA:984:C:OP2	2.21	0.40
1:AA:1053:G:H5''	1:AA:1055:A:OP1	2.21	0.40
1:AA:1239:A:H62	1:AA:1299:A:N6	2.19	0.40
9:AI:83:ILE:HG22	9:AI:87:LEU:HD13	2.04	0.40
1:BA:1081:A:H5'	5:BE:23:LYS:HG3	2.03	0.40
1:BA:1402:4OC:O2	1:BA:1402:4OC:H2'	2.22	0.40
6:BF:45:ARG:O	6:BF:56:LYS:HA	2.21	0.40
18:BR:23:TYR:HA	18:BR:58:ALA:HB1	2.03	0.40
22:CA:310:A:H5''	42:CV:15:THR:HG22	2.03	0.40
22:CA:1170:C:C2	22:CA:1171:G:N7	2.89	0.40
22:CA:1190:G:OP1	33:CM:32:GLY:HA2	2.21	0.40
25:CD:104:VAL:CG2	25:CD:105:LYS:N	2.84	0.40
25:CD:149:ASN:CG	25:CD:150:GLN:H	2.29	0.40
26:CE:31:VAL:HG21	26:CE:104:ALA:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CH:145:ASN:HB3	29:CH:147:VAL:HG23	2.03	0.40
31:CK:11:VAL:HG11	31:CK:50:THR:HA	2.03	0.40
34:CN:20:LEU:HD22	34:CN:20:LEU:N	2.35	0.40
38:CR:36:PHE:CE1	38:CR:40:ILE:HD11	2.56	0.40
48:C1:25:VAL:HG13	48:C1:26:THR:H	1.86	0.40
53:DA:634:C:H2'	53:DA:635:C:C6	2.56	0.40
53:DA:725:G:C6	53:DA:726:G:N1	2.90	0.40
53:DA:2534:A:C2'	53:DA:2535:G:O5'	2.70	0.40
24:DC:121:ASP:OD1	24:DC:121:ASP:N	2.55	0.40
27:DF:36:LEU:HD22	27:DF:154:ILE:HD13	2.03	0.40
55:DI:38:MET:O	55:DI:41:LEU:N	2.53	0.40
1:AA:7:A:H3'	5:AE:106:ILE:HD13	2.02	0.40
10:AJ:18:ILE:CG2	10:AJ:19:ASP:N	2.84	0.40
1:BA:158:G:H2'	1:BA:159:G:H5''	2.03	0.40
1:BA:736:C:OP1	18:BR:61:ARG:HD2	2.21	0.40
5:BE:81:LEU:CD1	5:BE:81:LEU:N	2.84	0.40
7:BG:91:VAL:O	7:BG:96:ARG:NH2	2.55	0.40
9:BI:83:ILE:O	9:BI:87:LEU:HD13	2.22	0.40
9:BI:124:ARG:HG3	9:BI:125:PRO:HD2	2.02	0.40
11:BK:36:ASP:CG	11:BK:38:GLN:HG2	2.46	0.40
15:BO:10:LYS:O	15:BO:14:GLU:HG3	2.21	0.40
19:BS:13:LEU:HD22	19:BS:16:LEU:HD23	2.03	0.40
22:CA:662:G:O2'	33:CM:14:LYS:HD3	2.22	0.40
22:CA:1651:G:H4'	35:CO:39:PRO:HG2	2.03	0.40
22:CA:1914:C:H2'	22:CA:1915:3TD:H5'A	2.02	0.40
22:CA:2365:G:H4'	44:CX:60:PHE:CE2	2.57	0.40
25:CD:19:GLY:O	32:CL:73:ASP:HB3	2.22	0.40
38:CR:9:ILE:C	38:CR:9:ILE:CD1	2.94	0.40
44:CX:34:GLY:N	44:CX:61:ALA:O	2.42	0.40
53:DA:839:U:H1'	53:DA:1191:G:H1'	2.03	0.40
61:DA:3200:PEG:H11	61:DA:3200:PEG:H32	1.70	0.40
54:DD:1:MET:HE2	54:DD:100:LEU:HD12	2.04	0.40
54:DD:18:ASP:HA	57:DQ:202:PG4:H42	2.02	0.40
32:DL:38:ILE:HD11	32:DL:112:PHE:HZ	1.86	0.40
35:DO:33:ILE:HD11	48:D1:55:ILE:CD1	2.51	0.40
45:DY:43:GLU:O	45:DY:44:LYS:C	2.63	0.40
1:AA:182:A:N1	1:AA:223:A:O2'	2.53	0.40
1:AA:234:C:H4'	17:AQ:66:PRO:HG3	2.03	0.40
1:AA:662:U:H2'	1:AA:663:A:C8	2.56	0.40
1:AA:977:A:H2'	1:AA:978:A:H5''	2.04	0.40
1:AA:1449:C:H2'	1:AA:1450:U:H5'	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:138:THR:O	2:AB:142:GLU:N	2.42	0.40
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	2.03	0.40
9:AI:57:MET:HG3	9:AI:61:LEU:H	1.85	0.40
9:AI:83:ILE:O	9:AI:86:ALA:N	2.55	0.40
14:AN:26:GLU:O	14:AN:30:ILE:HG13	2.22	0.40
1:BA:111:G:O6	1:BA:330:C:N4	2.55	0.40
1:BA:283:U:C4	1:BA:284:C:C4	3.09	0.40
1:BA:706:A:H1'	11:BK:31:ILE:HD11	2.04	0.40
1:BA:1111:A:O5'	1:BA:1111:A:H8	2.04	0.40
1:BA:1492:A:C5	1:BA:1493:A:C2	3.10	0.40
3:BC:11:ARG:HH21	3:BC:182:ILE:HG13	1.87	0.40
9:BI:52:LEU:CD1	9:BI:57:MET:HE2	2.51	0.40
10:BJ:28:THR:HG23	10:BJ:31:ARG:NH2	2.36	0.40
15:BO:67:LEU:CD2	15:BO:88:ARG:HH22	2.35	0.40
22:CA:523:C:H4'	22:CA:540:C:O2	2.21	0.40
22:CA:2680:U:H2'	22:CA:2681:C:C6	2.56	0.40
22:CA:2873:A:H4'	69:CA:3662:HOH:O	2.22	0.40
27:CF:21:ASN:O	27:CF:21:ASN:ND2	2.47	0.40
33:CM:111:ILE:C	33:CM:131:ALA:HB2	2.47	0.40
35:CO:17:ARG:O	35:CO:21:PHE:HD1	2.04	0.40
43:CW:9:ARG:NH2	43:CW:17:SER:OG	2.55	0.40
49:C2:50:LYS:O	49:C2:51:GLU:HB3	2.22	0.40
53:DA:362:A:H3'	53:DA:363:G:H8	1.86	0.40
53:DA:905:A:C6	53:DA:906:U:C5	3.09	0.40
53:DA:1167:C:H2'	53:DA:1168:G:H5''	2.04	0.40
53:DA:2851:A:H2'	53:DA:2852:G:O4'	2.22	0.40
27:DF:158:THR:HG22	27:DF:160:ALA:N	2.34	0.40
29:DH:86:ASP:C	29:DH:88:GLY:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	209 (94%)	11 (5%)	2 (1%)	14	10
2	BB	222/224 (99%)	209 (94%)	11 (5%)	2 (1%)	14	10
3	AC	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	24	22
3	BC	204/206 (99%)	186 (91%)	10 (5%)	8 (4%)	2	0
4	AD	203/205 (99%)	199 (98%)	4 (2%)	0	100	100
4	BD	203/205 (99%)	199 (98%)	4 (2%)	0	100	100
5	AE	153/155 (99%)	145 (95%)	8 (5%)	0	100	100
5	BE	148/155 (96%)	122 (82%)	14 (10%)	12 (8%)	1	0
6	AF	104/106 (98%)	96 (92%)	8 (8%)	0	100	100
6	BF	98/106 (92%)	83 (85%)	12 (12%)	3 (3%)	3	1
7	AG	149/151 (99%)	138 (93%)	10 (7%)	1 (1%)	18	15
7	BG	149/151 (99%)	131 (88%)	15 (10%)	3 (2%)	6	2
8	AH	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
8	BH	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	16	12
9	AI	125/127 (98%)	111 (89%)	13 (10%)	1 (1%)	16	12
9	BI	125/127 (98%)	111 (89%)	13 (10%)	1 (1%)	16	12
10	AJ	97/99 (98%)	88 (91%)	8 (8%)	1 (1%)	12	9
10	BJ	96/99 (97%)	63 (66%)	22 (23%)	11 (12%)	0	0
11	AK	115/117 (98%)	104 (90%)	11 (10%)	0	100	100
11	BK	115/117 (98%)	100 (87%)	11 (10%)	4 (4%)	3	1
12	AL	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
12	BL	120/123 (98%)	110 (92%)	8 (7%)	2 (2%)	7	3
13	AM	112/114 (98%)	101 (90%)	8 (7%)	3 (3%)	4	1
13	BM	112/114 (98%)	95 (85%)	10 (9%)	7 (6%)	1	0
14	AN	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
14	BN	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
15	AO	86/88 (98%)	80 (93%)	3 (4%)	3 (4%)	3	1
15	BO	86/88 (98%)	79 (92%)	2 (2%)	5 (6%)	1	0
16	AP	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	9	6
16	BP	80/82 (98%)	66 (82%)	11 (14%)	3 (4%)	2	1
17	AQ	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
17	BQ	78/80 (98%)	64 (82%)	10 (13%)	4 (5%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	53/55 (96%)	51 (96%)	1 (2%)	1 (2%)	6	3
18	BR	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	6	3
19	AS	77/79 (98%)	69 (90%)	7 (9%)	1 (1%)	9	6
19	BS	77/79 (98%)	65 (84%)	9 (12%)	3 (4%)	2	0
20	AT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
20	BT	83/86 (96%)	77 (93%)	3 (4%)	3 (4%)	2	1
21	AU	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
21	BU	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
24	CC	269/271 (99%)	251 (93%)	15 (6%)	3 (1%)	11	8
24	DC	269/271 (99%)	253 (94%)	15 (6%)	1 (0%)	30	28
25	CD	207/209 (99%)	193 (93%)	11 (5%)	3 (1%)	9	5
26	CE	199/201 (99%)	186 (94%)	9 (4%)	4 (2%)	6	2
26	DE	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
27	CF	175/177 (99%)	155 (89%)	14 (8%)	6 (3%)	3	1
27	DF	175/177 (99%)	165 (94%)	10 (6%)	0	100	100
28	CG	174/176 (99%)	135 (78%)	33 (19%)	6 (3%)	3	1
28	DG	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
29	CH	147/149 (99%)	116 (79%)	22 (15%)	9 (6%)	1	0
29	DH	147/149 (99%)	129 (88%)	16 (11%)	2 (1%)	9	5
30	CJ	132/134 (98%)	117 (89%)	11 (8%)	4 (3%)	3	1
30	DJ	132/134 (98%)	117 (89%)	11 (8%)	4 (3%)	3	1
31	CK	140/142 (99%)	127 (91%)	11 (8%)	2 (1%)	9	5
31	DK	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
32	CL	120/123 (98%)	112 (93%)	7 (6%)	1 (1%)	16	12
32	DL	121/123 (98%)	116 (96%)	4 (3%)	1 (1%)	16	12
33	CM	142/144 (99%)	128 (90%)	8 (6%)	6 (4%)	2	0
33	DM	142/144 (99%)	138 (97%)	3 (2%)	1 (1%)	18	15
34	CN	133/136 (98%)	125 (94%)	7 (5%)	1 (1%)	16	12
34	DN	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
35	CO	118/125 (94%)	110 (93%)	5 (4%)	3 (2%)	4	1
35	DO	123/125 (98%)	116 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	CP	114/117 (97%)	105 (92%)	4 (4%)	5 (4%)	2	0
36	DP	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
37	CQ	112/114 (98%)	104 (93%)	7 (6%)	1 (1%)	14	10
37	DQ	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
38	CR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
38	DR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
39	CS	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	3	1
39	DS	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
40	CT	108/110 (98%)	101 (94%)	4 (4%)	3 (3%)	4	1
40	DT	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
41	CU	91/93 (98%)	81 (89%)	7 (8%)	3 (3%)	3	1
41	DU	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	11	8
42	CV	100/102 (98%)	81 (81%)	11 (11%)	8 (8%)	1	0
42	DV	100/102 (98%)	96 (96%)	3 (3%)	1 (1%)	12	9
43	CW	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
43	DW	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
44	CX	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
44	DX	75/76 (99%)	74 (99%)	1 (1%)	0	100	100
45	CY	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
45	DY	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
46	CZ	60/62 (97%)	52 (87%)	5 (8%)	3 (5%)	1	0
46	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
47	C0	56/58 (97%)	51 (91%)	4 (7%)	1 (2%)	6	3
47	D0	57/58 (98%)	54 (95%)	2 (4%)	1 (2%)	6	3
48	C1	54/56 (96%)	48 (89%)	4 (7%)	2 (4%)	2	1
48	D1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
49	C2	48/51 (94%)	41 (85%)	6 (12%)	1 (2%)	5	2
49	D2	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
50	C3	44/46 (96%)	40 (91%)	2 (4%)	2 (4%)	2	0
50	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
51	C4	62/64 (97%)	59 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	D4	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
52	C5	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
52	D5	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
54	DD	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
55	DI	133/135 (98%)	107 (80%)	19 (14%)	7 (5%)	1	0
All	All	11407/11629 (98%)	10507 (92%)	713 (6%)	187 (2%)	7	4

All (187) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	130	THR
3	AC	127	ARG
9	AI	25	ASN
10	AJ	57	VAL
13	AM	5	ALA
2	BB	130	THR
3	BC	66	VAL
3	BC	127	ARG
3	BC	139	GLN
3	BC	140	ASN
5	BE	24	THR
5	BE	45	ARG
5	BE	51	GLY
5	BE	102	GLY
5	BE	103	THR
5	BE	123	VAL
6	BF	53	LYS
6	BF	98	GLU
9	BI	25	ASN
10	BJ	93	ALA
11	BK	52	PHE
12	BL	44	LYS
13	BM	5	ALA
13	BM	14	HIS
16	BP	43	ALA
16	BP	79	ASN
16	BP	80	LYS
17	BQ	17	MET
18	BR	47	THR
19	BS	5	LEU

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Mol	Chain	Res	Type
25	CD	152	PRO
26	CE	42	GLY
26	CE	153	LEU
27	CF	62	GLY
27	CF	123	ASP
28	CG	119	ALA
29	CH	3	VAL
29	CH	9	VAL
29	CH	10	ALA
29	CH	137	GLU
30	CJ	15	ALA
30	CJ	19	ASN
31	CK	81	ILE
33	CM	82	LEU
33	CM	86	GLU
33	CM	111	ILE
35	CO	70	THR
36	CP	59	ALA
37	CQ	114	LEU
40	CT	65	ASP
41	CU	17	SER
42	CV	7	ARG
46	CZ	3	ALA
48	C1	56	ALA
50	C3	44	VAL
55	DI	67	THR
55	DI	104	ALA
55	DI	106	PHE
30	DJ	15	ALA
30	DJ	19	ASN
42	DV	52	LEU
13	AM	13	LYS
15	AO	88	ARG
3	BC	81	GLY
3	BC	141	ALA
3	BC	156	ARG
5	BE	111	MET
5	BE	155	ALA
5	BE	157	ARG
6	BF	52	ASN
7	BG	146	GLU
8	BH	89	LYS

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Mol	Chain	Res	Type
10	BJ	17	LEU
10	BJ	41	PRO
10	BJ	57	VAL
10	BJ	89	ARG
10	BJ	90	LEU
11	BK	89	PRO
11	BK	93	ARG
13	BM	4	ILE
13	BM	67	GLY
15	BO	88	ARG
17	BQ	70	THR
19	BS	6	LYS
20	BT	68	HIS
24	CC	253	LYS
25	CD	104	VAL
26	CE	82	GLY
27	CF	121	SER
27	CF	149	VAL
28	CG	92	VAL
28	CG	175	LYS
29	CH	16	GLY
30	CJ	25	GLY
31	CK	25	LEU
32	CL	35	VAL
33	CM	30	THR
35	CO	119	SER
36	CP	101	GLY
39	CS	29	THR
40	CT	62	ASP
40	CT	63	GLY
41	CU	18	GLU
41	CU	38	ALA
42	CV	19	LYS
42	CV	52	LEU
42	CV	75	ALA
42	CV	99	ASN
50	C3	45	SER
24	DC	253	LYS
29	DH	118	PRO
55	DI	108	VAL
30	DJ	25	GLY
32	DL	108	ARG

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Mol	Chain	Res	Type
2	AB	126	PHE
16	AP	48	GLU
18	AR	73	ARG
5	BE	138	ARG
10	BJ	43	PRO
10	BJ	95	GLY
11	BK	92	GLY
13	BM	114	LYS
15	BO	18	ASP
15	BO	46	HIS
15	BO	47	LYS
25	CD	86	GLU
28	CG	118	PRO
29	CH	2	GLN
29	CH	118	PRO
30	CJ	23	PRO
33	CM	29	LYS
33	CM	115	GLU
34	CN	69	PRO
36	CP	57	ALA
36	CP	66	GLY
39	CS	53	PHE
42	CV	55	PRO
42	CV	98	SER
46	CZ	37	LEU
47	C0	4	THR
55	DI	124	ASP
30	DJ	23	PRO
47	D0	4	THR
7	AG	80	VAL
15	AO	18	ASP
15	AO	21	ASP
2	BB	126	PHE
3	BC	80	LYS
10	BJ	36	VAL
10	BJ	101	SER
27	CF	174	ASP
27	CF	175	PHE
29	CH	33	GLN
35	CO	118	ARG
36	CP	100	HIS
48	C1	55	ILE

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Mol	Chain	Res	Type
55	DI	130	PRO
13	AM	105	ASN
5	BE	12	GLN
7	BG	80	VAL
7	BG	82	GLY
15	BO	21	ASP
17	BQ	18	GLU
28	CG	59	ALA
29	CH	31	VAL
49	C2	16	GLY
55	DI	68	PRO
33	DM	29	LYS
19	AS	29	LYS
10	BJ	34	ALA
13	BM	13	LYS
17	BQ	82	ALA
20	BT	4	ILE
20	BT	5	LYS
24	CC	261	LYS
42	CV	56	GLY
29	DH	122	LEU
19	BS	29	LYS
28	CG	28	GLY
24	CC	3	VAL
12	BL	45	PRO
13	BM	7	ILE
39	CS	50	GLY
46	CZ	46	VAL
5	BE	137	VAL
26	CE	83	VAL
41	DU	90	GLY

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/186 (100%)	181 (97%)	5 (3%)	39	45
2	BB	186/186 (100%)	179 (96%)	7 (4%)	29	32
3	AC	170/170 (100%)	160 (94%)	10 (6%)	18	16
3	BC	170/170 (100%)	140 (82%)	30 (18%)	2	1
4	AD	172/172 (100%)	165 (96%)	7 (4%)	27	29
4	BD	172/172 (100%)	167 (97%)	5 (3%)	37	42
5	AE	118/118 (100%)	108 (92%)	10 (8%)	10	7
5	BE	113/118 (96%)	88 (78%)	25 (22%)	1	0
6	AF	92/92 (100%)	88 (96%)	4 (4%)	26	27
6	BF	87/92 (95%)	71 (82%)	16 (18%)	1	1
7	AG	124/124 (100%)	118 (95%)	6 (5%)	23	23
7	BG	124/124 (100%)	99 (80%)	25 (20%)	1	0
8	AH	104/104 (100%)	101 (97%)	3 (3%)	37	42
8	BH	104/104 (100%)	86 (83%)	18 (17%)	2	1
9	AI	105/105 (100%)	102 (97%)	3 (3%)	37	42
9	BI	105/105 (100%)	102 (97%)	3 (3%)	37	42
10	AJ	87/87 (100%)	80 (92%)	7 (8%)	11	8
10	BJ	86/87 (99%)	64 (74%)	22 (26%)	0	0
11	AK	90/90 (100%)	87 (97%)	3 (3%)	33	37
11	BK	90/90 (100%)	79 (88%)	11 (12%)	5	2
12	AL	102/102 (100%)	97 (95%)	5 (5%)	22	22
12	BL	102/102 (100%)	85 (83%)	17 (17%)	2	1
13	AM	92/92 (100%)	88 (96%)	4 (4%)	26	27
13	BM	92/92 (100%)	78 (85%)	14 (15%)	3	1
14	AN	83/83 (100%)	83 (100%)	0	100	100
14	BN	83/83 (100%)	81 (98%)	2 (2%)	43	49
15	AO	76/76 (100%)	73 (96%)	3 (4%)	28	31
15	BO	76/76 (100%)	63 (83%)	13 (17%)	2	1
16	AP	65/65 (100%)	62 (95%)	3 (5%)	24	25
16	BP	65/65 (100%)	54 (83%)	11 (17%)	2	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AQ	74/74 (100%)	70 (95%)	4 (5%)	20	18
17	BQ	74/74 (100%)	55 (74%)	19 (26%)	0	0
18	AR	48/48 (100%)	48 (100%)	0	100	100
18	BR	48/48 (100%)	44 (92%)	4 (8%)	10	8
19	AS	70/70 (100%)	69 (99%)	1 (1%)	59	67
19	BS	70/70 (100%)	59 (84%)	11 (16%)	2	1
20	AT	65/65 (100%)	63 (97%)	2 (3%)	35	39
20	BT	65/65 (100%)	50 (77%)	15 (23%)	1	0
21	AU	48/48 (100%)	46 (96%)	2 (4%)	26	28
21	BU	48/48 (100%)	43 (90%)	5 (10%)	7	4
24	CC	216/216 (100%)	190 (88%)	26 (12%)	5	3
24	DC	216/216 (100%)	210 (97%)	6 (3%)	38	43
25	CD	164/164 (100%)	150 (92%)	14 (8%)	10	7
26	CE	165/165 (100%)	144 (87%)	21 (13%)	4	2
26	DE	165/165 (100%)	164 (99%)	1 (1%)	78	86
27	CF	148/148 (100%)	127 (86%)	21 (14%)	3	1
27	DF	148/148 (100%)	141 (95%)	7 (5%)	23	24
28	CG	137/137 (100%)	112 (82%)	25 (18%)	2	1
28	DG	137/137 (100%)	128 (93%)	9 (7%)	15	13
29	CH	114/114 (100%)	89 (78%)	25 (22%)	1	0
29	DH	114/114 (100%)	101 (89%)	13 (11%)	5	3
30	CJ	104/104 (100%)	99 (95%)	5 (5%)	23	23
30	DJ	104/104 (100%)	98 (94%)	6 (6%)	18	16
31	CK	116/116 (100%)	104 (90%)	12 (10%)	7	4
31	DK	116/116 (100%)	112 (97%)	4 (3%)	32	35
32	CL	103/104 (99%)	95 (92%)	8 (8%)	11	9
32	DL	104/104 (100%)	101 (97%)	3 (3%)	37	42
33	CM	103/103 (100%)	96 (93%)	7 (7%)	14	12
33	DM	103/103 (100%)	100 (97%)	3 (3%)	37	42
34	CN	108/108 (100%)	94 (87%)	14 (13%)	4	2
34	DN	109/108 (101%)	103 (94%)	6 (6%)	19	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	CO	100/102 (98%)	86 (86%)	14 (14%)	3	2
35	DO	102/102 (100%)	98 (96%)	4 (4%)	28	31
36	CP	86/87 (99%)	74 (86%)	12 (14%)	3	2
36	DP	87/87 (100%)	85 (98%)	2 (2%)	44	51
37	CQ	99/99 (100%)	88 (89%)	11 (11%)	6	3
37	DQ	99/99 (100%)	94 (95%)	5 (5%)	21	21
38	CR	89/89 (100%)	82 (92%)	7 (8%)	11	9
38	DR	89/89 (100%)	87 (98%)	2 (2%)	45	53
39	CS	84/84 (100%)	74 (88%)	10 (12%)	5	3
39	DS	84/84 (100%)	79 (94%)	5 (6%)	17	15
40	CT	93/93 (100%)	79 (85%)	14 (15%)	3	1
40	DT	93/93 (100%)	91 (98%)	2 (2%)	45	53
41	CU	80/80 (100%)	66 (82%)	14 (18%)	2	1
41	DU	80/80 (100%)	76 (95%)	4 (5%)	22	22
42	CV	83/83 (100%)	70 (84%)	13 (16%)	2	1
42	DV	83/83 (100%)	78 (94%)	5 (6%)	17	15
43	CW	78/78 (100%)	65 (83%)	13 (17%)	2	1
43	DW	78/78 (100%)	74 (95%)	4 (5%)	21	21
44	CX	56/58 (97%)	52 (93%)	4 (7%)	13	11
44	DX	58/58 (100%)	56 (97%)	2 (3%)	32	35
45	CY	67/67 (100%)	58 (87%)	9 (13%)	4	2
45	DY	67/67 (100%)	66 (98%)	1 (2%)	57	65
46	CZ	54/54 (100%)	46 (85%)	8 (15%)	3	1
46	DZ	54/54 (100%)	53 (98%)	1 (2%)	50	58
47	C0	48/48 (100%)	41 (85%)	7 (15%)	3	1
47	D0	49/48 (102%)	47 (96%)	2 (4%)	27	29
48	C1	47/47 (100%)	42 (89%)	5 (11%)	6	4
48	D1	47/47 (100%)	45 (96%)	2 (4%)	26	27
49	C2	45/46 (98%)	42 (93%)	3 (7%)	15	12
49	D2	45/46 (98%)	44 (98%)	1 (2%)	45	53
50	C3	38/38 (100%)	33 (87%)	5 (13%)	4	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	D3	38/38 (100%)	37 (97%)	1 (3%)	40	46
51	C4	51/51 (100%)	47 (92%)	4 (8%)	11	9
51	D4	51/51 (100%)	51 (100%)	0	100	100
52	C5	34/34 (100%)	31 (91%)	3 (9%)	9	7
52	D5	34/34 (100%)	33 (97%)	1 (3%)	37	42
54	DD	163/163 (100%)	161 (99%)	2 (1%)	63	72
55	DI	103/103 (100%)	100 (97%)	3 (3%)	37	42
All	All	9461/9478 (100%)	8665 (92%)	796 (8%)	10	7

All (796) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	5	SER
2	AB	20	THR
2	AB	73	LYS
2	AB	93	ASN
2	AB	129	LEU
3	AC	20	SER
3	AC	58	GLU
3	AC	64	ILE
3	AC	85	GLU
3	AC	101	ILE
3	AC	121	THR
3	AC	123	GLN
3	AC	125	GLU
3	AC	151	VAL
3	AC	186	THR
4	AD	5	LEU
4	AD	26	ARG
4	AD	132	ILE
4	AD	183	LYS
4	AD	194	ASP
4	AD	196	ASN
4	AD	197	GLU
5	AE	22	SER
5	AE	60	ILE
5	AE	74	VAL
5	AE	76	LEU
5	AE	80	THR
5	AE	94	VAL

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Mol	Chain	Res	Type
5	AE	105	ILE
5	AE	130	SER
5	AE	152	MET
5	AE	163	GLU
6	AF	71	ILE
6	AF	89	VAL
6	AF	90	MET
6	AF	98	GLU
7	AG	7	ILE
7	AG	15	ASP
7	AG	54	SER
7	AG	70	ARG
7	AG	75	VAL
7	AG	83	SER
8	AH	60	GLU
8	AH	75	ILE
8	AH	107	SER
9	AI	47	VAL
9	AI	66	THR
9	AI	94	LEU
10	AJ	7	ARG
10	AJ	8	ILE
10	AJ	19	ASP
10	AJ	27	GLU
10	AJ	35	GLN
10	AJ	80	THR
10	AJ	100	ILE
11	AK	23	ILE
11	AK	33	THR
11	AK	65	VAL
12	AL	24	LEU
12	AL	35	THR
12	AL	54	ARG
12	AL	55	VAL
12	AL	90	LEU
13	AM	53	ILE
13	AM	71	ARG
13	AM	107	ARG
13	AM	108	THR
15	AO	3	LEU
15	AO	40	GLN
15	AO	89	ARG

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Mol	Chain	Res	Type
16	AP	1	MET
16	AP	36	VAL
16	AP	44	SER
17	AQ	5	ILE
17	AQ	14	SER
17	AQ	42	THR
17	AQ	59	VAL
19	AS	18	LYS
20	AT	15	GLU
20	AT	40	GLU
21	AU	4	ILE
21	AU	20	LYS
2	BB	5	SER
2	BB	20	THR
2	BB	73	LYS
2	BB	93	ASN
2	BB	129	LEU
2	BB	146	ASN
2	BB	207	ILE
3	BC	3	GLN
3	BC	14	ILE
3	BC	20	SER
3	BC	27	LYS
3	BC	38	LYS
3	BC	43	LEU
3	BC	55	ILE
3	BC	58	GLU
3	BC	59	ARG
3	BC	75	ILE
3	BC	80	LYS
3	BC	82	GLU
3	BC	86	LYS
3	BC	101	ILE
3	BC	103	ILE
3	BC	121	THR
3	BC	123	GLN
3	BC	125	GLU
3	BC	127	ARG
3	BC	140	ASN
3	BC	152	GLU
3	BC	157	LEU
3	BC	165	THR

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Mol	Chain	Res	Type
3	BC	169	ARG
3	BC	175	LEU
3	BC	179	ARG
3	BC	186	THR
3	BC	192	THR
3	BC	200	VAL
3	BC	206	GLU
4	BD	5	LEU
4	BD	142	VAL
4	BD	173	VAL
4	BD	196	ASN
4	BD	206	LYS
5	BE	11	LEU
5	BE	12	GLN
5	BE	15	LEU
5	BE	22	SER
5	BE	26	LYS
5	BE	38	VAL
5	BE	46	VAL
5	BE	52	LYS
5	BE	60	ILE
5	BE	69	ARG
5	BE	78	ASN
5	BE	80	THR
5	BE	81	LEU
5	BE	93	ARG
5	BE	94	VAL
5	BE	96	MET
5	BE	101	GLU
5	BE	105	ILE
5	BE	114	VAL
5	BE	115	LEU
5	BE	120	VAL
5	BE	122	ASN
5	BE	149	SER
5	BE	151	GLU
5	BE	153	VAL
6	BF	7	VAL
6	BF	16	GLU
6	BF	29	ILE
6	BF	35	LYS
6	BF	51	ILE

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Mol	Chain	Res	Type
6	BF	53	LYS
6	BF	54	LEU
6	BF	56	LYS
6	BF	68	GLN
6	BF	69	GLU
6	BF	77	THR
6	BF	85	ILE
6	BF	86	ARG
6	BF	90	MET
6	BF	91	ARG
6	BF	93	LYS
7	BG	3	ARG
7	BG	5	ARG
7	BG	12	ILE
7	BG	22	LEU
7	BG	29	ILE
7	BG	47	LEU
7	BG	59	LEU
7	BG	60	GLU
7	BG	63	GLU
7	BG	66	LEU
7	BG	70	ARG
7	BG	73	VAL
7	BG	75	VAL
7	BG	77	SER
7	BG	78	ARG
7	BG	79	ARG
7	BG	89	VAL
7	BG	91	VAL
7	BG	97	ASN
7	BG	123	GLU
7	BG	129	GLU
7	BG	136	LYS
7	BG	140	ASP
7	BG	143	ARG
7	BG	144	MET
8	BH	3	MET
8	BH	18	GLN
8	BH	25	VAL
8	BH	26	THR
8	BH	51	VAL
8	BH	59	LEU

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Mol	Chain	Res	Type
8	BH	69	LYS
8	BH	75	ILE
8	BH	77	ARG
8	BH	83	LEU
8	BH	87	LYS
8	BH	90	ASP
8	BH	104	VAL
8	BH	107	SER
8	BH	111	MET
8	BH	114	ARG
8	BH	121	LEU
8	BH	125	ILE
9	BI	47	VAL
9	BI	66	THR
9	BI	94	LEU
10	BJ	5	ARG
10	BJ	9	ARG
10	BJ	16	ARG
10	BJ	22	THR
10	BJ	24	GLU
10	BJ	25	ILE
10	BJ	37	ARG
10	BJ	51	VAL
10	BJ	59	LYS
10	BJ	62	ARG
10	BJ	63	ASP
10	BJ	69	THR
10	BJ	73	LEU
10	BJ	77	VAL
10	BJ	82	LYS
10	BJ	83	THR
10	BJ	88	MET
10	BJ	90	LEU
10	BJ	98	VAL
10	BJ	99	GLN
10	BJ	100	ILE
10	BJ	102	LEU
11	BK	31	ILE
11	BK	38	GLN
11	BK	55	SER
11	BK	57	LYS
11	BK	65	VAL

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Mol	Chain	Res	Type
11	BK	82	LEU
11	BK	83	GLU
11	BK	100	LEU
11	BK	107	ILE
11	BK	109	ASN
11	BK	114	THR
12	BL	4	VAL
12	BL	9	ARG
12	BL	10	LYS
12	BL	12	ARG
12	BL	14	ARG
12	BL	18	LYS
12	BL	24	LEU
12	BL	35	THR
12	BL	44	LYS
12	BL	49	LEU
12	BL	54	ARG
12	BL	55	VAL
12	BL	58	THR
12	BL	88	LYS
12	BL	90	LEU
12	BL	94	ARG
12	BL	121	ARG
13	BM	4	ILE
13	BM	16	VAL
13	BM	25	VAL
13	BM	27	LYS
13	BM	29	ARG
13	BM	31	LYS
13	BM	48	LEU
13	BM	53	ILE
13	BM	59	GLU
13	BM	90	ARG
13	BM	91	HIS
13	BM	107	ARG
13	BM	110	LYS
13	BM	114	LYS
14	BN	26	GLU
14	BN	32	SER
15	BO	3	LEU
15	BO	6	GLU
15	BO	8	THR

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Mol	Chain	Res	Type
15	BO	17	ARG
15	BO	18	ASP
15	BO	35	GLN
15	BO	39	LEU
15	BO	64	ARG
15	BO	70	LEU
15	BO	83	GLU
15	BO	85	LEU
15	BO	87	LEU
15	BO	89	ARG
16	BP	1	MET
16	BP	2	VAL
16	BP	12	LYS
16	BP	18	GLN
16	BP	19	VAL
16	BP	20	VAL
16	BP	36	VAL
16	BP	46	LYS
16	BP	52	LEU
16	BP	63	GLN
16	BP	68	SER
17	BQ	5	ILE
17	BQ	7	THR
17	BQ	13	VAL
17	BQ	14	SER
17	BQ	16	LYS
17	BQ	17	MET
17	BQ	22	VAL
17	BQ	26	GLU
17	BQ	29	VAL
17	BQ	40	ARG
17	BQ	55	ILE
17	BQ	59	VAL
17	BQ	61	ILE
17	BQ	65	ARG
17	BQ	75	LEU
17	BQ	76	VAL
17	BQ	78	VAL
17	BQ	79	VAL
17	BQ	81	LYS
18	BR	21	ILE
18	BR	44	ILE

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Mol	Chain	Res	Type
18	BR	47	THR
18	BR	55	LEU
19	BS	5	LEU
19	BS	6	LYS
19	BS	7	LYS
19	BS	11	ILE
19	BS	13	LEU
19	BS	29	LYS
19	BS	33	THR
19	BS	37	ARG
19	BS	49	ILE
19	BS	58	VAL
19	BS	80	TYR
20	BT	10	ARG
20	BT	12	ILE
20	BT	15	GLU
20	BT	24	ARG
20	BT	27	MET
20	BT	30	THR
20	BT	36	TYR
20	BT	40	GLU
20	BT	54	MET
20	BT	58	VAL
20	BT	64	LYS
20	BT	66	LEU
20	BT	69	LYS
20	BT	84	ASN
20	BT	86	LEU
21	BU	4	ILE
21	BU	12	PHE
21	BU	20	LYS
21	BU	34	ARG
21	BU	56	HIS
24	CC	5	LYS
24	CC	14	ARG
24	CC	18	LYS
24	CC	36	LYS
24	CC	39	LYS
24	CC	59	LYS
24	CC	88	SER
24	CC	97	LYS
24	CC	105	LEU

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Mol	Chain	Res	Type
24	CC	130	LEU
24	CC	139	SER
24	CC	141	VAL
24	CC	156	ARG
24	CC	157	SER
24	CC	168	ASP
24	CC	174	LEU
24	CC	187	ASP
24	CC	195	VAL
24	CC	203	ARG
24	CC	204	VAL
24	CC	205	LEU
24	CC	213	TRP
24	CC	251	GLN
24	CC	265	LYS
24	CC	267	ILE
24	CC	269	ARG
25	CD	4	LEU
25	CD	12	THR
25	CD	32	ASN
25	CD	33	ARG
25	CD	39	ASP
25	CD	51	THR
25	CD	73	VAL
25	CD	91	THR
25	CD	95	SER
25	CD	104	VAL
25	CD	150	GLN
25	CD	157	LYS
25	CD	170	VAL
25	CD	177	VAL
26	CE	12	LEU
26	CE	25	GLU
26	CE	41	GLN
26	CE	44	ARG
26	CE	65	THR
26	CE	67	ARG
26	CE	69	ARG
26	CE	72	SER
26	CE	88	ARG
26	CE	93	SER
26	CE	108	ILE

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Mol	Chain	Res	Type
26	CE	109	LEU
26	CE	126	VAL
26	CE	133	LEU
26	CE	139	LYS
26	CE	146	VAL
26	CE	149	ILE
26	CE	150	THR
26	CE	164	LEU
26	CE	187	VAL
26	CE	200	LEU
27	CF	3	LYS
27	CF	18	THR
27	CF	19	GLU
27	CF	21	ASN
27	CF	26	MET
27	CF	31	VAL
27	CF	35	THR
27	CF	36	LEU
27	CF	46	ASP
27	CF	64	LYS
27	CF	72	LYS
27	CF	80	ARG
27	CF	89	VAL
27	CF	104	ILE
27	CF	117	LEU
27	CF	132	VAL
27	CF	133	ARG
27	CF	141	ILE
27	CF	149	VAL
27	CF	154	ILE
27	CF	158	THR
28	CG	6	LYS
28	CG	11	VAL
28	CG	17	VAL
28	CG	25	THR
28	CG	29	LYS
28	CG	30	ASN
28	CG	34	THR
28	CG	37	LEU
28	CG	43	VAL
28	CG	44	LYS
28	CG	45	HIS

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Mol	Chain	Res	Type
28	CG	49	THR
28	CG	73	ASN
28	CG	74	SER
28	CG	80	THR
28	CG	92	VAL
28	CG	98	VAL
28	CG	117	LEU
28	CG	127	THR
28	CG	137	ASP
28	CG	155	GLU
28	CG	160	LYS
28	CG	166	ASP
28	CG	168	VAL
28	CG	171	THR
29	CH	3	VAL
29	CH	6	LEU
29	CH	11	ASN
29	CH	12	LEU
29	CH	14	SER
29	CH	17	ASP
29	CH	20	ASN
29	CH	41	LYS
29	CH	42	LYS
29	CH	51	ARG
29	CH	72	ILE
29	CH	75	LEU
29	CH	77	THR
29	CH	78	VAL
29	CH	83	LYS
29	CH	87	GLU
29	CH	89	LYS
29	CH	97	ARG
29	CH	101	ASP
29	CH	117	LEU
29	CH	124	THR
29	CH	134	VAL
29	CH	142	VAL
29	CH	143	ILE
29	CH	144	VAL
30	CJ	35	ILE
30	CJ	59	ILE
30	CJ	61	VAL

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Mol	Chain	Res	Type
30	CJ	103	ARG
30	CJ	113	LYS
31	CK	3	THR
31	CK	28	LEU
31	CK	30	THR
31	CK	39	LYS
31	CK	57	LEU
31	CK	81	ILE
31	CK	95	ARG
31	CK	123	LYS
31	CK	124	VAL
31	CK	129	GLU
31	CK	131	ASN
31	CK	142	ILE
32	CL	49	ARG
32	CL	66	LYS
32	CL	67	LYS
32	CL	76	VAL
32	CL	90	ASN
32	CL	92	GLU
32	CL	107	LEU
32	CL	114	LYS
33	CM	19	LEU
33	CM	82	LEU
33	CM	92	LEU
33	CM	94	THR
33	CM	100	ILE
33	CM	115	GLU
33	CM	118	THR
34	CN	18	ARG
34	CN	20	LEU
34	CN	24	THR
34	CN	27	SER
34	CN	40	ARG
34	CN	47	GLU
34	CN	53	MET
34	CN	55	ARG
34	CN	58	LYS
34	CN	59	ARG
34	CN	78	LEU
34	CN	100	LYS
34	CN	111	GLU

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Mol	Chain	Res	Type
34	CN	115	GLU
35	CO	1	MET
35	CO	2	ARG
35	CO	20	MET
35	CO	51	LEU
35	CO	63	ARG
35	CO	69	ARG
35	CO	70	THR
35	CO	71	ARG
35	CO	76	VAL
35	CO	90	ARG
35	CO	95	THR
35	CO	97	ILE
35	CO	116	VAL
35	CO	118	ARG
36	CP	5	SER
36	CP	9	ARG
36	CP	16	ARG
36	CP	18	LEU
36	CP	25	ARG
36	CP	31	THR
36	CP	38	GLN
36	CP	47	VAL
36	CP	78	VAL
36	CP	85	LYS
36	CP	94	ARG
36	CP	103	VAL
37	CQ	6	LYS
37	CQ	8	LEU
37	CQ	19	SER
37	CQ	26	VAL
37	CQ	37	LYS
37	CQ	39	ARG
37	CQ	40	LEU
37	CQ	72	ARG
37	CQ	73	VAL
37	CQ	80	VAL
37	CQ	110	ILE
38	CR	5	LYS
38	CR	9	ILE
38	CR	11	ARG
38	CR	13	ARG

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Mol	Chain	Res	Type
38	CR	16	LYS
38	CR	41	LYS
38	CR	51	ARG
39	CS	10	LYS
39	CS	38	VAL
39	CS	45	GLU
39	CS	46	GLU
39	CS	47	VAL
39	CS	48	LYS
39	CS	58	VAL
39	CS	60	LYS
39	CS	62	GLU
39	CS	102	SER
40	CT	13	SER
40	CT	19	LEU
40	CT	30	SER
40	CT	41	LYS
40	CT	65	ASP
40	CT	66	ILE
40	CT	69	LEU
40	CT	76	VAL
40	CT	86	MET
40	CT	96	ILE
40	CT	97	LEU
40	CT	107	VAL
40	CT	109	ASP
40	CT	110	ARG
41	CU	2	ILE
41	CU	3	ARG
41	CU	5	GLU
41	CU	10	VAL
41	CU	18	GLU
41	CU	22	THR
41	CU	26	LYS
41	CU	30	ILE
41	CU	49	LYS
41	CU	50	LEU
41	CU	56	GLU
41	CU	69	ARG
41	CU	70	HIS
41	CU	77	ARG
42	CV	15	THR

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Mol	Chain	Res	Type
42	CV	19	LYS
42	CV	29	LEU
42	CV	35	ILE
42	CV	37	GLU
42	CV	41	LEU
42	CV	47	LYS
42	CV	53	ASN
42	CV	61	LYS
42	CV	68	SER
42	CV	72	ILE
42	CV	79	LYS
42	CV	101	GLU
43	CW	1	MET
43	CW	7	GLU
43	CW	10	LYS
43	CW	20	LEU
43	CW	29	ILE
43	CW	34	LYS
43	CW	40	ILE
43	CW	53	LYS
43	CW	61	LEU
43	CW	62	THR
43	CW	65	VAL
43	CW	66	ASP
43	CW	70	ILE
44	CX	30	SER
44	CX	38	VAL
44	CX	77	ARG
44	CX	82	ILE
45	CY	17	ASN
45	CY	20	HIS
45	CY	22	LEU
45	CY	35	SER
45	CY	48	THR
45	CY	56	MET
45	CY	71	LEU
45	CY	72	ARG
45	CY	76	GLU
46	CZ	2	LYS
46	CZ	8	GLU
46	CZ	18	LEU
46	CZ	19	LEU

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Mol	Chain	Res	Type
46	CZ	21	LEU
46	CZ	38	GLN
46	CZ	57	LEU
46	CZ	58	ASN
47	C0	3	LYS
47	C0	4	THR
47	C0	5	ILE
47	C0	10	THR
47	C0	19	LYS
47	C0	36	VAL
47	C0	57	VAL
48	C1	10	ARG
48	C1	26	THR
48	C1	28	LEU
48	C1	29	SER
48	C1	52	ARG
49	C2	8	LYS
49	C2	27	LYS
49	C2	47	VAL
50	C3	1	MET
50	C3	3	ARG
50	C3	4	THR
50	C3	42	LEU
50	C3	44	VAL
51	C4	13	ARG
51	C4	19	LYS
51	C4	30	ARG
51	C4	47	LYS
52	C5	3	VAL
52	C5	26	ILE
52	C5	36	ARG
24	DC	3	VAL
24	DC	39	LYS
24	DC	130	LEU
24	DC	139	SER
24	DC	182	ARG
24	DC	252	THR
54	DD	32	ASN
54	DD	95	SER
26	DE	7	ASP
27	DF	72	LYS
27	DF	89	VAL

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Mol	Chain	Res	Type
27	DF	105	THR
27	DF	132	VAL
27	DF	154	ILE
27	DF	158	THR
27	DF	174	ASP
28	DG	11	VAL
28	DG	26	ILE
28	DG	27	LYS
28	DG	45	HIS
28	DG	77	ILE
28	DG	85	LYS
28	DG	98	VAL
28	DG	104	ASN
28	DG	152	ARG
29	DH	14	SER
29	DH	15	LEU
29	DH	42	LYS
29	DH	44	ILE
29	DH	48	GLU
29	DH	50	ARG
29	DH	53	GLU
29	DH	60	GLU
29	DH	61	VAL
29	DH	76	GLU
29	DH	77	THR
29	DH	114	GLU
29	DH	125	THR
55	DI	16	SER
55	DI	71	CYS
55	DI	86	THR
30	DJ	24	VAL
30	DJ	35	ILE
30	DJ	59	ILE
30	DJ	61	VAL
30	DJ	103	ARG
30	DJ	113	LYS
31	DK	34	ARG
31	DK	39	LYS
31	DK	124	VAL
31	DK	142	ILE
32	DL	49	ARG
32	DL	58	LEU

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Mol	Chain	Res	Type
32	DL	90	ASN
33	DM	59	ARG
33	DM	92	LEU
33	DM	115	GLU
34	DN	27	SER
34	DN	47	GLU
34	DN	100	LYS
34	DN	115	GLU
34	DN	135	VAL
34	DN	136	MET
35	DO	69	ARG
35	DO	75	ILE
35	DO	76	VAL
35	DO	116	VAL
36	DP	31	THR
36	DP	78	VAL
37	DQ	7	GLN
37	DQ	19	SER
37	DQ	26	VAL
37	DQ	68	GLU
37	DQ	85	SER
38	DR	11	ARG
38	DR	51	ARG
39	DS	32	THR
39	DS	38	VAL
39	DS	45	GLU
39	DS	101	ILE
39	DS	102	SER
40	DT	86	MET
40	DT	109	ASP
41	DU	5	GLU
41	DU	10	VAL
41	DU	16	VAL
41	DU	93	LEU
42	DV	28	VAL
42	DV	58	ILE
42	DV	70	VAL
42	DV	79	LYS
42	DV	86	ARG
43	DW	7	GLU
43	DW	61	LEU
43	DW	66	ASP

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Mol	Chain	Res	Type
43	DW	70	ILE
44	DX	11	ARG
44	DX	82	ILE
45	DY	2	SER
46	DZ	2	LYS
47	D0	10	THR
47	D0	36	VAL
48	D1	29	SER
48	D1	52	ARG
49	D2	5	ILE
50	D3	1	MET
52	D5	36	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	51	ASN
3	AC	41	GLN
3	AC	139	GLN
5	AE	73	ASN
5	AE	89	HIS
6	AF	3	HIS
7	AG	148	ASN
11	AK	24	HIS
11	AK	118	HIS
15	AO	50	HIS
16	AP	9	HIS
3	BC	190	HIS
4	BD	40	GLN
4	BD	41	HIS
5	BE	97	GLN
6	BF	52	ASN
6	BF	68	GLN
8	BH	76	GLN
10	BJ	56	HIS
11	BK	15	GLN
11	BK	22	HIS
13	BM	12	HIS
14	BN	66	GLN
15	BO	28	GLN
21	BU	56	HIS
24	CC	70	ASN

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Mol	Chain	Res	Type
24	CC	251	GLN
25	CD	49	GLN
26	CE	46	GLN
26	CE	115	GLN
29	CH	28	ASN
34	CN	13	HIS
37	CQ	15	GLN
37	CQ	56	HIS
37	CQ	66	ASN
40	CT	31	GLN
43	CW	24	ASN
46	CZ	36	GLN
46	CZ	41	HIS
50	C3	29	GLN
54	DD	42	ASN
54	DD	49	GLN
27	DF	27	GLN
27	DF	81	GLN
28	DG	48	ASN
29	DH	43	ASN
55	DI	9	GLN
31	DK	47	HIS
32	DL	93	GLN
33	DM	35	HIS
36	DP	29	HIS
39	DS	6	GLN
43	DW	12	GLN
50	D3	26	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1533/1534 (99%)	259 (16%)	9 (0%)
1	BA	1532/1534 (99%)	269 (17%)	10 (0%)
22	CA	2896/2904 (99%)	424 (14%)	32 (1%)
23	CB	117/120 (97%)	11 (9%)	0
23	DB	119/120 (99%)	8 (6%)	0
53	DA	2887/2903 (99%)	384 (13%)	26 (0%)
All	All	9084/9115 (99%)	1355 (14%)	77 (0%)

All (1355) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	28	A
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	69	G
1	AA	70	U
1	AA	71	A
1	AA	72	A
1	AA	73	C
1	AA	74	A
1	AA	75	G
1	AA	76	G
1	AA	77	A
1	AA	78	A
1	AA	79	G
1	AA	80	A
1	AA	81	A
1	AA	82	G
1	AA	83	C
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	89	U
1	AA	90	C
1	AA	91	U
1	AA	94	G
1	AA	95	C
1	AA	97	G
1	AA	108	G
1	AA	119	A
1	AA	121	U
1	AA	122	G
1	AA	128	G
1	AA	130	A
1	AA	131	A
1	AA	137	U

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Mol	Chain	Res	Type
1	AA	142	G
1	AA	144	G
1	AA	158	G
1	AA	159	G
1	AA	163	C
1	AA	168	G
1	AA	173	U
1	AA	183	C
1	AA	201	G
1	AA	205	A
1	AA	208	U
1	AA	209	U
1	AA	210	C
1	AA	212	G
1	AA	240	G
1	AA	245	U
1	AA	247	G
1	AA	251	G
1	AA	262	A
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	346	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	382	A
1	AA	384	G
1	AA	406	G
1	AA	411	A
1	AA	412	A
1	AA	413	G
1	AA	421	U
1	AA	422	C
1	AA	429	U

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Mol	Chain	Res	Type
1	AA	430	A
1	AA	435	A
1	AA	439	U
1	AA	444	G
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	481	G
1	AA	486	U
1	AA	495	A
1	AA	496	A
1	AA	509	A
1	AA	511	C
1	AA	512	U
1	AA	527	G7M
1	AA	530	G
1	AA	532	A
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	562	U
1	AA	564	C
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	631	C
1	AA	632	U
1	AA	649	A
1	AA	650	G
1	AA	653	U
1	AA	654	G
1	AA	665	A
1	AA	682	G
1	AA	721	G
1	AA	723	U
1	AA	724	G
1	AA	733	G
1	AA	753	A

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Mol	Chain	Res	Type
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	815	A
1	AA	817	C
1	AA	827	U
1	AA	828	U
1	AA	832	G
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	845	A
1	AA	846	G
1	AA	887	G
1	AA	913	A
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	932	C
1	AA	934	C
1	AA	960	U
1	AA	969	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	992	U
1	AA	993	G
1	AA	1004	A
1	AA	1005	A
1	AA	1009	U
1	AA	1012	A
1	AA	1015	G
1	AA	1017	U
1	AA	1019	A
1	AA	1021	A
1	AA	1022	A
1	AA	1023	U
1	AA	1025	U
1	AA	1026	G
1	AA	1027	C
1	AA	1028	C

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Mol	Chain	Res	Type
1	AA	1029	U
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	G
1	AA	1034	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	1070	U
1	AA	1086	U
1	AA	1092	A
1	AA	1094	G
1	AA	1095	U
1	AA	1098	C
1	AA	1101	A
1	AA	1108	G
1	AA	1124	G
1	AA	1133	G
1	AA	1135	U
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	1152	A
1	AA	1158	C
1	AA	1159	U
1	AA	1160	G
1	AA	1167	A
1	AA	1168	U
1	AA	1184	G
1	AA	1196	A
1	AA	1197	A
1	AA	1212	U
1	AA	1213	A

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Mol	Chain	Res	Type
1	AA	1215	G
1	AA	1225	A
1	AA	1227	A
1	AA	1238	A
1	AA	1239	A
1	AA	1240	U
1	AA	1256	A
1	AA	1257	A
1	AA	1260	G
1	AA	1279	G
1	AA	1280	A
1	AA	1286	U
1	AA	1287	A
1	AA	1299	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1317	C
1	AA	1320	C
1	AA	1322	C
1	AA	1323	G
1	AA	1336	C
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1368	A
1	AA	1370	G
1	AA	1381	U
1	AA	1398	A
1	AA	1429	A
1	AA	1441	A
1	AA	1442	G
1	AA	1445	U
1	AA	1446	A
1	AA	1450	U
1	AA	1451	U
1	AA	1453	G
1	AA	1454	G
1	AA	1492	A
1	AA	1493	A
1	AA	1497	G
1	AA	1499	A

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Mol	Chain	Res	Type
1	AA	1503	A
1	AA	1505	G
1	AA	1506	U
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	BA	3	A
1	BA	4	U
1	BA	5	U
1	BA	7	A
1	BA	9	G
1	BA	22	G
1	BA	28	A
1	BA	32	A
1	BA	39	G
1	BA	47	C
1	BA	48	C
1	BA	50	A
1	BA	51	A
1	BA	69	G
1	BA	70	U
1	BA	71	A
1	BA	72	A
1	BA	74	A
1	BA	75	G
1	BA	76	G
1	BA	77	A
1	BA	78	A
1	BA	80	A
1	BA	81	A
1	BA	82	G
1	BA	83	C
1	BA	84	U
1	BA	85	U
1	BA	87	C
1	BA	88	U
1	BA	94	G
1	BA	95	C
1	BA	108	G
1	BA	119	A
1	BA	121	U
1	BA	122	G

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Mol	Chain	Res	Type
1	BA	128	G
1	BA	130	A
1	BA	131	A
1	BA	137	U
1	BA	142	G
1	BA	144	G
1	BA	158	G
1	BA	159	G
1	BA	163	C
1	BA	168	G
1	BA	173	U
1	BA	182	A
1	BA	183	C
1	BA	201	G
1	BA	204	G
1	BA	209	U
1	BA	210	C
1	BA	211	G
1	BA	212	G
1	BA	245	U
1	BA	247	G
1	BA	251	G
1	BA	262	A
1	BA	266	G
1	BA	267	C
1	BA	289	G
1	BA	321	A
1	BA	328	C
1	BA	329	A
1	BA	330	C
1	BA	332	G
1	BA	346	G
1	BA	347	G
1	BA	352	C
1	BA	354	G
1	BA	367	U
1	BA	372	C
1	BA	373	A
1	BA	382	A
1	BA	384	G
1	BA	406	G
1	BA	412	A

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Mol	Chain	Res	Type
1	BA	413	G
1	BA	421	U
1	BA	422	C
1	BA	429	U
1	BA	430	A
1	BA	435	A
1	BA	439	U
1	BA	444	G
1	BA	457	G
1	BA	458	U
1	BA	463	U
1	BA	467	U
1	BA	468	A
1	BA	469	C
1	BA	478	A
1	BA	479	U
1	BA	481	G
1	BA	485	U
1	BA	486	U
1	BA	495	A
1	BA	496	A
1	BA	509	A
1	BA	510	A
1	BA	511	C
1	BA	512	U
1	BA	527	G7M
1	BA	530	G
1	BA	532	A
1	BA	533	A
1	BA	547	A
1	BA	559	A
1	BA	562	U
1	BA	564	C
1	BA	568	G
1	BA	572	A
1	BA	573	A
1	BA	576	C
1	BA	577	G
1	BA	631	C
1	BA	632	U
1	BA	649	A
1	BA	650	G

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Mol	Chain	Res	Type
1	BA	653	U
1	BA	654	G
1	BA	665	A
1	BA	682	G
1	BA	723	U
1	BA	724	G
1	BA	733	G
1	BA	753	A
1	BA	755	G
1	BA	777	A
1	BA	793	U
1	BA	794	A
1	BA	815	A
1	BA	817	C
1	BA	827	U
1	BA	828	U
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	858	G
1	BA	887	G
1	BA	913	A
1	BA	914	A
1	BA	926	G
1	BA	932	C
1	BA	934	C
1	BA	942	G
1	BA	960	U
1	BA	969	A
1	BA	975	A
1	BA	976	G
1	BA	977	A
1	BA	988	G
1	BA	993	G
1	BA	1004	A
1	BA	1005	A
1	BA	1008	U
1	BA	1009	U
1	BA	1012	A

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Mol	Chain	Res	Type
1	BA	1015	G
1	BA	1017	U
1	BA	1020	G
1	BA	1021	A
1	BA	1023	U
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	1034	G
1	BA	1036	A
1	BA	1037	C
1	BA	1041	G
1	BA	1043	G
1	BA	1053	G
1	BA	1054	C
1	BA	1065	U
1	BA	1070	U
1	BA	1086	U
1	BA	1092	A
1	BA	1094	G
1	BA	1095	U
1	BA	1098	C
1	BA	1101	A
1	BA	1108	G
1	BA	1110	A
1	BA	1124	G
1	BA	1133	G
1	BA	1135	U
1	BA	1136	C
1	BA	1137	C
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

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Mol	Chain	Res	Type
1	BA	1158	C
1	BA	1159	U
1	BA	1160	G
1	BA	1167	A
1	BA	1168	U
1	BA	1183	U
1	BA	1184	G
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	1227	A
1	BA	1228	C
1	BA	1238	A
1	BA	1239	A
1	BA	1240	U
1	BA	1256	A
1	BA	1257	A
1	BA	1260	G
1	BA	1280	A
1	BA	1286	U
1	BA	1287	A
1	BA	1292	G
1	BA	1293	C
1	BA	1299	A
1	BA	1300	G
1	BA	1302	C
1	BA	1305	G
1	BA	1317	C
1	BA	1320	C
1	BA	1322	C
1	BA	1336	C
1	BA	1346	A
1	BA	1353	G
1	BA	1363	A
1	BA	1368	A
1	BA	1370	G
1	BA	1379	G
1	BA	1381	U

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Mol	Chain	Res	Type
1	BA	1398	A
1	BA	1419	G
1	BA	1429	A
1	BA	1441	A
1	BA	1442	G
1	BA	1445	U
1	BA	1446	A
1	BA	1452	C
1	BA	1453	G
1	BA	1454	G
1	BA	1491	G
1	BA	1492	A
1	BA	1493	A
1	BA	1494	G
1	BA	1497	G
1	BA	1503	A
1	BA	1505	G
1	BA	1506	U
1	BA	1517	G
1	BA	1529	G
1	BA	1530	G
1	BA	1533	C
1	BA	1534	A
22	CA	7	G
22	CA	10	A
22	CA	14	A
22	CA	15	G
22	CA	34	U
22	CA	42	A
22	CA	46	G
22	CA	58	G
22	CA	63	A
22	CA	71	A
22	CA	74	A
22	CA	75	G
22	CA	80	G
22	CA	83	A
22	CA	84	A
22	CA	101	A
22	CA	102	U
22	CA	119	A
22	CA	120	U

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Mol	Chain	Res	Type
22	CA	135	U
22	CA	136	G
22	CA	137	U
22	CA	138	U
22	CA	139	U
22	CA	140	C
22	CA	141	G
22	CA	142	A
22	CA	143	C
22	CA	196	A
22	CA	199	A
22	CA	200	U
22	CA	215	G
22	CA	216	A
22	CA	222	A
22	CA	248	G
22	CA	257	C
22	CA	265	A
22	CA	266	G
22	CA	272	A
22	CA	276	U
22	CA	279	A
22	CA	283	G
22	CA	285	G
22	CA	291	G
22	CA	311	A
22	CA	315	G
22	CA	325	G
22	CA	329	G
22	CA	330	A
22	CA	331	C
22	CA	336	C
22	CA	353	C
22	CA	354	A
22	CA	355	U
22	CA	361	G
22	CA	362	A
22	CA	370	G
22	CA	371	A
22	CA	372	G
22	CA	386	G
22	CA	404	A

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Mol	Chain	Res	Type
22	CA	405	U
22	CA	411	G
22	CA	412	A
22	CA	424	G
22	CA	425	G
22	CA	426	C
22	CA	435	C
22	CA	451	U
22	CA	480	A
22	CA	481	G
22	CA	491	G
22	CA	504	A
22	CA	505	A
22	CA	508	A
22	CA	531	C
22	CA	532	A
22	CA	533	G
22	CA	543	G
22	CA	546	U
22	CA	547	A
22	CA	548	G
22	CA	549	G
22	CA	550	C
22	CA	551	G
22	CA	563	A
22	CA	573	U
22	CA	575	A
22	CA	586	A
22	CA	603	A
22	CA	613	A
22	CA	614	A
22	CA	615	U
22	CA	618	G
22	CA	620	G
22	CA	627	A
22	CA	637	A
22	CA	645	C
22	CA	646	U
22	CA	647	G
22	CA	648	G
22	CA	654	A
22	CA	655	A

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Mol	Chain	Res	Type
22	CA	686	U
22	CA	730	A
22	CA	747	5MU
22	CA	764	A
22	CA	765	C
22	CA	775	G
22	CA	776	G
22	CA	782	A
22	CA	784	G
22	CA	785	G
22	CA	792	A
22	CA	805	G
22	CA	812	C
22	CA	819	A
22	CA	827	U
22	CA	828	U
22	CA	845	A
22	CA	846	U
22	CA	847	U
22	CA	858	G
22	CA	859	G
22	CA	866	A
22	CA	878	A
22	CA	883	G
22	CA	893	C
22	CA	896	A
22	CA	897	C
22	CA	910	A
22	CA	914	G
22	CA	915	C
22	CA	931	U
22	CA	934	U
22	CA	941	A
22	CA	946	C
22	CA	961	C
22	CA	974	G
22	CA	983	A
22	CA	984	A
22	CA	985	C
22	CA	995	C
22	CA	996	A
22	CA	1012	U

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Mol	Chain	Res	Type
22	CA	1013	C
22	CA	1022	G
22	CA	1026	G
22	CA	1033	U
22	CA	1046	A
22	CA	1047	G
22	CA	1053	C
22	CA	1070	A
22	CA	1083	U
22	CA	1084	A
22	CA	1088	A
22	CA	1090	A
22	CA	1110	G
22	CA	1111	A
22	CA	1112	G
22	CA	1122	G
22	CA	1128	G
22	CA	1129	A
22	CA	1132	U
22	CA	1133	A
22	CA	1135	C
22	CA	1136	G
22	CA	1138	G
22	CA	1142	A
22	CA	1143	A
22	CA	1168	G
22	CA	1169	A
22	CA	1171	G
22	CA	1172	C
22	CA	1174	U
22	CA	1175	A
22	CA	1176	U
22	CA	1177	G
22	CA	1179	G
22	CA	1180	U
22	CA	1182	G
22	CA	1186	G
22	CA	1208	C
22	CA	1230	A
22	CA	1231	U
22	CA	1238	G
22	CA	1253	A

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Mol	Chain	Res	Type
22	CA	1256	G
22	CA	1266	G
22	CA	1271	G
22	CA	1272	A
22	CA	1273	U
22	CA	1300	G
22	CA	1301	A
22	CA	1365	A
22	CA	1368	G
22	CA	1379	U
22	CA	1380	G
22	CA	1383	A
22	CA	1391	U
22	CA	1395	A
22	CA	1410	G
22	CA	1416	G
22	CA	1417	C
22	CA	1419	A
22	CA	1428	C
22	CA	1452	G
22	CA	1453	A
22	CA	1481	U
22	CA	1482	G
22	CA	1483	G
22	CA	1490	A
22	CA	1493	C
22	CA	1494	A
22	CA	1495	A
22	CA	1497	U
22	CA	1510	G
22	CA	1515	A
22	CA	1523	U
22	CA	1530	G
22	CA	1534	U
22	CA	1535	A
22	CA	1536	C
22	CA	1537	G
22	CA	1540	G
22	CA	1566	A
22	CA	1569	A
22	CA	1578	U
22	CA	1581	G

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Mol	Chain	Res	Type
22	CA	1583	A
22	CA	1584	U
22	CA	1585	C
22	CA	1586	A
22	CA	1587	G
22	CA	1606	C
22	CA	1608	A
22	CA	1610	A
22	CA	1647	U
22	CA	1648	U
22	CA	1649	G
22	CA	1674	G
22	CA	1714	U
22	CA	1715	G
22	CA	1725	U
22	CA	1727	C
22	CA	1729	U
22	CA	1730	C
22	CA	1731	G
22	CA	1732	C
22	CA	1738	G
22	CA	1739	A
22	CA	1740	G
22	CA	1744	A
22	CA	1755	A
22	CA	1764	C
22	CA	1773	A
22	CA	1782	U
22	CA	1799	G
22	CA	1800	C
22	CA	1801	A
22	CA	1807	G
22	CA	1808	A
22	CA	1816	C
22	CA	1829	A
22	CA	1858	A
22	CA	1859	U
22	CA	1870	C
22	CA	1871	A
22	CA	1872	A
22	CA	1873	G
22	CA	1874	C

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Mol	Chain	Res	Type
22	CA	1876	A
22	CA	1880	U
22	CA	1886	U
22	CA	1906	G
22	CA	1914	C
22	CA	1929	G
22	CA	1930	G
22	CA	1931	U
22	CA	1937	A
22	CA	1938	A
22	CA	1955	U
22	CA	1967	C
22	CA	1970	A
22	CA	1972	G
22	CA	1991	U
22	CA	1993	U
22	CA	1997	C
22	CA	2022	U
22	CA	2023	C
22	CA	2031	A
22	CA	2033	A
22	CA	2043	C
22	CA	2055	C
22	CA	2056	G
22	CA	2060	A
22	CA	2061	G
22	CA	2062	A
22	CA	2069	G7M
22	CA	2072	C
22	CA	2093	G
22	CA	2095	A
22	CA	2101	A
22	CA	2110	G
22	CA	2111	U
22	CA	2112	G
22	CA	2113	U
22	CA	2115	G
22	CA	2116	G
22	CA	2117	A
22	CA	2118	U
22	CA	2119	A
22	CA	2123	G

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Mol	Chain	Res	Type
22	CA	2124	G
22	CA	2125	G
22	CA	2126	A
22	CA	2127	G
22	CA	2128	G
22	CA	2131	U
22	CA	2132	U
22	CA	2133	G
22	CA	2137	U
22	CA	2147	A
22	CA	2157	G
22	CA	2158	A
22	CA	2163	A
22	CA	2164	C
22	CA	2165	C
22	CA	2169	A
22	CA	2171	A
22	CA	2172	U
22	CA	2173	A
22	CA	2182	U
22	CA	2183	A
22	CA	2189	U
22	CA	2190	G
22	CA	2198	A
22	CA	2204	G
22	CA	2211	A
22	CA	2212	A
22	CA	2225	A
22	CA	2226	C
22	CA	2238	G
22	CA	2239	G
22	CA	2268	A
22	CA	2273	A
22	CA	2283	C
22	CA	2286	G
22	CA	2287	A
22	CA	2305	U
22	CA	2308	G
22	CA	2311	A
22	CA	2324	U
22	CA	2325	G
22	CA	2327	A

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Mol	Chain	Res	Type
22	CA	2333	A
22	CA	2335	A
22	CA	2339	C
22	CA	2347	C
22	CA	2361	G
22	CA	2383	G
22	CA	2385	C
22	CA	2402	U
22	CA	2403	C
22	CA	2406	A
22	CA	2407	A
22	CA	2423	U
22	CA	2424	C
22	CA	2425	A
22	CA	2426	A
22	CA	2429	G
22	CA	2430	A
22	CA	2431	U
22	CA	2434	A
22	CA	2435	A
22	CA	2441	U
22	CA	2448	A
22	CA	2476	A
22	CA	2491	U
22	CA	2502	G
22	CA	2505	G
22	CA	2518	A
22	CA	2525	G
22	CA	2529	G
22	CA	2547	A
22	CA	2554	U
22	CA	2566	A
22	CA	2567	G
22	CA	2585	U
22	CA	2586	U
22	CA	2603	G
22	CA	2609	U
22	CA	2613	U
22	CA	2629	U
22	CA	2663	G
22	CA	2681	C
22	CA	2682	A

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Mol	Chain	Res	Type
22	CA	2689	U
22	CA	2690	U
22	CA	2714	G
22	CA	2718	G
22	CA	2726	A
22	CA	2744	G
22	CA	2748	A
22	CA	2765	A
22	CA	2778	A
22	CA	2791	G
22	CA	2794	C
22	CA	2798	U
22	CA	2799	A
22	CA	2803	G
22	CA	2811	G
22	CA	2820	A
22	CA	2821	A
22	CA	2825	G
22	CA	2867	G
22	CA	2873	A
22	CA	2874	C
22	CA	2883	A
22	CA	2884	U
22	CA	2891	U
22	CA	2894	G
22	CA	2903	U
22	CA	2904	U
23	CB	15	A
23	CB	23	G
23	CB	35	C
23	CB	45	A
23	CB	56	G
23	CB	66	A
23	CB	88	C
23	CB	89	U
23	CB	90	C
23	CB	99	A
23	CB	109	A
53	DA	10	A
53	DA	12	U
53	DA	14	A
53	DA	15	G

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Mol	Chain	Res	Type
53	DA	34	U
53	DA	46	G
53	DA	58	G
53	DA	63	A
53	DA	71	A
53	DA	74	A
53	DA	75	G
53	DA	80	G
53	DA	101	A
53	DA	102	U
53	DA	119	A
53	DA	120	U
53	DA	135	U
53	DA	136	G
53	DA	137	U
53	DA	138	U
53	DA	139	U
53	DA	140	C
53	DA	141	G
53	DA	142	A
53	DA	196	A
53	DA	216	A
53	DA	221	A
53	DA	222	A
53	DA	248	G
53	DA	257	C
53	DA	266	G
53	DA	272	A
53	DA	276	U
53	DA	277	G
53	DA	279	A
53	DA	283	G
53	DA	285	G
53	DA	291	G
53	DA	302	C
53	DA	311	A
53	DA	315	G
53	DA	325	G
53	DA	329	G
53	DA	330	A
53	DA	331	C
53	DA	353	C

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Mol	Chain	Res	Type
53	DA	355	U
53	DA	358	U
53	DA	361	G
53	DA	362	A
53	DA	370	G
53	DA	372	G
53	DA	386	G
53	DA	411	G
53	DA	412	A
53	DA	424	G
53	DA	425	G
53	DA	435	C
53	DA	451	U
53	DA	481	G
53	DA	491	G
53	DA	504	A
53	DA	505	A
53	DA	508	A
53	DA	531	C
53	DA	532	A
53	DA	533	G
53	DA	543	G
53	DA	546	U
53	DA	547	A
53	DA	548	G
53	DA	549	G
53	DA	550	C
53	DA	551	G
53	DA	563	A
53	DA	573	U
53	DA	575	A
53	DA	586	A
53	DA	603	A
53	DA	613	A
53	DA	614	A
53	DA	615	U
53	DA	620	G
53	DA	627	A
53	DA	637	A
53	DA	645	C
53	DA	646	U
53	DA	647	G

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Mol	Chain	Res	Type
53	DA	654	A
53	DA	655	A
53	DA	686	U
53	DA	730	A
53	DA	747	5MU
53	DA	764	A
53	DA	765	C
53	DA	775	G
53	DA	776	G
53	DA	782	A
53	DA	784	G
53	DA	785	G
53	DA	790	U
53	DA	792	A
53	DA	805	G
53	DA	812	C
53	DA	827	U
53	DA	828	U
53	DA	845	A
53	DA	846	U
53	DA	847	U
53	DA	858	G
53	DA	859	G
53	DA	866	A
53	DA	878	A
53	DA	885	C
53	DA	893	C
53	DA	896	A
53	DA	897	C
53	DA	910	A
53	DA	914	G
53	DA	915	C
53	DA	931	U
53	DA	934	U
53	DA	946	C
53	DA	961	C
53	DA	974	G
53	DA	983	A
53	DA	984	A
53	DA	985	C
53	DA	996	A
53	DA	1012	U

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Mol	Chain	Res	Type
53	DA	1013	C
53	DA	1022	G
53	DA	1026	G
53	DA	1033	U
53	DA	1046	A
53	DA	1047	G
53	DA	1070	A
53	DA	1083	U
53	DA	1084	A
53	DA	1088	A
53	DA	1090	A
53	DA	1112	G
53	DA	1130	U
53	DA	1132	U
53	DA	1133	A
53	DA	1135	C
53	DA	1136	G
53	DA	1138	G
53	DA	1142	A
53	DA	1143	A
53	DA	1168	G
53	DA	1171	G
53	DA	1172	C
53	DA	1174	U
53	DA	1175	A
53	DA	1176	U
53	DA	1177	G
53	DA	1182	G
53	DA	1238	G
53	DA	1253	A
53	DA	1256	G
53	DA	1271	G
53	DA	1272	A
53	DA	1273	U
53	DA	1300	G
53	DA	1301	A
53	DA	1352	U
53	DA	1365	A
53	DA	1379	U
53	DA	1383	A
53	DA	1410	G
53	DA	1416	G

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Mol	Chain	Res	Type
53	DA	1417	C
53	DA	1419	A
53	DA	1428	C
53	DA	1452	G
53	DA	1453	A
53	DA	1482	G
53	DA	1490	A
53	DA	1493	C
53	DA	1494	A
53	DA	1495	A
53	DA	1497	U
53	DA	1510	G
53	DA	1515	A
53	DA	1523	U
53	DA	1532	A
53	DA	1535	A
53	DA	1536	C
53	DA	1537	G
53	DA	1540	G
53	DA	1566	A
53	DA	1569	A
53	DA	1578	U
53	DA	1581	G
53	DA	1583	A
53	DA	1584	U
53	DA	1585	C
53	DA	1606	C
53	DA	1608	A
53	DA	1647	U
53	DA	1648	U
53	DA	1649	G
53	DA	1674	G
53	DA	1714	U
53	DA	1715	G
53	DA	1725	U
53	DA	1727	C
53	DA	1729	U
53	DA	1730	C
53	DA	1731	G
53	DA	1732	C
53	DA	1738	G
53	DA	1739	A

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Mol	Chain	Res	Type
53	DA	1740	G
53	DA	1744	A
53	DA	1755	A
53	DA	1764	C
53	DA	1773	A
53	DA	1782	U
53	DA	1800	C
53	DA	1801	A
53	DA	1808	A
53	DA	1816	C
53	DA	1829	A
53	DA	1858	A
53	DA	1859	U
53	DA	1870	C
53	DA	1871	A
53	DA	1872	A
53	DA	1873	G
53	DA	1874	C
53	DA	1876	A
53	DA	1880	U
53	DA	1886	U
53	DA	1906	G
53	DA	1907	G
53	DA	1913	A
53	DA	1914	C
53	DA	1929	G
53	DA	1930	G
53	DA	1931	U
53	DA	1937	A
53	DA	1938	A
53	DA	1955	U
53	DA	1967	C
53	DA	1970	A
53	DA	1972	G
53	DA	1991	U
53	DA	1993	U
53	DA	1997	C
53	DA	2023	C
53	DA	2031	A
53	DA	2033	A
53	DA	2043	C
53	DA	2055	C

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Mol	Chain	Res	Type
53	DA	2056	G
53	DA	2060	A
53	DA	2061	G
53	DA	2062	A
53	DA	2069	G7M
53	DA	2085	U
53	DA	2093	G
53	DA	2097	A
53	DA	2101	A
53	DA	2105	U
53	DA	2108	A
53	DA	2111	U
53	DA	2112	G
53	DA	2113	U
53	DA	2115	G
53	DA	2116	G
53	DA	2117	A
53	DA	2118	U
53	DA	2119	A
53	DA	2123	G
53	DA	2126	A
53	DA	2127	G
53	DA	2128	G
53	DA	2131	U
53	DA	2132	U
53	DA	2133	G
53	DA	2134	A
53	DA	2136	G
53	DA	2137	U
53	DA	2145	C
53	DA	2146	C
53	DA	2147	A
53	DA	2148	G
53	DA	2149	U
53	DA	2159	G
53	DA	2160	C
53	DA	2161	C
53	DA	2162	G
53	DA	2163	A
53	DA	2164	C
53	DA	2165	C
53	DA	2167	U

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Mol	Chain	Res	Type
53	DA	2168	G
53	DA	2169	A
53	DA	2170	A
53	DA	2171	A
53	DA	2172	U
53	DA	2173	A
53	DA	2177	C
53	DA	2178	C
53	DA	2179	C
53	DA	2181	U
53	DA	2185	U
53	DA	2187	U
53	DA	2188	U
53	DA	2190	G
53	DA	2198	A
53	DA	2204	G
53	DA	2211	A
53	DA	2225	A
53	DA	2238	G
53	DA	2239	G
53	DA	2268	A
53	DA	2283	C
53	DA	2286	G
53	DA	2287	A
53	DA	2305	U
53	DA	2308	G
53	DA	2324	U
53	DA	2325	G
53	DA	2327	A
53	DA	2333	A
53	DA	2335	A
53	DA	2339	C
53	DA	2347	C
53	DA	2383	G
53	DA	2385	C
53	DA	2406	A
53	DA	2407	A
53	DA	2424	C
53	DA	2425	A
53	DA	2431	U
53	DA	2434	A
53	DA	2435	A

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Mol	Chain	Res	Type
53	DA	2441	U
53	DA	2448	A
53	DA	2476	A
53	DA	2491	U
53	DA	2502	G
53	DA	2505	G
53	DA	2518	A
53	DA	2525	G
53	DA	2529	G
53	DA	2547	A
53	DA	2554	U
53	DA	2566	A
53	DA	2567	G
53	DA	2573	C
53	DA	2585	U
53	DA	2586	U
53	DA	2603	G
53	DA	2609	U
53	DA	2613	U
53	DA	2629	U
53	DA	2663	G
53	DA	2682	A
53	DA	2689	U
53	DA	2690	U
53	DA	2714	G
53	DA	2726	A
53	DA	2744	G
53	DA	2748	A
53	DA	2765	A
53	DA	2778	A
53	DA	2791	G
53	DA	2798	U
53	DA	2799	A
53	DA	2803	G
53	DA	2811	G
53	DA	2820	A
53	DA	2821	A
53	DA	2825	G
53	DA	2867	G
53	DA	2873	A
53	DA	2874	C
53	DA	2883	A

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Mol	Chain	Res	Type
53	DA	2891	U
53	DA	2894	G
23	DB	25	U
23	DB	35	C
23	DB	45	A
23	DB	56	G
23	DB	66	A
23	DB	89	U
23	DB	90	C
23	DB	109	A

All (77) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	209	U
1	AA	412	A
1	AA	429	U
1	AA	653	U
1	AA	793	U
1	AA	1024	G
1	AA	1031	C
1	AA	1211	U
1	BA	4	U
1	BA	83	C
1	BA	209	U
1	BA	429	U
1	BA	653	U
1	BA	793	U
1	BA	1028	C
1	BA	1183	U
1	BA	1211	U
1	BA	1493	A
22	CA	199	A
22	CA	271	G
22	CA	335	C
22	CA	404	A
22	CA	627	A
22	CA	645	C
22	CA	647	G
22	CA	764	A
22	CA	776	G

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Mol	Chain	Res	Type
22	CA	784	G
22	CA	846	U
22	CA	960	A
22	CA	984	A
22	CA	1128	G
22	CA	1142	A
22	CA	1379	U
22	CA	1647	U
22	CA	1730	C
22	CA	1738	G
22	CA	2118	U
22	CA	2146	C
22	CA	2162	G
22	CA	2225	A
22	CA	2286	G
22	CA	2324	U
22	CA	2326	C
22	CA	2406	A
22	CA	2425	A
22	CA	2585	U
22	CA	2680	U
22	CA	2873	A
22	CA	2903	U
53	DA	199	A
53	DA	627	A
53	DA	645	C
53	DA	764	A
53	DA	776	G
53	DA	784	G
53	DA	846	U
53	DA	859	G
53	DA	984	A
53	DA	1046	A
53	DA	1128	G
53	DA	1142	A
53	DA	1253	A
53	DA	1494	A
53	DA	1647	U
53	DA	1730	C
53	DA	1738	G
53	DA	1929	G
53	DA	2118	U

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Mol	Chain	Res	Type
53	DA	2127	G
53	DA	2130	U
53	DA	2158	A
53	DA	2324	U
53	DA	2406	A
53	DA	2585	U
53	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$
12	D2T	BL	89	12	8,9,10	0.95	0	6,11,13	2.18	3 (50%)
22	PSU	CA	1911	22	18,21,22	1.12	2 (11%)	21,30,33	1.83	4 (19%)
1	2MG	AA	1516	1	23,26,27	1.19	3 (13%)	33,38,41	2.23	10 (30%)
22	PSU	CA	2457	22	18,21,22	1.05	2 (11%)	21,30,33	2.03	5 (23%)
53	G7M	DA	2069	53	23,26,27	1.47	4 (17%)	34,39,42	1.66	5 (14%)
53	PSU	DA	2457	53	18,21,22	0.86	1 (5%)	21,30,33	1.53	3 (14%)
1	PSU	BA	516	1	18,21,22	1.02	2 (11%)	21,30,33	1.83	5 (23%)
1	2MG	BA	966	1	23,26,27	1.27	3 (13%)	33,38,41	2.27	5 (15%)
22	5MU	CA	747	22	19,22,23	1.31	4 (21%)	27,32,35	2.36	6 (22%)
1	4OC	BA	1402	1	20,23,24	0.81	0	25,32,35	1.07	2 (8%)
53	OMU	DA	2552	53	19,22,23	1.21	3 (15%)	25,31,34	1.85	6 (24%)
1	UR3	AA	1498	1	19,22,23	0.97	1 (5%)	26,32,35	1.90	5 (19%)
54	MEQ	DD	150[A]	54	8,9,10	0.94	0	5,10,12	1.38	2 (40%)
1	2MG	AA	1207	1	23,26,27	1.27	5 (21%)	33,38,41	2.17	8 (24%)
53	PSU	DA	955	53	18,21,22	1.15	1 (5%)	21,30,33	1.61	3 (14%)
53	2MG	DA	2445	53	23,26,27	1.32	2 (8%)	33,38,41	2.12	8 (24%)
53	PSU	DA	2580	53	18,21,22	0.81	1 (5%)	21,30,33	1.60	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	6MZ	CA	2030	22	22,25,26	1.60	4 (18%)	29,36,39	2.25	11 (37%)
53	5MC	DA	1962	53	19,22,23	1.48	3 (15%)	26,32,35	1.34	5 (19%)
1	5MC	AA	967	1	19,22,23	1.53	2 (10%)	26,32,35	1.12	3 (11%)
22	5MU	CA	1939	22	19,22,23	1.34	3 (15%)	27,32,35	2.10	6 (22%)
53	OMG	DA	2251	53	23,26,27	1.18	3 (13%)	32,38,41	1.95	7 (21%)
1	UR3	BA	1498	1	19,22,23	1.04	1 (5%)	26,32,35	1.73	3 (11%)
1	MA6	AA	1518	1	23,26,27	1.50	5 (21%)	33,38,41	1.98	8 (24%)
22	2MG	CA	2445	22	23,26,27	1.27	3 (13%)	33,38,41	2.17	8 (24%)
1	MA6	BA	1519	1	23,26,27	1.43	5 (21%)	33,38,41	2.24	12 (36%)
53	3TD	DA	1915	53	19,22,23	1.61	3 (15%)	23,32,35	2.18	3 (13%)
53	5MU	DA	1939	53	19,22,23	1.38	4 (21%)	27,32,35	1.99	7 (25%)
22	PSU	CA	2605	22	18,21,22	0.97	2 (11%)	21,30,33	2.00	4 (19%)
53	H2U	DA	2449	53	18,21,22	1.31	2 (11%)	19,30,33	1.51	4 (21%)
34	4D4	DN	81[A]	-	9,11,12	2.10	2 (22%)	7,13,15	0.93	0
1	5MC	BA	1407	1	19,22,23	1.92	2 (10%)	26,32,35	1.14	3 (11%)
53	PSU	DA	2604	53	18,21,22	1.05	1 (5%)	21,30,33	1.75	5 (23%)
53	PSU	DA	2605	53	18,21,22	0.97	1 (5%)	21,30,33	1.78	3 (14%)
22	G7M	CA	2069	22	23,26,27	1.51	3 (13%)	34,39,42	1.75	5 (14%)
22	PSU	CA	955	22	18,21,22	0.98	1 (5%)	21,30,33	1.81	3 (14%)
12	D2T	AL	89	12	8,9,10	2.48	2 (25%)	6,11,13	1.57	2 (33%)
53	6MZ	DA	2030	53	22,25,26	1.41	6 (27%)	29,36,39	2.16	12 (41%)
53	PSU	DA	1911	53	18,21,22	1.00	1 (5%)	21,30,33	1.90	4 (19%)
1	2MG	BA	1516	1	23,26,27	1.27	4 (17%)	33,38,41	2.37	12 (36%)
1	5MC	AA	1407	1	19,22,23	1.91	2 (10%)	26,32,35	1.14	2 (7%)
53	PSU	DA	1917	53	18,21,22	1.04	2 (11%)	21,30,33	1.90	5 (23%)
53	2MA	DA	2503	56,53	22,25,26	1.26	5 (22%)	32,37,40	2.39	9 (28%)
22	PSU	CA	1917	22	18,21,22	1.08	1 (5%)	21,30,33	1.69	4 (19%)
1	MA6	AA	1519	1	23,26,27	1.43	5 (21%)	33,38,41	2.07	10 (30%)
22	PSU	CA	2504	22	18,21,22	1.07	2 (11%)	21,30,33	1.96	5 (23%)
22	OMG	CA	2251	22	23,26,27	1.19	1 (4%)	32,38,41	2.01	7 (21%)
1	4OC	AA	1402	1	20,23,24	0.78	0	25,32,35	0.97	1 (4%)
53	PSU	DA	2504	53	18,21,22	0.91	0	21,30,33	1.64	3 (14%)
54	MEQ	DD	150[B]	54	8,9,10	1.24	1 (12%)	5,10,12	1.03	0
22	3TD	CA	1915	22	19,22,23	1.61	3 (15%)	23,32,35	2.14	5 (21%)
53	1MG	DA	745	53	23,26,27	1.14	3 (13%)	33,39,42	1.74	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	5MU	DA	747	53	19,22,23	1.48	4 (21%)	27,32,35	2.33	6 (22%)
1	G7M	BA	527	1	23,26,27	1.56	3 (13%)	34,39,42	1.79	4 (11%)
22	OMC	CA	2498	22,56	19,22,23	0.80	0	25,31,34	0.87	1 (4%)
22	2MG	CA	1835	22	23,26,27	1.29	4 (17%)	33,38,41	2.14	6 (18%)
34	4D4	CN	81	34	9,11,12	2.16	2 (22%)	7,13,15	0.69	0
53	6MZ	DA	1618	53	22,25,26	1.55	5 (22%)	29,36,39	2.11	10 (34%)
53	OMC	DA	2498	56,53	19,22,23	0.91	1 (5%)	25,31,34	1.08	1 (4%)
22	1MG	CA	745	22	23,26,27	1.26	3 (13%)	33,39,42	1.86	5 (15%)
22	PSU	CA	2580	22	18,21,22	1.07	2 (11%)	21,30,33	1.99	6 (28%)
22	5MC	CA	1962	22	19,22,23	1.68	3 (15%)	26,32,35	1.19	2 (7%)
22	6MZ	CA	1618	22	22,25,26	1.57	3 (13%)	29,36,39	2.31	11 (37%)
53	2MG	DA	1835	53	23,26,27	1.03	2 (8%)	33,38,41	2.57	11 (33%)
22	PSU	CA	746	22,56	18,21,22	1.24	1 (5%)	21,30,33	2.06	5 (23%)
34	4D4	DN	81[B]	-	9,11,12	2.02	2 (22%)	7,13,15	0.74	0
1	PSU	AA	516	56,1	18,21,22	0.96	2 (11%)	21,30,33	2.02	4 (19%)
1	2MG	AA	966	1	23,26,27	1.24	2 (8%)	33,38,41	2.12	8 (24%)
1	2MG	BA	1207	1	23,26,27	1.20	3 (13%)	33,38,41	2.26	8 (24%)
53	PSU	DA	746	56,53	18,21,22	1.25	4 (22%)	21,30,33	2.22	5 (23%)
1	MA6	BA	1518	1	23,26,27	1.47	5 (21%)	33,38,41	2.07	8 (24%)
1	5MC	BA	967	1	19,22,23	1.72	3 (15%)	26,32,35	1.07	2 (7%)
22	OMU	CA	2552	22	19,22,23	1.17	2 (10%)	25,31,34	1.81	5 (20%)
22	2MA	CA	2503	22	22,25,26	1.68	4 (18%)	32,37,40	2.27	9 (28%)
1	G7M	AA	527	1	23,26,27	1.44	5 (21%)	34,39,42	1.84	5 (14%)

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
12	D2T	BL	89	12	-	4/7/12/14	-
22	PSU	CA	1911	22	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3
22	PSU	CA	2457	22	-	0/7/25/26	0/2/2/2
53	G7M	DA	2069	53	-	2/7/25/26	0/3/3/3
53	PSU	DA	2457	53	-	0/7/25/26	0/2/2/2
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	BA	966	1	-	0/9/27/28	0/3/3/3
22	5MU	CA	747	22	-	0/7/25/26	0/2/2/2
1	4OC	BA	1402	1	-	3/9/29/30	0/2/2/2
53	OMU	DA	2552	53	-	0/9/27/28	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
54	MEQ	DD	150[A]	54	-	2/8/9/11	-
1	2MG	AA	1207	1	-	0/9/27/28	0/3/3/3
53	PSU	DA	955	53	-	0/7/25/26	0/2/2/2
53	2MG	DA	2445	53	-	0/9/27/28	0/3/3/3
53	PSU	DA	2580	53	-	0/7/25/26	0/2/2/2
22	6MZ	CA	2030	22	-	2/9/27/28	0/3/3/3
53	5MC	DA	1962	53	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
22	5MU	CA	1939	22	-	0/7/25/26	0/2/2/2
53	OMG	DA	2251	53	-	0/9/27/28	0/3/3/3
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/11/29/30	0/3/3/3
22	2MG	CA	2445	22	-	0/9/27/28	0/3/3/3
1	MA6	BA	1519	1	-	2/11/29/30	0/3/3/3
53	3TD	DA	1915	53	-	0/7/25/26	0/2/2/2
53	5MU	DA	1939	53	-	0/7/25/26	0/2/2/2
22	PSU	CA	2605	22	-	0/7/25/26	0/2/2/2
53	H2U	DA	2449	53	-	0/7/38/39	0/2/2/2
34	4D4	DN	81[A]	-	-	0/11/12/14	-
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
53	PSU	DA	2604	53	-	0/7/25/26	0/2/2/2
53	PSU	DA	2605	53	-	0/7/25/26	0/2/2/2
22	G7M	CA	2069	22	-	1/7/25/26	0/3/3/3
22	PSU	CA	955	22	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	1/7/12/14	-
53	6MZ	DA	2030	53	-	2/9/27/28	0/3/3/3
53	PSU	DA	1911	53	-	0/7/25/26	0/2/2/2
1	2MG	BA	1516	1	-	0/9/27/28	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
53	PSU	DA	1917	53	-	0/7/25/26	0/2/2/2
53	2MA	DA	2503	56,53	-	1/7/25/26	0/3/3/3
22	PSU	CA	1917	22	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	1/11/29/30	0/3/3/3
22	PSU	CA	2504	22	-	0/7/25/26	0/2/2/2
22	OMG	CA	2251	22	-	1/9/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	PSU	DA	2504	53	-	0/7/25/26	0/2/2/2
54	MEQ	DD	150[B]	54	-	4/8/9/11	-
22	3TD	CA	1915	22	-	2/7/25/26	0/2/2/2
53	1MG	DA	745	53	-	0/7/25/26	0/3/3/3
53	5MU	DA	747	53	-	1/7/25/26	0/2/2/2
1	G7M	BA	527	1	-	2/7/25/26	0/3/3/3
22	OMC	CA	2498	22,56	-	0/9/27/28	0/2/2/2
22	2MG	CA	1835	22	-	2/9/27/28	0/3/3/3
34	4D4	CN	81	34	-	6/11/12/14	-
53	6MZ	DA	1618	53	-	0/9/27/28	0/3/3/3
53	OMC	DA	2498	56,53	-	1/9/27/28	0/2/2/2
22	1MG	CA	745	22	-	0/7/25/26	0/3/3/3
22	PSU	CA	2580	22	-	0/7/25/26	0/2/2/2
22	5MC	CA	1962	22	-	0/7/25/26	0/2/2/2
22	6MZ	CA	1618	22	-	0/9/27/28	0/3/3/3
53	2MG	DA	1835	53	-	0/9/27/28	0/3/3/3
22	PSU	CA	746	22,56	-	2/7/25/26	0/2/2/2
34	4D4	DN	81[B]	-	-	5/11/12/14	-
1	PSU	AA	516	56,1	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	2/9/27/28	0/3/3/3
1	2MG	BA	1207	1	-	0/9/27/28	0/3/3/3
53	PSU	DA	746	56,53	-	2/7/25/26	0/2/2/2
1	MA6	BA	1518	1	-	1/11/29/30	0/3/3/3
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
22	OMU	CA	2552	22	-	1/9/27/28	0/2/2/2
22	2MA	CA	2503	22	-	1/7/25/26	0/3/3/3
1	G7M	AA	527	1	-	0/7/25/26	0/3/3/3

All (187) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	1407	5MC	C5-C4	7.09	1.49	1.44
1	AA	1407	5MC	C5-C4	7.02	1.49	1.44
1	BA	967	5MC	C5-C4	6.25	1.48	1.44
22	CA	1962	5MC	C5-C4	6.12	1.48	1.44
12	AL	89	D2T	CB-CA	5.75	1.56	1.54
22	CA	2503	2MA	C5-C4	5.34	1.48	1.39
1	AA	967	5MC	C5-C4	5.17	1.48	1.44
22	CA	2030	6MZ	C5-C4	4.89	1.47	1.39
22	CA	1618	6MZ	C5-C4	4.88	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	DA	1962	5MC	C5-C4	4.86	1.47	1.44
34	CN	81	4D4	CZ-NE	4.70	1.42	1.33
53	DA	2069	G7M	C5-N7	-4.69	1.33	1.39
34	DN	81[A]	4D4	CZ-NE	4.55	1.42	1.33
22	CA	2069	G7M	C5-N7	-4.53	1.34	1.39
1	AA	1518	MA6	C5-C4	4.51	1.47	1.39
1	BA	527	G7M	C5-N7	-4.49	1.34	1.39
1	BA	1518	MA6	C5-C4	4.48	1.47	1.39
53	DA	1618	6MZ	C5-C4	4.47	1.47	1.39
34	DN	81[B]	4D4	CZ-NE	4.43	1.41	1.33
1	AA	527	G7M	C5-N7	-4.37	1.34	1.39
53	DA	1915	3TD	C6-C5	4.22	1.40	1.35
1	BA	1519	MA6	C5-C4	4.22	1.46	1.39
22	CA	746	PSU	C6-C5	4.04	1.39	1.35
1	AA	1519	MA6	C5-C4	3.99	1.46	1.39
22	CA	1911	PSU	C6-C5	3.87	1.39	1.35
22	CA	1915	3TD	C10-N3	3.76	1.53	1.47
22	CA	1917	PSU	C6-C5	3.74	1.39	1.35
53	DA	2449	H2U	C2-N1	3.70	1.40	1.35
53	DA	747	5MU	C4-N3	-3.69	1.31	1.38
53	DA	955	PSU	C6-C5	3.60	1.39	1.35
53	DA	1915	3TD	C10-N3	3.47	1.53	1.47
22	CA	1939	5MU	C6-C5	3.42	1.40	1.34
22	CA	2069	G7M	C5-C4	3.40	1.46	1.38
53	DA	1911	PSU	C6-C5	3.38	1.39	1.35
22	CA	2251	OMG	C5-C4	3.36	1.48	1.38
53	DA	2503	2MA	C5-C4	3.35	1.45	1.39
1	AA	1518	MA6	C5-N7	-3.34	1.33	1.39
1	BA	1516	2MG	C5-C4	3.33	1.47	1.38
53	DA	2030	6MZ	C5-C4	3.29	1.45	1.39
22	CA	2445	2MG	C5-C4	3.29	1.47	1.38
1	BA	527	G7M	C6-N1	-3.27	1.32	1.38
22	CA	745	1MG	C5-C4	3.27	1.47	1.38
22	CA	1915	3TD	C6-C5	3.26	1.38	1.35
1	AA	966	2MG	C5-C4	3.24	1.47	1.38
53	DA	1917	PSU	C6-C5	3.24	1.38	1.35
1	BA	966	2MG	C5-C4	3.21	1.47	1.38
1	BA	1407	5MC	C6-C5	3.19	1.39	1.34
53	DA	2604	PSU	C4-C5	-3.19	1.35	1.44
22	CA	2580	PSU	C6-C5	3.18	1.38	1.35
34	CN	81	4D4	CZ-NH2	3.14	1.43	1.32
22	CA	1618	6MZ	C5-C6	3.14	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CA	1835	2MG	C5-C4	3.12	1.47	1.38
53	DA	2445	2MG	C5-C4	3.12	1.47	1.38
22	CA	2030	6MZ	C5-C6	3.10	1.49	1.41
22	CA	2504	PSU	C6-C5	3.09	1.38	1.35
1	BA	1207	2MG	C5-C4	3.06	1.47	1.38
1	AA	1407	5MC	C6-C5	3.05	1.39	1.34
1	AA	967	5MC	C6-C5	3.04	1.39	1.34
1	AA	1207	2MG	C5-C4	3.04	1.47	1.38
53	DA	747	5MU	C6-C5	3.02	1.39	1.34
1	BA	527	G7M	C5-C4	2.99	1.45	1.38
53	DA	2251	OMG	C5-C4	2.91	1.46	1.38
1	AA	1516	2MG	C5-C4	2.90	1.46	1.38
1	BA	967	5MC	C6-C5	2.89	1.39	1.34
22	CA	2457	PSU	C6-C5	2.88	1.38	1.35
53	DA	745	1MG	C5-C4	2.87	1.46	1.38
1	AA	1519	MA6	C8-N7	2.87	1.37	1.31
22	CA	1618	6MZ	C8-N7	2.85	1.37	1.31
34	DN	81[A]	4D4	CZ-NH2	2.83	1.42	1.32
1	BA	1518	MA6	C5-C6	2.82	1.48	1.41
53	DA	2445	2MG	C6-N1	-2.82	1.33	1.38
53	DA	1915	3TD	C4-N3	-2.79	1.34	1.40
1	AA	516	PSU	C6-C5	2.77	1.38	1.35
22	CA	2503	2MA	C5-C6	2.76	1.48	1.41
1	BA	516	PSU	C6-C5	2.76	1.38	1.35
22	CA	2503	2MA	C8-N7	2.74	1.37	1.31
53	DA	1962	5MC	C6-C5	2.74	1.39	1.34
22	CA	955	PSU	C6-C5	2.73	1.38	1.35
34	DN	81[B]	4D4	CZ-NH2	2.72	1.42	1.32
53	DA	2605	PSU	C4-C5	-2.72	1.36	1.44
53	DA	1939	5MU	C6-N1	-2.70	1.33	1.38
12	AL	89	D2T	CB-SB	2.70	1.85	1.82
53	DA	1618	6MZ	C8-N9	-2.69	1.33	1.37
53	DA	2457	PSU	C4-C5	-2.66	1.37	1.44
53	DA	747	5MU	C6-N1	-2.65	1.33	1.38
53	DA	1939	5MU	C6-C5	2.65	1.38	1.34
53	DA	1618	6MZ	C5-C6	2.64	1.48	1.41
22	CA	1915	3TD	C4-N3	-2.63	1.35	1.40
22	CA	747	5MU	C4-C5	2.62	1.49	1.44
22	CA	747	5MU	C6-C5	2.61	1.38	1.34
22	CA	2030	6MZ	C8-N7	2.60	1.36	1.31
22	CA	745	1MG	C2-N1	2.60	1.42	1.37
54	DD	150[B]	MEQ	OE1-CD	2.60	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	DA	2069	G7M	C5-C4	2.59	1.44	1.38
1	BA	966	2MG	C6-N1	-2.58	1.34	1.38
1	AA	527	G7M	C5-C4	2.58	1.44	1.38
1	BA	1519	MA6	C5-C6	2.57	1.48	1.41
53	DA	1939	5MU	C4-N3	-2.56	1.34	1.38
1	AA	1519	MA6	C5-C6	2.54	1.47	1.41
22	CA	2605	PSU	C6-C5	2.53	1.38	1.35
53	DA	2552	OMU	C4-N3	-2.51	1.34	1.38
53	DA	2069	G7M	C4-N9	-2.49	1.31	1.38
1	BA	1516	2MG	C2-N3	2.49	1.36	1.32
22	CA	2552	OMU	C4-N3	-2.48	1.34	1.38
22	CA	1939	5MU	C4-C5	2.46	1.48	1.44
53	DA	746	PSU	C4-C5	-2.45	1.37	1.44
22	CA	1835	2MG	C2-N3	2.43	1.36	1.32
53	DA	2030	6MZ	C8-N7	2.43	1.36	1.31
53	DA	1618	6MZ	C8-N7	2.43	1.36	1.31
53	DA	1939	5MU	C2-N3	-2.41	1.33	1.38
53	DA	1962	5MC	C6-N1	-2.40	1.33	1.38
22	CA	2605	PSU	C4-C5	-2.40	1.37	1.44
53	DA	2552	OMU	C2-N3	-2.40	1.33	1.38
1	AA	966	2MG	C2-N3	2.39	1.36	1.32
1	AA	527	G7M	C6-N1	-2.39	1.34	1.38
1	BA	966	2MG	C2-N3	2.39	1.36	1.32
1	AA	1518	MA6	C4-N9	-2.37	1.32	1.37
1	BA	1518	MA6	C8-N7	2.37	1.36	1.31
22	CA	2504	PSU	C4-C5	-2.37	1.37	1.44
53	DA	1618	6MZ	C5-N7	-2.36	1.34	1.39
53	DA	2030	6MZ	C8-N9	-2.34	1.33	1.37
1	AA	1207	2MG	C5-N7	-2.34	1.34	1.39
22	CA	1962	5MC	C6-C5	2.34	1.38	1.34
53	DA	2449	H2U	C4-N3	-2.33	1.33	1.37
22	CA	2580	PSU	C4-C5	-2.33	1.37	1.44
53	DA	1835	2MG	C5-C4	2.32	1.45	1.38
1	AA	516	PSU	C4-C5	-2.31	1.37	1.44
22	CA	2030	6MZ	C4-N9	-2.31	1.32	1.37
53	DA	2503	2MA	C5-N7	-2.31	1.34	1.39
22	CA	1835	2MG	C6-N1	-2.31	1.34	1.38
1	BA	1516	2MG	C6-N1	-2.30	1.34	1.38
53	DA	2030	6MZ	C5-C6	2.30	1.47	1.41
53	DA	2580	PSU	C4-C5	-2.29	1.38	1.44
53	DA	2503	2MA	C8-N7	2.29	1.36	1.31
1	AA	1207	2MG	C2-N3	2.29	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1516	2MG	C2-N3	2.28	1.36	1.32
1	BA	1519	MA6	C8-N7	2.28	1.36	1.31
53	DA	745	1MG	C4-N9	-2.28	1.32	1.38
53	DA	2503	2MA	C4-N9	-2.28	1.33	1.37
22	CA	1962	5MC	C6-N1	-2.26	1.34	1.38
22	CA	2445	2MG	C2-N3	2.26	1.36	1.32
1	AA	1207	2MG	C6-N1	-2.25	1.34	1.38
1	BA	1519	MA6	C5-N7	-2.25	1.35	1.39
53	DA	2498	OMC	C6-N1	-2.24	1.32	1.38
1	BA	516	PSU	C4-C5	-2.24	1.38	1.44
1	AA	1518	MA6	C8-N7	2.23	1.36	1.31
53	DA	2552	OMU	C5-C4	-2.22	1.38	1.43
53	DA	746	PSU	C6-C5	2.22	1.37	1.35
53	DA	2251	OMG	C6-N1	-2.22	1.34	1.38
53	DA	1835	2MG	C6-N1	-2.20	1.34	1.38
22	CA	2503	2MA	C4-N3	2.20	1.37	1.34
1	BA	1207	2MG	C2-N3	2.19	1.36	1.32
1	AA	1519	MA6	C5-N7	-2.19	1.35	1.39
53	DA	1917	PSU	C4-C5	-2.16	1.38	1.44
22	CA	745	1MG	C2-N3	2.16	1.37	1.33
53	DA	746	PSU	O4'-C1'	-2.16	1.40	1.43
1	AA	1516	2MG	C6-N1	-2.16	1.34	1.38
1	BA	1518	MA6	C4-N9	-2.16	1.33	1.37
22	CA	1835	2MG	C5-N7	-2.13	1.34	1.39
22	CA	2445	2MG	C6-N1	-2.13	1.34	1.38
53	DA	2251	OMG	C4-N9	-2.13	1.32	1.38
22	CA	747	5MU	C6-N1	-2.12	1.34	1.38
53	DA	747	5MU	C4-C5	2.12	1.48	1.44
1	BA	1518	MA6	C5-N7	-2.12	1.35	1.39
22	CA	1911	PSU	C4-C5	-2.11	1.38	1.44
22	CA	2457	PSU	C4-C5	-2.11	1.38	1.44
1	BA	1516	2MG	C5-N7	-2.09	1.34	1.39
1	BA	1498	UR3	C5-C4	-2.08	1.38	1.43
1	AA	1207	2MG	C4-N9	-2.08	1.32	1.38
1	BA	967	5MC	C6-N1	-2.07	1.34	1.38
1	AA	1518	MA6	C5-C6	2.07	1.46	1.41
22	CA	2552	OMU	C2-N1	2.07	1.41	1.38
53	DA	745	1MG	C5-N7	-2.07	1.34	1.39
53	DA	2069	G7M	C6-N1	-2.06	1.35	1.38
53	DA	746	PSU	C2'-C1'	-2.06	1.50	1.53
53	DA	2030	6MZ	C6-N6	2.05	1.36	1.34
22	CA	747	5MU	C2-N3	-2.05	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	1207	2MG	C6-N1	-2.05	1.35	1.38
1	AA	527	G7M	C5-C6	2.04	1.48	1.43
1	BA	1519	MA6	C4-N9	-2.04	1.33	1.37
22	CA	1939	5MU	C4-N3	-2.04	1.35	1.38
1	AA	527	G7M	C4-N9	-2.03	1.32	1.38
1	AA	1519	MA6	C4-N9	-2.02	1.33	1.37
1	AA	1498	UR3	C5-C4	-2.02	1.38	1.43
53	DA	2503	2MA	C5-C6	2.01	1.46	1.41
53	DA	2030	6MZ	C5-N7	-2.01	1.35	1.39
22	CA	2069	G7M	C5-C6	2.00	1.48	1.43

All (395) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	1915	3TD	N1-C2-N3	8.35	122.20	116.13
53	DA	1835	2MG	C2-N3-C4	8.25	122.32	112.00
22	CA	1915	3TD	N1-C2-N3	7.77	121.78	116.13
1	BA	966	2MG	C2-N3-C4	7.48	121.36	112.00
53	DA	2503	2MA	C5-C4-N3	-7.35	119.44	127.18
1	BA	1207	2MG	C2-N3-C4	7.28	121.10	112.00
22	CA	1835	2MG	C2-N3-C4	7.22	121.03	112.00
1	BA	1516	2MG	C2-N3-C4	7.18	120.98	112.00
22	CA	2503	2MA	C5-C4-N3	-7.09	119.71	127.18
22	CA	2445	2MG	C2-N3-C4	7.01	120.77	112.00
1	AA	1498	UR3	C4-N3-C2	-7.00	118.95	124.58
1	AA	1207	2MG	C2-N3-C4	6.83	120.54	112.00
1	BA	1516	2MG	C5-C4-N3	-6.65	117.81	128.39
1	AA	966	2MG	C2-N3-C4	6.65	120.31	112.00
1	AA	1516	2MG	C2-N3-C4	6.49	120.12	112.00
53	DA	2445	2MG	C2-N3-C4	6.48	120.11	112.00
1	BA	966	2MG	C5-C4-N3	-6.46	118.10	128.39
53	DA	746	PSU	N1-C2-N3	6.24	121.75	115.17
1	BA	1498	UR3	C4-N3-C2	-6.23	119.56	124.58
53	DA	1835	2MG	C5-C4-N3	-6.09	118.70	128.39
22	CA	1835	2MG	C5-C4-N3	-6.03	118.79	128.39
22	CA	2503	2MA	N3-C4-N9	6.01	134.62	126.99
53	DA	747	5MU	N3-C2-N1	5.96	122.65	114.89
22	CA	745	1MG	C5-C4-N3	-5.93	118.95	128.39
22	CA	2445	2MG	C5-C4-N3	-5.87	119.05	128.39
22	CA	747	5MU	C4-N3-C2	-5.83	119.69	127.34
53	DA	2503	2MA	N3-C4-N9	5.79	134.33	126.99
22	CA	2251	OMG	C5-C4-N3	-5.74	119.25	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1516	2MG	C5-C4-N3	-5.73	119.28	128.39
1	BA	527	G7M	C5-C4-N3	-5.71	117.36	128.15
1	AA	966	2MG	C5-C4-N3	-5.69	119.33	128.39
1	AA	1518	MA6	C5-C4-N3	-5.68	118.89	126.72
53	DA	747	5MU	C4-N3-C2	-5.59	120.01	127.34
1	AA	1207	2MG	C5-C4-N3	-5.59	119.50	128.39
1	BA	1518	MA6	C5-C4-N3	-5.58	119.03	126.72
53	DA	2251	OMG	C5-C4-N3	-5.57	119.53	128.39
22	CA	746	PSU	N1-C2-N3	5.55	121.02	115.17
1	BA	1207	2MG	C5-C4-N3	-5.53	119.58	128.39
22	CA	2069	G7M	N9-C4-N3	5.47	136.89	125.95
1	BA	527	G7M	N9-C4-N3	5.42	136.80	125.95
53	DA	1911	PSU	C4-N3-C2	-5.40	118.93	126.37
53	DA	2445	2MG	C5-C4-N3	-5.27	120.00	128.39
53	DA	1939	5MU	N3-C2-N1	5.26	121.74	114.89
22	CA	1618	6MZ	C5-C4-N3	-5.25	119.49	126.72
1	AA	527	G7M	C2-N3-C4	5.18	121.22	112.30
22	CA	2069	G7M	C5-C4-N3	-5.15	118.42	128.15
22	CA	747	5MU	N3-C2-N1	5.14	121.58	114.89
1	AA	516	PSU	C4-N3-C2	-5.13	119.30	126.37
22	CA	1939	5MU	N3-C2-N1	5.13	121.57	114.89
22	CA	955	PSU	C4-N3-C2	-5.09	119.36	126.37
1	AA	1519	MA6	C5-C4-N3	-5.08	119.73	126.72
1	AA	527	G7M	C5-C4-N3	-5.07	118.56	128.15
53	DA	1618	6MZ	C5-C4-N3	-5.05	119.76	126.72
53	DA	2605	PSU	C4-N3-C2	-5.05	119.41	126.37
53	DA	2503	2MA	N6-C6-N1	5.04	123.83	117.03
1	BA	1519	MA6	C5-C4-N3	-5.04	119.78	126.72
53	DA	745	1MG	C5-C4-N3	-5.03	120.39	128.39
53	DA	2552	OMU	C4-N3-C2	-5.02	120.38	126.61
53	DA	747	5MU	O2-C2-N1	-5.02	116.27	122.80
1	BA	1516	2MG	N9-C4-N3	5.00	135.96	125.95
53	DA	746	PSU	C4-N3-C2	-4.99	119.50	126.37
53	DA	2030	6MZ	C5-C4-N3	-4.97	119.87	126.72
22	CA	2457	PSU	N1-C2-N3	4.97	120.41	115.17
22	CA	2605	PSU	C4-N3-C2	-4.97	119.53	126.37
22	CA	747	5MU	O4-C4-C5	-4.93	119.28	124.92
53	DA	2069	G7M	N9-C4-N3	4.90	135.75	125.95
22	CA	2504	PSU	C4-N3-C2	-4.89	119.63	126.37
22	CA	1939	5MU	C4-N3-C2	-4.87	120.95	127.34
22	CA	2580	PSU	C4-N3-C2	-4.86	119.67	126.37
22	CA	1911	PSU	C4-N3-C2	-4.85	119.69	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CA	2552	OMU	C4-N3-C2	-4.85	120.59	126.61
22	CA	746	PSU	C4-N3-C2	-4.81	119.75	126.37
53	DA	1835	2MG	N1-C2-N2	4.80	121.46	116.56
22	CA	2457	PSU	C4-N3-C2	-4.79	119.77	126.37
22	CA	1618	6MZ	C6-C5-N7	4.76	137.62	132.43
1	AA	527	G7M	N9-C4-N3	4.76	135.47	125.95
1	BA	966	2MG	N9-C4-N3	4.76	135.47	125.95
22	CA	2251	OMG	C2-N3-C4	4.75	120.48	112.30
22	CA	745	1MG	C2-N3-C4	4.73	122.62	111.98
22	CA	2030	6MZ	C5-C4-N3	-4.72	120.21	126.72
1	BA	527	G7M	C2-N3-C4	4.72	120.43	112.30
53	DA	745	1MG	C2-N3-C4	4.72	122.58	111.98
22	CA	2030	6MZ	C6-C5-N7	4.70	137.55	132.43
22	CA	2251	OMG	N9-C4-N3	4.70	135.35	125.95
22	CA	747	5MU	C5-C4-N3	4.70	119.41	115.32
22	CA	2580	PSU	N1-C2-N3	4.69	120.12	115.17
53	DA	2604	PSU	C4-N3-C2	-4.68	119.92	126.37
22	CA	2605	PSU	N1-C2-N3	4.68	120.11	115.17
22	CA	2504	PSU	N1-C2-N3	4.68	120.10	115.17
22	CA	745	1MG	N9-C4-N3	4.63	135.21	125.95
22	CA	2069	G7M	C2-N3-C4	4.62	120.25	112.30
53	DA	1917	PSU	N1-C2-N3	4.59	120.00	115.17
1	AA	516	PSU	O2-C2-N1	-4.58	118.07	122.79
1	AA	516	PSU	N1-C2-N3	4.57	119.99	115.17
22	CA	1911	PSU	N1-C2-N3	4.51	119.93	115.17
22	CA	1835	2MG	N9-C4-N3	4.51	134.97	125.95
53	DA	1911	PSU	N1-C2-N3	4.51	119.92	115.17
53	DA	1939	5MU	C4-N3-C2	-4.49	121.45	127.34
53	DA	1917	PSU	C4-N3-C2	-4.48	120.20	126.37
53	DA	2069	G7M	C2-N3-C4	4.46	119.98	112.30
22	CA	1917	PSU	C4-N3-C2	-4.44	120.25	126.37
1	AA	1516	2MG	N9-C4-N3	4.44	134.84	125.95
53	DA	2251	OMG	C2-N3-C4	4.43	119.93	112.30
1	BA	516	PSU	C4-N3-C2	-4.41	120.29	126.37
22	CA	1939	5MU	O2-C2-N1	-4.41	117.06	122.80
1	AA	1518	MA6	N3-C4-N9	4.37	134.60	127.17
1	BA	1519	MA6	C2-N1-C6	4.34	122.44	111.83
22	CA	747	5MU	C5-C6-N1	-4.34	118.59	123.31
1	BA	516	PSU	N1-C2-N3	4.33	119.74	115.17
22	CA	955	PSU	N1-C2-N3	4.32	119.73	115.17
53	DA	2457	PSU	C4-N3-C2	-4.31	120.44	126.37
53	DA	1835	2MG	N9-C4-N3	4.31	134.56	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	747	5MU	C5-C4-N3	4.30	119.06	115.32
1	AA	966	2MG	N9-C4-N3	4.29	134.53	125.95
1	BA	1519	MA6	N3-C4-N9	4.28	134.45	127.17
53	DA	2069	G7M	C5-C4-N3	-4.27	120.08	128.15
1	BA	1518	MA6	N3-C4-N9	4.24	134.38	127.17
1	AA	1207	2MG	N9-C4-N3	4.22	134.39	125.95
22	CA	1917	PSU	N1-C2-N3	4.22	119.62	115.17
53	DA	2251	OMG	N9-C4-N3	4.21	134.37	125.95
53	DA	2504	PSU	C4-N3-C2	-4.21	120.58	126.37
22	CA	1939	5MU	C5-C4-N3	4.19	118.97	115.32
22	CA	1939	5MU	O4-C4-C5	-4.18	120.14	124.92
22	CA	2552	OMU	N3-C2-N1	4.17	120.32	114.89
53	DA	2552	OMU	N3-C2-N1	4.16	120.31	114.89
1	BA	1518	MA6	C2-N1-C6	4.15	121.97	111.83
53	DA	2605	PSU	N1-C2-N3	4.15	119.54	115.17
22	CA	1618	6MZ	C4-C5-N7	-4.13	105.86	110.58
1	AA	1519	MA6	C2-N1-C6	4.13	121.92	111.83
53	DA	1618	6MZ	N3-C4-N9	4.12	134.17	127.17
22	CA	747	5MU	O2-C2-N1	-4.11	117.44	122.80
22	CA	2445	2MG	N9-C4-N3	4.09	134.13	125.95
1	BA	1207	2MG	N9-C4-N3	4.08	134.12	125.95
22	CA	2552	OMU	C5-C4-N3	4.06	120.49	114.80
22	CA	2030	6MZ	C4-C5-N7	-4.01	106.00	110.58
53	DA	2030	6MZ	N1-C2-N3	-3.99	122.54	128.58
22	CA	2503	2MA	N6-C6-N1	3.98	122.40	117.03
22	CA	1915	3TD	C4-N3-C2	-3.97	120.41	124.61
1	BA	1519	MA6	N1-C2-N3	-3.96	122.58	128.58
53	DA	2580	PSU	C4-N3-C2	-3.96	120.91	126.37
1	BA	1207	2MG	C6-C5-N7	3.94	137.47	130.29
53	DA	2030	6MZ	C6-C5-N7	3.94	136.73	132.43
53	DA	1939	5MU	O4-C4-C5	-3.93	120.42	124.92
1	AA	1519	MA6	C4-C5-N7	-3.92	106.10	110.58
1	AA	1518	MA6	C2-N1-C6	3.91	121.39	111.83
53	DA	2445	2MG	C6-C5-N7	3.91	137.40	130.29
53	DA	2552	OMU	C5-C4-N3	3.86	120.21	114.80
1	BA	1518	MA6	C2-N3-C4	3.81	121.14	111.83
53	DA	1618	6MZ	C4-C5-N7	-3.79	106.25	110.58
53	DA	2504	PSU	N1-C2-N3	3.74	119.11	115.17
53	DA	1915	3TD	C4-N3-C2	-3.73	120.67	124.61
22	CA	1618	6MZ	C2-N3-C4	3.72	120.92	111.83
1	BA	1519	MA6	C4-N9-C8	3.71	109.64	105.74
22	CA	1618	6MZ	N3-C4-N9	3.69	133.44	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	1519	MA6	C2-N3-C4	3.67	120.81	111.83
1	BA	1518	MA6	N1-C2-N3	-3.66	123.04	128.58
53	DA	2030	6MZ	N3-C4-N9	3.66	133.39	127.17
53	DA	2503	2MA	C4-N9-C8	3.65	109.57	105.74
22	CA	1962	5MC	C5-C6-N1	-3.64	119.36	123.31
1	BA	1498	UR3	C5-C4-N3	3.64	119.83	115.04
1	AA	1407	5MC	C5-C4-N3	-3.63	118.03	121.75
1	AA	1519	MA6	N1-C2-N3	-3.63	123.09	128.58
53	DA	955	PSU	C4-N3-C2	-3.61	121.40	126.37
12	BL	89	D2T	OD1-CG-CB	-3.61	114.88	122.44
1	AA	1519	MA6	C2-N3-C4	3.61	120.64	111.83
53	DA	1618	6MZ	C6-C5-N7	3.60	136.35	132.43
53	DA	2445	2MG	N1-C2-N2	3.60	120.23	116.56
53	DA	1835	2MG	C6-C5-N7	3.60	136.83	130.29
53	DA	2449	H2U	N3-C2-N1	3.59	120.25	116.65
53	DA	1939	5MU	O2-C2-N1	-3.59	118.13	122.80
53	DA	955	PSU	N1-C2-N3	3.57	118.94	115.17
22	CA	1618	6MZ	C9-N6-C6	-3.57	119.54	122.85
1	BA	1518	MA6	C4-C5-N7	-3.56	106.51	110.58
53	DA	1962	5MC	C5-C4-N3	-3.56	118.11	121.75
53	DA	746	PSU	C6-N1-C2	-3.53	119.41	122.69
53	DA	2030	6MZ	C2-N3-C4	3.53	120.45	111.83
22	CA	1618	6MZ	N1-C2-N3	-3.51	123.26	128.58
53	DA	745	1MG	N9-C4-N3	3.51	132.97	125.95
1	AA	1518	MA6	C2-N3-C4	3.48	120.34	111.83
22	CA	2445	2MG	C6-C5-N7	3.48	136.62	130.29
22	CA	2457	PSU	C6-C5-C4	3.48	120.52	118.17
22	CA	2030	6MZ	N1-C2-N3	-3.46	123.34	128.58
22	CA	2030	6MZ	N3-C4-N9	3.45	133.03	127.17
53	DA	2030	6MZ	C4-C5-N7	-3.45	106.64	110.58
22	CA	2030	6MZ	C9-N6-C6	-3.44	119.66	122.85
1	AA	1519	MA6	N3-C4-N9	3.42	132.98	127.17
22	CA	2030	6MZ	C2-N3-C4	3.39	120.11	111.83
53	DA	747	5MU	O4-C4-C5	-3.39	121.04	124.92
1	BA	966	2MG	C6-C5-N7	3.38	136.44	130.29
22	CA	2605	PSU	C6-C5-C4	3.37	120.45	118.17
1	AA	967	5MC	C5-C6-N1	-3.35	119.67	123.31
1	BA	1519	MA6	C4-C5-N7	-3.34	106.76	110.58
53	DA	2445	2MG	N9-C4-N3	3.34	132.63	125.95
53	DA	2503	2MA	N9-C8-N7	-3.34	109.20	113.94
53	DA	2580	PSU	O2-C2-N1	-3.31	119.38	122.79
53	DA	2498	OMC	C2'-C1'-N1	-3.30	107.98	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CA	2503	2MA	C4-C5-N7	-3.29	106.82	110.58
22	CA	2503	2MA	C4-N9-C8	3.29	109.19	105.74
53	DA	747	5MU	C5-C6-N1	-3.26	119.78	123.31
1	BA	1519	MA6	N1-C6-N6	3.25	120.81	116.86
53	DA	2251	OMG	C6-C5-N7	3.24	136.19	130.29
53	DA	745	1MG	C6-C5-N7	3.23	136.54	129.36
1	BA	967	5MC	C5-C6-N1	-3.23	119.81	123.31
53	DA	1835	2MG	N2-C2-N3	-3.20	116.43	120.51
22	CA	2503	2MA	C2-N1-C6	3.19	123.01	118.10
53	DA	2503	2MA	C4-C5-N7	-3.18	106.94	110.58
53	DA	1917	PSU	O2-C2-N1	-3.18	119.51	122.79
1	AA	1498	UR3	C5-C4-N3	3.17	119.22	115.04
1	BA	1407	5MC	C5-C6-N1	-3.16	119.88	123.31
53	DA	1939	5MU	C5-C4-N3	3.16	118.07	115.32
53	DA	2445	2MG	C4-C5-N7	-3.15	105.68	110.67
22	CA	2251	OMG	C6-C5-N7	3.14	136.01	130.29
1	AA	1207	2MG	C6-C5-N7	3.14	136.00	130.29
1	AA	1518	MA6	C4-C5-N7	-3.12	107.01	110.58
53	DA	1618	6MZ	C2-N3-C4	3.11	119.43	111.83
22	CA	746	PSU	C6-C5-C4	3.10	120.27	118.17
1	AA	1498	UR3	C1'-N1-C2	3.10	122.11	117.04
22	CA	2030	6MZ	C4-N9-C8	3.09	108.99	105.74
1	BA	1407	5MC	C5-C4-N3	-3.09	118.59	121.75
53	DA	746	PSU	O2-C2-N1	-3.09	119.60	122.79
53	DA	2449	H2U	C5-C4-N3	3.08	119.97	116.69
1	AA	1407	5MC	C5-C6-N1	-3.08	119.97	123.31
53	DA	1835	2MG	C2-N1-C6	-3.07	120.84	124.55
22	CA	2552	OMU	O4-C4-C5	-3.07	119.86	125.16
1	BA	516	PSU	O2-C2-N1	-3.07	119.62	122.79
1	AA	1498	UR3	C3U-N3-C2	3.07	122.68	117.33
53	DA	2552	OMU	O2-C2-N1	-3.07	118.80	122.80
22	CA	1835	2MG	C6-C5-N7	3.06	135.86	130.29
1	AA	1516	2MG	C6-C5-N7	3.03	135.81	130.29
1	AA	1207	2MG	N1-C2-N2	3.03	119.65	116.56
1	BA	1207	2MG	N1-C2-N2	3.00	119.62	116.56
53	DA	2445	2MG	N2-C2-N3	-2.99	116.70	120.51
53	DA	2604	PSU	N1-C2-N3	2.98	118.31	115.17
1	BA	1516	2MG	C6-C5-N7	2.97	135.70	130.29
1	AA	966	2MG	C6-C5-N7	2.96	135.68	130.29
53	DA	1618	6MZ	C4-N9-C8	2.96	108.84	105.74
53	DA	1618	6MZ	C9-N6-C6	-2.96	120.11	122.85
53	DA	1962	5MC	CM5-C5-C6	-2.95	118.86	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	1618	6MZ	N1-C2-N3	-2.95	124.12	128.58
1	AA	1518	MA6	N1-C2-N3	-2.93	124.15	128.58
53	DA	2503	2MA	C5-N7-C8	2.91	108.03	103.45
53	DA	1962	5MC	C5-C6-N1	-2.91	120.15	123.31
53	DA	2030	6MZ	C4-N9-C8	2.90	108.78	105.74
1	AA	1516	2MG	O6-C6-C5	-2.90	118.88	126.53
53	DA	1911	PSU	O2-C2-N1	-2.90	119.80	122.79
22	CA	2069	G7M	O6-C6-C5	-2.89	121.56	128.01
53	DA	2069	G7M	O6-C6-C5	-2.88	121.58	128.01
22	CA	2504	PSU	C6-N1-C2	-2.88	120.02	122.69
22	CA	2457	PSU	O2-C2-N1	-2.85	119.84	122.79
53	DA	2604	PSU	O2-C2-N1	-2.85	119.85	122.79
22	CA	1618	6MZ	C5-N7-C8	2.84	107.92	103.45
1	BA	1402	4OC	C6-C5-C4	2.84	120.43	117.00
22	CA	2445	2MG	C4-C5-N7	-2.83	106.19	110.67
53	DA	745	1MG	C4-C5-N7	-2.82	106.21	110.67
53	DA	2552	OMU	O4-C4-C5	-2.81	120.32	125.16
1	BA	1519	MA6	C5-N7-C8	2.80	107.85	103.45
1	BA	1519	MA6	N9-C8-N7	-2.79	109.97	113.94
22	CA	746	PSU	C6-N1-C2	-2.79	120.10	122.69
1	BA	1516	2MG	CM2-N2-C2	-2.78	117.68	123.65
53	DA	2457	PSU	N1-C2-N3	2.78	118.09	115.17
1	AA	1516	2MG	C2-N1-C6	-2.77	121.20	124.55
1	BA	1207	2MG	C4-C5-N7	-2.76	106.29	110.67
1	BA	966	2MG	C4-C5-N7	-2.75	106.31	110.67
22	CA	1939	5MU	C5-C6-N1	-2.75	120.33	123.31
22	CA	1618	6MZ	C4-N9-C8	2.73	108.60	105.74
53	DA	1618	6MZ	C5-N7-C8	2.72	107.73	103.45
22	CA	2030	6MZ	C5-N7-C8	2.72	107.72	103.45
22	CA	1915	3TD	C1'-C5-C4	2.70	121.71	117.61
53	DA	2457	PSU	O2-C2-N1	-2.70	120.00	122.79
1	BA	1518	MA6	C4-N9-C8	2.70	108.57	105.74
53	DA	2449	H2U	O2-C2-N1	-2.69	119.87	123.10
53	DA	1915	3TD	C1'-C5-C4	2.68	121.67	117.61
53	DA	955	PSU	C6-N1-C2	-2.67	120.21	122.69
12	BL	89	D2T	CB-CA-N	2.67	114.50	109.10
22	CA	2504	PSU	O2-C2-N1	-2.67	120.04	122.79
1	BA	1516	2MG	C4-C5-N7	-2.65	106.47	110.67
22	CA	2445	2MG	N1-C2-N2	2.65	119.26	116.56
22	CA	2457	PSU	C6-N1-C2	-2.63	120.25	122.69
53	DA	2604	PSU	O4-C4-C5	-2.63	117.48	124.01
53	DA	1835	2MG	O6-C6-C5	-2.62	119.62	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CA	2605	PSU	O2-C2-N1	-2.62	120.09	122.79
22	CA	745	1MG	C6-C5-N7	2.62	135.17	129.36
22	CA	1917	PSU	O2-C2-N1	-2.61	120.10	122.79
1	AA	1519	MA6	C5-N7-C8	2.61	107.55	103.45
22	CA	2503	2MA	C5-N7-C8	2.61	107.55	103.45
1	AA	527	G7M	C5-C6-N1	2.58	117.18	111.84
1	BA	1498	UR3	C1'-N1-C2	2.58	121.25	117.04
53	DA	1835	2MG	C4-C5-N7	-2.57	106.59	110.67
22	CA	745	1MG	C4-C5-N7	-2.57	106.60	110.67
22	CA	2580	PSU	O2-C2-N1	-2.55	120.16	122.79
22	CA	2251	OMG	O6-C6-C5	-2.55	119.80	126.53
22	CA	2580	PSU	O4'-C1'-C2'	2.55	108.68	105.15
22	CA	746	PSU	O2-C2-N1	-2.54	120.16	122.79
53	DA	2251	OMG	C4-C5-N7	-2.54	106.64	110.67
22	CA	2504	PSU	C6-C5-C4	2.54	119.89	118.17
1	AA	1498	UR3	C6-N1-C2	-2.54	119.73	121.80
1	BA	1519	MA6	C5-C6-N6	-2.53	121.32	125.33
53	DA	1917	PSU	C6-N1-C2	-2.53	120.34	122.69
53	DA	2605	PSU	O2-C2-N1	-2.53	120.18	122.79
53	DA	2504	PSU	O2-C2-N1	-2.53	120.18	122.79
1	AA	1519	MA6	C4-N9-C8	2.51	108.37	105.74
1	BA	967	5MC	C5-C4-N3	-2.51	119.19	121.75
1	AA	1402	4OC	CM4-N4-C4	-2.50	117.57	122.45
53	DA	1917	PSU	C6-C5-C4	2.49	119.86	118.17
1	AA	1516	2MG	N1-C2-N2	2.49	119.10	116.56
1	BA	1516	2MG	C2-N1-C6	-2.48	121.55	124.55
1	AA	966	2MG	C4-C5-N7	-2.48	106.74	110.67
22	CA	1962	5MC	C5-C4-N3	-2.47	119.22	121.75
22	CA	1911	PSU	O2-C2-N1	-2.47	120.24	122.79
53	DA	2030	6MZ	C2-N1-C6	2.47	123.41	115.24
22	CA	955	PSU	O2-C2-N1	-2.46	120.25	122.79
1	BA	527	G7M	C5-C6-N1	2.46	116.92	111.84
12	BL	89	D2T	OD2-CG-CB	2.45	118.44	113.15
1	AA	966	2MG	O6-C6-C5	-2.45	120.08	126.53
53	DA	2251	OMG	O6-C6-C5	-2.44	120.09	126.53
53	DA	1835	2MG	C5-C6-N1	2.43	119.45	113.25
22	CA	2580	PSU	C6-C5-C4	2.43	119.81	118.17
1	AA	1207	2MG	O6-C6-C5	-2.42	120.14	126.53
53	DA	1939	5MU	C5-C6-N1	-2.41	120.69	123.31
1	BA	516	PSU	C6-N1-C2	-2.41	120.45	122.69
53	DA	745	1MG	C6-C5-C4	-2.41	117.25	119.97
12	AL	89	D2T	OD1-CG-CB	-2.40	117.40	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	1518	MA6	C5-N7-C8	2.40	107.23	103.45
53	DA	2069	G7M	C5-C6-N1	2.40	116.81	111.84
22	CA	2030	6MZ	C2-N1-C6	2.40	123.20	115.24
1	AA	1516	2MG	N2-C2-N3	-2.40	117.46	120.51
22	CA	2030	6MZ	N9-C8-N7	-2.39	110.54	113.94
1	AA	1519	MA6	C6-C5-N7	2.39	137.25	133.43
22	CA	1618	6MZ	N9-C8-N7	-2.38	110.55	113.94
1	AA	1207	2MG	C4-C5-N7	-2.38	106.90	110.67
1	AA	966	2MG	CM2-N2-C2	-2.38	118.54	123.65
22	CA	2580	PSU	C6-N1-C2	-2.37	120.50	122.69
53	DA	2030	6MZ	C9-N6-C6	-2.34	120.68	122.85
1	BA	516	PSU	C6-C5-C4	2.32	119.74	118.17
1	AA	1518	MA6	C5-N7-C8	2.32	107.09	103.45
53	DA	2030	6MZ	C5-N7-C8	2.31	107.09	103.45
1	AA	1519	MA6	N9-C8-N7	-2.31	110.66	113.94
1	AA	1207	2MG	CM2-N2-C2	-2.31	118.69	123.65
22	CA	2552	OMU	O2-C2-N1	-2.31	119.79	122.80
12	AL	89	D2T	CB-CA-N	2.31	113.77	109.10
1	AA	527	G7M	O6-C6-C5	-2.30	122.88	128.01
22	CA	1835	2MG	C4-C5-N7	-2.30	107.03	110.67
22	CA	1915	3TD	C5-C6-N1	-2.30	118.95	122.14
53	DA	2604	PSU	C5-C4-N3	2.29	121.60	116.55
1	AA	1516	2MG	C4-C5-N7	-2.28	107.05	110.67
1	AA	967	5MC	C5-C4-N3	-2.28	119.42	121.75
53	DA	1835	2MG	CM2-N2-C2	-2.28	118.76	123.65
1	BA	1516	2MG	N1-C2-N2	2.26	118.87	116.56
22	CA	1915	3TD	O4'-C1'-C2'	2.25	108.27	105.15
1	BA	1516	2MG	O6-C6-C5	-2.25	120.61	126.53
22	CA	1911	PSU	C6-N1-C2	-2.24	120.61	122.69
22	CA	2069	G7M	C5-C6-N1	2.24	116.47	111.84
54	DD	150[A]	MEQ	OE1-CD-CG	-2.23	117.97	122.02
22	CA	1835	2MG	O6-C6-C5	-2.23	120.64	126.53
22	CA	2503	2MA	N9-C8-N7	-2.23	110.77	113.94
53	DA	2030	6MZ	N9-C8-N7	-2.23	110.78	113.94
53	DA	746	PSU	C6-C5-C4	2.23	119.68	118.17
22	CA	2251	OMG	CM2-O2'-C2'	-2.21	108.80	114.47
53	DA	2580	PSU	N1-C2-N3	2.21	117.50	115.17
1	BA	1516	2MG	N2-C2-N3	-2.21	117.69	120.51
22	CA	2251	OMG	C4-C5-N7	-2.20	107.18	110.67
53	DA	1962	5MC	O2-C2-N3	-2.20	118.86	122.33
1	AA	516	PSU	C6-N1-C2	-2.19	120.66	122.69
53	DA	2030	6MZ	C4-N9-C1'	-2.19	121.51	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	2580	PSU	C6-C5-C4	-2.18	116.70	118.17
1	AA	1516	2MG	C5-C6-N1	2.18	118.81	113.25
53	DA	1911	PSU	C5-C4-N3	2.18	121.35	116.55
1	AA	966	2MG	N1-C2-N2	2.17	118.78	116.56
1	BA	1516	2MG	C8-N7-C5	2.17	108.12	104.26
22	CA	1618	6MZ	C2-N1-C6	2.13	122.31	115.24
53	DA	2503	2MA	C5-C6-N6	-2.13	118.01	123.29
1	BA	1207	2MG	O6-C6-C5	-2.12	120.93	126.53
53	DA	2580	PSU	O4'-C1'-C2'	2.11	108.07	105.15
53	DA	1618	6MZ	C2-N1-C6	2.11	122.22	115.24
1	BA	1407	5MC	CM5-C5-C6	-2.10	120.01	122.85
53	DA	2552	OMU	C5-C6-N1	-2.09	118.44	121.84
1	BA	1402	4OC	CM2-O2'-C2'	-2.08	109.14	114.47
1	BA	1207	2MG	C8-N7-C5	2.07	107.95	104.26
53	DA	2449	H2U	C5-C6-N1	-2.07	105.26	111.52
1	AA	1518	MA6	C4-N9-C8	2.06	107.90	105.74
22	CA	1917	PSU	C6-N1-C2	-2.06	120.78	122.69
1	BA	1519	MA6	C6-C5-N7	2.05	136.71	133.43
22	CA	2503	2MA	C6-C5-N7	2.05	136.03	132.09
53	DA	2251	OMG	C8-N9-C4	2.04	109.84	106.03
22	CA	2498	OMC	O2-C2-N3	-2.03	119.13	122.33
22	CA	2445	2MG	N2-C2-N3	-2.03	117.92	120.51
53	DA	2503	2MA	C2-N1-C6	2.03	121.22	118.10
53	DA	2580	PSU	C5-C4-N3	2.03	121.02	116.55
53	DA	2445	2MG	C8-N7-C5	2.03	107.87	104.26
53	DA	1962	5MC	N1-C2-N3	2.02	122.31	118.80
22	CA	2445	2MG	CM2-N2-C2	-2.02	119.31	123.65
1	BA	1516	2MG	C5-C6-N1	2.02	118.39	113.25
54	DD	150[A]	MEQ	CG-CD-NE2	2.01	119.21	116.39
53	DA	1939	5MU	C5M-C5-C4	2.01	120.92	118.78
1	AA	967	5MC	C5-C4-N4	-2.00	118.57	121.39

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	966	2MG	N1-C2-N2-CM2
1	AA	966	2MG	N3-C2-N2-CM2
1	BA	527	G7M	O4'-C4'-C5'-O5'
12	BL	89	D2T	CA-CB-SB-CB1
12	BL	89	D2T	CA-CB-CG-OD1
12	BL	89	D2T	CA-CB-CG-OD2

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Mol	Chain	Res	Type	Atoms
22	CA	2251	OMG	C1'-C2'-O2'-CM2
34	CN	81	4D4	C-CA-CB-CG
34	CN	81	4D4	N-CA-CB-CG
34	CN	81	4D4	OB-CB-CG-CD
54	DD	150[B]	MEQ	CG-CD-NE2-CE
54	DD	150[B]	MEQ	OE1-CD-NE2-CE
34	DN	81[B]	4D4	CA-CB-CG-CD
34	DN	81[B]	4D4	NE-CD-CG-CB
1	BA	527	G7M	C3'-C4'-C5'-O5'
54	DD	150[A]	MEQ	OE1-CD-CG-CB
54	DD	150[A]	MEQ	NE2-CD-CG-CB
1	BA	1519	MA6	O4'-C4'-C5'-O5'
34	DN	81[B]	4D4	OB-CB-CG-CD
54	DD	150[B]	MEQ	CA-CB-CG-CD
53	DA	2030	6MZ	O4'-C4'-C5'-O5'
22	CA	1835	2MG	O4'-C4'-C5'-O5'
53	DA	2030	6MZ	C3'-C4'-C5'-O5'
1	BA	1402	4OC	O4'-C4'-C5'-O5'
22	CA	1835	2MG	C3'-C4'-C5'-O5'
1	BA	1518	MA6	O4'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1
54	DD	150[B]	MEQ	C-CA-CB-CG
1	BA	1519	MA6	C3'-C4'-C5'-O5'
34	CN	81	4D4	C-CA-CB-OB
34	CN	81	4D4	CA-CB-CG-CD
1	AA	1519	MA6	O4'-C4'-C5'-O5'
22	CA	2030	6MZ	O4'-C4'-C5'-O5'
34	DN	81[B]	4D4	CG-CD-NE-CZ
53	DA	2503	2MA	C4'-C5'-O5'-P
53	DA	2069	G7M	C4'-C5'-O5'-P
22	CA	746	PSU	O4'-C1'-C5-C6
53	DA	746	PSU	O4'-C1'-C5-C6
22	CA	1915	3TD	C3'-C4'-C5'-O5'
12	BL	89	D2T	CG-CB-SB-CB1
22	CA	746	PSU	C2'-C1'-C5-C6
53	DA	746	PSU	C2'-C1'-C5-C6
53	DA	2069	G7M	O4'-C4'-C5'-O5'
22	CA	2503	2MA	C4'-C5'-O5'-P
22	CA	2552	OMU	C3'-C2'-O2'-CM2
34	CN	81	4D4	O-C-CA-CB
34	DN	81[B]	4D4	O-C-CA-CB
22	CA	1915	3TD	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
53	DA	747	5MU	C3'-C4'-C5'-O5'
1	BA	1402	4OC	C2'-C1'-N1-C2
22	CA	2030	6MZ	C3'-C4'-C5'-O5'
53	DA	2498	OMC	C4'-C5'-O5'-P
1	BA	1402	4OC	C3'-C4'-C5'-O5'
22	CA	2069	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

32 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	BA	516	PSU	1	0
1	BA	966	2MG	1	0
22	CA	747	5MU	1	0
1	BA	1402	4OC	2	0
54	DD	150[A]	MEQ	2	0
22	CA	2030	6MZ	2	0
22	CA	1939	5MU	1	0
53	DA	2251	OMG	2	0
1	BA	1498	UR3	1	0
1	AA	1518	MA6	2	0
22	CA	2445	2MG	2	0
1	BA	1519	MA6	4	0
34	DN	81[A]	4D4	1	0
1	BA	1407	5MC	2	0
22	CA	2069	G7M	1	0
12	AL	89	D2T	1	0
53	DA	2030	6MZ	2	0
1	BA	1516	2MG	1	0
1	AA	1519	MA6	3	0
22	CA	2251	OMG	1	0
1	AA	1402	4OC	1	0
54	DD	150[B]	MEQ	1	0
22	CA	1915	3TD	4	0
22	CA	2498	OMC	2	0
34	CN	81	4D4	1	0
53	DA	2498	OMC	2	0
22	CA	1962	5MC	1	0
22	CA	1618	6MZ	1	0
1	BA	1518	MA6	2	0
1	BA	967	5MC	1	0
22	CA	2503	2MA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	527	G7M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 546 ligands modelled in this entry, 466 are monoatomic - leaving 80 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	PUT	DA	3188	-	5,5,5	0.19	0	4,4,4	0.27	0
61	PEG	DA	3219	-	6,6,6	1.03	0	5,5,5	0.44	0
66	EDO	DA	3210	-	3,3,3	0.30	0	2,2,2	0.51	0
62	SPD	DA	3187	-	9,9,9	0.42	0	8,8,8	0.93	0
59	PUT	AA	1673	-	5,5,5	0.22	0	4,4,4	0.48	0
61	PEG	DA	3201	-	6,6,6	1.04	0	5,5,5	0.49	0
64	PGE	D1	102	-	9,9,9	1.05	0	8,8,8	0.31	0
64	PGE	DS	201	-	9,9,9	0.96	0	8,8,8	0.31	0
59	PUT	DA	3213	-	5,5,5	0.26	0	4,4,4	0.20	0
59	PUT	DA	3206	-	5,5,5	0.28	0	4,4,4	0.51	0
61	PEG	AL	201	-	6,6,6	0.96	0	5,5,5	0.45	0
62	SPD	DA	3183	-	9,9,9	0.42	0	8,8,8	0.77	0
58	MPD	DS	203	-	7,7,7	1.01	1 (14%)	9,10,10	0.60	0
57	PG4	DA	3217	-	12,12,12	0.74	0	11,11,11	0.54	0
64	PGE	DA	3226	-	9,9,9	0.97	0	8,8,8	0.26	0
64	PGE	DA	3215	-	9,9,9	0.94	0	8,8,8	0.30	0
58	MPD	DA	3208	-	7,7,7	0.53	0	9,10,10	0.37	0
66	EDO	D1	101	-	3,3,3	0.25	0	2,2,2	0.45	0
59	PUT	AA	1672	-	5,5,5	0.21	0	4,4,4	0.54	0
64	PGE	D3	101	-	9,9,9	0.92	0	8,8,8	0.37	0
66	EDO	DA	3198	-	3,3,3	0.33	0	2,2,2	0.41	0
59	PUT	DA	3214	-	5,5,5	0.23	0	4,4,4	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	PEG	DA	3227	-	6,6,6	0.97	0	5,5,5	0.42	0
64	PGE	DA	3218	-	9,9,9	0.84	0	8,8,8	0.38	0
58	MPD	DE	302	-	7,7,7	0.53	0	9,10,10	0.58	0
57	PG4	DQ	202	-	12,12,12	0.67	0	11,11,11	0.56	0
58	MPD	DA	3205	-	7,7,7	0.77	0	9,10,10	1.15	1 (11%)
67	GUN	DA	3212	-	12,12,12	1.65	2 (16%)	15,17,17	3.23	9 (60%)
58	MPD	DA	3190	-	7,7,7	0.67	0	9,10,10	0.68	0
66	EDO	DA	3209	-	3,3,3	0.35	0	2,2,2	0.34	0
66	EDO	D0	101	-	3,3,3	0.34	0	2,2,2	0.46	0
68	TRS	DA	3221	-	7,7,7	0.38	0	9,9,9	0.80	0
59	PUT	DA	3224	-	5,5,5	0.25	0	4,4,4	0.71	0
59	PUT	DA	3189	-	5,5,5	0.30	0	4,4,4	0.41	0
64	PGE	DA	3204	-	9,9,9	0.97	0	8,8,8	0.55	0
65	ACY	DA	3191	-	3,3,3	0.91	0	3,3,3	0.80	0
66	EDO	DA	3194	-	3,3,3	0.29	0	2,2,2	0.49	0
64	PGE	DU	101	-	9,9,9	0.97	0	8,8,8	0.43	0
66	EDO	DB	210	-	3,3,3	0.27	0	2,2,2	0.76	0
58	MPD	DN	201	-	7,7,7	0.54	0	9,10,10	0.91	0
61	PEG	DA	3200	-	6,6,6	1.07	0	5,5,5	0.53	0
62	SPD	DA	3207	-	9,9,9	0.50	0	8,8,8	0.65	0
57	PG4	DR	202	-	12,12,12	0.84	0	11,11,11	0.43	0
59	PUT	DA	3184	-	5,5,5	0.29	0	4,4,4	0.30	0
61	PEG	DA	3228	-	6,6,6	1.05	0	5,5,5	0.18	0
57	PG4	AA	1670	-	12,12,12	0.81	0	11,11,11	0.41	0
58	MPD	DT	201	-	7,7,7	0.86	1 (14%)	9,10,10	1.09	0
59	PUT	DA	3223	-	5,5,5	0.32	0	4,4,4	0.42	0
66	EDO	DR	203	-	3,3,3	0.29	0	2,2,2	0.42	0
58	MPD	DK	201	-	7,7,7	0.55	0	9,10,10	0.75	0
58	MPD	AA	1671	-	7,7,7	0.55	0	9,10,10	0.61	0
58	MPD	AA	1676	-	7,7,7	0.72	0	9,10,10	0.62	0
59	PUT	DA	3222	-	5,5,5	0.22	0	4,4,4	0.41	0
61	PEG	DP	201	-	6,6,6	0.98	0	5,5,5	0.41	0
57	PG4	BA	1642	-	12,12,12	0.80	0	11,11,11	0.43	0
59	PUT	DM	201	-	5,5,5	0.27	0	4,4,4	0.66	0
63	1PE	DA	3203	-	15,15,15	0.66	0	14,14,14	0.32	0
59	PUT	DA	3220	-	5,5,5	0.19	0	4,4,4	0.46	0
58	MPD	DA	3192	-	7,7,7	0.41	0	9,10,10	1.38	1 (11%)
64	PGE	DA	3186	-	9,9,9	0.94	0	8,8,8	0.30	0
59	PUT	AA	1674	-	5,5,5	0.21	0	4,4,4	0.52	0
57	PG4	DA	3193	-	12,12,12	0.79	0	11,11,11	0.59	0
61	PEG	D3	102	-	6,6,6	1.00	0	5,5,5	0.40	0
58	MPD	DA	3211	-	7,7,7	0.53	0	9,10,10	0.95	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	MPD	DE	301	-	7,7,7	0.64	0	9,10,10	0.73	0
66	EDO	DB	211	-	3,3,3	0.35	0	2,2,2	0.52	0
61	PEG	DL	201	-	6,6,6	0.87	0	5,5,5	0.55	0
59	PUT	AA	1675	-	5,5,5	0.28	0	4,4,4	0.33	0
66	EDO	DA	3197	-	3,3,3	0.26	0	2,2,2	0.57	0
66	EDO	DA	3216	-	3,3,3	0.36	0	2,2,2	0.39	0
66	EDO	DB	212	-	3,3,3	0.32	0	2,2,2	0.48	0
62	SPD	DA	3225	-	9,9,9	0.56	0	8,8,8	1.10	1 (12%)
65	ACY	DA	3196	-	3,3,3	1.00	0	3,3,3	0.86	0
63	1PE	DA	3185	-	15,15,15	0.55	0	14,14,14	0.49	0
61	PEG	DA	3199	-	6,6,6	0.92	0	5,5,5	0.58	0
59	PUT	DA	3195	-	5,5,5	0.25	0	4,4,4	0.38	0
57	PG4	DS	202	-	12,12,12	0.76	0	11,11,11	0.32	0
65	ACY	DA	3202	-	3,3,3	0.95	0	3,3,3	0.64	0
58	MPD	DT	202	-	7,7,7	0.54	0	9,10,10	0.58	0
61	PEG	DQ	201	-	6,6,6	1.01	0	5,5,5	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PUT	DA	3188	-	-	0/3/3/3	-
61	PEG	DA	3219	-	-	1/4/4/4	-
66	EDO	DA	3210	-	-	0/1/1/1	-
62	SPD	DA	3187	-	-	0/7/7/7	-
59	PUT	AA	1673	-	-	0/3/3/3	-
61	PEG	DA	3201	-	-	3/4/4/4	-
64	PGE	D1	102	-	-	1/7/7/7	-
64	PGE	DS	201	-	-	2/7/7/7	-
59	PUT	DA	3213	-	-	0/3/3/3	-
59	PUT	DA	3206	-	-	1/3/3/3	-
61	PEG	AL	201	-	-	2/4/4/4	-
62	SPD	DA	3183	-	-	3/7/7/7	-
58	MPD	DS	203	-	-	0/5/5/5	-
57	PG4	DA	3217	-	-	5/10/10/10	-
64	PGE	DA	3226	-	-	4/7/7/7	-
64	PGE	DA	3215	-	-	3/7/7/7	-
58	MPD	DA	3208	-	-	1/5/5/5	-
66	EDO	D1	101	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PUT	AA	1672	-	-	0/3/3/3	-
64	PGE	D3	101	-	-	3/7/7/7	-
66	EDO	DA	3198	-	-	0/1/1/1	-
59	PUT	DA	3214	-	-	1/3/3/3	-
61	PEG	DA	3227	-	-	3/4/4/4	-
64	PGE	DA	3218	-	-	3/7/7/7	-
58	MPD	DE	302	-	-	1/5/5/5	-
57	PG4	DQ	202	-	-	0/10/10/10	-
58	MPD	DA	3205	-	-	4/5/5/5	-
67	GUN	DA	3212	-	-	-	0/2/2/2
58	MPD	DA	3190	-	-	2/5/5/5	-
66	EDO	DA	3209	-	-	1/1/1/1	-
66	EDO	D0	101	-	-	1/1/1/1	-
68	TRS	DA	3221	-	-	6/9/9/9	-
59	PUT	DA	3224	-	-	0/3/3/3	-
59	PUT	DA	3189	-	-	0/3/3/3	-
64	PGE	DA	3204	-	-	5/7/7/7	-
66	EDO	DA	3194	-	-	0/1/1/1	-
64	PGE	DU	101	-	-	2/7/7/7	-
66	EDO	DB	210	-	-	1/1/1/1	-
58	MPD	DN	201	-	-	3/5/5/5	-
61	PEG	DA	3200	-	-	2/4/4/4	-
62	SPD	DA	3207	-	-	5/7/7/7	-
57	PG4	DR	202	-	-	5/10/10/10	-
59	PUT	DA	3184	-	-	1/3/3/3	-
61	PEG	DA	3228	-	-	1/4/4/4	-
57	PG4	AA	1670	-	-	6/10/10/10	-
58	MPD	DT	201	-	-	1/5/5/5	-
59	PUT	DA	3223	-	-	1/3/3/3	-
66	EDO	DR	203	-	-	1/1/1/1	-
58	MPD	DK	201	-	-	1/5/5/5	-
58	MPD	AA	1671	-	-	1/5/5/5	-
58	MPD	AA	1676	-	-	2/5/5/5	-
59	PUT	DA	3222	-	-	2/3/3/3	-
61	PEG	DP	201	-	-	4/4/4/4	-
57	PG4	BA	1642	-	-	2/10/10/10	-
59	PUT	DM	201	-	-	3/3/3/3	-
63	1PE	DA	3203	-	-	6/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PUT	DA	3220	-	-	0/3/3/3	-
58	MPD	DA	3192	-	-	5/5/5/5	-
64	PGE	DA	3186	-	-	2/7/7/7	-
59	PUT	AA	1674	-	-	1/3/3/3	-
57	PG4	DA	3193	-	-	7/10/10/10	-
61	PEG	D3	102	-	-	3/4/4/4	-
58	MPD	DA	3211	-	-	4/5/5/5	-
58	MPD	DE	301	-	-	3/5/5/5	-
66	EDO	DB	211	-	-	1/1/1/1	-
61	PEG	DL	201	-	-	3/4/4/4	-
59	PUT	AA	1675	-	-	2/3/3/3	-
66	EDO	DA	3197	-	-	1/1/1/1	-
66	EDO	DA	3216	-	-	1/1/1/1	-
66	EDO	DB	212	-	-	0/1/1/1	-
62	SPD	DA	3225	-	-	2/7/7/7	-
63	1PE	DA	3185	-	-	7/13/13/13	-
61	PEG	DA	3199	-	-	2/4/4/4	-
59	PUT	DA	3195	-	-	2/3/3/3	-
57	PG4	DS	202	-	-	3/10/10/10	-
58	MPD	DT	202	-	-	3/5/5/5	-
61	PEG	DQ	201	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	DA	3212	GUN	C5-C4	3.07	1.48	1.39
58	DS	203	MPD	O2-C2	-2.19	1.39	1.44
58	DT	201	MPD	O2-C2	-2.03	1.39	1.44
67	DA	3212	GUN	C2-N3	2.00	1.38	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	DA	3212	GUN	N9-C4-N3	8.02	135.75	125.99
67	DA	3212	GUN	C2-N3-C4	4.99	122.17	113.36
67	DA	3212	GUN	C6-C5-N7	3.92	137.42	130.29
67	DA	3212	GUN	C8-N7-C5	3.65	109.31	104.38
58	DA	3192	MPD	CM-C2-C1	-3.31	103.22	110.63
67	DA	3212	GUN	N9-C8-N7	-3.29	109.16	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	DA	3212	GUN	C4-C5-N7	-2.78	105.82	110.17
67	DA	3212	GUN	C8-N9-C4	2.63	109.17	106.25
58	DA	3205	MPD	CM-C2-C1	2.61	116.47	110.63
62	DA	3225	SPD	C7-C8-C9	-2.50	105.22	114.17
67	DA	3212	GUN	C5-C6-N1	2.31	119.14	113.25
58	DA	3211	MPD	CM-C2-C1	-2.28	105.52	110.63
67	DA	3212	GUN	C2-N1-C6	-2.02	121.44	125.11

There are no chirality outliers.

All (160) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AA	1671	MPD	C2-C3-C4-O4
58	DA	3190	MPD	C2-C3-C4-O4
58	DA	3190	MPD	C2-C3-C4-C5
58	DA	3192	MPD	O2-C2-C3-C4
58	DA	3192	MPD	CM-C2-C3-C4
58	DA	3192	MPD	C2-C3-C4-C5
58	DN	201	MPD	O2-C2-C3-C4
58	DN	201	MPD	CM-C2-C3-C4
58	DT	202	MPD	C2-C3-C4-O4
68	DA	3221	TRS	N-C-C1-O1
63	DA	3203	1PE	C15-C25-OH5-C14
61	DA	3199	PEG	C4-C3-O2-C2
61	DP	201	PEG	C4-C3-O2-C2
57	DA	3217	PG4	C3-C4-O3-C5
57	DR	202	PG4	C5-C6-O4-C7
64	DA	3204	PGE	C1-C2-O2-C3
57	DR	202	PG4	O2-C3-C4-O3
63	DA	3203	1PE	OH4-C13-C23-OH3
64	DA	3215	PGE	O2-C3-C4-O3
62	DA	3207	SPD	C3-C4-C5-N6
57	DA	3193	PG4	O2-C3-C4-O3
62	DA	3225	SPD	C3-C4-C5-N6
63	DA	3203	1PE	OH6-C15-C25-OH5
57	DR	202	PG4	O3-C5-C6-O4
59	DA	3222	PUT	C1-C2-C3-C4
63	DA	3185	1PE	OH4-C13-C23-OH3
61	D3	102	PEG	O1-C1-C2-O2
64	DA	3204	PGE	O2-C3-C4-O3
64	D3	101	PGE	O2-C3-C4-O3
61	DA	3201	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
61	DL	201	PEG	O2-C3-C4-O4
64	DA	3186	PGE	O3-C5-C6-O4
64	DA	3204	PGE	O3-C5-C6-O4
64	DA	3226	PGE	O1-C1-C2-O2
64	DU	101	PGE	O1-C1-C2-O2
62	DA	3207	SPD	C8-C7-N6-C5
57	DA	3193	PG4	O4-C7-C8-O5
61	DP	201	PEG	O1-C1-C2-O2
63	DA	3185	1PE	OH2-C12-C22-OH3
63	DA	3203	1PE	OH2-C12-C22-OH3
64	DA	3215	PGE	O3-C5-C6-O4
64	DU	101	PGE	O3-C5-C6-O4
57	DA	3217	PG4	O3-C5-C6-O4
62	DA	3207	SPD	C4-C5-N6-C7
64	DS	201	PGE	O2-C3-C4-O3
57	AA	1670	PG4	O2-C3-C4-O3
57	AA	1670	PG4	O1-C1-C2-O2
61	AL	201	PEG	O1-C1-C2-O2
61	DA	3199	PEG	O1-C1-C2-O2
61	DA	3227	PEG	O2-C3-C4-O4
61	DP	201	PEG	O2-C3-C4-O4
66	DB	211	EDO	O1-C1-C2-O2
62	DA	3207	SPD	C2-C3-C4-C5
62	DA	3183	SPD	C8-C7-N6-C5
57	BA	1642	PG4	O3-C5-C6-O4
62	DA	3183	SPD	C2-C3-C4-C5
59	AA	1674	PUT	C1-C2-C3-C4
59	AA	1675	PUT	C1-C2-C3-C4
61	DA	3201	PEG	O1-C1-C2-O2
61	DA	3219	PEG	O2-C3-C4-O4
61	DL	201	PEG	O1-C1-C2-O2
57	DS	202	PG4	O3-C5-C6-O4
57	AA	1670	PG4	O4-C7-C8-O5
66	DA	3216	EDO	O1-C1-C2-O2
66	DB	210	EDO	O1-C1-C2-O2
66	D0	101	EDO	O1-C1-C2-O2
61	DA	3200	PEG	C1-C2-O2-C3
61	DQ	201	PEG	O1-C1-C2-O2
64	DA	3226	PGE	O3-C5-C6-O4
59	DA	3206	PUT	C1-C2-C3-C4
59	DA	3214	PUT	C1-C2-C3-C4
68	DA	3221	TRS	C1-C-C2-O2

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Mol	Chain	Res	Type	Atoms
59	DA	3195	PUT	C2-C3-C4-N2
61	D3	102	PEG	C1-C2-O2-C3
64	DS	201	PGE	C6-C5-O3-C4
57	DA	3217	PG4	C6-C5-O3-C4
61	DA	3227	PEG	C1-C2-O2-C3
63	DA	3185	1PE	C16-C26-OH6-C15
63	DA	3185	1PE	C12-C22-OH3-C23
61	DA	3201	PEG	C1-C2-O2-C3
63	DA	3185	1PE	C24-C14-OH5-C25
57	DA	3193	PG4	C3-C4-O3-C5
64	DA	3226	PGE	C1-C2-O2-C3
64	D1	102	PGE	C3-C4-O3-C5
57	DR	202	PG4	C6-C5-O3-C4
57	DA	3193	PG4	C4-C3-O2-C2
61	DA	3227	PEG	O1-C1-C2-O2
57	AA	1670	PG4	C3-C4-O3-C5
59	AA	1675	PUT	C2-C3-C4-N2
58	DA	3205	MPD	O2-C2-C3-C4
58	DA	3208	MPD	O2-C2-C3-C4
58	DK	201	MPD	O2-C2-C3-C4
58	DT	202	MPD	O2-C2-C3-C4
61	D3	102	PEG	C4-C3-O2-C2
63	DA	3185	1PE	C23-C13-OH4-C24
57	DA	3217	PG4	O1-C1-C2-O2
57	DS	202	PG4	O4-C7-C8-O5
61	DA	3200	PEG	O2-C3-C4-O4
64	DA	3186	PGE	O1-C1-C2-O2
64	D3	101	PGE	O3-C5-C6-O4
58	DA	3211	MPD	CM-C2-C3-C4
58	DN	201	MPD	C1-C2-C3-C4
57	AA	1670	PG4	C5-C6-O4-C7
63	DA	3203	1PE	C13-C23-OH3-C22
68	DA	3221	TRS	C3-C-C2-O2
64	D3	101	PGE	O1-C1-C2-O2
57	DA	3193	PG4	C1-C2-O2-C3
61	DQ	201	PEG	C4-C3-O2-C2
58	DA	3205	MPD	C2-C3-C4-C5
58	DE	301	MPD	C2-C3-C4-C5
58	DT	202	MPD	C2-C3-C4-C5
59	DA	3195	PUT	N1-C1-C2-C3
59	DM	201	PUT	N1-C1-C2-C3
64	DA	3218	PGE	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
57	AA	1670	PG4	O3-C5-C6-O4
57	DA	3193	PG4	C8-C7-O4-C6
66	DR	203	EDO	O1-C1-C2-O2
59	DA	3222	PUT	C2-C3-C4-N2
59	DM	201	PUT	C1-C2-C3-C4
61	DL	201	PEG	C4-C3-O2-C2
64	DA	3218	PGE	C1-C2-O2-C3
68	DA	3221	TRS	N-C-C2-O2
68	DA	3221	TRS	C1-C-C3-O3
62	DA	3183	SPD	C3-C4-C5-N6
61	DA	3228	PEG	C1-C2-O2-C3
59	DA	3223	PUT	C1-C2-C3-C4
57	DA	3193	PG4	C6-C5-O3-C4
64	DA	3204	PGE	C4-C3-O2-C2
64	DA	3215	PGE	C4-C3-O2-C2
66	DA	3197	EDO	O1-C1-C2-O2
66	DA	3209	EDO	O1-C1-C2-O2
63	DA	3203	1PE	OH5-C14-C24-OH4
57	DA	3217	PG4	O2-C3-C4-O3
61	AL	201	PEG	C1-C2-O2-C3
63	DA	3185	1PE	C13-C23-OH3-C22
59	DM	201	PUT	C2-C3-C4-N2
64	DA	3218	PGE	O2-C3-C4-O3
61	DP	201	PEG	C1-C2-O2-C3
58	AA	1676	MPD	O2-C2-C3-C4
58	DA	3211	MPD	O2-C2-C3-C4
57	DS	202	PG4	C4-C3-O2-C2
64	DA	3204	PGE	O1-C1-C2-O2
57	DR	202	PG4	C4-C3-O2-C2
58	DA	3192	MPD	C2-C3-C4-O4
58	DA	3205	MPD	C2-C3-C4-O4
58	DA	3211	MPD	C2-C3-C4-O4
58	DE	302	MPD	C2-C3-C4-O4
58	AA	1676	MPD	C1-C2-C3-C4
58	DA	3192	MPD	C1-C2-C3-C4
58	DA	3205	MPD	CM-C2-C3-C4
58	DA	3211	MPD	C1-C2-C3-C4
58	DE	301	MPD	C1-C2-C3-C4
58	DE	301	MPD	CM-C2-C3-C4
58	DT	201	MPD	CM-C2-C3-C4
62	DA	3225	SPD	C8-C7-N6-C5
57	BA	1642	PG4	C5-C6-O4-C7

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Mol	Chain	Res	Type	Atoms
59	DA	3184	PUT	C2-C3-C4-N2
62	DA	3207	SPD	N1-C2-C3-C4
68	DA	3221	TRS	N-C-C3-O3
64	DA	3226	PGE	O2-C3-C4-O3

There are no ring outliers.

42 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
66	DA	3210	EDO	3	0
62	DA	3187	SPD	1	0
59	AA	1673	PUT	1	0
61	DA	3201	PEG	1	0
59	DA	3213	PUT	1	0
62	DA	3183	SPD	1	0
57	DA	3217	PG4	1	0
66	DA	3198	EDO	3	0
59	DA	3214	PUT	2	0
61	DA	3227	PEG	1	0
64	DA	3218	PGE	1	0
57	DQ	202	PG4	3	0
58	DA	3205	MPD	3	0
67	DA	3212	GUN	1	0
58	DA	3190	MPD	1	0
66	DA	3209	EDO	1	0
59	DA	3224	PUT	2	0
59	DA	3189	PUT	1	0
64	DA	3204	PGE	2	0
66	DA	3194	EDO	3	0
64	DU	101	PGE	1	0
58	DN	201	MPD	6	0
61	DA	3200	PEG	1	0
57	DR	202	PG4	10	0
57	AA	1670	PG4	1	0
59	DA	3223	PUT	4	0
59	DA	3222	PUT	2	0
61	DP	201	PEG	4	0
57	BA	1642	PG4	2	0
63	DA	3203	1PE	3	0
59	DA	3220	PUT	1	0
57	DA	3193	PG4	7	0
61	D3	102	PEG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	DA	3211	MPD	1	0
66	DA	3197	EDO	1	0
66	DB	212	EDO	1	0
62	DA	3225	SPD	5	0
63	DA	3185	1PE	1	0
59	DA	3195	PUT	3	0
57	DS	202	PG4	2	0
65	DA	3202	ACY	1	0
61	DQ	201	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1523/1534 (99%)	0.00	19 (1%) 76 78	50, 82, 132, 172	0
1	BA	1522/1534 (99%)	0.94	85 (5%) 30 32	64, 105, 192, 222	0
2	AB	224/224 (100%)	1.88	96 (42%) 0 1	74, 117, 124, 132	0
2	BB	224/224 (100%)	2.43	136 (60%) 0 0	74, 114, 123, 130	0
3	AC	206/206 (100%)	1.16	16 (7%) 19 20	77, 88, 100, 105	0
3	BC	206/206 (100%)	2.40	115 (55%) 0 0	100, 117, 150, 166	0
4	AD	205/205 (100%)	1.28	32 (15%) 5 5	70, 91, 116, 125	0
4	BD	205/205 (100%)	1.80	77 (37%) 1 1	64, 76, 86, 91	0
5	AE	155/155 (100%)	1.35	32 (20%) 2 3	68, 79, 89, 95	0
5	BE	150/155 (96%)	2.71	106 (70%) 0 0	77, 91, 103, 114	0
6	AF	106/106 (100%)	1.47	25 (23%) 2 2	65, 92, 100, 102	0
6	BF	100/106 (94%)	2.35	55 (55%) 0 0	92, 104, 113, 117	0
7	AG	151/151 (100%)	2.13	68 (45%) 0 1	90, 117, 127, 132	0
7	BG	151/151 (100%)	2.99	113 (74%) 0 0	111, 153, 177, 185	0
8	AH	129/129 (100%)	1.05	9 (6%) 22 24	69, 82, 95, 103	0
8	BH	129/129 (100%)	2.54	84 (65%) 0 0	72, 111, 132, 139	0
9	AI	127/127 (100%)	2.24	74 (58%) 0 0	81, 111, 124, 130	0
9	BI	127/127 (100%)	3.28	104 (81%) 0 0	130, 152, 171, 177	0
10	AJ	99/99 (100%)	2.22	57 (57%) 0 0	60, 70, 76, 77	0
10	BJ	98/99 (98%)	3.58	90 (91%) 0 0	69, 76, 80, 81	0
11	AK	117/117 (100%)	1.41	25 (21%) 2 2	60, 90, 104, 108	0
11	BK	117/117 (100%)	1.93	55 (47%) 0 0	75, 102, 115, 118	0
12	AL	122/123 (99%)	1.08	16 (13%) 7 7	55, 67, 77, 88	0
12	BL	122/123 (99%)	2.54	79 (64%) 0 0	72, 84, 92, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	2.12	58 (50%)	0	0	84, 112, 124, 128	0
13	BM	114/114 (100%)	3.48	91 (79%)	0	0	190, 219, 233, 235	0
14	AN	100/100 (100%)	2.21	46 (46%)	0	0	80, 100, 134, 140	0
14	BN	100/100 (100%)	3.17	86 (86%)	0	0	126, 174, 220, 227	0
15	AO	88/88 (100%)	1.33	14 (15%)	5	5	69, 82, 93, 98	0
15	BO	88/88 (100%)	2.23	53 (60%)	0	0	80, 105, 118, 125	0
16	AP	82/82 (100%)	1.42	14 (17%)	4	4	70, 85, 104, 113	0
16	BP	82/82 (100%)	3.67	75 (91%)	0	0	84, 106, 122, 126	0
17	AQ	80/80 (100%)	1.29	16 (20%)	3	3	69, 83, 96, 101	0
17	BQ	80/80 (100%)	3.18	62 (77%)	0	0	89, 120, 129, 133	0
18	AR	55/55 (100%)	1.58	12 (21%)	2	2	79, 86, 96, 98	0
18	BR	55/55 (100%)	2.17	27 (49%)	0	0	83, 90, 98, 100	0
19	AS	79/79 (100%)	2.04	36 (45%)	0	1	91, 110, 123, 127	0
19	BS	79/79 (100%)	2.96	60 (75%)	0	0	199, 217, 228, 231	0
20	AT	86/86 (100%)	1.59	21 (24%)	2	2	58, 84, 101, 107	0
20	BT	85/86 (98%)	3.62	69 (81%)	0	0	107, 131, 142, 144	0
21	AU	56/56 (100%)	1.79	21 (37%)	1	1	67, 80, 103, 113	0
21	BU	56/56 (100%)	2.13	27 (48%)	0	0	65, 85, 106, 113	0
22	CA	2876/2904 (99%)	1.31	429 (14%)	5	5	77, 118, 180, 217	0
23	CB	118/120 (98%)	0.73	0	100	100	108, 157, 167, 168	0
23	DB	120/120 (100%)	-0.13	0	100	100	37, 58, 73, 81	0
24	CC	271/271 (100%)	3.70	243 (89%)	0	0	83, 107, 126, 131	0
24	DC	271/271 (100%)	1.26	49 (18%)	3	3	35, 59, 71, 78	0
25	CD	209/209 (100%)	3.28	178 (85%)	0	0	87, 108, 121, 126	0
26	CE	201/201 (100%)	3.73	171 (85%)	0	0	90, 157, 187, 196	0
26	DE	201/201 (100%)	0.55	5 (2%)	58	61	33, 57, 72, 78	0
27	CF	177/177 (100%)	2.40	110 (62%)	0	0	167, 172, 174, 176	0
27	DF	177/177 (100%)	1.53	45 (25%)	1	2	58, 75, 91, 94	0
28	CG	176/176 (100%)	2.61	114 (64%)	0	0	108, 120, 130, 134	0
28	DG	176/176 (100%)	1.00	16 (9%)	15	15	49, 62, 71, 75	0
29	CH	149/149 (100%)	2.75	100 (67%)	0	0	96, 121, 141, 223	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	DH	149/149 (100%)	2.25	83 (55%) 0 0	65, 128, 133, 154	0
30	CJ	134/134 (100%)	3.05	97 (72%) 0 0	202, 219, 225, 228	0
30	DJ	134/134 (100%)	3.52	106 (79%) 0 0	155, 183, 202, 208	0
31	CK	142/142 (100%)	2.92	103 (72%) 0 0	98, 110, 115, 120	0
31	DK	142/142 (100%)	0.19	5 (3%) 47 49	33, 41, 51, 60	0
32	CL	122/123 (99%)	2.78	89 (72%) 0 0	94, 107, 113, 114	0
32	DL	123/123 (100%)	0.42	2 (1%) 70 73	37, 48, 59, 68	0
33	CM	144/144 (100%)	4.02	126 (87%) 0 0	100, 137, 162, 166	0
33	DM	144/144 (100%)	0.63	4 (2%) 55 57	28, 53, 69, 73	0
34	CN	135/136 (99%)	3.01	110 (81%) 0 0	95, 122, 142, 150	0
34	DN	135/136 (99%)	0.33	2 (1%) 72 74	23, 44, 57, 63	1 (0%)
35	CO	120/125 (96%)	3.64	110 (91%) 0 0	103, 120, 137, 142	0
35	DO	125/125 (100%)	0.47	8 (6%) 25 27	35, 44, 60, 69	0
36	CP	116/117 (99%)	2.61	65 (56%) 0 0	146, 155, 162, 164	0
36	DP	117/117 (100%)	1.02	5 (4%) 40 41	49, 59, 69, 73	0
37	CQ	114/114 (100%)	3.13	90 (78%) 0 0	110, 116, 124, 131	0
37	DQ	114/114 (100%)	0.75	9 (7%) 18 20	40, 52, 63, 73	0
38	CR	117/117 (100%)	3.51	91 (77%) 0 0	100, 115, 126, 128	0
38	DR	117/117 (100%)	0.10	3 (2%) 57 60	30, 40, 49, 64	0
39	CS	103/103 (100%)	3.31	85 (82%) 0 0	103, 125, 133, 137	0
39	DS	103/103 (100%)	0.46	2 (1%) 66 69	29, 48, 59, 73	0
40	CT	110/110 (100%)	3.81	99 (90%) 0 0	91, 121, 146, 150	0
40	DT	110/110 (100%)	0.14	1 (0%) 81 83	33, 39, 52, 68	0
41	CU	93/93 (100%)	4.19	83 (89%) 0 0	117, 149, 169, 176	0
41	DU	93/93 (100%)	1.18	15 (16%) 4 5	41, 57, 76, 83	0
42	CV	102/102 (100%)	5.01	98 (96%) 0 0	151, 176, 205, 210	0
42	DV	102/102 (100%)	1.08	13 (12%) 8 8	48, 60, 69, 80	0
43	CW	94/94 (100%)	2.21	50 (53%) 0 0	129, 148, 161, 165	0
43	DW	94/94 (100%)	0.70	2 (2%) 63 66	40, 54, 65, 71	0
44	CX	75/76 (98%)	2.99	63 (84%) 0 0	109, 118, 122, 126	0
44	DX	76/76 (100%)	0.62	5 (6%) 24 26	22, 46, 59, 65	1 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	CY	77/77 (100%)	4.00	72 (93%) 0 0	99, 116, 133, 135	0
45	DY	77/77 (100%)	1.10	12 (15%) 5 5	42, 59, 73, 78	0
46	CZ	62/62 (100%)	3.72	55 (88%) 0 0	158, 174, 193, 199	0
46	DZ	62/62 (100%)	1.47	15 (24%) 2 2	56, 66, 81, 82	0
47	C0	58/58 (100%)	2.99	41 (70%) 0 0	119, 130, 142, 143	0
47	D0	58/58 (100%)	0.50	5 (8%) 16 17	24, 42, 50, 56	2 (3%)
48	C1	56/56 (100%)	3.68	49 (87%) 0 0	92, 123, 140, 144	0
48	D1	56/56 (100%)	0.34	4 (7%) 22 23	27, 44, 58, 64	0
49	C2	50/51 (98%)	2.83	29 (58%) 0 0	113, 122, 128, 132	0
49	D2	51/51 (100%)	1.00	8 (15%) 5 5	50, 59, 66, 67	0
50	C3	46/46 (100%)	4.45	45 (97%) 0 0	95, 108, 115, 117	0
50	D3	46/46 (100%)	0.66	1 (2%) 62 65	35, 44, 53, 62	0
51	C4	64/64 (100%)	4.50	63 (98%) 0 0	109, 119, 126, 127	0
51	D4	64/64 (100%)	0.39	2 (3%) 51 54	39, 45, 51, 57	0
52	C5	38/38 (100%)	4.15	36 (94%) 0 0	106, 114, 120, 125	0
52	D5	38/38 (100%)	0.45	2 (5%) 32 34	42, 48, 58, 63	0
53	DA	2873/2903 (98%)	-0.30	67 (2%) 61 64	22, 49, 130, 199	8 (0%)
54	DD	208/209 (99%)	0.23	3 (1%) 73 75	29, 44, 58, 63	0
55	DI	135/135 (100%)	3.63	114 (84%) 0 0	76, 123, 152, 159	1 (0%)
All	All	20634/20744 (99%)	1.42	6063 (29%) 1 1	22, 96, 176, 235	13 (0%)

All (6063) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	BT	4	ILE	11.7
7	AG	5	ARG	11.4
42	CV	78	GLY	10.8
26	CE	73	ILE	10.6
38	CR	8	VAL	10.2
7	BG	62	PHE	10.1
13	BM	112	PRO	10.0
51	C4	15	LYS	9.9
38	CR	4	VAL	9.9
26	CE	77	ILE	9.8
20	BT	69	LYS	9.6

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Mol	Chain	Res	Type	RSRZ
38	CR	9	ILE	9.5
14	AN	21	PHE	9.5
30	DJ	54	PRO	9.3
42	CV	5	ILE	9.1
30	DJ	53	LEU	9.1
42	CV	35	ILE	9.0
42	CV	58	ILE	9.0
9	BI	116	VAL	9.0
13	BM	96	PRO	8.9
12	AL	124	ALA	8.8
40	CT	99	ARG	8.8
20	BT	68	HIS	8.8
32	CL	122	VAL	8.7
45	CY	49	LEU	8.7
26	CE	178	VAL	8.7
33	CM	19	LEU	8.6
3	BC	193	TYR	8.5
42	CV	36	VAL	8.4
9	BI	48	VAL	8.4
39	CS	51	VAL	8.4
32	CL	35	VAL	8.3
20	BT	67	ILE	8.3
26	CE	104	ALA	8.3
33	CM	71	ALA	8.3
24	CC	9	THR	8.2
26	CE	164	LEU	8.1
42	CV	2	ALA	8.0
35	CO	60	VAL	8.0
38	CR	39	VAL	8.0
46	CZ	43	LEU	8.0
42	CV	12	ILE	8.0
33	CM	28	GLY	8.0
33	CM	61	LEU	8.0
33	CM	30	THR	7.9
38	CR	2	ALA	7.9
42	CV	75	ALA	7.9
52	C5	10	LEU	7.8
25	CD	8	LYS	7.8
55	DI	131	THR	7.8
24	CC	202	LEU	7.8
42	CV	67	VAL	7.8
51	C4	25	LYS	7.8

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Mol	Chain	Res	Type	RSRZ
40	CT	97	LEU	7.7
26	CE	36	ALA	7.7
40	CT	46	LEU	7.7
41	CU	62	VAL	7.7
33	CM	21	ARG	7.6
33	CM	27	LEU	7.6
13	BM	98	ARG	7.6
42	CV	25	VAL	7.6
51	C4	22	PHE	7.5
24	CC	233	GLY	7.5
38	CR	38	ALA	7.5
26	CE	108	ILE	7.5
41	CU	74	ILE	7.5
24	CC	242	LYS	7.5
50	C3	42	LEU	7.5
14	BN	82	ILE	7.5
45	CY	35	SER	7.5
33	CM	75	ALA	7.4
41	CU	32	LEU	7.4
8	BH	2	SER	7.4
30	CJ	76	ALA	7.4
42	CV	80	ALA	7.4
25	CD	6	GLY	7.4
55	DI	84	TYR	7.3
31	CK	48	VAL	7.3
9	AI	130	ARG	7.3
55	DI	83	ALA	7.3
55	DI	106	PHE	7.3
42	CV	79	LYS	7.3
42	CV	3	ALA	7.3
42	CV	83	VAL	7.3
17	BQ	78	VAL	7.2
24	CC	250	VAL	7.2
39	CS	75	VAL	7.2
24	CC	12	GLY	7.2
33	CM	72	ALA	7.2
34	CN	116	ALA	7.2
52	C5	26	ILE	7.2
46	CZ	32	ALA	7.2
42	CV	59	VAL	7.1
37	CQ	92	VAL	7.1
31	CK	119	PHE	7.1

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Mol	Chain	Res	Type	RSRZ
41	CU	36	LYS	7.1
52	C5	31	PRO	7.0
31	CK	81	ILE	7.0
12	BL	7	LEU	7.0
55	DI	95	LEU	7.0
41	CU	43	ILE	7.0
46	CZ	11	VAL	7.0
47	C0	29	LEU	7.0
30	DJ	13	VAL	7.0
13	BM	106	ALA	7.0
33	CM	20	GLY	7.0
26	CE	147	LEU	7.0
24	CC	213	TRP	7.0
38	CR	5	LYS	7.0
26	CE	33	VAL	6.9
13	BM	99	GLY	6.9
26	CE	83	VAL	6.9
33	CM	92	LEU	6.9
50	C3	31	LEU	6.9
24	CC	254	GLY	6.9
9	BI	16	ALA	6.9
12	BL	2	ALA	6.9
31	CK	117	ALA	6.9
10	BJ	102	LEU	6.9
45	CY	31	PRO	6.8
34	CN	84	LYS	6.8
24	CC	216	VAL	6.8
20	BT	66	LEU	6.8
34	CN	95	LEU	6.8
33	CM	25	SER	6.8
29	CH	47	PHE	6.8
18	BR	20	GLU	6.8
46	CZ	53	VAL	6.8
41	CU	7	LEU	6.8
41	CU	50	LEU	6.8
30	DJ	67	PHE	6.8
6	BF	54	LEU	6.8
41	CU	10	VAL	6.8
42	CV	70	VAL	6.8
51	C4	58	VAL	6.8
42	CV	31	SER	6.8
33	CM	101	ILE	6.7

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Mol	Chain	Res	Type	RSRZ
25	CD	192	ALA	6.7
33	CM	53	GLY	6.7
26	CE	119	ILE	6.7
7	BG	59	LEU	6.7
24	CC	27	GLY	6.7
42	CV	13	VAL	6.7
10	BJ	44	THR	6.7
13	BM	108	THR	6.7
51	C4	52	LYS	6.7
33	CM	23	ILE	6.6
39	CS	49	ILE	6.6
42	CV	64	ALA	6.6
41	CU	93	LEU	6.6
19	AS	9	PRO	6.6
41	CU	57	VAL	6.6
24	CC	47	GLY	6.6
39	CS	73	LYS	6.6
16	BP	54	LEU	6.6
47	C0	15	GLY	6.6
19	BS	74	PHE	6.6
55	DI	92	ALA	6.6
42	CV	29	LEU	6.6
45	CY	30	LEU	6.6
48	C1	3	VAL	6.6
40	CT	80	PRO	6.6
10	BJ	71	LEU	6.6
46	CZ	19	LEU	6.6
26	CE	96	VAL	6.6
42	CV	77	THR	6.5
26	CE	101	TYR	6.5
42	CV	26	LYS	6.5
48	C1	12	LYS	6.5
21	BU	57	ALA	6.5
55	DI	59	LEU	6.5
28	CG	9	VAL	6.5
40	CT	73	LYS	6.5
33	CM	8	PRO	6.5
2	BB	135	LEU	6.5
30	DJ	129	ILE	6.5
49	C2	36	LEU	6.5
50	C3	10	LEU	6.5
52	C5	23	ILE	6.5

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Mol	Chain	Res	Type	RSRZ
30	DJ	118	THR	6.5
50	C3	24	THR	6.5
20	BT	63	ALA	6.5
25	CD	23	PRO	6.5
46	DZ	63	ALA	6.5
48	C1	2	ALA	6.5
16	BP	4	ILE	6.5
30	DJ	11	LEU	6.5
42	CV	39	ILE	6.5
30	CJ	54	PRO	6.4
26	CE	39	ALA	6.4
30	DJ	14	ALA	6.4
17	BQ	8	LEU	6.4
35	CO	38	LEU	6.4
33	CM	26	GLY	6.4
33	CM	49	GLY	6.4
13	BM	27	LYS	6.4
17	BQ	29	VAL	6.4
41	CU	63	VAL	6.4
3	BC	192	THR	6.4
42	CV	76	ALA	6.4
51	C4	60	ALA	6.4
51	C4	57	LEU	6.4
9	BI	127	PHE	6.4
42	CV	65	ILE	6.4
42	CV	103	ILE	6.4
7	BG	6	VAL	6.4
24	CC	228	VAL	6.4
48	C1	8	PRO	6.4
26	CE	159	LEU	6.4
26	CE	180	LEU	6.4
13	BM	22	ILE	6.4
26	CE	175	ILE	6.4
40	CT	96	ILE	6.4
55	DI	82	ILE	6.4
24	CC	220	VAL	6.4
33	CM	67	THR	6.4
31	CK	111	LYS	6.4
5	BE	110	ALA	6.4
42	CV	14	LEU	6.4
36	CP	8	ILE	6.3
33	CM	29	LYS	6.3

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Mol	Chain	Res	Type	RSRZ
9	BI	124	ARG	6.3
30	DJ	76	ALA	6.3
35	CO	19	ALA	6.3
50	C3	23	ALA	6.3
13	BM	95	LEU	6.3
24	CC	49	ILE	6.3
30	CJ	129	ILE	6.3
49	C2	22	THR	6.3
50	C3	36	ALA	6.3
24	CC	54	ILE	6.3
31	CK	103	ILE	6.3
40	CT	85	ILE	6.3
19	BS	49	ILE	6.3
24	CC	245	VAL	6.2
26	CE	89	PRO	6.2
35	CO	98	LEU	6.2
41	CU	61	LEU	6.2
55	DI	41	LEU	6.2
33	CM	105	ILE	6.2
41	CU	30	ILE	6.2
42	CV	85	PHE	6.2
42	CV	96	PHE	6.2
51	C4	14	PHE	6.2
41	CU	47	VAL	6.2
42	CV	23	GLY	6.2
55	DI	90	GLY	6.2
24	CC	34	LEU	6.2
41	CU	11	LEU	6.2
8	AH	2	SER	6.2
14	AN	30	ILE	6.2
24	CC	246	THR	6.2
42	CV	15	THR	6.2
50	D3	46	LYS	6.2
41	DU	1	MET	6.2
13	BM	16	VAL	6.2
9	BI	119	ARG	6.2
31	CK	47	HIS	6.2
42	CV	21	LYS	6.2
26	CE	182	ALA	6.1
26	CE	105	LEU	6.1
26	CE	143	LEU	6.1
33	CM	66	PHE	6.1

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Mol	Chain	Res	Type	RSRZ
30	CJ	80	LEU	6.1
50	C3	43	THR	6.1
30	DJ	55	ILE	6.1
35	CO	34	ILE	6.1
29	CH	108	VAL	6.1
13	BM	89	LEU	6.1
51	C4	23	LYS	6.1
25	CD	10	GLY	6.1
24	CC	240	PHE	6.1
26	CE	183	PHE	6.1
28	CG	10	VAL	6.1
40	CT	98	LYS	6.1
46	CZ	18	LEU	6.1
51	C4	59	ILE	6.0
24	CC	248	TRP	6.0
24	CC	20	VAL	6.0
32	CL	32	TYR	6.0
4	AD	2	ALA	6.0
35	CO	25	ALA	6.0
31	CK	109	LEU	6.0
16	BP	21	VAL	6.0
24	CC	30	PHE	6.0
36	CP	97	PHE	6.0
36	CP	103	VAL	6.0
14	BN	36	ALA	6.0
46	CZ	33	ALA	6.0
7	BG	22	LEU	6.0
16	BP	52	LEU	6.0
46	CZ	28	LEU	6.0
55	DI	72	LEU	6.0
30	CJ	122	ILE	6.0
31	CK	8	PRO	6.0
16	BP	20	VAL	6.0
9	AI	72	ILE	6.0
10	BJ	76	ILE	6.0
7	BG	80	VAL	5.9
51	C4	37	ALA	5.9
55	DI	93	ALA	5.9
24	CC	255	LYS	5.9
2	BB	98	GLY	5.9
26	CE	42	GLY	5.9
24	CC	247	PRO	5.9

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Mol	Chain	Res	Type	RSRZ
33	CM	73	ILE	5.9
33	CM	103	ILE	5.9
45	CY	13	VAL	5.9
33	CM	107	PHE	5.9
37	CQ	102	GLU	5.9
30	DJ	115	ALA	5.9
30	DJ	109	ILE	5.9
42	CV	72	ILE	5.9
36	CP	7	ARG	5.9
30	DJ	58	VAL	5.9
45	CY	7	VAL	5.9
41	CU	33	LYS	5.9
40	CT	19	LEU	5.9
9	BI	64	TYR	5.9
24	CC	11	PRO	5.9
36	CP	32	PRO	5.9
51	C4	46	PRO	5.9
16	BP	65	ALA	5.8
7	BG	5	ARG	5.8
50	C3	35	ARG	5.8
14	BN	31	ILE	5.8
42	CV	43	LYS	5.8
25	CD	155	VAL	5.8
41	CU	58	VAL	5.8
17	BQ	70	THR	5.8
55	DI	99	PHE	5.8
30	DJ	80	LEU	5.8
45	CY	20	HIS	5.8
9	BI	128	SER	5.8
24	CC	251	GLN	5.8
17	BQ	79	VAL	5.8
24	CC	165	VAL	5.8
52	C5	3	VAL	5.8
33	CM	74	THR	5.8
3	BC	37	PHE	5.8
28	CG	170	ARG	5.8
43	CW	23	ALA	5.8
10	BJ	73	LEU	5.8
50	C3	1	MET	5.8
4	BD	77	LYS	5.8
34	CN	2	LEU	5.8
34	CN	41	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
51	C4	33	LEU	5.8
39	CS	74	ILE	5.7
16	BP	60	TRP	5.7
45	CY	14	THR	5.7
24	CC	272	SER	5.7
24	CC	64	ILE	5.7
27	CF	156	ILE	5.7
45	CY	64	ILE	5.7
40	CT	102	HIS	5.7
28	CG	92	VAL	5.7
42	CV	34	VAL	5.7
55	DI	77	VAL	5.7
25	CD	132	ALA	5.7
48	C1	18	SER	5.7
26	CE	177	PRO	5.7
42	CV	4	LYS	5.7
55	DI	39	THR	5.7
24	CC	237	GLY	5.7
26	CE	78	TRP	5.7
5	BE	123	VAL	5.7
7	BG	69	VAL	5.7
10	BJ	77	VAL	5.7
24	CC	204	VAL	5.7
26	CE	52	VAL	5.7
30	DJ	110	ALA	5.7
37	CQ	108	ALA	5.7
25	CD	201	LEU	5.7
26	CE	85	PHE	5.7
35	CO	113	ILE	5.7
24	CC	3	VAL	5.6
50	C3	33	ARG	5.6
41	CU	46	ALA	5.6
24	CC	105	LEU	5.6
41	CU	81	LYS	5.6
24	CC	41	GLY	5.6
25	CD	112	THR	5.6
33	CM	34	GLY	5.6
38	CR	45	TYR	5.6
5	BE	99	ALA	5.6
14	BN	99	ALA	5.6
45	CY	4	VAL	5.6
9	BI	118	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
12	BL	15	LYS	5.6
34	CN	118	LYS	5.6
55	DI	126	LEU	5.6
55	DI	96	PHE	5.6
14	AN	31	ILE	5.6
35	CO	97	ILE	5.6
39	CS	88	GLY	5.6
13	BM	86	TYR	5.6
55	DI	24	SER	5.6
20	AT	2	ALA	5.6
35	CO	104	ALA	5.6
42	CV	44	LYS	5.6
17	BQ	22	VAL	5.6
34	CN	20	LEU	5.6
35	CO	21	PHE	5.6
45	CY	29	PHE	5.6
30	DJ	10	LYS	5.6
38	CR	41	LYS	5.6
7	BG	152	ALA	5.6
30	CJ	58	VAL	5.6
40	CT	107	VAL	5.6
45	CY	67	VAL	5.6
46	CZ	50	VAL	5.6
50	C3	44	VAL	5.6
14	AN	27	LEU	5.5
30	DJ	106	LEU	5.5
46	CZ	22	LEU	5.5
46	CZ	42	LEU	5.5
17	BQ	28	PHE	5.5
25	CD	156	PHE	5.5
26	CE	90	GLN	5.5
41	CU	73	ARG	5.5
24	CC	179	GLY	5.5
12	AL	2	ALA	5.5
29	DH	81	ALA	5.5
16	BP	36	VAL	5.5
24	CC	52	ARG	5.5
26	CE	109	LEU	5.5
30	DJ	70	VAL	5.5
30	DJ	78	VAL	5.5
33	CM	18	ARG	5.5
39	CS	20	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
40	CT	11	ARG	5.5
45	CY	22	LEU	5.5
55	DI	23	LEU	5.5
25	CD	118	PHE	5.5
42	CV	73	PHE	5.5
50	C3	18	PHE	5.5
34	CN	8	LYS	5.5
50	C3	25	LYS	5.5
20	BT	65	GLY	5.5
51	C4	61	CYS	5.5
33	CM	15	ALA	5.5
41	CU	41	ALA	5.5
7	BG	32	VAL	5.5
25	CD	9	VAL	5.5
16	BP	32	PHE	5.5
25	CD	166	GLY	5.5
38	CR	7	GLY	5.5
12	BL	14	ARG	5.5
16	BP	57	ILE	5.5
40	CT	74	ILE	5.5
42	CV	6	ARG	5.5
48	C1	21	ALA	5.5
50	C3	40	ALA	5.5
20	BT	58	VAL	5.5
29	CH	15	LEU	5.5
40	CT	76	VAL	5.5
39	CS	76	LYS	5.5
26	CE	88	ARG	5.4
37	CQ	104	THR	5.4
3	BC	162	ILE	5.4
16	BP	27	ALA	5.4
49	C2	10	LYS	5.4
30	CJ	11	LEU	5.4
5	BE	157	ARG	5.4
26	CE	23	PHE	5.4
51	C4	32	ILE	5.4
24	CC	61	ALA	5.4
26	CE	34	ALA	5.4
37	CQ	91	ALA	5.4
28	CG	148	LEU	5.4
29	CH	12	LEU	5.4
8	BH	3	MET	5.4

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Mol	Chain	Res	Type	RSRZ
30	CJ	70	VAL	5.4
26	CE	67	ARG	5.4
29	CH	11	ASN	5.4
45	CY	2	SER	5.4
24	DC	240	PHE	5.4
24	CC	265	LYS	5.4
35	CO	99	LYS	5.4
42	CV	33	LYS	5.4
51	C4	47	LYS	5.4
25	CD	96	ILE	5.4
28	CG	103	ILE	5.4
39	DS	103	ALA	5.4
35	CO	46	ARG	5.4
38	CR	11	ARG	5.4
10	BJ	52	LEU	5.4
38	CR	18	LEU	5.4
9	BI	111	VAL	5.4
42	CV	28	VAL	5.4
55	DI	85	VAL	5.4
26	CE	71	GLY	5.4
35	CO	105	GLY	5.4
38	CR	25	TYR	5.4
9	AI	129	LYS	5.4
20	BT	5	LYS	5.4
24	CC	256	LYS	5.4
42	CV	95	PHE	5.4
45	CY	38	PHE	5.4
9	BI	125	PRO	5.3
24	CC	48	ARG	5.3
26	CE	49	ARG	5.3
26	CE	50	ALA	5.3
7	BG	23	LEU	5.3
45	CY	33	LEU	5.3
51	C4	29	LEU	5.3
25	CD	5	VAL	5.3
42	CV	42	VAL	5.3
40	CT	75	PHE	5.3
36	CP	2	ASP	5.3
12	BL	124	ALA	5.3
24	CC	210	ALA	5.3
42	CV	71	ALA	5.3
10	BJ	42	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
34	CN	119	LEU	5.3
36	CP	5	SER	5.3
12	BL	16	VAL	5.3
14	BN	45	VAL	5.3
26	CE	47	LYS	5.3
33	CM	11	GLY	5.3
36	CP	3	LYS	5.3
55	DI	54	VAL	5.3
38	CR	47	TYR	5.3
16	BP	31	ARG	5.3
38	CR	44	GLN	5.3
44	CX	74	PRO	5.3
9	BI	21	ILE	5.3
34	CN	56	ALA	5.3
37	CQ	95	ALA	5.3
3	BC	33	LEU	5.3
9	AI	63	LEU	5.3
30	CJ	128	SER	5.3
33	CM	46	VAL	5.3
40	CT	105	VAL	5.3
45	CY	18	ARG	5.3
41	CU	39	THR	5.3
48	C1	9	THR	5.3
16	BP	17	TYR	5.3
52	C5	1	MET	5.3
16	BP	33	ILE	5.3
27	CF	67	ILE	5.3
37	CQ	64	ILE	5.3
47	C0	7	ILE	5.3
38	CR	22	LYS	5.3
13	AM	5	ALA	5.3
31	CK	94	ALA	5.3
36	CP	6	ALA	5.3
41	CU	45	ALA	5.3
2	AB	57	LEU	5.3
24	CC	33	LEU	5.3
32	CL	86	LEU	5.3
34	CN	15	GLY	5.3
46	CZ	57	LEU	5.3
50	C3	27	GLY	5.3
5	BE	137	VAL	5.2
25	CD	142	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
40	CT	45	VAL	5.2
44	CX	38	VAL	5.2
10	BJ	69	THR	5.2
26	CE	53	THR	5.2
38	CR	61	TRP	5.2
40	CT	100	THR	5.2
9	BI	20	PHE	5.2
39	CS	52	PRO	5.2
42	CV	24	LYS	5.2
9	BI	72	ILE	5.2
10	BJ	40	ILE	5.2
30	CJ	109	ILE	5.2
16	BP	25	ARG	5.2
16	BP	58	ALA	5.2
37	CQ	49	ALA	5.2
44	CX	49	ALA	5.2
14	BN	96	LEU	5.2
38	CR	26	GLY	5.2
42	CV	16	GLY	5.2
26	CE	196	VAL	5.2
42	CV	97	LYS	5.2
2	BB	126	PHE	5.2
10	BJ	41	PRO	5.2
44	CX	26	PHE	5.2
38	CR	17	ILE	5.2
24	CC	159	GLY	5.2
31	CK	133	ALA	5.2
55	DI	91	ALA	5.2
19	BS	31	LEU	5.2
19	BS	71	LEU	5.2
47	C0	17	LEU	5.2
35	CO	76	VAL	5.2
41	CU	85	VAL	5.2
52	C5	25	VAL	5.2
24	CC	5	LYS	5.2
42	CV	55	PRO	5.2
49	C2	21	TYR	5.2
10	BJ	6	ILE	5.2
10	BJ	100	ILE	5.2
13	BM	7	ILE	5.2
37	CQ	84	ILE	5.2
39	CS	27	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
24	CC	234	GLY	5.2
24	CC	241	GLY	5.2
33	CM	9	ALA	5.2
33	CM	102	GLY	5.2
40	CT	43	ALA	5.2
18	BR	67	LEU	5.2
30	CJ	79	LEU	5.2
30	DJ	79	LEU	5.2
37	CQ	114	LEU	5.2
30	CJ	10	LYS	5.2
13	BM	97	VAL	5.2
30	CJ	13	VAL	5.2
24	CC	8	PRO	5.1
29	CH	136	SER	5.1
30	CJ	69	PHE	5.1
52	C5	28	SER	5.1
33	CM	22	GLY	5.1
36	CP	40	ILE	5.1
48	C1	55	ILE	5.1
30	DJ	114	ALA	5.1
40	CT	5	ALA	5.1
45	CY	24	ALA	5.1
24	CC	176	LEU	5.1
36	CP	48	LEU	5.1
49	C2	11	LEU	5.1
13	BM	109	ARG	5.1
10	BJ	74	VAL	5.1
16	BP	2	VAL	5.1
28	CG	169	VAL	5.1
41	CU	67	VAL	5.1
55	DI	33	VAL	5.1
55	DI	50	VAL	5.1
40	CT	86	MET	5.1
33	CM	68	SER	5.1
3	AC	168	TYR	5.1
13	BM	4	ILE	5.1
14	BN	101	TRP	5.1
33	CM	31	GLY	5.1
39	CS	50	GLY	5.1
42	CV	20	GLY	5.1
42	CV	38	GLY	5.1
47	C0	14	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
5	BE	26	LYS	5.1
12	BL	44	LYS	5.1
30	CJ	14	ALA	5.1
40	CT	42	LYS	5.1
26	CE	27	LEU	5.1
27	CF	152	LEU	5.1
29	CH	75	LEU	5.1
38	CR	6	ARG	5.1
39	CS	39	LEU	5.1
42	CV	27	ASN	5.1
55	DI	58	THR	5.1
44	CX	23	VAL	5.1
14	BN	70	PRO	5.1
53	DA	654	A	5.1
9	BI	14	SER	5.1
24	CC	39	LYS	5.1
42	DV	56	GLY	5.1
48	C1	14	GLY	5.1
17	BQ	61	ILE	5.1
20	BT	36	TYR	5.1
45	CY	46	PHE	5.1
42	CV	22	ARG	5.1
10	BJ	12	ALA	5.1
31	CK	6	ALA	5.1
36	CP	14	ALA	5.1
24	CC	205	LEU	5.1
25	CD	126	ASN	5.1
24	CC	65	VAL	5.1
26	CE	28	VAL	5.1
30	CJ	24	VAL	5.1
30	CJ	78	VAL	5.1
31	CK	100	VAL	5.1
31	CK	46	PRO	5.1
6	BF	100	SER	5.1
52	C5	33	HIS	5.1
50	C3	14	ARG	5.1
52	C5	12	ARG	5.1
35	CO	102	PHE	5.0
7	BG	39	ALA	5.0
7	BG	134	ALA	5.0
16	BP	22	ALA	5.0
27	DF	83	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
50	C3	13	ASN	5.0
7	AG	13	LEU	5.0
19	BS	15	LEU	5.0
20	BT	86	LEU	5.0
55	DI	67	THR	5.0
45	CY	77	LYS	5.0
48	C1	27	SER	5.0
33	CM	35	HIS	5.0
30	DJ	52	GLY	5.0
31	CK	83	GLY	5.0
2	BB	171	ILE	5.0
16	BP	67	ILE	5.0
24	CC	67	PHE	5.0
24	CC	239	ASN	5.0
26	CE	172	ALA	5.0
30	DJ	49	ILE	5.0
33	CM	77	ILE	5.0
38	CR	10	ALA	5.0
43	CW	94	ALA	5.0
3	BC	178	LEU	5.0
14	BN	60	GLN	5.0
28	CG	157	TYR	5.0
40	CT	36	LEU	5.0
33	CM	1	MET	5.0
55	DI	38	MET	5.0
7	BG	38	THR	5.0
24	CC	252	THR	5.0
40	CT	3	THR	5.0
3	BC	167	TRP	5.0
25	CD	80	TRP	5.0
46	CZ	44	LYS	5.0
41	CU	12	ARG	5.0
26	CE	179	SER	5.0
29	CH	138	VAL	5.0
55	DI	130	PRO	5.0
20	BT	3	ASN	5.0
17	BQ	37	PHE	5.0
26	CE	37	ALA	5.0
30	DJ	38	PHE	5.0
7	AG	23	LEU	5.0
13	BM	19	LEU	5.0
13	BM	34	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
25	CD	187	LEU	5.0
37	CQ	97	LEU	5.0
46	CZ	6	LEU	5.0
46	CZ	21	LEU	5.0
4	BD	206	LYS	5.0
19	BS	7	LYS	5.0
20	BT	64	LYS	5.0
26	CE	43	THR	5.0
51	C4	39	LYS	5.0
4	BD	44	ARG	5.0
26	CE	70	SER	5.0
5	BE	120	VAL	5.0
24	CC	16	VAL	5.0
39	CS	54	VAL	5.0
14	BN	29	ALA	5.0
14	BN	30	ILE	5.0
16	AP	82	ALA	5.0
29	DH	80	ILE	5.0
33	CM	39	LYS	5.0
41	CU	44	LYS	5.0
53	DA	1172	C	5.0
24	CC	32	PRO	4.9
50	C3	7	PRO	4.9
24	CC	4	VAL	4.9
25	CD	37	VAL	4.9
39	CS	47	VAL	4.9
9	BI	117	GLY	4.9
40	CT	40	ASN	4.9
51	C4	28	ASN	4.9
44	CX	78	LYS	4.9
33	CM	69	ARG	4.9
36	CP	16	ARG	4.9
39	CS	36	ALA	4.9
41	CU	13	ALA	4.9
51	C4	4	ILE	4.9
26	CE	112	LEU	4.9
33	CM	57	LEU	4.9
33	CM	64	PHE	4.9
6	BF	92	THR	4.9
19	BS	33	THR	4.9
48	C1	28	LEU	4.9
20	BT	6	SER	4.9

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Mol	Chain	Res	Type	RSRZ
10	BJ	43	PRO	4.9
14	BN	57	PRO	4.9
38	CR	59	GLN	4.9
7	BG	43	VAL	4.9
28	CG	161	GLY	4.9
37	CQ	105	GLY	4.9
38	CR	23	GLY	4.9
48	C1	6	ASN	4.9
9	BI	68	LYS	4.9
17	BQ	21	ILE	4.9
24	CC	135	ILE	4.9
24	CC	164	ILE	4.9
37	CQ	110	ILE	4.9
7	AG	38	THR	4.9
8	BH	86	TYR	4.9
26	CE	35	TYR	4.9
51	C4	49	MET	4.9
38	CR	16	LYS	4.9
25	CD	26	VAL	4.9
30	CJ	9	VAL	4.9
42	CV	93	VAL	4.9
54	DD	209	ALA	4.9
1	AA	121	U	4.9
35	CO	51	LEU	4.9
51	C4	62	LEU	4.9
30	DJ	128	SER	4.9
41	CU	72	GLN	4.9
50	C3	5	PHE	4.9
29	CH	35	LYS	4.9
31	CK	116	ARG	4.9
47	C0	56	LYS	4.9
48	C1	7	LYS	4.9
48	C1	15	MET	4.9
26	CE	32	VAL	4.9
26	CE	186	VAL	4.9
29	CH	3	VAL	4.9
7	BG	65	ALA	4.8
10	BJ	61	ALA	4.8
3	BC	175	LEU	4.8
7	BG	7	ILE	4.8
13	AM	7	ILE	4.8
16	BP	6	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
44	CX	21	LEU	4.8
41	CU	78	SER	4.8
41	DU	69	ARG	4.8
33	CM	52	GLY	4.8
33	CM	58	TYR	4.8
41	CU	84	TYR	4.8
9	BI	104	VAL	4.8
12	BL	98	VAL	4.8
35	CO	29	VAL	4.8
35	CO	47	VAL	4.8
37	CQ	46	VAL	4.8
39	CS	72	VAL	4.8
45	CY	51	VAL	4.8
51	C4	7	VAL	4.8
52	C5	7	VAL	4.8
38	CR	35	ALA	4.8
39	CS	28	ALA	4.8
51	C4	34	THR	4.8
55	DI	48	ALA	4.8
7	BG	42	ILE	4.8
8	BH	125	ILE	4.8
20	BT	19	LYS	4.8
26	CE	98	LYS	4.8
26	CE	200	LEU	4.8
30	DJ	138	LEU	4.8
49	C2	38	LYS	4.8
44	CX	60	PHE	4.8
24	CC	249	GLY	4.8
28	CG	168	VAL	4.8
34	CN	36	VAL	4.8
41	CU	31	VAL	4.8
48	C1	54	VAL	4.8
49	C2	47	VAL	4.8
50	C3	9	VAL	4.8
46	CZ	47	ARG	4.8
33	CM	83	ALA	4.8
35	CO	91	ALA	4.8
26	CE	153	LEU	4.8
35	CO	10	LEU	4.8
10	BJ	67	ILE	4.8
25	CD	14	ILE	4.8
53	DA	138	U	4.8

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Mol	Chain	Res	Type	RSRZ
14	BN	77	PHE	4.8
28	CG	52	PHE	4.8
37	CQ	23	GLY	4.8
30	DJ	12	GLN	4.8
30	DJ	24	VAL	4.8
36	CP	9	ARG	4.8
39	CS	81	LYS	4.8
40	CT	6	LYS	4.8
26	CE	80	SER	4.8
20	BT	7	ALA	4.8
5	BE	11	LEU	4.7
10	BJ	92	LEU	4.7
20	BT	79	LEU	4.7
24	CC	110	LEU	4.7
31	CK	93	ILE	4.7
37	CQ	4	ILE	4.7
5	BE	91	GLY	4.7
19	BS	76	PRO	4.7
25	CD	194	PRO	4.7
51	C4	26	HIS	4.7
41	CU	49	LYS	4.7
13	BM	60	VAL	4.7
24	CC	83	TYR	4.7
29	CH	142	VAL	4.7
55	DI	132	TYR	4.7
3	BC	44	THR	4.7
20	BT	70	ASN	4.7
26	CE	131	THR	4.7
25	CD	209	ALA	4.7
47	C0	13	ALA	4.7
7	BG	66	LEU	4.7
14	BN	27	LEU	4.7
30	CJ	53	LEU	4.7
19	BS	9	PRO	4.7
24	CC	235	GLY	4.7
37	CQ	22	PRO	4.7
6	BF	80	PHE	4.7
10	BJ	49	PHE	4.7
33	CM	50	PHE	4.7
25	CD	157	LYS	4.7
37	CQ	63	LYS	4.7
10	BJ	36	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
25	CD	170	VAL	4.7
26	CE	146	VAL	4.7
29	DH	147	VAL	4.7
40	CT	20	VAL	4.7
42	CV	11	VAL	4.7
45	CY	47	VAL	4.7
26	CE	55	SER	4.7
20	BT	80	THR	4.7
45	CY	48	THR	4.7
35	CO	68	ALA	4.7
55	DI	44	ALA	4.7
39	CS	82	HIS	4.7
7	AG	7	ILE	4.7
24	CC	148	PRO	4.7
24	DC	233	GLY	4.7
30	CJ	55	ILE	4.7
30	DJ	86	ILE	4.7
40	CT	79	GLY	4.7
36	CP	4	LYS	4.7
37	CQ	94	LYS	4.7
52	C5	32	LYS	4.7
42	CV	9	ASP	4.7
13	BM	25	VAL	4.7
40	CT	47	VAL	4.7
13	BM	105	ASN	4.7
35	CO	112	TYR	4.7
16	BP	3	THR	4.7
35	DO	122	ALA	4.7
43	CW	22	ALA	4.7
25	CD	116	LYS	4.7
33	CM	70	LYS	4.7
3	BC	196	ILE	4.7
5	BE	30	ILE	4.7
40	CT	66	ILE	4.7
55	DI	123	ILE	4.7
53	DA	1175	A	4.6
6	BF	8	PHE	4.6
47	C0	53	PHE	4.6
40	CT	13	SER	4.6
52	C5	13	ASN	4.6
24	CC	19	VAL	4.6
25	CD	24	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
31	CK	105	VAL	4.6
37	CQ	73	VAL	4.6
39	CS	96	VAL	4.6
41	CU	16	VAL	4.6
24	CC	13	ARG	4.6
38	CR	28	ARG	4.6
18	AR	51	TYR	4.6
43	CW	82	TYR	4.6
13	BM	32	ALA	4.6
14	AN	12	LYS	4.6
25	CD	119	ALA	4.6
35	CO	111	ALA	4.6
35	DO	125	ALA	4.6
52	C5	9	LYS	4.6
12	BL	92	GLY	4.6
14	BN	79	LEU	4.6
42	CV	41	LEU	4.6
47	C0	18	PRO	4.6
10	BJ	18	ILE	4.6
20	BT	57	ILE	4.6
35	CO	63	ARG	4.6
41	CU	80	TRP	4.6
9	BI	114	LYS	4.6
17	BQ	23	VAL	4.6
29	CH	130	VAL	4.6
52	C5	15	LYS	4.6
14	BN	2	ALA	4.6
16	BP	82	ALA	4.6
24	CC	2	ALA	4.6
24	CC	198	ALA	4.6
42	CV	63	ALA	4.6
45	CY	9	GLY	4.6
51	C4	21	GLY	4.6
2	BB	85	LEU	4.6
25	CD	186	LEU	4.6
29	CH	149	GLU	4.6
13	AM	11	ASP	4.6
3	BC	207	ILE	4.6
7	BG	104	ILE	4.6
9	BI	65	ILE	4.6
12	BL	82	ILE	4.6
44	CX	37	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
47	C0	32	ILE	4.6
35	CO	22	ARG	4.6
27	CF	20	PHE	4.6
29	CH	20	ASN	4.6
24	CC	178	SER	4.6
35	CO	14	SER	4.6
40	CT	12	SER	4.6
17	BQ	46	VAL	4.6
24	CC	184	VAL	4.6
30	CJ	132	THR	4.6
35	CO	48	VAL	4.6
41	CU	55	VAL	4.6
16	BP	64	GLY	4.6
24	CC	112	ALA	4.6
32	CL	83	ALA	4.6
33	CM	44	GLY	4.6
35	DO	124	ALA	4.6
41	CU	71	GLY	4.6
7	BG	118	LEU	4.6
13	AM	19	LEU	4.6
13	AM	80	LEU	4.6
30	DJ	20	PRO	4.6
42	DV	52	LEU	4.6
40	CT	103	ILE	4.6
41	DU	2	ILE	4.6
35	CO	11	ASN	4.6
35	CO	62	ASN	4.6
16	BP	12	LYS	4.6
20	BT	16	LYS	4.6
40	CT	81	SER	4.6
42	CV	47	LYS	4.6
51	C4	16	LYS	4.6
18	AR	74	HIS	4.6
29	CH	29	PHE	4.6
24	CC	223	THR	4.5
10	BJ	51	VAL	4.5
25	CD	50	VAL	4.5
49	C2	42	VAL	4.5
55	DI	26	VAL	4.5
12	BL	84	GLY	4.5
24	CC	224	ALA	4.5
30	DJ	23	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
55	DI	79	PRO	4.5
14	BN	46	LEU	4.5
20	BT	10	ARG	4.5
34	CN	112	LEU	4.5
49	C2	34	LEU	4.5
5	BE	60	ILE	4.5
18	BR	21	ILE	4.5
28	CG	77	ILE	4.5
55	DI	136	ILE	4.5
17	BQ	20	SER	4.5
40	CT	7	HIS	4.5
38	CR	57	PHE	4.5
30	DJ	117	MET	4.5
7	AG	94	VAL	4.5
7	BG	64	VAL	4.5
24	CC	137	VAL	4.5
25	CD	172	VAL	4.5
28	CG	23	VAL	4.5
29	CH	144	VAL	4.5
45	CY	58	VAL	4.5
55	DI	64	VAL	4.5
30	DJ	18	ALA	4.5
52	C5	29	ALA	4.5
17	BQ	73	TRP	4.5
24	CC	174	LEU	4.5
35	CO	28	LEU	4.5
46	CZ	14	LEU	4.5
17	AQ	5	ILE	4.5
24	CC	37	ASN	4.5
12	BL	3	THR	4.5
13	BM	113	ARG	4.5
34	CN	6	ARG	4.5
27	CF	93	GLY	4.5
2	BB	199	VAL	4.5
5	BE	46	VAL	4.5
17	BQ	58	VAL	4.5
26	CE	126	VAL	4.5
28	CG	76	VAL	4.5
33	CM	38	GLN	4.5
25	CD	196	ALA	4.5
55	DI	110	ALA	4.5
55	DI	111	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
36	CP	17	LYS	4.5
44	CX	75	LYS	4.5
9	BI	61	LEU	4.5
15	BO	56	LEU	4.5
29	CH	6	LEU	4.5
34	CN	124	LEU	4.5
10	BJ	70	HIS	4.5
35	CO	23	ASN	4.5
10	AJ	6	ILE	4.5
39	CS	80	ARG	4.5
5	BE	103	THR	4.5
25	CD	25	THR	4.5
41	CU	51	PHE	4.5
42	CV	87	PHE	4.5
16	BP	10	GLY	4.5
34	CN	19	GLY	4.5
5	BE	23	LYS	4.5
41	CU	66	LYS	4.5
10	BJ	26	VAL	4.5
25	CD	152	PRO	4.5
28	CG	112	PRO	4.5
7	BG	51	ALA	4.5
7	BG	61	ALA	4.5
28	CG	174	ALA	4.5
41	CU	83	ALA	4.5
8	BH	92	LEU	4.5
13	BM	83	LEU	4.5
40	CT	23	LEU	4.5
46	CZ	15	ASN	4.5
48	C1	11	SER	4.4
2	BB	67	ILE	4.4
2	BB	164	ILE	4.4
38	CR	13	ARG	4.4
39	CS	55	ASP	4.4
26	CE	84	THR	4.4
30	DJ	112	THR	4.4
2	BB	149	GLY	4.4
5	BE	104	GLY	4.4
24	CC	55	GLY	4.4
39	CS	77	PHE	4.4
52	C5	34	LYS	4.4
2	AB	4	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
28	CG	102	VAL	4.4
2	BB	34	ALA	4.4
2	BB	134	ALA	4.4
24	CC	211	ALA	4.4
26	CE	26	ALA	4.4
29	CH	23	ALA	4.4
29	DH	64	ALA	4.4
30	CJ	77	ALA	4.4
30	DJ	77	ALA	4.4
33	CM	113	ALA	4.4
48	C1	39	LEU	4.4
55	DI	117	LEU	4.4
4	BD	153	SER	4.4
13	BM	30	SER	4.4
20	BT	24	ARG	4.4
33	CM	33	ARG	4.4
10	AJ	40	ILE	4.4
13	BM	100	GLN	4.4
53	DA	1176	U	4.4
2	BB	130	THR	4.4
7	BG	133	THR	4.4
24	CC	51	THR	4.4
26	CE	81	GLY	4.4
26	CE	173	THR	4.4
36	CP	12	THR	4.4
13	BM	63	PHE	4.4
16	BP	16	PHE	4.4
26	CE	124	PHE	4.4
51	C4	43	HIS	4.4
31	CK	113	PRO	4.4
21	AU	57	ALA	4.4
50	C3	20	ALA	4.4
51	C4	27	ALA	4.4
7	BG	13	LEU	4.4
30	CJ	138	LEU	4.4
39	CS	79	ARG	4.4
45	CY	50	ARG	4.4
55	DI	81	LEU	4.4
53	DA	139	U	4.4
3	AC	207	ILE	4.4
14	BN	93	ILE	4.4
29	CH	94	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
17	BQ	30	LYS	4.4
5	BE	50	TYR	4.4
51	C4	64	TYR	4.4
14	AN	42	TRP	4.4
53	DA	549	G	4.4
40	CT	60	HIS	4.4
24	CC	266	PHE	4.4
37	CQ	43	PHE	4.4
43	CW	84	PRO	4.4
24	CC	175	ARG	4.4
24	CC	238	ARG	4.4
45	CY	3	ARG	4.4
45	CY	56	MET	4.4
7	AG	105	VAL	4.4
29	CH	37	VAL	4.4
38	CR	31	VAL	4.4
19	AS	5	LEU	4.4
25	CD	188	LEU	4.4
26	CE	72	SER	4.4
26	CE	157	LEU	4.4
31	CK	114	LEU	4.4
45	CY	71	LEU	4.4
8	AH	76	GLN	4.4
27	CF	72	LYS	4.4
35	CO	100	CYS	4.4
41	CU	9	LYS	4.4
41	CU	40	LYS	4.4
13	BM	77	ILE	4.4
17	BQ	38	ILE	4.4
47	C0	48	ILE	4.4
7	BG	44	TYR	4.3
24	CC	62	TYR	4.3
32	CL	81	GLY	4.3
24	CC	14	ARG	4.3
41	CU	76	ARG	4.3
42	CV	94	ARG	4.3
45	CY	32	ASN	4.3
20	BT	31	PHE	4.3
26	CE	158	PHE	4.3
7	BG	150	ALA	4.3
11	BK	86	VAL	4.3
16	BP	19	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
20	BT	11	ALA	4.3
30	DJ	57	VAL	4.3
35	CO	55	ALA	4.3
7	AG	25	LYS	4.3
52	C5	8	LYS	4.3
42	CV	10	GLU	4.3
2	BB	151	ILE	4.3
25	CD	146	ILE	4.3
27	CF	79	ILE	4.3
36	CP	58	ILE	4.3
37	CQ	48	ILE	4.3
5	BE	42	GLY	4.3
26	CE	40	ARG	4.3
33	CM	16	GLY	4.3
35	CO	2	ARG	4.3
42	CV	84	GLY	4.3
48	C1	16	ARG	4.3
27	CF	84	PRO	4.3
7	AG	26	PHE	4.3
7	BG	151	PHE	4.3
35	CO	67	PHE	4.3
24	CC	18	LYS	4.3
32	CL	66	LYS	4.3
16	BP	72	ALA	4.3
29	CH	106	ALA	4.3
30	DJ	15	ALA	4.3
42	CV	51	ALA	4.3
29	CH	31	VAL	4.3
7	BG	50	LEU	4.3
37	DQ	114	LEU	4.3
42	CV	52	LEU	4.3
51	C4	54	ASP	4.3
38	CR	30	ARG	4.3
11	BK	107	ILE	4.3
30	DJ	59	ILE	4.3
33	CM	100	ILE	4.3
35	CO	52	ILE	4.3
38	CR	90	ILE	4.3
51	C4	24	HIS	4.3
55	DI	52	MET	4.3
31	CK	53	TYR	4.3
9	BI	13	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
41	CU	64	LYS	4.3
50	C3	46	LYS	4.3
14	BN	21	PHE	4.3
26	CE	135	ALA	4.3
29	CH	10	ALA	4.3
30	CJ	110	ALA	4.3
35	CO	108	ALA	4.3
49	C2	52	ALA	4.3
7	AG	32	VAL	4.3
7	BG	141	VAL	4.3
8	BH	34	VAL	4.3
9	AI	58	VAL	4.3
25	CD	107	VAL	4.3
29	DH	121	VAL	4.3
32	CL	8	LEU	4.3
34	CN	78	LEU	4.3
35	CO	65	LEU	4.3
36	CP	18	LEU	4.3
6	BF	91	ARG	4.3
26	CE	92	HIS	4.3
3	BC	159	GLY	4.3
13	BM	45	ILE	4.3
20	BT	12	ILE	4.3
24	CC	267	ILE	4.3
33	CM	32	GLY	4.3
33	CM	111	ILE	4.3
34	CN	73	ILE	4.3
41	CU	2	ILE	4.3
20	BT	13	GLN	4.3
37	CQ	12	GLN	4.3
9	BI	129	LYS	4.3
13	BM	31	LYS	4.3
25	CD	123	LYS	4.3
31	CK	72	LYS	4.3
41	CU	82	LYS	4.3
44	CX	44	LYS	4.3
5	BE	150	PRO	4.3
7	BG	117	ALA	4.2
20	BT	73	ALA	4.2
30	CJ	120	ALA	4.2
30	DJ	42	PHE	4.2
33	CM	108	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
35	CO	61	ALA	4.2
41	CU	35	ALA	4.2
44	CX	45	PHE	4.2
45	CY	53	ALA	4.2
12	AL	9	ARG	4.2
29	CH	27	ARG	4.2
38	CR	3	ARG	4.2
48	C1	10	ARG	4.2
7	BG	47	LEU	4.2
9	BI	47	VAL	4.2
10	BJ	96	VAL	4.2
24	CC	17	VAL	4.2
24	CC	172	VAL	4.2
24	CC	192	LEU	4.2
26	CE	31	VAL	4.2
26	CE	138	LEU	4.2
26	CE	167	VAL	4.2
28	CG	43	VAL	4.2
37	CQ	8	LEU	4.2
40	CT	50	VAL	4.2
52	C5	22	VAL	4.2
17	BQ	17	MET	4.2
26	CE	38	GLY	4.2
29	CH	92	GLY	4.2
32	CL	26	GLY	4.2
34	CN	61	GLY	4.2
50	C3	17	GLY	4.2
13	BM	33	ILE	4.2
25	CD	22	ILE	4.2
26	CE	57	LYS	4.2
50	C3	37	LYS	4.2
26	CE	48	THR	4.2
30	CJ	118	THR	4.2
45	CY	66	THR	4.2
51	C4	17	THR	4.2
7	BG	71	PRO	4.2
30	DJ	22	PRO	4.2
12	BL	9	ARG	4.2
13	BM	29	ARG	4.2
19	BS	3	ARG	4.2
48	C1	17	ARG	4.2
25	CD	140	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
55	DI	113	PHE	4.2
27	CF	74	VAL	4.2
30	DJ	98	VAL	4.2
35	CO	44	LEU	4.2
41	CU	87	LEU	4.2
39	CS	92	TRP	4.2
47	C0	36	VAL	4.2
26	CE	97	ASN	4.2
41	CU	68	LYS	4.2
5	BE	158	GLY	4.2
13	AM	99	GLY	4.2
24	DC	237	GLY	4.2
26	CE	82	GLY	4.2
27	CF	76	GLY	4.2
51	C4	53	GLY	4.2
44	DX	10	THR	4.2
48	C1	43	ILE	4.2
10	BJ	45	ARG	4.2
14	BN	81	ARG	4.2
51	C4	42	ARG	4.2
38	CR	24	TYR	4.2
14	AN	29	ALA	4.2
32	CL	16	ALA	4.2
34	CN	121	ALA	4.2
48	C1	45	ALA	4.2
12	BL	81	LEU	4.2
17	BQ	67	LEU	4.2
17	BQ	75	LEU	4.2
25	CD	40	LEU	4.2
28	CG	87	LEU	4.2
46	CZ	37	LEU	4.2
51	C4	55	LEU	4.2
6	AF	89	VAL	4.2
13	BM	43	VAL	4.2
14	BN	97	LYS	4.2
29	DH	146	VAL	4.2
30	DJ	9	VAL	4.2
33	CM	13	LYS	4.2
35	CO	116	VAL	4.2
38	CR	34	VAL	4.2
41	CU	34	VAL	4.2
35	CO	7	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
35	DO	123	GLU	4.2
39	CS	9	GLY	4.2
45	CY	15	GLY	4.2
52	C5	21	GLY	4.2
10	BJ	50	THR	4.2
25	CD	129	THR	4.2
30	DJ	71	THR	4.2
34	CN	40	ARG	4.2
39	CS	78	ARG	4.2
40	CT	18	ARG	4.2
50	C3	12	ARG	4.2
7	AG	2	PRO	4.2
19	BS	4	SER	4.2
24	CC	15	HIS	4.2
46	CZ	30	MET	4.2
37	CQ	98	TYR	4.2
17	BQ	16	LYS	4.2
33	CM	14	LYS	4.2
55	DI	75	ALA	4.2
3	BC	43	LEU	4.2
33	CM	3	LEU	4.2
38	CR	101	PHE	4.2
7	BG	27	VAL	4.2
19	AS	58	VAL	4.2
30	DJ	119	GLY	4.1
33	CM	37	GLY	4.1
41	CU	65	GLY	4.1
42	CV	32	GLY	4.1
24	CC	203	ARG	4.1
40	CT	92	ARG	4.1
47	C0	16	ARG	4.1
48	C1	13	ARG	4.1
47	C0	10	THR	4.1
10	BJ	8	ILE	4.1
13	AM	45	ILE	4.1
16	BP	42	ILE	4.1
35	CO	33	ILE	4.1
8	BH	6	PRO	4.1
9	AI	128	SER	4.1
19	BS	12	ASP	4.1
13	AM	115	PRO	4.1
24	DC	272	SER	4.1

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Mol	Chain	Res	Type	RSRZ
38	CR	29	SER	4.1
41	CU	1	MET	4.1
35	CO	40	LYS	4.1
45	CY	26	LYS	4.1
3	BC	30	ALA	4.1
3	BC	168	TYR	4.1
8	BH	130	ALA	4.1
13	AM	2	ALA	4.1
20	AT	62	ALA	4.1
30	CJ	114	ALA	4.1
30	DJ	63	ALA	4.1
31	CK	42	ALA	4.1
37	CQ	99	TYR	4.1
33	CM	79	LEU	4.1
24	CC	212	ARG	4.1
25	CD	60	VAL	4.1
25	CD	122	VAL	4.1
25	CD	144	GLY	4.1
30	DJ	61	VAL	4.1
33	CM	110	VAL	4.1
37	CQ	93	ARG	4.1
10	BJ	38	GLY	4.1
39	CS	63	VAL	4.1
9	BI	105	THR	4.1
42	CV	102	THR	4.1
45	CY	8	THR	4.1
41	CU	79	ASP	4.1
17	BQ	55	ILE	4.1
26	CE	181	ILE	4.1
31	CK	118	MET	4.1
42	CV	48	PRO	4.1
26	CE	41	GLN	4.1
6	BF	57	ALA	4.1
20	BT	72	ALA	4.1
46	CZ	3	ALA	4.1
9	BI	54	LEU	4.1
18	BR	51	TYR	4.1
24	CC	93	LEU	4.1
38	CR	32	TYR	4.1
45	CY	78	TYR	4.1
32	CL	101	GLY	4.1
55	DI	15	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
55	DI	55	VAL	4.1
24	CC	257	THR	4.1
35	CO	36	THR	4.1
55	DI	34	THR	4.1
9	BI	110	GLN	4.1
20	AT	4	ILE	4.1
26	CE	166	LYS	4.1
40	CT	55	ILE	4.1
49	C2	5	ILE	4.1
50	C3	2	LYS	4.1
55	DI	37	LYS	4.1
55	DI	43	LYS	4.1
33	CM	10	GLU	4.1
24	CC	43	ARG	4.1
50	C3	21	ARG	4.1
8	BH	97	ALA	4.1
29	CH	39	ALA	4.1
38	CR	27	ALA	4.1
40	CT	44	ALA	4.1
55	DI	104	ALA	4.1
55	DI	135	ALA	4.1
13	BM	94	GLY	4.1
14	BN	48	LEU	4.1
14	BN	74	LEU	4.1
38	CR	60	LEU	4.1
39	CS	8	GLY	4.1
9	BI	38	TYR	4.1
2	BB	210	VAL	4.1
4	BD	137	VAL	4.1
9	BI	19	VAL	4.1
17	AQ	83	VAL	4.1
25	CD	200	ASP	4.1
31	CK	49	ASP	4.1
34	CN	70	ASP	4.1
40	CT	82	MET	4.1
26	CE	185	LYS	4.1
25	CD	174	SER	4.1
29	CH	4	ILE	4.1
30	CJ	59	ILE	4.1
55	DI	118	ILE	4.1
33	CM	78	ARG	4.0
34	CN	18	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
6	BF	83	ALA	4.0
13	AM	36	ALA	4.0
13	BM	37	ALA	4.0
24	CC	56	GLY	4.0
49	C2	4	GLY	4.0
10	AJ	10	LEU	4.0
27	CF	117	LEU	4.0
33	CM	82	LEU	4.0
38	CR	109	LEU	4.0
45	CY	68	LEU	4.0
42	CV	92	LYS	4.0
10	BJ	57	VAL	4.0
21	AU	53	VAL	4.0
24	CC	144	VAL	4.0
25	CD	20	VAL	4.0
25	CD	189	VAL	4.0
25	CD	193	VAL	4.0
27	CF	25	VAL	4.0
27	DF	74	VAL	4.0
30	DJ	140	VAL	4.0
32	CL	19	VAL	4.0
38	CR	36	PHE	4.0
33	CM	106	GLU	4.0
55	DI	35	VAL	4.0
10	BJ	22	THR	4.0
25	CD	199	SER	4.0
7	AG	109	ARG	4.0
11	AK	13	ARG	4.0
27	CF	80	ARG	4.0
40	CT	95	ARG	4.0
24	CC	227	PRO	4.0
3	BC	94	ILE	4.0
6	BF	85	ILE	4.0
25	CD	27	ILE	4.0
38	CR	65	ILE	4.0
49	D2	54	ILE	4.0
53	DA	143	C	4.0
10	BJ	46	LYS	4.0
19	BS	8	GLY	4.0
25	CD	19	GLY	4.0
30	DJ	27	ALA	4.0
40	CT	26	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
43	CW	6	ALA	4.0
52	C5	5	ALA	4.0
24	CC	261	LYS	4.0
35	CO	18	GLN	4.0
13	BM	48	LEU	4.0
33	CM	6	LEU	4.0
46	DZ	8	GLU	4.0
9	AI	127	PHE	4.0
16	BP	38	PHE	4.0
18	BR	64	TYR	4.0
29	DH	108	VAL	4.0
30	DJ	62	TYR	4.0
35	CO	4	ARG	4.0
36	CP	27	VAL	4.0
37	DQ	2	SER	4.0
35	CO	85	PRO	4.0
13	AM	9	ILE	4.0
13	AM	33	ILE	4.0
24	CC	46	ASN	4.0
34	CN	65	ILE	4.0
33	CM	84	LYS	4.0
40	CT	16	LYS	4.0
49	C2	53	LYS	4.0
5	BE	108	GLY	4.0
10	BJ	29	ALA	4.0
12	BL	23	ALA	4.0
20	AT	47	ALA	4.0
20	BT	22	ALA	4.0
39	CS	37	GLU	4.0
26	CE	168	ASP	4.0
44	CX	63	ALA	4.0
47	D0	2[A]	ALA	4.0
48	C1	56	ALA	4.0
50	C3	32	ALA	4.0
9	BI	11	ARG	4.0
9	BI	113	ARG	4.0
18	AR	73	ARG	4.0
33	CM	125	LEU	4.0
55	DI	5	LEU	4.0
22	CA	2585	U	4.0
31	CK	50	THR	4.0
2	BB	32	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
7	BG	135	VAL	4.0
9	BI	55	VAL	4.0
9	BI	103	PHE	4.0
10	AJ	74	VAL	4.0
30	CJ	98	VAL	4.0
33	CM	122	VAL	4.0
34	CN	57	VAL	4.0
24	CC	161	TYR	4.0
10	AJ	79	PRO	4.0
31	CK	97	PRO	4.0
51	C4	63	PRO	4.0
8	BH	36	ILE	4.0
13	BM	53	ILE	4.0
25	CD	48	ILE	4.0
29	DH	143	ILE	4.0
31	CK	84	ILE	4.0
39	CS	101	ILE	4.0
49	C2	48	ILE	4.0
25	CD	114	LYS	4.0
39	CS	71	LYS	4.0
35	CO	1	MET	4.0
2	BB	139	ARG	4.0
24	CC	42	GLY	4.0
25	CD	176	ASP	4.0
40	CT	94	ASP	4.0
41	CU	75	GLY	4.0
55	DI	42	ARG	4.0
16	BP	81	ALA	3.9
24	CC	166	ALA	3.9
28	CG	7	ALA	3.9
29	CH	140	ALA	3.9
30	CJ	83	ALA	3.9
55	DI	112	ALA	3.9
5	BE	115	LEU	3.9
31	CK	25	LEU	3.9
24	CC	259	SER	3.9
42	CV	30	SER	3.9
9	BI	43	THR	3.9
10	BJ	80	THR	3.9
30	DJ	68	THR	3.9
45	CY	25	THR	3.9
7	AG	141	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
30	CJ	42	PHE	3.9
39	CS	14	VAL	3.9
35	CO	107	ASN	3.9
37	CQ	74	PHE	3.9
10	BJ	39	PRO	3.9
13	BM	103	LYS	3.9
26	CE	139	LYS	3.9
40	CT	48	LYS	3.9
44	CX	24	LYS	3.9
17	BQ	5	ILE	3.9
20	BT	83	ILE	3.9
15	AO	17	ARG	3.9
5	BE	109	GLY	3.9
33	CM	124	GLY	3.9
51	C4	18	GLY	3.9
29	DH	10	ALA	3.9
41	CU	38	ALA	3.9
51	C4	65	ALA	3.9
19	BS	35	SER	3.9
13	BM	20	THR	3.9
48	C1	33	THR	3.9
3	BC	195	VAL	3.9
8	BH	95	VAL	3.9
11	BK	20	VAL	3.9
12	BL	8	VAL	3.9
14	AN	45	VAL	3.9
25	CD	203	VAL	3.9
27	CF	40	VAL	3.9
29	CH	110	VAL	3.9
30	DJ	139	VAL	3.9
53	DA	1171	G	3.9
2	BB	174	LYS	3.9
9	AI	20	PHE	3.9
10	BJ	59	LYS	3.9
35	CO	109	PRO	3.9
45	CY	6	GLN	3.9
55	DI	68	PRO	3.9
55	DI	89	PRO	3.9
55	DI	119	PRO	3.9
8	AH	3	MET	3.9
39	CS	83	TYR	3.9
2	BB	21	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
25	CD	141	ARG	3.9
31	CK	120	ARG	3.9
45	CY	27	ARG	3.9
3	BC	10	ILE	3.9
3	BC	155	GLY	3.9
13	BM	84	GLY	3.9
24	CC	209	GLY	3.9
33	CM	24	GLY	3.9
55	DI	115	GLY	3.9
13	AM	35	ALA	3.9
28	CG	46	ALA	3.9
29	CH	81	ALA	3.9
10	BJ	90	LEU	3.9
12	BL	24	LEU	3.9
16	BP	74	LEU	3.9
25	CD	138	LEU	3.9
26	CE	118	LEU	3.9
28	CG	50	LEU	3.9
29	CH	30	LEU	3.9
3	BC	26	THR	3.9
24	CC	173	THR	3.9
25	CD	185	ASN	3.9
14	BN	47	LYS	3.9
2	BB	70	VAL	3.9
3	BC	39	VAL	3.9
7	BG	105	VAL	3.9
8	BH	78	VAL	3.9
10	BJ	84	VAL	3.9
14	BN	14	VAL	3.9
25	CD	104	VAL	3.9
25	CD	207	VAL	3.9
29	CH	121	VAL	3.9
33	CM	62	PRO	3.9
35	CO	39	PRO	3.9
40	CT	87	PRO	3.9
42	CV	50	PRO	3.9
32	CL	112	PHE	3.9
30	DJ	8	TYR	3.9
5	BE	16	ILE	3.9
15	BO	36	ILE	3.9
32	CL	2	ILE	3.9
39	DS	26	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
39	CS	56	GLY	3.9
44	CX	13	GLY	3.9
44	CX	42	GLY	3.9
2	BB	185	ALA	3.9
5	BE	53	ALA	3.9
10	BJ	93	ALA	3.9
12	BL	13	ALA	3.9
13	BM	18	ALA	3.9
13	BM	40	ALA	3.9
1	BA	211	G	3.9
5	BE	122	ASN	3.9
14	BN	83	LYS	3.9
24	CC	24	LEU	3.9
26	CE	133	LEU	3.9
31	CK	106	LYS	3.9
35	CO	35	LYS	3.9
41	CU	8	LEU	3.9
46	CZ	27	ASN	3.9
25	CD	133	THR	3.9
16	BP	1	MET	3.9
39	CS	84	ARG	3.9
42	CV	82	ARG	3.9
7	BG	93	PRO	3.9
30	DJ	56	PRO	3.9
51	C4	2	PRO	3.9
2	BB	163	VAL	3.8
3	BC	52	VAL	3.8
19	BS	34	TRP	3.8
24	CC	58	HIS	3.8
24	CC	141	VAL	3.8
26	CE	60	TRP	3.8
28	CG	11	VAL	3.8
30	CJ	140	VAL	3.8
34	CN	92	TRP	3.8
40	CT	106	VAL	3.8
29	CH	139	PHE	3.8
30	CJ	67	PHE	3.8
30	DJ	69	PHE	3.8
31	CK	4	PHE	3.8
31	CK	74	TYR	3.8
7	BG	12	ILE	3.8
13	BM	111	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
24	CC	57	GLY	3.8
25	CD	195	GLY	3.8
27	CF	85	ILE	3.8
27	CF	124	GLY	3.8
30	DJ	35	ILE	3.8
34	CN	96	ILE	3.8
4	BD	45	LYS	3.8
20	BT	9	LYS	3.8
28	CG	6	LYS	3.8
30	DJ	66	SER	3.8
51	C4	5	LYS	3.8
7	BG	46	ALA	3.8
9	AI	121	ALA	3.8
13	BM	2	ALA	3.8
2	AB	135	LEU	3.8
17	BQ	65	ARG	3.8
19	BS	13	LEU	3.8
24	CC	177	ARG	3.8
25	CD	4	LEU	3.8
32	CL	107	LEU	3.8
33	CM	59	ARG	3.8
35	CO	79	LEU	3.8
36	CP	26	LEU	3.8
45	CY	37	ARG	3.8
3	BC	165	THR	3.8
33	CM	55	MET	3.8
41	CU	60	THR	3.8
41	CU	15	HIS	3.8
10	BJ	98	VAL	3.8
31	CK	124	VAL	3.8
34	CN	108	VAL	3.8
36	CP	93	ASP	3.8
2	BB	198	PHE	3.8
25	CD	127	PHE	3.8
1	BA	1364	U	3.8
55	DI	32	GLY	3.8
2	BB	40	ILE	3.8
10	BJ	25	ILE	3.8
13	BM	23	TYR	3.8
27	CF	44	ILE	3.8
29	DH	94	ILE	3.8
30	CJ	49	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
32	CL	22	ILE	3.8
40	CT	38	TYR	3.8
48	C1	49	TYR	3.8
34	CN	14	LYS	3.8
39	CS	48	LYS	3.8
42	CV	37	GLU	3.8
51	C4	3	LYS	3.8
35	CO	9	GLN	3.8
9	BI	130	ARG	3.8
46	CZ	23	ARG	3.8
50	C3	41	ARG	3.8
50	C3	26	ASN	3.8
2	BB	136	MET	3.8
9	BI	108	ALA	3.8
25	CD	75	ALA	3.8
26	CE	128	ALA	3.8
38	CR	115	ALA	3.8
47	C0	50	ALA	3.8
6	BF	39	LEU	3.8
7	BG	124	LEU	3.8
9	AI	54	LEU	3.8
35	CO	83	LEU	3.8
55	DI	129	LEU	3.8
24	CC	231	PRO	3.8
25	CD	143	PRO	3.8
32	CL	120	PRO	3.8
20	BT	59	ASP	3.8
3	BC	66	VAL	3.8
5	BE	18	VAL	3.8
7	BG	94	VAL	3.8
13	AM	64	VAL	3.8
28	CG	113	VAL	3.8
46	CZ	26	PHE	3.8
12	AL	15	LYS	3.8
24	CC	138	GLY	3.8
24	CC	147	LYS	3.8
26	CE	132	LYS	3.8
37	CQ	9	GLU	3.8
51	C4	36	LYS	3.8
26	CE	94	GLN	3.8
8	BH	75	ILE	3.8
24	CC	156	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
24	CC	221	ARG	3.8
24	CC	270	ARG	3.8
25	CD	128	ARG	3.8
27	DF	85	ILE	3.8
28	CG	141	ILE	3.8
29	CH	44	ILE	3.8
32	CL	30	ARG	3.8
36	CP	15	ARG	3.8
38	CR	33	ARG	3.8
46	CZ	48	ARG	3.8
51	C4	30	ARG	3.8
19	BS	80	TYR	3.8
24	CC	96	TYR	3.8
24	CC	103	TYR	3.8
50	C3	45	SER	3.8
16	BP	26	ASN	3.8
2	BB	61	ALA	3.8
10	BJ	86	ALA	3.8
21	AU	50	ALA	3.8
25	CD	65	ALA	3.8
28	CG	40	ALA	3.8
29	DH	65	ALA	3.8
37	CQ	107	ALA	3.8
38	CR	12	ALA	3.8
2	BB	129	LEU	3.8
9	BI	35	LEU	3.8
26	CE	165	HIS	3.8
27	CF	36	LEU	3.8
28	CG	133	LEU	3.8
34	CN	129	THR	3.8
36	CP	21	LEU	3.8
37	CQ	25	THR	3.8
10	BJ	75	ASP	3.8
19	BS	30	PRO	3.8
30	CJ	75	PRO	3.8
2	BB	221	VAL	3.8
9	BI	58	VAL	3.8
20	BT	33	LYS	3.8
25	CD	177	VAL	3.8
26	CE	74	LYS	3.8
30	CJ	61	VAL	3.8
33	CM	89	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
39	CS	10	LYS	3.8
51	C4	12	LYS	3.8
55	DI	18	VAL	3.8
5	BE	102	GLY	3.8
24	CC	214	ARG	3.8
26	CE	56	GLY	3.8
27	CF	131	GLY	3.8
28	CG	153	ARG	3.8
36	CP	96	GLY	3.8
44	CX	25	ARG	3.8
2	AB	30	PHE	3.8
29	CH	132	PHE	3.8
55	DI	69	PHE	3.8
2	BB	111	ILE	3.7
5	BE	106	ILE	3.7
22	CA	2602	A	3.7
29	DH	4	ILE	3.7
34	CN	82	MET	3.8
35	CO	13	ASN	3.7
40	CT	4	ILE	3.7
31	CK	75	TYR	3.7
7	BG	128	ALA	3.7
9	BI	44	ALA	3.7
14	AN	2	ALA	3.7
25	CD	54	ALA	3.7
26	CE	87	ALA	3.7
29	DH	39	ALA	3.7
29	DH	105	ALA	3.7
38	CR	21	ALA	3.7
48	C1	19	HIS	3.7
15	BO	25	THR	3.7
25	CD	171	THR	3.7
28	CG	36	THR	3.7
2	AB	68	LEU	3.7
2	BB	148	LEU	3.7
14	BN	16	LEU	3.7
15	BO	67	LEU	3.7
26	CE	134	LEU	3.7
28	CG	105	LEU	3.7
37	CQ	55	LEU	3.7
43	CW	38	LEU	3.7
10	BJ	79	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
30	CJ	23	PRO	3.7
30	DJ	26	PRO	3.7
30	DJ	74	PRO	3.7
4	BD	148	LYS	3.7
9	BI	120	LYS	3.7
24	CC	253	LYS	3.7
38	CR	15	LYS	3.7
32	CL	31	ARG	3.7
34	CN	60	GLN	3.7
36	CP	98	GLN	3.7
17	BQ	83	VAL	3.7
24	CC	268	VAL	3.7
1	AA	412	A	3.7
24	DC	235	GLY	3.7
25	CD	158	GLY	3.7
38	CR	100	VAL	3.7
53	DA	2602	A	3.7
7	BG	26	PHE	3.7
21	BU	12	PHE	3.7
26	CE	75	SER	3.7
26	CE	93	SER	3.7
29	CH	91	PHE	3.7
39	CS	53	PHE	3.7
55	DI	76	PHE	3.7
7	AG	29	ILE	3.7
9	AI	21	ILE	3.7
30	DJ	122	ILE	3.7
31	CK	142	ILE	3.7
37	CQ	50	ILE	3.7
36	CP	99	TYR	3.7
28	CG	68	ALA	3.7
41	CU	23	ALA	3.7
51	C4	48	ALA	3.7
25	CD	197	THR	3.7
2	BB	117	LEU	3.7
6	BF	47	LEU	3.7
9	BI	63	LEU	3.7
18	BR	68	LEU	3.7
20	AT	66	LEU	3.7
20	BT	71	LYS	3.7
29	CH	41	LYS	3.7
31	DK	9	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
33	CM	17	LYS	3.7
14	AN	49	GLN	3.7
16	BP	18	GLN	3.7
26	CE	59	PRO	3.7
30	CJ	74	PRO	3.7
36	CP	94	ARG	3.7
11	BK	19	GLY	3.7
24	CC	109	GLY	3.7
24	CC	222	GLY	3.7
25	CD	135	GLY	3.7
30	DJ	125	MET	3.7
35	CO	24	MET	3.7
3	BC	138	VAL	3.7
25	CD	109	VAL	3.7
27	CF	146	VAL	3.7
55	DI	27	VAL	3.7
41	CU	70	HIS	3.7
6	BF	36	ILE	3.7
24	DC	74	ILE	3.7
30	CJ	35	ILE	3.7
40	CT	24	ILE	3.7
2	BB	218	ALA	3.7
17	BQ	26	GLU	3.7
16	BP	50	THR	3.7
19	BS	79	THR	3.7
20	BT	17	ALA	3.7
25	CD	151	THR	3.7
31	CK	104	ALA	3.7
32	CL	33	ALA	3.7
42	CV	81	ASP	3.7
52	C5	18	LYS	3.7
55	DI	36	ASP	3.7
13	BM	107	ARG	3.7
14	BN	9	ARG	3.7
2	AB	161	LEU	3.7
9	BI	87	LEU	3.7
24	CC	154	LEU	3.7
25	CD	79	LEU	3.7
26	CE	62	GLN	3.7
27	CF	66	LEU	3.7
27	CF	81	GLN	3.7
40	CT	51	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
47	C0	25	LEU	3.7
10	BJ	88	MET	3.7
9	BI	31	ASN	3.7
9	BI	67	VAL	3.7
25	CD	92	VAL	3.7
37	CQ	65	SER	3.7
42	CV	49	VAL	3.7
47	C0	51	VAL	3.7
8	BH	45	PHE	3.7
28	CG	83	PHE	3.7
5	AE	163	GLU	3.7
10	AJ	100	ILE	3.7
13	BM	39	ILE	3.7
17	BQ	25	ILE	3.7
20	BT	32	ILE	3.7
30	DJ	82	LYS	3.7
40	CT	83	LYS	3.7
42	CV	60	GLU	3.7
45	CY	62	LYS	3.7
38	CR	37	GLN	3.7
46	CZ	39	GLN	3.7
10	BJ	94	ALA	3.7
13	BM	15	ALA	3.7
13	BM	35	ALA	3.7
14	AN	22	ALA	3.7
24	CC	50	THR	3.7
22	CA	1175	A	3.7
24	CC	186	ALA	3.7
30	CJ	27	ALA	3.7
40	CT	21	ALA	3.7
40	CT	56	ALA	3.7
45	CY	73	ALA	3.7
55	DI	80	THR	3.7
13	BM	69	LEU	3.6
14	BN	20	TYR	3.7
17	BQ	34	TYR	3.7
19	BS	16	LEU	3.6
31	CK	44	TYR	3.7
48	C1	48	TYR	3.7
24	CC	29	PRO	3.6
19	BS	44	MET	3.6
24	CC	225	MET	3.6

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Mol	Chain	Res	Type	RSRZ
19	BS	68	GLY	3.6
24	CC	143	ASN	3.6
51	C4	56	GLY	3.6
7	BG	91	VAL	3.6
10	AJ	26	VAL	3.6
28	CG	162	VAL	3.6
30	CJ	139	VAL	3.6
34	CN	135	VAL	3.6
16	BP	47	GLU	3.6
37	CQ	88	ARG	3.6
46	CZ	54	LYS	3.6
19	BS	41	PHE	3.6
26	DE	7	ASP	3.6
34	CN	68	PHE	3.6
2	AB	186	ILE	3.6
11	BK	110	ILE	3.6
22	CA	12	U	3.6
22	CA	810	U	3.6
22	CA	2402	U	3.6
29	CH	143	ILE	3.6
36	CP	35	ILE	3.6
41	CU	37	ASP	3.6
44	CX	36	ILE	3.6
53	DA	2165	C	3.6
13	BM	28	THR	3.6
33	CM	117	THR	3.6
50	C3	4	THR	3.6
3	BC	160	ALA	3.6
16	BP	11	ALA	3.6
17	BQ	82	ALA	3.6
24	CC	92	ALA	3.6
34	CN	52	ALA	3.6
34	CN	79	ALA	3.6
38	CR	63	ALA	3.6
7	AG	66	LEU	3.6
7	AG	118	LEU	3.6
8	BH	32	LEU	3.6
8	BH	83	LEU	3.6
9	BI	98	LEU	3.6
9	BI	6	TYR	3.6
24	CC	244	PRO	3.6
25	CD	175	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
29	CH	38	PRO	3.6
30	CJ	56	PRO	3.6
35	CO	54	LEU	3.6
41	CU	14	PRO	3.6
9	BI	40	GLY	3.6
14	BN	95	GLY	3.6
25	CD	78	GLY	3.6
32	CL	82	ASN	3.6
33	CM	65	GLY	3.6
44	CX	54	GLY	3.6
35	CO	27	SER	3.6
3	AC	170	GLU	3.6
24	CC	180	GLU	3.6
2	BB	131	LYS	3.6
10	BJ	68	ARG	3.6
13	BM	90	ARG	3.6
45	CY	10	LYS	3.6
45	CY	11	ARG	3.6
47	C0	19	LYS	3.6
14	BN	34	VAL	3.6
21	BU	6	VAL	3.6
25	CD	178	VAL	3.6
37	CQ	17	VAL	3.6
10	AJ	75	ASP	3.6
2	BB	90	PHE	3.6
3	BC	103	ILE	3.6
7	AG	12	ILE	3.6
9	BI	39	PHE	3.6
19	BS	61	PHE	3.6
27	CF	111	ILE	3.6
44	CX	79	PHE	3.6
45	CY	59	ILE	3.6
49	C2	9	ILE	3.6
22	CA	2250	G	3.6
30	CJ	60	THR	3.6
37	CQ	13	MET	3.6
40	CT	39	THR	3.6
30	DJ	120	ALA	3.6
21	AU	2	PRO	3.6
30	CJ	22	PRO	3.6
55	DI	60	LEU	3.6
24	CC	44	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
55	DI	51	TYR	3.6
7	BG	81	GLY	3.6
24	CC	53	HIS	3.6
34	CN	83	GLY	3.6
42	CV	45	HIS	3.6
5	BE	112	ARG	3.6
24	CC	258	ARG	3.6
27	CF	73	SER	3.6
41	CU	19	LYS	3.6
2	BB	96	TRP	3.6
2	AB	92	VAL	3.6
3	BC	84	VAL	3.6
12	AL	16	VAL	3.6
12	BL	4	VAL	3.6
14	AN	11	VAL	3.6
19	BS	58	VAL	3.6
28	CG	98	VAL	3.6
29	CH	9	VAL	3.6
40	CT	29	VAL	3.6
48	C1	20	ASP	3.6
3	BC	55	ILE	3.6
5	AE	164	ILE	3.6
19	BS	10	PHE	3.6
30	CJ	86	ILE	3.6
55	DI	11	ILE	3.6
5	BE	24	THR	3.6
7	BG	49	THR	3.6
30	DJ	132	THR	3.6
31	CK	45	THR	3.6
9	BI	17	ALA	3.6
10	BJ	21	ALA	3.6
24	CC	208	ALA	3.6
36	CP	11	ALA	3.6
36	CP	57	ALA	3.6
37	CQ	58	ALA	3.6
38	CR	68	ALA	3.6
55	DI	25	ALA	3.6
21	BU	11	PRO	3.6
3	BC	12	LEU	3.6
7	AG	99	LEU	3.6
10	BJ	17	LEU	3.6
46	CZ	56	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
24	CC	45	ASN	3.6
24	DC	239	ASN	3.6
33	CM	41	ARG	3.6
53	DA	1094	U	3.6
45	CY	54	LYS	3.6
24	CC	127	GLY	3.6
1	BA	1534	A	3.6
9	AI	96	SER	3.6
26	CE	30	GLN	3.6
33	CM	104	GLN	3.6
5	BE	152	MET	3.5
6	BF	10	VAL	3.5
32	CL	57	VAL	3.5
49	C2	12	VAL	3.5
51	C4	50	VAL	3.5
5	BE	134	ILE	3.5
7	BG	72	THR	3.5
26	CE	19	PHE	3.5
28	CG	121	ILE	3.5
29	DH	91	PHE	3.5
30	CJ	101	ILE	3.5
35	CO	70	THR	3.5
35	CO	75	ILE	3.5
38	CR	80	ILE	3.5
12	BL	17	ALA	3.5
27	CF	75	ALA	3.5
38	CR	50	ARG	3.5
41	CU	69	ARG	3.5
25	CD	154	LYS	3.5
25	CD	160	LYS	3.5
26	CE	63	LYS	3.5
32	CL	89	ASN	3.5
34	CN	109	PRO	3.5
46	CZ	61	ALA	3.5
24	CC	90	ASN	3.5
40	CT	9	HIS	3.5
40	CT	49	LYS	3.5
5	BE	76	LEU	3.5
6	BF	74	LEU	3.5
39	CS	25	LEU	3.5
13	AM	26	GLY	3.5
25	CD	111	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
26	CE	66	GLY	3.5
31	CK	112	GLY	3.5
20	BT	14	SER	3.5
8	BH	128	TYR	3.5
42	CV	8	ASP	3.5
36	DP	1	MET	3.5
6	BF	89	VAL	3.5
7	BG	75	VAL	3.5
8	BH	110	VAL	3.5
19	BS	19	VAL	3.5
24	CC	78	VAL	3.5
28	CG	4	VAL	3.5
3	BC	127	ARG	3.5
17	BQ	40	ARG	3.5
33	CM	51	GLU	3.5
35	CO	103	ARG	3.5
38	CR	51	ARG	3.5
12	BL	40	THR	3.5
27	CF	155	THR	3.5
40	CT	104	THR	3.5
4	AD	132	ILE	3.5
25	CD	202	ILE	3.5
32	CL	47	ILE	3.5
38	CR	40	ILE	3.5
52	C5	2	LYS	3.5
55	DI	8	LYS	3.5
20	BT	51	PHE	3.5
9	BI	23	PRO	3.5
9	BI	101	ALA	3.5
14	AN	36	ALA	3.5
14	AN	52	PRO	3.5
16	BP	7	ALA	3.5
25	CD	167	ASN	3.5
24	CC	126	PRO	3.5
24	CC	218	PRO	3.5
27	CF	171	ALA	3.5
30	DJ	124	ALA	3.5
40	CT	10	ALA	3.5
45	CY	12	PRO	3.5
51	C4	11	ALA	3.5
10	AJ	71	LEU	3.5
13	BM	80	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
14	AN	96	LEU	3.5
29	DH	122	LEU	3.5
11	AK	19	GLY	3.5
33	CM	88	GLY	3.5
37	CQ	69	GLY	3.5
25	CD	137	SER	3.5
40	CT	101	SER	3.5
25	CD	131	ASP	3.5
35	CO	20	MET	3.5
43	CW	57	TYR	3.5
7	AG	4	ARG	3.5
10	BJ	47	GLU	3.5
19	BS	37	ARG	3.5
26	CE	61	ARG	3.5
36	CP	10	ARG	3.5
40	CT	25	ARG	3.5
13	AM	97	VAL	3.5
14	BN	84	VAL	3.5
19	BS	23	VAL	3.5
29	CH	8	LYS	3.5
29	CH	21	VAL	3.5
32	CL	44	LYS	3.5
32	CL	103	VAL	3.5
34	CN	80	VAL	3.5
37	CQ	61	VAL	3.5
39	CS	58	VAL	3.5
42	CV	91	LYS	3.5
44	CX	71	VAL	3.5
51	C4	35	LYS	3.5
24	CC	232	HIS	3.5
37	CQ	60	THR	3.5
17	BQ	9	GLN	3.5
24	CC	124	ILE	3.5
29	DH	44	ILE	3.5
31	CK	101	ILE	3.5
3	BC	24	ALA	3.5
11	BK	21	ALA	3.5
26	CE	86	ALA	3.5
30	CJ	41	ALA	3.5
32	CL	100	PHE	3.5
33	CM	56	PRO	3.5
8	BH	17	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
13	BM	56	LEU	3.5
43	CW	20	LEU	3.5
2	AB	6	MET	3.5
13	BM	81	MET	3.5
24	CC	6	CYS	3.5
9	BI	122	ARG	3.5
27	CF	128	TYR	3.5
35	CO	17	ARG	3.5
8	BH	56	LYS	3.5
19	AS	7	LYS	3.5
24	CC	26	LYS	3.5
24	CC	59	LYS	3.5
42	CV	17	LYS	3.5
24	CC	230	HIS	3.5
41	DU	70	HIS	3.5
5	AE	161	VAL	3.5
5	BE	74	VAL	3.5
19	BS	51	VAL	3.5
24	CC	120	VAL	3.5
24	CC	195	VAL	3.5
29	DH	142	VAL	3.5
32	CL	65	THR	3.5
35	CO	53	THR	3.5
45	CY	16	ASN	3.5
47	C0	8	THR	3.5
6	AF	42	TRP	3.4
16	BP	41	PRO	3.4
27	DF	67	ILE	3.4
31	CK	55	ILE	3.4
5	BE	31	PHE	3.4
5	BE	118	ALA	3.4
9	BI	76	ALA	3.4
10	BJ	23	ALA	3.4
14	BN	22	ALA	3.4
19	AS	61	PHE	3.4
25	CD	31	ALA	3.4
25	CD	57	ALA	3.4
25	CD	69	ALA	3.4
25	CD	206	ALA	3.4
41	CU	20	ALA	3.4
2	BB	97	LEU	3.4
2	BB	141	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
3	BC	111	LEU	3.4
3	BC	144	LEU	3.4
4	AD	5	LEU	3.4
5	BE	15	LEU	3.4
8	BH	40	LEU	3.4
8	BH	61	LEU	3.4
10	BJ	87	LEU	3.4
13	AM	48	LEU	3.4
14	AN	51	LEU	3.4
14	AN	55	SER	3.4
26	CE	103	GLY	3.4
34	CN	23	GLY	3.4
34	CN	107	GLY	3.4
15	BO	87	LEU	3.4
46	CZ	40	SER	3.4
19	BS	66	MET	3.4
4	BD	47	ARG	3.4
8	BH	91	GLU	3.4
15	BO	58	ARG	3.4
15	BO	72	ARG	3.4
29	CH	97	ARG	3.4
33	CM	48	ARG	3.4
35	CO	43	GLU	3.4
1	BA	948	C	3.4
7	BG	137	LYS	3.4
14	AN	23	LYS	3.4
22	CA	1606	C	3.4
22	CA	1808	A	3.4
25	CD	7	LYS	3.4
33	CM	36	LYS	3.4
53	DA	140	C	3.4
20	BT	20	HIS	3.4
34	CN	91	TYR	3.4
38	CR	56	GLN	3.4
29	DH	11	ASN	3.4
19	AS	39	THR	3.4
29	DH	144	VAL	3.4
49	C2	43	VAL	3.4
2	BB	186	ILE	3.4
13	BM	73	ILE	3.4
18	BR	26	ILE	3.4
29	DH	118	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
32	CL	39	ILE	3.4
4	BD	2	ALA	3.4
9	AI	102	GLY	3.4
9	BI	74	GLY	3.4
13	BM	26	GLY	3.4
24	CC	170	ALA	3.4
26	CE	142	ALA	3.4
29	DH	13	GLY	3.4
30	CJ	99	GLY	3.4
30	DJ	84	ALA	3.4
33	CM	43	GLY	3.4
38	CR	42	ALA	3.4
46	DZ	62	GLY	3.4
48	C1	51	GLY	3.4
52	C5	38	GLY	3.4
3	BC	23	PHE	3.4
13	AM	63	PHE	3.4
32	CL	79	PHE	3.4
11	BK	82	LEU	3.4
12	AL	14	ARG	3.4
18	AR	55	LEU	3.4
29	CH	117	LEU	3.4
35	CO	115	LEU	3.4
9	AI	68	LYS	3.4
24	CC	7	LYS	3.4
36	CP	19	GLN	3.4
28	CG	111	HIS	3.4
53	DA	546	U	3.4
9	AI	90	TYR	3.4
20	AT	3	ASN	3.4
27	CF	83	TYR	3.4
28	CG	151	TYR	3.4
2	BB	119	THR	3.4
4	BD	169	THR	3.4
5	BE	21	VAL	3.4
7	AG	27	VAL	3.4
10	AJ	36	VAL	3.4
13	AM	43	VAL	3.4
17	BQ	59	VAL	3.4
24	DC	250	VAL	3.4
28	CG	80	THR	3.4
33	CM	85	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
42	DV	49	VAL	3.4
7	BG	14	PRO	3.4
12	BL	28	PRO	3.4
13	BM	115	PRO	3.4
26	CE	199	MET	3.4
22	CA	46	G	3.4
22	CA	561	G	3.4
2	AB	75	ALA	3.4
2	AB	166	ALA	3.4
8	BH	7	ILE	3.4
8	BH	85	ILE	3.4
9	AI	28	ILE	3.4
13	BM	9	ILE	3.4
15	BO	82	ILE	3.4
24	CC	88	SER	3.4
24	CC	217	ARG	3.4
24	DC	38	SER	3.4
25	CD	103	ASP	3.4
27	CF	82	GLY	3.4
30	CJ	25	GLY	3.4
25	CD	162	ALA	3.4
27	CF	106	ILE	3.4
28	CG	131	ILE	3.4
30	DJ	41	ALA	3.4
30	DJ	133	ALA	3.4
32	CL	99	ILE	3.4
33	CM	45	GLY	3.4
42	CV	57	GLY	3.4
44	CX	52	GLY	3.4
46	CZ	62	GLY	3.4
51	C4	40	ARG	3.4
24	CC	155	ALA	3.4
2	BB	161	LEU	3.4
5	BE	124	LEU	3.4
7	AG	22	LEU	3.4
9	AI	100	LYS	3.4
17	BQ	39	LYS	3.4
27	CF	170	LEU	3.4
39	CS	22	LEU	3.4
38	CR	52	GLN	3.4
13	BM	91	HIS	3.4
28	DG	111	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
4	AD	74	ASN	3.4
16	BP	40	ASN	3.4
9	BI	66	THR	3.4
15	BO	22	THR	3.4
19	BS	39	THR	3.4
24	CC	219	THR	3.4
16	BP	5	ARG	3.4
24	CC	271	ARG	3.4
26	CE	44	ARG	3.4
33	CM	47	ARG	3.4
35	CO	110	MET	3.4
38	CR	53	ARG	3.4
3	BC	173	VAL	3.4
4	BD	25	VAL	3.4
9	AI	47	VAL	3.4
9	AI	55	VAL	3.4
29	CH	103	VAL	3.4
29	DH	103	VAL	3.4
29	DH	138	VAL	3.4
32	CL	24	VAL	3.4
3	BC	7	PRO	3.4
4	BD	205	SER	3.4
9	BI	69	GLY	3.4
24	CC	40	SER	3.4
25	CD	21	SER	3.4
28	CG	8	PRO	3.4
29	DH	38	PRO	3.4
35	CO	15	SER	3.4
36	CP	42	PRO	3.4
36	CP	95	SER	3.4
40	CT	77	ASP	3.4
40	CT	91	GLY	3.4
42	CV	68	SER	3.4
46	CZ	35	GLY	3.4
34	CN	62	LYS	3.4
2	AB	164	ILE	3.4
6	AF	95	ALA	3.4
17	AQ	33	ILE	3.4
24	CC	89	ALA	3.4
28	CG	26	ILE	3.4
31	CK	134	ALA	3.4
34	CN	21	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
35	CO	77	ALA	3.4
36	CP	87	ILE	3.4
40	CT	14	ALA	3.4
47	C0	2	ALA	3.4
19	AS	13	LEU	3.4
25	CD	101	PHE	3.4
27	DF	122	PHE	3.4
36	CP	92	PHE	3.4
39	CS	86	GLN	3.4
43	CW	91	PHE	3.4
45	CY	39	TRP	3.3
12	BL	20	ASN	3.3
9	BI	12	ARG	3.3
12	BL	12	ARG	3.3
14	BN	85	ARG	3.3
21	BU	33	ARG	3.3
24	CC	181	MET	3.3
27	CF	71	ARG	3.3
34	CN	16	ARG	3.3
35	CO	71	ARG	3.3
45	CY	28	ARG	3.3
45	CY	74	ARG	3.3
1	BA	108	G	3.3
5	BE	131	THR	3.3
10	BJ	83	THR	3.3
22	CA	214	G	3.3
30	CJ	68	THR	3.3
30	DJ	73	THR	3.3
31	CK	3	THR	3.3
49	C2	17	THR	3.3
30	CJ	8	TYR	3.3
30	DJ	51	LYS	3.3
34	CN	11	LYS	3.3
37	CQ	29	LYS	3.3
44	CX	62	LYS	3.3
18	AR	40	VAL	3.3
18	BR	40	VAL	3.3
24	CC	162	VAL	3.3
25	CD	63	PRO	3.3
26	CE	120	VAL	3.3
28	CG	90	VAL	3.3
28	CG	132	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
30	DJ	25	GLY	3.3
35	CO	6	SER	3.3
37	CQ	70	VAL	3.3
39	CS	69	GLY	3.3
41	CU	53	VAL	3.3
2	AB	41	ILE	3.3
2	AB	134	ALA	3.3
19	BS	45	ILE	3.3
20	BT	41	ALA	3.3
24	CC	31	ALA	3.3
28	CG	63	ALA	3.3
38	CR	46	ALA	3.3
49	D2	52	ALA	3.3
2	BB	214	LEU	3.3
7	BG	120	LEU	3.3
14	AN	48	LEU	3.3
20	AT	86	LEU	3.3
32	CL	29	HIS	3.3
37	CQ	100	LEU	3.3
45	CY	34	HIS	3.3
47	C0	24	LEU	3.3
49	C2	20	PHE	3.3
14	BN	35	ASN	3.3
14	BN	42	TRP	3.3
35	CO	73	ASN	3.3
2	AB	7	ARG	3.3
7	BG	4	ARG	3.3
14	BN	75	ARG	3.3
20	BT	18	ARG	3.3
24	CC	167	ARG	3.3
37	CQ	103	ARG	3.3
9	BI	112	GLU	3.3
41	CU	4	GLU	3.3
53	DA	142	A	3.3
22	CA	559	G	3.3
24	CC	28	LYS	3.3
19	BS	63	THR	3.3
35	CO	95	THR	3.3
16	BP	24	SER	3.3
32	CL	28	SER	3.3
42	CV	98	SER	3.3
2	BB	193	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
6	AF	103	VAL	3.3
7	AG	80	VAL	3.3
9	AI	48	VAL	3.3
11	BK	113	VAL	3.3
24	CC	171	TYR	3.3
27	DF	128	TYR	3.3
29	CH	13	GLY	3.3
30	DJ	33	VAL	3.3
50	C3	30	VAL	3.3
55	DI	12	VAL	3.3
10	AJ	76	ILE	3.3
27	DF	34	ILE	3.3
27	DF	79	ILE	3.3
29	DH	111	ALA	3.3
32	CL	115	ILE	3.3
34	CN	63	ILE	3.3
34	CN	126	ILE	3.3
40	CT	54	ALA	3.3
44	CX	80	ILE	3.3
46	CZ	51	ALA	3.3
52	C5	16	ILE	3.3
2	BB	57	LEU	3.3
9	AI	35	LEU	3.3
30	CJ	28	LEU	3.3
34	CN	33	LEU	3.3
40	CT	69	LEU	3.3
2	BB	30	PHE	3.3
16	BP	39	PHE	3.3
24	CC	260	ASN	3.3
25	CD	15	PHE	3.3
35	CO	69	ARG	3.3
35	CO	87	PHE	3.3
40	CT	61	ASN	3.3
46	CZ	29	ARG	3.3
51	C4	45	ARG	3.3
2	AB	136	MET	3.3
31	CK	1	MET	3.3
1	BA	1235	U	3.3
14	BN	12	LYS	3.3
20	BT	85	LYS	3.3
34	CN	127	LYS	3.3
30	CJ	73	THR	3.3

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Mol	Chain	Res	Type	RSRZ
52	C5	27	CYS	3.3
5	BE	44	GLY	3.3
10	BJ	95	GLY	3.3
11	BK	90	GLY	3.3
41	CU	90	GLY	3.3
49	D2	16	GLY	3.3
8	BH	25	VAL	3.3
10	AJ	57	VAL	3.3
12	BL	21	VAL	3.3
24	CC	142	HIS	3.3
29	CH	19	VAL	3.3
29	CH	135	HIS	3.3
31	CK	77	HIS	3.3
33	CM	116	VAL	3.3
44	CX	31	VAL	3.3
10	BJ	34	ALA	3.3
26	CE	161	ALA	3.3
39	CS	103	ALA	3.3
12	BL	67	ILE	3.3
27	CF	104	ILE	3.3
32	CL	41	ILE	3.3
38	CR	74	ILE	3.3
2	BB	212	LEU	3.3
8	BH	11	LEU	3.3
9	BI	18	ARG	3.3
10	AJ	102	LEU	3.3
14	AN	24	ARG	3.3
15	BO	32	LEU	3.3
24	CC	81	LEU	3.3
29	DH	12	LEU	3.3
50	C3	34	ARG	3.3
52	C5	36	ARG	3.3
25	CD	136	ASN	3.3
34	CN	17	ASN	3.3
40	CT	78	GLU	3.3
30	DJ	136	MET	3.3
22	CA	1250	G	3.3
22	CA	1382	G	3.3
24	DC	242	LYS	3.3
26	CE	58	LYS	3.3
15	BO	62	GLN	3.3
27	CF	123	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
47	C0	9	GLN	3.3
3	BC	186	THR	3.2
14	AN	32	SER	3.2
14	BN	64	CYS	3.2
14	BN	80	SER	3.2
33	CM	12	SER	3.2
25	CD	147	GLY	3.2
20	BT	75	HIS	3.2
21	AU	56	HIS	3.2
43	CW	81	PRO	3.2
5	BE	117	VAL	3.2
14	BN	61	ARG	3.2
24	CC	269	ARG	3.2
25	CD	29	VAL	3.2
26	CE	69	ARG	3.2
26	CE	162	ARG	3.2
29	DH	78	VAL	3.2
34	CN	55	ARG	3.2
36	CP	28	VAL	3.2
40	CT	17	VAL	3.2
44	CX	55	ARG	3.2
44	DX	11	ARG	3.2
50	C3	39	ARG	3.2
1	BA	4	U	3.2
4	BD	175	ALA	3.2
8	BH	20	ALA	3.2
9	BI	90	TYR	3.2
9	BI	121	ALA	3.2
20	BT	77	ALA	3.2
28	CG	5	ALA	3.2
31	CK	59	ALA	3.2
34	CN	94	ALA	3.2
52	C5	30	GLU	3.2
2	BB	181	ILE	3.2
22	CA	61	C	3.2
22	CA	680	C	3.2
26	CE	149	ILE	3.2
27	CF	137	ILE	3.2
43	CW	40	ILE	3.2
2	BB	43	LEU	3.2
15	AO	57	LEU	3.2
15	BO	57	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
34	CN	12	MET	3.2
22	CA	583	G	3.2
22	CA	801	G	3.2
22	CA	1324	G	3.2
35	DO	121	LYS	3.2
50	C3	11	LYS	3.2
51	C4	41	LYS	3.2
55	DI	105	LYS	3.2
19	AS	41	PHE	3.2
21	AU	37	PHE	3.2
27	CF	177	PHE	3.2
50	C3	29	GLN	3.2
9	BI	9	THR	3.2
12	BL	58	THR	3.2
16	BP	66	THR	3.2
49	C2	23	THR	3.2
6	BF	58	HIS	3.2
7	AG	81	GLY	3.2
21	BU	56	HIS	3.2
25	CD	76	GLY	3.2
45	CY	36	HIS	3.2
45	CY	75	GLY	3.2
48	C1	47	GLY	3.2
4	BD	46	PRO	3.2
5	AE	93	ARG	3.2
12	BL	11	PRO	3.2
13	BM	93	ARG	3.2
17	BQ	27	ARG	3.2
31	CK	15	TRP	3.2
32	CL	84	CYS	3.2
35	CO	12	ARG	3.2
55	DI	31	ARG	3.2
22	CA	1323	C	3.2
7	AG	73	VAL	3.2
7	BG	89	VAL	3.2
10	AJ	77	VAL	3.2
15	BO	59	MET	3.2
28	CG	15	VAL	3.2
50	C3	22	MET	3.2
2	BB	83	ALA	3.2
4	AD	122	ALA	3.2
7	BG	149	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
12	BL	18	LYS	3.2
14	AN	25	ALA	3.2
18	BR	49	ALA	3.2
19	BS	50	ALA	3.2
20	AT	5	LYS	3.2
24	CC	183	LYS	3.2
24	DC	253	LYS	3.2
26	CE	201	ALA	3.2
27	CF	70	ALA	3.2
27	CF	161	LYS	3.2
37	CQ	111	LYS	3.2
38	CR	113	ALA	3.2
43	CW	14	LYS	3.2
55	DI	2	ALA	3.2
8	BH	14	ILE	3.2
8	BH	99	LEU	3.2
9	AI	30	ILE	3.2
27	CF	4	LEU	3.2
31	CK	32	LEU	3.2
53	DA	2133	G	3.2
37	CQ	7	GLN	3.2
25	CD	108	ASP	3.2
7	AG	62	PHE	3.2
37	CQ	59	PHE	3.2
9	BI	81	HIS	3.2
10	AJ	45	ARG	3.2
11	BK	118	HIS	3.2
15	BO	2	SER	3.2
16	BP	8	ARG	3.2
25	CD	77	ARG	3.2
25	CD	134	HIS	3.2
26	CE	102	ARG	3.2
44	CX	11	ARG	3.2
52	C5	24	ARG	3.2
5	BE	119	GLY	3.2
7	AG	8	GLY	3.2
22	CA	941	A	3.2
51	C4	20	GLY	3.2
55	DI	47	GLU	3.2
1	BA	63	C	3.2
22	CA	946	C	3.2
22	CA	1117	C	3.2

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Mol	Chain	Res	Type	RSRZ
13	BM	85	CYS	3.2
2	AB	132	LYS	3.2
4	BD	151	LYS	3.2
12	BL	30	LYS	3.2
17	AQ	4	LYS	3.2
30	CJ	81	LYS	3.2
46	CZ	2	LYS	3.2
42	CV	40	ASN	3.2
42	CV	74	ASN	3.2
45	CY	23	ASN	3.2
46	CZ	58	ASN	3.2
2	BB	14	VAL	3.2
3	BC	15	VAL	3.2
12	BL	107	VAL	3.2
20	BT	35	VAL	3.2
27	CF	132	VAL	3.2
32	CL	63	VAL	3.2
34	CN	67	VAL	3.2
37	CQ	30	VAL	3.2
40	CT	71	VAL	3.2
2	BB	166	ALA	3.2
2	AB	97	LEU	3.2
3	BC	101	ILE	3.2
10	AJ	73	LEU	3.2
13	AM	83	LEU	3.2
21	BU	29	LEU	3.2
24	CC	104	ILE	3.2
29	CH	62	LEU	3.2
32	CL	77	ILE	3.2
34	CN	102	LEU	3.2
34	CN	103	TYR	3.2
48	C1	22	LEU	3.2
49	D2	5	ILE	3.2
16	BP	23	ASP	3.2
33	CM	81	ASP	3.2
2	BB	69	PHE	3.2
3	BC	29	PHE	3.2
4	BD	107	PHE	3.2
14	BN	59	ARG	3.2
24	DC	238	ARG	3.2
25	CD	82	PHE	3.2
29	CH	123	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
33	CM	60	ARG	3.2
35	CO	64	ARG	3.2
42	CV	7	ARG	3.2
52	C5	19	ARG	3.2
26	DE	165	HIS	3.2
45	DY	20	HIS	3.2
5	BE	116	GLU	3.2
27	CF	164	GLU	3.2
5	BE	27	GLY	3.2
16	BP	62	GLY	3.2
24	CC	263	THR	3.2
30	CJ	126	THR	3.2
32	CL	27	GLY	3.2
34	CN	85	GLY	3.2
50	C3	38	GLY	3.2
12	BL	91	PRO	3.2
14	BN	52	PRO	3.2
28	CG	156	PRO	3.2
34	CN	125	PRO	3.2
42	DV	50	PRO	3.2
14	AN	28	LYS	3.2
24	CC	146	MET	3.2
39	CS	85	LYS	3.2
42	CV	61	LYS	3.2
43	CW	48	MET	3.2
31	CK	131	ASN	3.2
37	DQ	115	ASN	3.2
25	CD	148	GLN	3.2
8	BH	115	ALA	3.1
9	AI	111	VAL	3.1
12	BL	93	VAL	3.1
20	AT	41	ALA	3.1
26	CE	45	ALA	3.1
27	CF	119	ALA	3.1
34	CN	113	ALA	3.1
44	CX	47	ALA	3.1
55	DI	13	ALA	3.1
2	AB	173	ILE	3.1
6	AF	61	LEU	3.1
9	BI	107	ASP	3.1
10	BJ	10	LEU	3.1
13	BM	17	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
15	BO	66	LEU	3.1
25	CD	2	ILE	3.1
27	CF	154	ILE	3.1
28	CG	33	LEU	3.1
28	CG	107	LEU	3.1
29	DH	117	LEU	3.1
32	CL	118	LEU	3.1
33	CM	112	LEU	3.1
39	CS	59	ILE	3.1
44	CX	32	LEU	3.1
55	DI	3	LEU	3.1
27	DF	80	ARG	3.1
13	AM	12	HIS	3.1
35	CO	3	HIS	3.1
46	CZ	41	HIS	3.1
22	CA	2691	C	3.1
5	AE	31	PHE	3.1
12	BL	61	PHE	3.1
14	BN	32	SER	3.1
21	BU	37	PHE	3.1
24	CC	38	SER	3.1
39	CS	35	PHE	3.1
7	BG	112	GLY	3.1
12	BL	64	THR	3.1
14	BN	78	GLY	3.1
14	BN	98	LYS	3.1
15	BO	5	THR	3.1
29	DH	125	THR	3.1
32	CL	68	GLY	3.1
35	CO	26	GLY	3.1
37	CQ	106	LYS	3.1
4	AD	46	PRO	3.1
8	BH	81	PRO	3.1
19	AS	30	PRO	3.1
27	CF	176	PRO	3.1
30	DJ	75	PRO	3.1
31	CK	110	PRO	3.1
5	AE	70	ASN	3.1
53	DA	548	G	3.1
55	DI	103	ASN	3.1
38	CR	20	GLN	3.1
46	CZ	25	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
13	AM	85	CYS	3.1
17	BQ	64	CYS	3.1
44	CX	53	CYS	3.1
2	AB	199	VAL	3.1
3	BC	5	VAL	3.1
3	BC	61	ALA	3.1
3	BC	153	VAL	3.1
5	BE	136	VAL	3.1
10	AJ	12	ALA	3.1
21	BU	53	VAL	3.1
24	CC	106	ALA	3.1
27	DF	2	ALA	3.1
30	DJ	104	ALA	3.1
31	CK	33	ALA	3.1
39	CS	13	ARG	3.1
40	DT	110	ARG	3.1
48	C1	46	ASP	3.1
1	BA	532	A	3.1
1	BA	1362	A	3.1
2	AB	67	ILE	3.1
4	BD	132	ILE	3.1
4	BD	191	LEU	3.1
9	BI	79	ILE	3.1
9	BI	94	LEU	3.1
19	BS	47	LEU	3.1
26	CE	12	LEU	3.1
44	CX	59	LEU	3.1
4	BD	166	GLU	3.1
22	CA	2021	C	3.1
2	BB	64	LYS	3.1
10	BJ	11	LYS	3.1
13	BM	110	LYS	3.1
13	BM	114	LYS	3.1
14	BN	3	LYS	3.1
25	CD	190	LYS	3.1
30	DJ	72	LYS	3.1
2	AB	91	PHE	3.1
3	BC	197	GLY	3.1
8	BH	55	THR	3.1
11	BK	120	GLY	3.1
15	BO	15	PHE	3.1
19	AS	74	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
30	CJ	117	MET	3.1
20	BT	30	THR	3.1
24	CC	151	GLY	3.1
24	DC	241	GLY	3.1
26	CE	54	GLY	3.1
27	DF	105	THR	3.1
29	CH	24	GLY	3.1
30	CJ	112	THR	3.1
30	DJ	60	THR	3.1
32	CL	104	THR	3.1
36	CP	117	PHE	3.1
48	C1	23	THR	3.1
48	C1	26	THR	3.1
49	C2	24	THR	3.1
22	CA	1537	G	3.1
24	CC	153	GLN	3.1
34	CN	69	PRO	3.1
53	DA	141	G	3.1
53	DA	653	U	3.1
26	CE	79	ARG	3.1
2	BB	79	ALA	3.1
2	BB	219	ALA	3.1
3	BC	91	VAL	3.1
7	AG	6	VAL	3.1
11	AK	129	VAL	3.1
14	AN	34	VAL	3.1
21	BU	52	ALA	3.1
27	CF	54	ALA	3.1
27	CF	108	VAL	3.1
29	DH	63	ALA	3.1
29	DH	148	ALA	3.1
30	CJ	57	VAL	3.1
31	CK	9	GLU	3.1
36	CP	41	ALA	3.1
39	CS	64	VAL	3.1
43	CW	54	ALA	3.1
46	CZ	46	VAL	3.1
55	DI	120	ALA	3.1
3	BC	157	LEU	3.1
7	AG	30	LEU	3.1
10	BJ	53	ILE	3.1
11	BK	79	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
20	BT	39	ILE	3.1
39	CS	41	ILE	3.1
44	CX	82	ILE	3.1
7	BG	114	LYS	3.1
7	BG	136	LYS	3.1
13	AM	114	LYS	3.1
13	BM	44	LYS	3.1
20	BT	8	LYS	3.1
26	CE	99	LYS	3.1
28	CG	85	LYS	3.1
28	CG	158	LYS	3.1
42	CV	19	LYS	3.1
26	CE	107	SER	3.1
27	CF	130	MET	3.1
28	CG	2	SER	3.1
35	CO	59	SER	3.1
37	CQ	2	SER	3.1
1	BA	121	U	3.1
2	BB	195	GLY	3.1
3	BC	158	GLY	3.1
24	CC	152	GLY	3.1
26	CE	17	THR	3.1
28	CG	171	THR	3.1
2	AB	69	PHE	3.1
2	BB	162	PHE	3.1
8	BH	49	PHE	3.1
44	CX	69	PHE	3.1
2	AB	158	PRO	3.1
3	BC	60	PRO	3.1
24	DC	247	PRO	3.1
44	CX	76	ASN	3.1
1	AA	1534	A	3.1
9	AI	41	ARG	3.1
10	BJ	72	ARG	3.1
14	BN	65	ARG	3.1
32	CL	98	ARG	3.1
41	CU	3	ARG	3.1
46	DZ	7	ARG	3.1
53	DA	1847	A	3.1
3	BC	161	GLU	3.1
16	BP	53	ASP	3.1
28	CG	166	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
14	BN	8	ALA	3.1
19	AS	22	ALA	3.1
20	BT	47	ALA	3.1
26	CE	160	ALA	3.1
28	CG	97	ALA	3.1
28	CG	136	ALA	3.1
29	CH	69	ALA	3.1
30	CJ	133	ALA	3.1
33	CM	131	ALA	3.1
43	CW	28	ALA	3.1
8	BH	129	VAL	3.1
9	AI	13	LYS	3.1
14	AN	19	LYS	3.1
17	BQ	13	VAL	3.1
27	DF	72	LYS	3.1
47	C0	55	VAL	3.1
2	BB	68	LEU	3.1
51	C4	44	LEU	3.1
2	AB	60	ILE	3.1
3	BC	202	ILE	3.1
31	CK	54	ILE	3.1
32	CL	75	SER	3.1
33	CM	80	SER	3.1
22	CA	215	G	3.0
29	CH	133	GLN	3.1
3	BC	184	TYR	3.0
9	BI	70	GLY	3.0
24	DC	234	GLY	3.0
29	CH	120	GLY	3.0
9	BI	84	THR	3.0
24	CC	226	ASN	3.0
6	BF	79	ARG	3.0
10	BJ	5	ARG	3.0
13	BM	87	ARG	3.0
14	BN	63	ARG	3.0
22	CA	1301	A	3.0
31	CK	13	ARG	3.0
34	CN	117	PHE	3.0
37	CQ	109	ARG	3.0
39	CS	5	PHE	3.0
43	CW	2	PHE	3.0
50	C3	19	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
53	DA	1090	A	3.0
30	DJ	50	GLU	3.0
37	CQ	68	GLU	3.0
8	BH	94	LYS	3.0
14	AN	47	LYS	3.0
16	BP	13	LYS	3.0
30	DJ	45	LYS	3.0
39	CS	97	LYS	3.0
15	BO	7	ALA	3.0
28	CG	150	ALA	3.0
28	CG	165	ALA	3.0
30	CJ	63	ALA	3.0
36	CP	77	ALA	3.0
44	CX	61	ALA	3.0
55	DI	100	ALA	3.0
2	BB	183	VAL	3.0
5	AE	115	LEU	3.0
5	BE	56	VAL	3.0
6	BF	61	LEU	3.0
7	AG	135	VAL	3.0
8	BH	51	VAL	3.0
8	BH	63	LEU	3.0
16	BP	61	VAL	3.0
32	CL	1	MET	3.0
32	CL	7	MET	3.0
27	CF	103	LEU	3.0
36	CP	62	LEU	3.0
43	CW	65	VAL	3.0
8	BH	126	ILE	3.0
9	BI	73	SER	3.0
27	CF	34	ILE	3.0
33	CM	42	SER	3.0
34	CN	22	GLN	3.0
42	CV	46	GLN	3.0
9	BI	83	ILE	3.0
13	AM	73	ILE	3.0
16	AP	4	ILE	3.0
22	CA	822	G	3.0
24	CC	91	ILE	3.0
45	CY	52	SER	3.0
48	C1	34	SER	3.0
52	C5	6	SER	3.0

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Mol	Chain	Res	Type	RSRZ
12	BL	86	ARG	3.0
13	BM	24	GLY	3.0
14	BN	68	GLY	3.0
24	CC	86	ASN	3.0
25	CD	163	GLY	3.0
44	CX	39	ARG	3.0
50	C3	3	ARG	3.0
24	CC	160	THR	3.0
25	CD	52	THR	3.0
29	CH	79	THR	3.0
34	CN	24	THR	3.0
29	CH	25	TYR	3.0
1	BA	135	C	3.0
16	BP	15	PRO	3.0
24	CC	85	PRO	3.0
42	CV	101	GLU	3.0
46	CZ	17	GLU	3.0
5	BE	33	PHE	3.0
7	BG	18	PHE	3.0
27	CF	77	PHE	3.0
30	CJ	38	PHE	3.0
34	CN	9	PHE	3.0
38	CR	49	ASP	3.0
5	AE	86	LYS	3.0
6	BF	55	HIS	3.0
7	BG	36	LYS	3.0
27	CF	88	LYS	3.0
30	CJ	87	LYS	3.0
25	CD	11	MET	3.0
7	BG	121	ALA	3.0
13	BM	61	ALA	3.0
20	AT	87	ALA	3.0
25	CD	102	ALA	3.0
27	CF	55	ALA	3.0
29	CH	148	ALA	3.0
30	CJ	115	ALA	3.0
38	CR	69	ALA	3.0
9	BI	29	VAL	3.0
10	AJ	98	VAL	3.0
11	BK	129	VAL	3.0
12	BL	57	LEU	3.0
15	BO	39	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
24	CC	10	SER	3.0
24	DC	137	VAL	3.0
27	CF	28	VAL	3.0
31	CK	64	VAL	3.0
33	CM	95	LEU	3.0
46	DZ	56	LEU	3.0
38	CR	55	ARG	3.0
2	AB	207	ILE	3.0
13	AM	4	ILE	3.0
17	AQ	38	ILE	3.0
21	BU	4	ILE	3.0
43	CW	89	ILE	3.0
31	CK	79	GLY	3.0
31	CK	115	GLY	3.0
41	DU	56	GLU	3.0
5	AE	24	THR	3.0
9	AI	105	THR	3.0
26	CE	13	THR	3.0
27	CF	35	THR	3.0
28	CG	49	THR	3.0
33	CM	118	THR	3.0
34	CN	54	THR	3.0
44	CX	43	THR	3.0
47	C0	35	THR	3.0
24	CC	22	PRO	3.0
35	CO	50	PRO	3.0
37	CQ	18	PRO	3.0
2	BB	116	ASP	3.0
9	BI	7	TYR	3.0
13	BM	13	LYS	3.0
14	BN	71	HIS	3.0
25	CD	105	LYS	3.0
31	CK	39	LYS	3.0
27	DF	114	PHE	3.0
34	CN	31	PHE	3.0
24	CC	132	MET	3.0
24	CC	163	GLN	3.0
33	CM	54	GLN	3.0
40	CT	15	GLN	3.0
16	BP	56	ARG	3.0
22	CA	325	G	3.0
2	BB	172	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
4	AD	153	SER	3.0
7	BG	115	SER	3.0
8	BH	24	ALA	3.0
22	CA	1246	A	3.0
31	CK	63	ALA	3.0
31	CK	95	ARG	3.0
30	DJ	21	SER	3.0
33	CM	97	ALA	3.0
33	CM	133	ALA	3.0
34	DN	59	ARG	3.0
35	CO	96	ARG	3.0
37	CQ	53	ARG	3.0
46	DZ	3	ALA	3.0
53	DA	2886[A]	A	3.0
2	AB	129	LEU	3.0
4	BD	125	VAL	3.0
5	BE	114	VAL	3.0
7	AG	59	LEU	3.0
7	BG	30	LEU	3.0
7	BG	87	VAL	3.0
28	CG	79	VAL	3.0
29	DH	19	VAL	3.0
30	DJ	28	LEU	3.0
31	CK	122	LEU	3.0
34	CN	93	VAL	3.0
55	DI	108	VAL	3.0
5	AE	148	ASN	3.0
8	BH	21	ASN	3.0
37	CQ	44	GLU	3.0
41	CU	5	GLU	3.0
44	CX	17	GLU	3.0
2	AB	71	GLY	3.0
6	BF	51	ILE	3.0
32	CL	43	ILE	3.0
33	CM	114	GLY	3.0
36	CP	22	GLY	3.0
49	C2	18	GLY	3.0
10	AJ	80	THR	3.0
32	CL	6	THR	3.0
40	CT	37	THR	3.0
46	CZ	55	THR	3.0
6	BF	56	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
14	BN	7	LYS	3.0
17	BQ	36	LYS	3.0
7	BG	85	TYR	3.0
7	AG	103	TRP	3.0
9	AI	119	ARG	2.9
10	BJ	9	ARG	2.9
14	BN	53	ARG	2.9
22	CA	93	G	2.9
26	CE	21	ARG	2.9
31	CK	37	ARG	2.9
1	BA	1325	C	2.9
2	AB	34	ALA	2.9
4	BD	149	ALA	2.9
7	BG	145	ALA	2.9
22	CA	2000	C	2.9
30	CJ	44	ALA	2.9
30	DJ	135	SER	2.9
33	CM	98	ALA	2.9
36	DP	51	ALA	2.9
37	CQ	11	GLU	2.9
39	CS	7	SER	2.9
40	CT	30	SER	2.9
55	DI	30	SER	2.9
3	BC	47	LEU	2.9
19	AS	16	LEU	2.9
19	BS	5	LEU	2.9
20	BT	21	ASN	2.9
20	BT	84	ASN	2.9
29	CH	5	LEU	2.9
31	CK	28	LEU	2.9
37	CQ	66	ASN	2.9
55	DI	57	ASN	2.9
55	DI	71	CYS	2.9
5	BE	25	VAL	2.9
5	BE	88	VAL	2.9
7	AG	69	VAL	2.9
21	AU	3	VAL	2.9
21	BU	14	VAL	2.9
25	CD	98	VAL	2.9
34	CN	89	VAL	2.9
43	CW	92	VAL	2.9
24	CC	206	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
41	DU	71	GLY	2.9
2	AB	171	ILE	2.9
3	BC	68	ILE	2.9
10	AJ	8	ILE	2.9
32	DL	116	ILE	2.9
8	BH	31	LYS	2.9
11	AK	14	LYS	2.9
13	AM	13	LYS	2.9
31	CK	2	LYS	2.9
46	DZ	4	LYS	2.9
51	C4	19	LYS	2.9
3	BC	191	THR	2.9
4	BD	99	ASP	2.9
8	BH	112	THR	2.9
9	AI	43	THR	2.9
10	BJ	60	ASP	2.9
26	CE	65	THR	2.9
28	CG	51	THR	2.9
31	CK	76	HIS	2.9
13	AM	10	PRO	2.9
20	AT	61	GLN	2.9
25	CD	130	GLN	2.9
39	CS	87	GLN	2.9
2	BB	35	ARG	2.9
13	BM	92	ARG	2.9
21	AU	47	ARG	2.9
22	CA	532	A	2.9
22	CA	1322	A	2.9
22	CA	2003	A	2.9
2	BB	16	PHE	2.9
3	BC	42	TYR	2.9
10	BJ	65	TYR	2.9
28	CG	58	TYR	2.9
31	CK	96	ARG	2.9
37	CQ	62	ARG	2.9
51	C4	8	ARG	2.9
55	DI	46	ARG	2.9
22	CA	45	G	2.9
22	CA	798	G	2.9
1	BA	136	C	2.9
6	BF	42	TRP	2.9
7	BG	103	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
22	CA	1325	U	2.9
45	CY	70	GLU	2.9
2	BB	147	SER	2.9
12	BL	19	SER	2.9
24	CC	157	SER	2.9
25	CD	97	SER	2.9
2	BB	12	ALA	2.9
4	BD	122	ALA	2.9
12	AL	73	ASN	2.9
13	AM	106	ALA	2.9
14	BN	44	ALA	2.9
19	AS	50	ALA	2.9
24	CC	70	ASN	2.9
24	CC	197	ASN	2.9
26	CE	192	ALA	2.9
29	DH	20	ASN	2.9
37	DQ	66	ASN	2.9
55	DI	22	ALA	2.9
2	BB	87	CYS	2.9
4	BD	91	LEU	2.9
7	BG	76	LYS	2.9
12	BL	10	LYS	2.9
19	BS	21	LYS	2.9
19	BS	29	LYS	2.9
29	CH	90	LEU	2.9
25	CD	115	GLY	2.9
29	DH	120	GLY	2.9
30	DJ	97	LYS	2.9
43	CW	42	LEU	2.9
43	CW	33	GLY	2.9
55	DI	66	GLY	2.9
2	BB	196	VAL	2.9
26	CE	193	VAL	2.9
2	AB	82	ASP	2.9
6	BF	6	ILE	2.9
18	BR	33	ILE	2.9
29	CH	72	ILE	2.9
39	CS	89	HIS	2.9
43	CW	70	ILE	2.9
5	BE	80	THR	2.9
44	CX	58	THR	2.9
11	BK	89	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
32	CL	48	PRO	2.9
48	C1	5	GLN	2.9
2	AB	21	ARG	2.9
5	BE	93	ARG	2.9
7	BG	79	ARG	2.9
25	CD	169	ARG	2.9
1	BA	1116	U	2.9
22	CA	431	U	2.9
22	CA	1249	U	2.9
55	DI	134	GLU	2.9
2	BB	91	PHE	2.9
2	BB	213	TYR	2.9
4	BD	182	PHE	2.9
27	CF	175	PHE	2.9
28	CG	164	TYR	2.9
39	CS	93	PHE	2.9
9	BI	15	SER	2.9
25	CD	95	SER	2.9
26	CE	163	ASN	2.9
31	CK	85	LYS	2.9
36	CP	63	LYS	2.9
2	AB	76	ALA	2.9
16	BP	43	ALA	2.9
20	BT	62	ALA	2.9
24	DC	122	ALA	2.9
25	CD	182	ALA	2.9
30	CJ	124	ALA	2.9
46	DZ	33	ALA	2.9
51	C4	10	ALA	2.9
2	BB	33	GLY	2.9
3	BC	124	LEU	2.9
5	BE	51	GLY	2.9
10	AJ	52	LEU	2.9
15	BO	81	LEU	2.9
24	CC	130	LEU	2.9
26	CE	3	LEU	2.9
26	CE	151	GLY	2.9
29	CH	16	GLY	2.9
30	CJ	106	LEU	2.9
24	DC	243	HIS	2.9
27	CF	31	VAL	2.9
27	CF	163	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
38	CR	14	HIS	2.9
45	CY	5	CYS	2.9
47	C0	20	HIS	2.9
47	C0	34	HIS	2.9
48	C1	42	HIS	2.9
2	AB	14	VAL	2.9
5	BE	38	VAL	2.9
7	BG	73	VAL	2.9
11	AK	16	VAL	2.9
17	BQ	76	VAL	2.9
20	AT	58	VAL	2.9
28	CG	144	VAL	2.9
29	DH	134	VAL	2.9
32	CL	62	VAL	2.9
33	CM	120	VAL	2.9
34	CN	101	VAL	2.9
2	BB	9	MET	2.9
4	BD	145	ILE	2.9
6	BF	46	GLN	2.9
3	BC	21	THR	2.9
5	BE	140	THR	2.9
14	BN	50	THR	2.9
14	BN	67	THR	2.9
16	BP	75	ILE	2.9
17	BQ	7	THR	2.9
20	BT	27	MET	2.9
10	BJ	48	ARG	2.9
19	AS	37	ARG	2.9
21	AU	55	ARG	2.9
22	CA	528	A	2.9
22	CA	2082	A	2.9
30	DJ	17	MET	2.9
28	CG	69	ARG	2.9
29	CH	80	ILE	2.9
37	CQ	75	GLN	2.9
39	CS	1	MET	2.9
50	C3	6	GLN	2.9
29	DH	97	ARG	2.9
31	CK	34	ARG	2.9
53	DA	2167	U	2.9
2	AB	201	PRO	2.9
7	AG	93	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
11	BK	123	PRO	2.9
17	BQ	66	PRO	2.9
22	CA	1	G	2.9
22	CA	531	C	2.9
22	CA	682	G	2.9
22	CA	805	G	2.9
22	CA	953	G	2.9
22	CA	1644	C	2.9
24	CC	236	GLU	2.9
36	CP	20	GLU	2.9
6	BF	49	TYR	2.9
17	BQ	43	LYS	2.9
19	AS	10	PHE	2.9
19	BS	17	LYS	2.9
29	DH	139	PHE	2.9
27	CF	127	ASN	2.9
30	CJ	97	LYS	2.9
38	CR	106	PHE	2.9
39	CS	24	LYS	2.9
45	CY	42	SER	2.9
8	AH	24	ALA	2.9
11	AK	66	ALA	2.9
12	BL	113	ALA	2.9
15	BO	76	ALA	2.9
27	DF	119	ALA	2.9
33	CM	134	ALA	2.9
9	BI	71	GLY	2.9
12	BL	118	GLY	2.9
14	AN	101	TRP	2.9
30	CJ	131	GLY	2.9
37	CQ	67	GLY	2.9
3	BC	131	ARG	2.8
5	BE	36	LEU	2.8
8	BH	13	ARG	2.8
9	AI	50	GLN	2.8
13	AM	113	ARG	2.8
22	CA	448	U	2.8
22	CA	1365	A	2.8
27	CF	125	ARG	2.8
31	DK	1	MET	2.8
32	CL	78	ARG	2.8
41	CU	48	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
41	DU	73	ARG	2.8
44	CX	20	ARG	2.8
50	C3	28	ARG	2.8
51	C4	13	ARG	2.8
8	BH	72	VAL	2.8
25	CD	180	VAL	2.8
29	DH	130	VAL	2.8
32	CL	61	VAL	2.8
39	CS	38	VAL	2.8
47	C0	57	VAL	2.8
2	BB	138	THR	2.8
6	AF	97	THR	2.8
12	BL	97	THR	2.8
18	BR	71	THR	2.8
24	CC	191	THR	2.8
4	AD	28	ILE	2.8
15	AO	82	ILE	2.8
32	CL	116	ILE	2.8
33	DM	103	ILE	2.8
1	AA	844	G	2.8
2	BB	158	PRO	2.8
29	CH	118	PRO	2.8
21	BU	54	LYS	2.8
25	CD	62	LYS	2.8
43	CW	10	LYS	2.8
48	C1	53	LYS	2.8
3	BC	154	SER	2.8
5	BE	32	SER	2.8
7	BG	77	SER	2.8
19	BS	43	ASN	2.8
37	CQ	85	SER	2.8
47	C0	52	SER	2.8
2	AB	126	PHE	2.8
2	AB	162	PHE	2.8
38	CR	79	PHE	2.8
1	AA	1492	A	2.8
1	BA	632	U	2.8
2	BB	22	TYR	2.8
22	CA	150	U	2.8
9	BI	49	ARG	2.8
10	AJ	35	GLN	2.8
10	AJ	70	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
2	AB	172	ALA	2.8
2	BB	192	ASP	2.8
3	BC	133	ALA	2.8
3	BC	163	ALA	2.8
3	BC	180	ALA	2.8
7	AG	98	ALA	2.8
7	AG	144	MET	2.8
8	BH	5	ASP	2.8
16	BP	28	ARG	2.8
24	CC	133	ARG	2.8
26	CE	46	GLN	2.8
27	CF	30	ARG	2.8
34	CN	13	HIS	2.8
9	AI	82	GLY	2.8
11	BK	67	ALA	2.8
15	AO	19	ALA	2.8
17	BQ	35	GLY	2.8
20	BT	87	ALA	2.8
26	CE	68	ALA	2.8
27	CF	153	ASP	2.8
30	CJ	15	ALA	2.8
30	DJ	32	GLY	2.8
39	CS	65	ALA	2.8
47	C0	22	ALA	2.8
1	BA	222	C	2.8
5	AE	11	LEU	2.8
11	AK	100	LEU	2.8
18	BR	65	LEU	2.8
19	AS	71	LEU	2.8
5	BE	10	GLU	2.8
11	BK	44	TRP	2.8
22	CA	41	C	2.8
22	CA	57	C	2.8
29	DH	75	LEU	2.8
14	BN	10	GLU	2.8
45	CY	76	GLU	2.8
1	BA	1032	G	2.8
5	BE	94	VAL	2.8
5	BE	153	VAL	2.8
6	BF	60	VAL	2.8
6	BF	64	VAL	2.8
6	BF	97	THR	2.8

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Mol	Chain	Res	Type	RSRZ
8	BH	39	VAL	2.8
9	AI	104	VAL	2.8
11	BK	121	CYS	2.8
15	BO	27	VAL	2.8
22	CA	389	G	2.8
22	CA	530	G	2.8
25	CD	34	VAL	2.8
26	CE	187	VAL	2.8
28	CG	41	VAL	2.8
32	CL	69	VAL	2.8
3	AC	103	ILE	2.8
10	BJ	55	PRO	2.8
29	DH	72	ILE	2.8
37	CQ	5	ILE	2.8
38	CR	94	ILE	2.8
12	BL	123	LYS	2.8
42	CV	99	ASN	2.8
9	BI	41	ARG	2.8
14	BN	66	GLN	2.8
16	BP	35	ARG	2.8
20	BT	29	ARG	2.8
25	CD	184	ARG	2.8
37	CQ	72	ARG	2.8
40	CT	84	ARG	2.8
19	BS	14	HIS	2.8
24	CC	200	HIS	2.8
46	CZ	36	GLN	2.8
48	C1	38	HIS	2.8
2	BB	123	ASP	2.8
3	BC	130	PHE	2.8
37	CQ	20	PHE	2.8
2	BB	156	GLY	2.8
5	BE	129	GLY	2.8
22	CA	679	C	2.8
7	BG	129	GLU	2.8
8	BH	19	ALA	2.8
16	AP	45	GLU	2.8
20	AT	50	ALA	2.8
30	DJ	83	ALA	2.8
15	BO	3	LEU	2.8
22	CA	1271	G	2.8
38	CR	83	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
40	CT	33	LEU	2.8
53	DA	283	G	2.8
53	DA	1177	G	2.8
3	AC	165	THR	2.8
7	AG	133	THR	2.8
30	DJ	126	THR	2.8
31	CK	30	THR	2.8
2	AB	23	TRP	2.8
3	AC	167	TRP	2.8
12	BL	87	VAL	2.8
24	DC	248	TRP	2.8
27	CF	97	TRP	2.8
4	BD	177	LYS	2.8
5	BE	105	ILE	2.8
5	BE	159	LYS	2.8
7	AG	104	ILE	2.8
9	BI	100	LYS	2.8
12	BL	88	LYS	2.8
14	AN	3	LYS	2.8
19	BS	6	LYS	2.8
21	AU	5	LYS	2.8
21	AU	54	LYS	2.8
32	CL	111	LYS	2.8
34	CN	76	LYS	2.8
35	CO	5	LYS	2.8
38	CR	62	ILE	2.8
40	CT	41	LYS	2.8
47	C0	44	ILE	2.8
1	AA	1	A	2.8
42	CV	69	ASN	2.8
14	BN	69	ARG	2.8
35	CO	86	ARG	2.8
36	CP	13	ARG	2.8
41	CU	6	ARG	2.8
20	BT	55	GLN	2.8
17	BQ	31	HIS	2.8
7	BG	144	MET	2.8
14	BN	54	ASP	2.8
40	CT	59	GLU	2.8
6	BF	78	PHE	2.8
7	BG	132	GLY	2.8
10	AJ	49	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
16	BP	30	GLY	2.8
27	CF	62	GLY	2.8
27	CF	173	PHE	2.8
1	AA	1305	G	2.8
13	AM	40	ALA	2.8
21	AU	48	ALA	2.8
22	CA	468	G	2.8
22	CA	1131	G	2.8
22	CA	1248	G	2.8
24	CC	190	ALA	2.8
29	CH	111	ALA	2.8
40	CT	32	ALA	2.8
24	DC	33	LEU	2.8
28	CG	37	LEU	2.8
43	CW	86	LEU	2.8
7	BG	84	THR	2.8
8	BH	26	THR	2.8
10	AJ	44	THR	2.8
10	BJ	32	THR	2.8
13	BM	104	THR	2.8
19	AS	33	THR	2.8
22	CA	1199	U	2.8
22	CA	2904	U	2.8
26	CE	150	THR	2.8
28	CG	172	LYS	2.8
34	CN	42	THR	2.8
53	DA	2585	U	2.8
55	DI	86	THR	2.8
4	BD	186	PRO	2.8
13	AM	112	PRO	2.8
32	CL	102	PRO	2.8
2	BB	47	VAL	2.8
5	AE	46	VAL	2.8
7	AG	43	VAL	2.8
13	BM	64	VAL	2.8
24	DC	120	VAL	2.8
28	CG	17	VAL	2.8
30	DJ	39	CYS	2.8
37	CQ	86	VAL	2.8
44	CX	51	VAL	2.8
2	BB	41	ILE	2.8
2	BB	207	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
3	BC	64	ILE	2.8
5	AE	60	ILE	2.8
9	BI	28	ILE	2.8
15	AO	11	ILE	2.8
22	CA	821	A	2.8
22	CA	1214	A	2.8
24	DC	164	ILE	2.8
33	CM	142	ILE	2.8
3	BC	164	ARG	2.7
10	BJ	7	ARG	2.7
25	CD	125	TRP	2.8
31	DK	95	ARG	2.7
36	CP	33	ARG	2.7
29	CH	28	ASN	2.7
45	CY	17	ASN	2.7
4	BD	144	SER	2.7
47	C0	12	SER	2.7
6	AF	55	HIS	2.7
16	BP	9	HIS	2.7
22	CA	1600	C	2.7
24	CC	201	MET	2.7
26	CE	141	MET	2.7
29	CH	1	MET	2.7
19	AS	65	GLU	2.7
35	CO	106	ASP	2.7
35	DO	120	GLU	2.7
55	DI	114	GLU	2.7
2	BB	65	GLY	2.7
6	BF	31	GLY	2.7
16	BP	37	GLY	2.7
22	CA	1332	G	2.7
22	CA	1642	G	2.7
22	CA	1797	G	2.7
22	CA	1823	G	2.7
25	CD	198	GLY	2.7
26	CE	174	GLY	2.7
30	CJ	52	GLY	2.7
31	CK	107	GLY	2.7
49	D2	4	GLY	2.7
1	AA	842	U	2.7
22	CA	29	U	2.7
22	CA	790	U	2.7

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Mol	Chain	Res	Type	RSRZ
27	CF	100	PHE	2.7
29	CH	46	PHE	2.7
7	BG	110	LYS	2.7
10	AJ	34	ALA	2.7
12	BL	26	ALA	2.7
28	CG	44	LYS	2.7
38	CR	84	LYS	2.7
48	C1	37	LYS	2.7
49	C2	37	LYS	2.7
8	BH	121	LEU	2.7
11	BK	100	LEU	2.7
29	DH	62	LEU	2.7
35	CO	94	TYR	2.7
36	CP	36	TYR	2.7
13	AM	108	THR	2.7
22	CA	631	A	2.7
22	CA	2406	A	2.7
25	CD	110	THR	2.7
28	CG	84	THR	2.7
30	CJ	46	THR	2.7
37	CQ	76	THR	2.7
6	AF	50	PRO	2.7
14	BN	90	ARG	2.7
16	BP	51	ARG	2.7
34	CN	98	PRO	2.7
45	CY	57	ARG	2.7
2	AB	196	VAL	2.7
3	BC	200	VAL	2.7
8	BH	104	VAL	2.7
10	AJ	84	VAL	2.7
19	AS	19	VAL	2.7
29	CH	78	VAL	2.7
29	CH	146	VAL	2.7
29	DH	61	VAL	2.7
34	CN	131	VAL	2.7
43	CW	8	VAL	2.7
2	AB	151	ILE	2.7
3	BC	149	ILE	2.7
11	AK	31	ILE	2.7
11	BK	34	ILE	2.7
32	CL	38	ILE	2.7
43	CW	49	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
22	CA	517	C	2.7
10	BJ	54	SER	2.7
10	BJ	101	SER	2.7
28	CG	115	HIS	2.7
25	CD	168	GLU	2.7
41	CU	27	SER	2.7
42	CV	100	SER	2.7
49	C2	51	GLU	2.7
8	BH	90	ASP	2.7
9	AI	56	ASP	2.7
10	BJ	91	ASP	2.7
16	BP	55	ASP	2.7
22	CA	180	G	2.7
22	CA	914	G	2.7
22	CA	1355	G	2.7
22	CA	1778	U	2.7
22	CA	2321	U	2.7
3	AC	171	GLY	2.7
3	BC	2	GLY	2.7
28	CG	120	GLY	2.7
29	DH	16	GLY	2.7
39	CS	57	GLY	2.7
43	DW	67	GLY	2.7
51	C4	9	GLY	2.7
9	AI	27	LYS	2.7
11	AK	75	LYS	2.7
12	AL	10	LYS	2.7
14	BN	76	LYS	2.7
33	CM	63	LYS	2.7
51	D4	15	LYS	2.7
55	DI	20	LYS	2.7
3	BC	48	ALA	2.7
4	BD	162	ALA	2.7
7	AG	39	ALA	2.7
7	AG	151	PHE	2.7
8	BH	23	ALA	2.7
15	BO	34	ALA	2.7
21	AU	52	ALA	2.7
22	CA	1008	A	2.7
29	CH	84	ALA	2.7
30	CJ	84	ALA	2.7
30	DJ	44	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
34	CN	122	ALA	2.7
43	CW	39	ALA	2.7
2	AB	157	LEU	2.7
47	C0	27	LEU	2.7
52	C5	4	ARG	2.7
15	BO	33	THR	2.7
24	DC	252	THR	2.7
33	CM	94	THR	2.7
33	CM	121	THR	2.7
51	C4	38	THR	2.7
7	AG	85	TYR	2.7
2	BB	48	PRO	2.7
9	BI	37	GLN	2.7
27	CF	143	TYR	2.7
31	CK	125	TYR	2.7
30	CJ	26	PRO	2.7
32	CL	3	GLN	2.7
43	CW	31	TYR	2.7
11	BK	115	PRO	2.7
13	BM	10	PRO	2.7
11	BK	119	ASN	2.7
22	CA	1297	C	2.7
26	CE	156	ASN	2.7
53	DA	1870	C	2.7
5	BE	85	VAL	2.7
6	BF	7	VAL	2.7
12	BL	96	HIS	2.7
16	BP	34	GLU	2.7
25	CD	81	GLU	2.7
29	CH	147	VAL	2.7
39	CS	34	GLU	2.7
39	CS	70	GLU	2.7
55	DI	40	GLU	2.7
11	BK	97	ILE	2.7
17	BQ	33	ILE	2.7
19	BS	11	ILE	2.7
47	C0	5	ILE	2.7
27	CF	129	SER	2.7
46	CZ	34	SER	2.7
1	BA	1286	U	2.7
22	CA	533	G	2.7
22	CA	630	G	2.7

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Mol	Chain	Res	Type	RSRZ
2	BB	66	LYS	2.7
9	AI	120	LYS	2.7
13	BM	78	LYS	2.7
24	CC	68	LYS	2.7
34	CN	123	LYS	2.7
44	CX	19	LYS	2.7
2	AB	98	GLY	2.7
10	AJ	33	GLY	2.7
10	AJ	95	GLY	2.7
29	DH	126	GLY	2.7
55	DI	45	GLY	2.7
22	CA	2020	A	2.7
2	AB	225	ARG	2.7
3	AC	127	ARG	2.7
25	CD	59	ARG	2.7
38	CR	48	ARG	2.7
39	CS	90	ARG	2.7
5	BE	95	PHE	2.7
6	AF	80	PHE	2.7
25	CD	68	PHE	2.7
29	CH	36	ALA	2.7
35	CO	66	ALA	2.7
44	CX	18	ALA	2.7
37	CQ	10	GLN	2.7
2	BB	157	LEU	2.7
6	AF	47	LEU	2.7
12	AL	74	LEU	2.7
13	AM	89	LEU	2.7
14	AN	50	THR	2.7
22	CA	183	C	2.7
22	CA	584	C	2.7
22	CA	1868	C	2.7
27	DF	117	LEU	2.7
38	CR	95	LEU	2.7
53	DA	885	C	2.7
3	BC	174	PRO	2.7
9	AI	6	TYR	2.7
9	BI	4	ASN	2.7
10	BJ	27	GLU	2.7
15	BO	6	GLU	2.7
19	BS	59	PRO	2.7
25	CD	74	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
26	CE	127	GLU	2.7
28	DG	8	PRO	2.7
29	CH	137	GLU	2.7
41	DU	92	ASN	2.7
44	CX	70	GLU	2.7
55	DI	133	GLU	2.7
12	BL	66	TYR	2.7
31	CK	40	HIS	2.7
2	AB	187	VAL	2.7
2	BB	4	VAL	2.7
4	BD	130	VAL	2.7
6	BF	70	VAL	2.7
7	BG	41	SER	2.7
15	AO	2	SER	2.7
20	BT	23	SER	2.7
2	AB	123	ASP	2.7
7	BG	15	ASP	2.7
8	BH	46	ILE	2.7
24	DC	165	VAL	2.7
27	DF	121	SER	2.7
35	CO	89	SER	2.7
37	CQ	47	VAL	2.7
37	CQ	83	SER	2.7
16	BP	69	ASP	2.7
18	BR	39	ILE	2.7
28	CG	19	ILE	2.7
12	BL	27	CYS	2.7
22	CA	1277	G	2.7
9	BI	115	LYS	2.7
25	CD	208	LYS	2.7
28	CG	160	LYS	2.7
32	CL	54	LYS	2.7
37	CQ	38	LYS	2.7
37	CQ	96	LYS	2.7
40	CT	28	LYS	2.7
44	CX	66	LYS	2.7
1	BA	101	A	2.7
22	CA	1654	A	2.7
5	BE	54	ARG	2.7
7	BG	78	ARG	2.7
9	BI	26	GLY	2.7
9	BI	102	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
24	CC	87	ARG	2.7
24	CC	262	ARG	2.7
32	CL	55	GLY	2.7
34	CN	114	ARG	2.7
38	CR	92	ARG	2.7
45	CY	63	GLY	2.7
15	BO	28	GLN	2.6
25	CD	164	GLN	2.6
42	CV	66	GLN	2.6
1	BA	233	C	2.6
1	BA	1234	C	2.6
22	CA	509	C	2.6
22	CA	1615	C	2.6
5	BE	151	GLU	2.6
24	CC	158	ALA	2.6
24	DC	194	GLU	2.6
34	CN	43	ALA	2.6
37	CQ	27	GLU	2.6
40	CT	58	ALA	2.6
40	CT	93	ALA	2.6
42	DV	76	ALA	2.6
2	AB	10	LEU	2.6
4	BD	110	THR	2.6
5	BE	37	THR	2.6
5	BE	111	MET	2.6
11	BK	52	PHE	2.6
14	BN	73	PHE	2.6
22	CA	803	U	2.6
17	BQ	44	LEU	2.6
19	BS	48	THR	2.6
25	CD	12	THR	2.6
29	DH	6	LEU	2.6
34	CN	53	MET	2.6
12	BL	45	PRO	2.6
13	AM	105	ASN	2.6
14	AN	57	PRO	2.6
19	AS	42	PRO	2.6
26	CE	76	PRO	2.6
37	CQ	56	HIS	2.6
40	CT	57	ASN	2.6
55	DI	88	HIS	2.6
27	CF	8	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
30	CJ	21	SER	2.6
30	CJ	135	SER	2.6
32	CL	37	ASP	2.6
33	DM	91	ASP	2.6
46	CZ	49	ASP	2.6
1	BA	292	G	2.6
2	BB	132	LYS	2.6
2	BB	187	VAL	2.6
3	BC	77	ILE	2.6
5	AE	120	VAL	2.6
6	AF	93	LYS	2.6
6	AF	51	ILE	2.6
9	BI	30	ILE	2.6
11	BK	16	VAL	2.6
12	BL	119	VAL	2.6
20	BT	76	LYS	2.6
22	CA	2360	G	2.6
29	CH	83	LYS	2.6
27	DF	106	ILE	2.6
27	DF	137	ILE	2.6
29	DH	37	VAL	2.6
31	CK	73	VAL	2.6
39	CS	33	VAL	2.6
43	CW	46	LYS	2.6
55	DI	73	LYS	2.6
24	DC	135	ILE	2.6
1	AA	845	A	2.6
22	CA	1237	A	2.6
17	AQ	27	ARG	2.6
17	BQ	11	ARG	2.6
21	BU	55	ARG	2.6
38	CR	64	ARG	2.6
44	CX	14	ARG	2.6
5	BE	79	GLY	2.6
24	CC	99	GLY	2.6
28	CG	159	GLY	2.6
30	DJ	85	GLY	2.6
31	CK	82	GLY	2.6
34	CN	39	GLY	2.6
1	BA	132	C	2.6
1	BA	234	C	2.6
22	CA	678	C	2.6

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Mol	Chain	Res	Type	RSRZ
22	CA	944	C	2.6
39	CS	91	GLN	2.6
1	BA	723	U	2.6
6	BF	90	MET	2.6
5	BE	19	ASN	2.6
5	BE	70	ASN	2.6
6	BF	48	ALA	2.6
7	AG	134	ALA	2.6
9	AI	81	HIS	2.6
10	BJ	28	THR	2.6
11	BK	33	THR	2.6
12	BL	5	ASN	2.6
15	BO	19	ALA	2.6
27	CF	107	ALA	2.6
38	CR	99	ALA	2.6
43	CW	36	ALA	2.6
43	CW	52	ALA	2.6
44	CX	33	ALA	2.6
44	CX	57	HIS	2.6
50	C3	16	HIS	2.6
17	BQ	41	THR	2.6
27	CF	159	THR	2.6
41	CU	86	THR	2.6
49	C2	29	THR	2.6
2	BB	184	PHE	2.6
8	BH	28	PRO	2.6
9	AI	39	PHE	2.6
11	AK	82	LEU	2.6
19	AS	31	LEU	2.6
26	DE	153	LEU	2.6
27	CF	138	PHE	2.6
35	CO	80	PHE	2.6
49	C2	39	PHE	2.6
1	AA	1019	A	2.6
1	AA	1441	A	2.6
1	BA	102	G	2.6
2	BB	110	SER	2.6
3	BC	62	LYS	2.6
4	AD	148	LYS	2.6
7	BG	11	LYS	2.6
7	BG	17	LYS	2.6
7	BG	25	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
12	AL	18	LYS	2.6
22	CA	777	G	2.6
22	CA	947	A	2.6
22	CA	1247	A	2.6
22	CA	2029	G	2.6
22	CA	2046	G	2.6
27	CF	69	LYS	2.6
30	DJ	48	SER	2.6
38	CR	19	LYS	2.6
38	CR	54	LYS	2.6
43	CW	45	ASP	2.6
53	DA	613	A	2.6
53	DA	1093	G	2.6
53	DA	2163	A	2.6
8	BH	65	TYR	2.6
10	BJ	16	ARG	2.6
14	AN	61	ARG	2.6
19	BS	78	ARG	2.6
32	CL	18	ARG	2.6
5	BE	72	ILE	2.6
11	BK	84	VAL	2.6
12	BL	80	ILE	2.6
13	AM	17	ILE	2.6
13	AM	39	ILE	2.6
18	BR	59	ILE	2.6
24	DC	116	ILE	2.6
29	CH	134	VAL	2.6
43	CW	30	ILE	2.6
24	CC	188	CYS	2.6
2	BB	215	GLY	2.6
9	AI	117	GLY	2.6
10	AJ	4	GLN	2.6
22	CA	209	C	2.6
24	CC	73	GLY	2.6
25	CD	53	GLY	2.6
27	CF	86	GLY	2.6
30	DJ	107	GLN	2.6
41	CU	54	GLU	2.6
26	CE	188	MET	2.6
40	CT	1	MET	2.6
7	BG	130	ASN	2.6
11	AK	119	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	BB	104	TRP	2.6
8	BH	37	ALA	2.6
16	AP	22	ALA	2.6
25	CD	16	THR	2.6
27	CF	2	ALA	2.6
28	CG	123	ALA	2.6
29	DH	106	ALA	2.6
31	CK	29	ALA	2.6
45	CY	69	ALA	2.6
51	C4	6	THR	2.6
2	AB	85	LEU	2.6
5	AE	23	LYS	2.6
5	BE	98	PRO	2.6
2	BB	82	ASP	2.6
7	AG	120	LEU	2.6
7	BG	33	ASP	2.6
9	AI	61	LEU	2.6
18	BR	69	PRO	2.6
17	BQ	48	ASP	2.6
22	CA	125	A	2.6
26	CE	130	LYS	2.6
28	DG	56	ASP	2.6
29	DH	58	LEU	2.6
30	DJ	95	LYS	2.6
32	CL	87	LEU	2.6
37	CQ	87	LYS	2.6
38	CR	112	LYS	2.6
43	CW	37	PRO	2.6
4	AD	20	PHE	2.6
22	CA	535	G	2.6
22	CA	1407	G	2.6
24	CC	264	ASP	2.6
40	CT	22	ASP	2.6
40	CT	67	ASP	2.6
53	DA	2168	G	2.6
5	BE	100	SER	2.6
5	BE	130	SER	2.6
15	AO	89	ARG	2.6
15	BO	4	SER	2.6
19	AS	3	ARG	2.6
33	CM	40	SER	2.6
35	CO	45	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
36	CP	25	ARG	2.6
40	CT	110	ARG	2.6
44	CX	30	SER	2.6
44	CX	41	ARG	2.6
1	BA	843	U	2.6
2	AB	200	ILE	2.6
2	BB	38	VAL	2.6
3	BC	120	ILE	2.6
4	AD	25	VAL	2.6
5	BE	97	GLN	2.6
22	CA	2045	C	2.6
53	DA	2132	U	2.6
6	AF	64	VAL	2.6
9	AI	64	TYR	2.6
28	CG	24	ILE	2.6
30	CJ	12	GLN	2.6
30	DJ	101	ILE	2.6
30	DJ	111	GLN	2.6
31	DK	142	ILE	2.6
24	CC	199	GLU	2.6
42	CV	62	GLU	2.6
2	AB	180	GLY	2.6
9	AI	69	GLY	2.6
17	BQ	10	GLY	2.6
37	CQ	45	GLY	2.6
43	CW	15	GLY	2.6
44	CX	22	GLY	2.6
13	BM	75	MET	2.6
14	BN	89	MET	2.6
3	BC	176	HIS	2.6
10	BJ	56	HIS	2.6
3	BC	4	LYS	2.6
6	BF	93	LYS	2.6
22	CA	666	A	2.6
22	CA	2725	A	2.6
30	CJ	113	LYS	2.6
48	C1	57	LYS	2.6
3	BC	99	ALA	2.6
3	BC	156	ARG	2.6
4	AD	73	ARG	2.6
4	AD	175	ALA	2.6
6	BF	99	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
8	BH	35	ALA	2.6
8	BH	102	ALA	2.6
10	BJ	62	ARG	2.6
11	BK	47	ALA	2.6
11	BK	127	ARG	2.6
13	BM	5	ALA	2.6
20	AT	7	ALA	2.6
22	CA	585	G	2.6
22	CA	836	G	2.6
22	CA	1093	G	2.6
22	CA	2623	G	2.6
27	CF	43	ALA	2.6
31	CK	87	ALA	2.6
34	CN	128	THR	2.6
38	CR	96	ALA	2.6
46	CZ	16	THR	2.6
14	BN	94	PRO	2.6
24	CC	229	ASP	2.6
29	CH	32	PRO	2.6
2	BB	62	SER	2.6
3	BC	201	TRP	2.6
4	BD	90	LEU	2.6
4	BD	161	LEU	2.6
9	BI	52	LEU	2.6
10	AJ	17	LEU	2.6
11	BK	55	SER	2.6
44	CX	16	SER	2.6
46	CZ	10	SER	2.6
22	CA	665	U	2.6
27	CF	122	PHE	2.5
29	DH	46	PHE	2.5
22	CA	672	C	2.5
22	CA	1030	C	2.5
22	CA	1607	C	2.5
18	BR	54	GLN	2.5
25	CD	36	GLN	2.5
25	CD	150	GLN	2.5
14	AN	26	GLU	2.5
16	BP	45	GLU	2.5
3	AC	162	ILE	2.5
5	AE	18	VAL	2.5
5	AE	74	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
8	BH	101	ILE	2.5
11	AK	20	VAL	2.5
27	CF	136	ILE	2.5
36	CP	39	VAL	2.5
43	CW	63	ILE	2.5
6	BF	59	TYR	2.5
6	BF	9	MET	2.5
8	BH	100	GLY	2.5
8	BH	122	GLY	2.5
9	AI	71	GLY	2.5
9	BI	82	GLY	2.5
14	AN	20	TYR	2.5
18	AR	46	GLY	2.5
29	DH	34	GLY	2.5
31	CK	108	MET	2.5
26	CE	29	HIS	2.5
35	CO	31	HIS	2.5
1	BA	262	A	2.5
2	BB	128	LYS	2.5
4	BD	74	ASN	2.5
7	AG	35	LYS	2.5
22	CA	586	A	2.5
22	CA	2726	A	2.5
26	CE	24	ASN	2.5
26	CE	95	LYS	2.5
26	CE	106	LYS	2.5
30	DJ	81	LYS	2.5
32	CL	67	LYS	2.5
35	CO	78	LYS	2.5
45	DY	77	LYS	2.5
1	BA	134	G	2.5
1	BA	202	G	2.5
7	BG	109	ARG	2.5
20	BT	25	ARG	2.5
22	CA	60	G	2.5
27	CF	167	ARG	2.5
32	CL	64	ARG	2.5
33	CM	126	ARG	2.5
35	CO	118	ARG	2.5
37	CQ	21	ARG	2.5
3	BC	189	ALA	2.5
6	AF	105	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
6	BF	28	ALA	2.5
7	AG	72	THR	2.5
11	BK	30	THR	2.5
29	DH	96	THR	2.5
35	CO	58	ASP	2.5
42	CV	18	ASP	2.5
5	BE	22	SER	2.5
8	BH	93	PRO	2.5
9	AI	125	PRO	2.5
14	BN	25	ALA	2.5
35	CO	41	ALA	2.5
42	DV	51	ALA	2.5
19	BS	38	SER	2.5
22	CA	587	C	2.5
22	CA	1556	C	2.5
4	BD	48	LEU	2.5
8	BH	76	GLN	2.5
9	BI	32	GLN	2.5
15	BO	31	LEU	2.5
27	CF	50	LEU	2.5
29	DH	5	LEU	2.5
46	CZ	31	GLN	2.5
14	BN	39	GLU	2.5
41	CU	18	GLU	2.5
21	AU	12	PHE	2.5
5	BE	64	MET	2.5
30	DJ	36	MET	2.5
2	BB	31	ILE	2.5
2	BB	124	GLY	2.5
2	BB	173	ILE	2.5
3	BC	75	ILE	2.5
3	BC	116	VAL	2.5
6	BF	22	ILE	2.5
9	AI	19	VAL	2.5
11	BK	23	ILE	2.5
25	CD	191	GLY	2.5
26	CE	113	VAL	2.5
27	DF	76	GLY	2.5
29	DH	3	VAL	2.5
32	CL	76	VAL	2.5
34	CN	46	ILE	2.5
34	CN	99	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
37	CQ	81	VAL	2.5
43	CW	64	VAL	2.5
48	C1	25	VAL	2.5
1	BA	1492	A	2.5
16	BP	59	HIS	2.5
2	AB	22	TYR	2.5
6	BF	25	TYR	2.5
22	CA	529	A	2.5
22	CA	781	A	2.5
22	CA	1773	A	2.5
16	BP	80	LYS	2.5
19	AS	6	LYS	2.5
29	DH	25	TYR	2.5
1	BA	1307	U	2.5
7	AG	10	ARG	2.5
9	BI	99	ARG	2.5
9	BI	123	ARG	2.5
10	AJ	89	ARG	2.5
10	BJ	89	ARG	2.5
12	BL	59	ASN	2.5
13	BM	101	ARG	2.5
15	BO	17	ARG	2.5
16	BP	29	ASN	2.5
21	AU	45	ARG	2.5
22	CA	1647	U	2.5
48	C1	50	ARG	2.5
22	CA	379	G	2.5
22	CA	780	G	2.5
22	CA	1573	G	2.5
53	DA	277	G	2.5
8	BH	113	ASP	2.5
10	BJ	85	ASP	2.5
13	BM	58	ASP	2.5
53	DA	1072	C	2.5
53	DA	2161	C	2.5
15	BO	8	THR	2.5
28	CG	34	THR	2.5
2	AB	147	SER	2.5
3	BC	109	PRO	2.5
7	BG	107	ALA	2.5
14	AN	5	SER	2.5
16	BP	44	SER	2.5

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Mol	Chain	Res	Type	RSRZ
17	AQ	82	ALA	2.5
18	BR	58	ALA	2.5
24	CC	35	GLU	2.5
24	DC	236	GLU	2.5
27	CF	172	ALA	2.5
29	CH	56	ALA	2.5
37	CQ	42	ALA	2.5
37	DQ	68	GLU	2.5
37	DQ	102	GLU	2.5
46	CZ	24	GLU	2.5
2	BB	179	LEU	2.5
3	AC	12	LEU	2.5
3	BC	87	LEU	2.5
4	BD	68	LEU	2.5
8	BH	59	LEU	2.5
37	CQ	40	LEU	2.5
2	AB	184	PHE	2.5
3	BC	129	MET	2.5
8	BH	27	MET	2.5
9	AI	57	MET	2.5
22	CA	504	A	2.5
22	CA	1307	A	2.5
37	CQ	31	TRP	2.5
2	AB	131	LYS	2.5
2	BB	71	GLY	2.5
7	BG	8	GLY	2.5
8	BH	108	LYS	2.5
28	CG	91	GLY	2.5
30	CJ	82	LYS	2.5
30	DJ	40	LYS	2.5
34	CN	71	LYS	2.5
34	CN	133	LYS	2.5
38	CR	93	LYS	2.5
39	CS	12	HIS	2.5
49	C2	19	HIS	2.5
53	DA	2402	U	2.5
3	BC	56	VAL	2.5
3	BC	76	VAL	2.5
4	AD	129	VAL	2.5
4	BD	128	ARG	2.5
4	BD	173	VAL	2.5
5	AE	141	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
9	AI	29	VAL	2.5
9	AI	49	ARG	2.5
11	AK	113	VAL	2.5
21	AU	34	ARG	2.5
21	BU	32	VAL	2.5
25	CD	13	ARG	2.5
28	CG	55	ARG	2.5
28	DG	170	ARG	2.5
31	CK	11	VAL	2.5
31	CK	56	VAL	2.5
35	CO	8	ARG	2.5
37	CQ	101	ARG	2.5
46	CZ	52	ARG	2.5
55	DI	56	ARG	2.5
55	DI	61	ARG	2.5
55	DI	94	ARG	2.5
12	BL	117	TYR	2.5
22	CA	55	G	2.5
22	CA	289	G	2.5
22	CA	338	G	2.5
22	CA	356	G	2.5
22	CA	524	G	2.5
22	CA	799	G	2.5
27	DF	143	TYR	2.5
28	CG	94	TYR	2.5
30	CJ	62	TYR	2.5
38	CR	76	TYR	2.5
53	DA	1537	G	2.5
17	BQ	53	CYS	2.5
52	C5	11	CYS	2.5
22	CA	2073	C	2.5
22	CA	2527	C	2.5
8	BH	9	ASP	2.5
5	AE	145	GLU	2.5
7	AG	58	GLU	2.5
7	AG	106	GLU	2.5
14	BN	92	GLU	2.5
24	DC	251	GLN	2.5
52	C5	37	GLN	2.5
5	AE	22	SER	2.5
5	AE	160	SER	2.5
9	BI	96	SER	2.5

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Mol	Chain	Res	Type	RSRZ
15	BO	13	SER	2.5
17	BQ	74	THR	2.5
20	AT	6	SER	2.5
13	BM	36	ALA	2.5
20	AT	63	ALA	2.5
21	BU	15	ALA	2.5
21	BU	41	PRO	2.5
24	DC	31	ALA	2.5
28	CG	54	PRO	2.5
28	CG	154	PRO	2.5
32	CL	11	ALA	2.5
32	CL	46	ALA	2.5
35	CO	88	ALA	2.5
42	DV	64	ALA	2.5
2	AB	179	LEU	2.5
12	BL	102	LEU	2.5
13	AM	34	LEU	2.5
14	BN	51	LEU	2.5
27	CF	57	LEU	2.5
9	BI	88	MET	2.5
1	AA	1016	A	2.5
22	CA	213	A	2.5
22	CA	783	A	2.5
22	CA	1779	U	2.5
53	DA	2131	U	2.5
2	AB	32	PHE	2.5
2	BB	28	LYS	2.5
17	BQ	4	LYS	2.5
19	AS	28	LYS	2.5
25	CD	124	ARG	2.5
27	CF	5	HIS	2.5
27	CF	99	PHE	2.5
27	CF	114	PHE	2.5
43	CW	25	LYS	2.5
35	CO	90	ARG	2.5
36	CP	100	HIS	2.5
44	CX	72	LYS	2.5
46	CZ	4	LYS	2.5
48	C1	32	LYS	2.5
48	D1	57	LYS	2.5
7	BG	92	ARG	2.5
12	BL	83	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
15	BO	89	ARG	2.5
40	CT	8	ARG	2.5
47	C0	11	ARG	2.5
19	AS	8	GLY	2.5
24	CC	215	GLY	2.5
28	CG	57	GLY	2.5
28	CG	135	GLY	2.5
39	CS	17	GLY	2.5
1	BA	201	G	2.5
2	BB	60	ILE	2.5
2	BB	80	VAL	2.4
3	BC	14	ILE	2.5
3	BC	182	ILE	2.5
7	AG	91	VAL	2.4
13	BM	65	VAL	2.4
19	BS	60	VAL	2.4
22	CA	245	G	2.5
22	CA	1296	G	2.5
22	CA	1319	C	2.4
22	CA	1574	C	2.4
27	DF	111	ILE	2.5
29	DH	110	VAL	2.4
30	CJ	33	VAL	2.4
45	CY	40	VAL	2.4
45	DY	64	ILE	2.5
3	BC	41	GLN	2.4
4	BD	35	GLU	2.4
7	BG	58	GLU	2.4
10	AJ	91	ASP	2.4
27	CF	32	GLU	2.4
33	CM	76	GLU	2.4
41	CU	42	GLU	2.4
18	AR	23	TYR	2.4
21	AU	38	TYR	2.4
2	BB	125	THR	2.4
3	AC	192	THR	2.4
5	BE	149	SER	2.4
11	BK	108	THR	2.4
24	DC	259	SER	2.4
25	CD	35	THR	2.4
25	CD	61	THR	2.4
28	CG	129	THR	2.4

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Mol	Chain	Res	Type	RSRZ
30	CJ	71	THR	2.4
31	CK	65	THR	2.4
32	CL	97	THR	2.4
41	CU	22	THR	2.4
2	BB	182	PRO	2.4
7	BG	2	PRO	2.4
19	BS	42	PRO	2.4
43	CW	27	PRO	2.4
1	BA	949	A	2.4
1	BA	1151	A	2.4
2	BB	84	ALA	2.4
9	BI	57	MET	2.4
22	CA	44	A	2.4
22	CA	453	A	2.4
22	CA	626	A	2.4
22	CA	1321	A	2.4
22	CA	1598	A	2.4
29	CH	26	ALA	2.4
30	CJ	17	MET	2.4
31	CK	92	MET	2.4
31	CK	126	ALA	2.4
34	CN	35	ALA	2.4
34	CN	105	MET	2.4
53	DA	846	U	2.4
53	DA	2166	U	2.4
4	BD	159	LEU	2.4
6	AF	106	LYS	2.4
12	BL	108	LYS	2.4
25	CD	56	LYS	2.4
30	CJ	45	LYS	2.4
31	CK	121	LYS	2.4
6	BF	86	ARG	2.4
15	BO	51	HIS	2.4
27	CF	92	ARG	2.4
28	CG	45	HIS	2.4
32	CL	17	ARG	2.4
36	CP	30	ARG	2.4
4	BD	20	PHE	2.4
7	AG	82	GLY	2.4
11	AK	27	PHE	2.4
15	BO	43	PHE	2.4
25	CD	72	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
25	CD	120	GLY	2.4
27	DF	131	GLY	2.4
28	CG	109	PHE	2.4
30	DJ	131	GLY	2.4
42	CV	90	GLY	2.4
54	DD	87	GLY	2.4
1	BA	112	G	2.4
22	CA	68	G	2.4
22	CA	110	G	2.4
22	CA	455	C	2.4
22	CA	549	G	2.4
22	CA	1236	G	2.4
22	CA	1251	C	2.4
22	CA	1643	G	2.4
22	CA	2405	G	2.4
31	CK	67	ASN	2.4
3	BC	57	ILE	2.4
7	AG	9	GLN	2.4
7	BG	106	GLU	2.4
9	AI	97	GLU	2.4
26	CE	115	GLN	2.4
32	DL	110	GLU	2.4
26	CE	169	VAL	2.4
26	CE	176	ASP	2.4
27	CF	13	VAL	2.4
28	DG	121	ILE	2.4
41	DU	91	GLN	2.4
4	BD	170	TRP	2.4
6	AF	60	VAL	2.4
14	AN	33	ASP	2.4
24	CC	66	ASP	2.4
24	CC	84	ASP	2.4
29	DH	21	VAL	2.4
31	CK	60	ASP	2.4
32	CL	85	VAL	2.4
48	C1	30	VAL	2.4
48	D1	55	ILE	2.4
3	AC	184	TYR	2.4
4	BD	103	TYR	2.4
22	CA	1176	U	2.4
22	CA	1624	U	2.4
24	DC	171	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
29	CH	93	SER	2.4
2	BB	220	THR	2.4
13	BM	102	THR	2.4
22	CA	354	A	2.4
22	CA	675	A	2.4
22	CA	804	A	2.4
22	CA	1272	A	2.4
24	CC	140	THR	2.4
48	C1	44	THR	2.4
53	DA	1089	A	2.4
27	CF	65	PRO	2.4
29	DH	1	MET	2.4
55	DI	128	THR	2.4
7	BG	88	PRO	2.4
11	BK	124	PRO	2.4
2	AB	79	ALA	2.4
2	BB	216	ALA	2.4
3	BC	38	LYS	2.4
3	BC	45	LYS	2.4
4	BD	92	ALA	2.4
4	BD	165	ARG	2.4
5	BE	156	LYS	2.4
9	AI	16	ALA	2.4
9	AI	22	LYS	2.4
10	BJ	37	ARG	2.4
13	AM	32	ALA	2.4
14	BN	15	ALA	2.4
14	BN	28	LYS	2.4
15	BO	47	LYS	2.4
15	BO	88	ARG	2.4
18	AR	56	ALA	2.4
21	BU	48	ALA	2.4
24	CC	182	ARG	2.4
24	CC	207	LYS	2.4
25	CD	83	ARG	2.4
26	CE	170	ARG	2.4
27	CF	45	ALA	2.4
27	CF	58	ALA	2.4
28	CG	96	ALA	2.4
29	DH	83	LYS	2.4
31	CK	12	LYS	2.4
33	CM	138	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
34	CN	10	ARG	2.4
36	CP	37	ALA	2.4
36	CP	113	ALA	2.4
43	CW	21	ARG	2.4
43	CW	85	LYS	2.4
44	CX	84	ALA	2.4
55	DI	19	ALA	2.4
55	DI	127	ALA	2.4
11	AK	118	HIS	2.4
13	AM	56	LEU	2.4
13	AM	95	LEU	2.4
13	BM	12	HIS	2.4
18	BR	29	LEU	2.4
26	DE	164	LEU	2.4
28	CG	89	LEU	2.4
29	DH	30	LEU	2.4
32	CL	25	LEU	2.4
39	CS	66	HIS	2.4
1	BA	1533	C	2.4
22	CA	440	C	2.4
22	CA	456	C	2.4
22	CA	1638	C	2.4
1	BA	230	G	2.4
1	BA	1356	G	2.4
2	BB	17	GLY	2.4
9	BI	10	GLY	2.4
22	CA	952	G	2.4
22	CA	974	G	2.4
22	CA	1197	G	2.4
22	CA	1216	G	2.4
22	CA	1560	G	2.4
28	CG	93	GLY	2.4
31	CK	127	GLY	2.4
27	DF	77	PHE	2.4
31	CK	89	PHE	2.4
34	CN	115	GLU	2.4
46	CZ	38	GLN	2.4
2	AB	192	ASP	2.4
13	AM	82	ASP	2.4
14	BN	38	ASP	2.4
28	DG	47	ASP	2.4
29	DH	86	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
5	AE	106	ILE	2.4
5	BE	39	VAL	2.4
8	AH	78	VAL	2.4
10	AJ	53	ILE	2.4
10	AJ	96	VAL	2.4
12	BL	63	VAL	2.4
16	AP	75	ILE	2.4
19	AS	11	ILE	2.4
22	CA	2584	U	2.4
26	CE	121	VAL	2.4
27	DF	89	VAL	2.4
29	CH	99	ILE	2.4
37	CQ	80	VAL	2.4
41	DU	53	VAL	2.4
42	DV	103	ILE	2.4
52	C5	17	VAL	2.4
1	BA	1357	A	2.4
1	BA	1368	A	2.4
22	CA	2706	A	2.4
53	DA	1098	A	2.4
6	BF	88	MET	2.4
8	BH	105	SER	2.4
19	AS	34	TRP	2.4
8	BH	111	MET	2.4
9	BI	46	MET	2.4
25	CD	1	MET	2.4
25	CD	113	SER	2.4
27	DF	129	SER	2.4
34	CN	136	MET	2.4
51	C4	51	SER	2.4
4	AD	151	LYS	2.4
6	BF	2	ARG	2.4
9	BI	60	LYS	2.4
10	AJ	5	ARG	2.4
10	AJ	83	THR	2.4
12	AL	44	LYS	2.4
14	AN	53	ARG	2.4
16	BP	70	ARG	2.4
19	BS	77	THR	2.4
25	CD	70	LYS	2.4
31	CK	5	THR	2.4
31	CK	123	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
32	CL	23	LYS	2.4
34	CN	58	LYS	2.4
27	DF	176	PRO	2.4
31	CK	16	TYR	2.4
41	CU	29	THR	2.4
47	D0	10	THR	2.4
24	CC	107	PRO	2.4
42	DV	55	PRO	2.4
2	AB	176	ALA	2.4
9	AI	101	ALA	2.4
20	AT	45	ALA	2.4
22	CA	268	C	2.4
22	CA	335	C	2.4
22	CA	560	C	2.4
22	CA	982	C	2.4
22	CA	1200	C	2.4
22	CA	1612	C	2.4
22	CA	1822	C	2.4
27	DF	75	ALA	2.4
29	DH	67	ALA	2.4
46	CZ	63	ALA	2.4
55	DI	28	ALA	2.4
4	BD	199	LEU	2.4
7	AG	124	LEU	2.4
10	AJ	87	LEU	2.4
29	CH	54	LEU	2.4
22	CA	438	G	2.4
22	CA	446	G	2.4
22	CA	649	G	2.4
22	CA	775	G	2.4
22	CA	1202	G	2.4
22	CA	1215	G	2.4
22	CA	1331	G	2.4
22	CA	1622	G	2.4
22	CA	1792	G	2.4
24	CC	194	GLU	2.4
46	DZ	59	GLU	2.4
4	BD	164	GLN	2.4
5	BE	78	ASN	2.4
5	BE	148	ASN	2.4
9	AI	70	GLY	2.4
11	BK	109	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
12	BL	29	GLN	2.4
16	BP	63	GLN	2.4
25	CD	94	GLN	2.4
25	CD	173	GLN	2.4
27	CF	41	GLY	2.4
28	CG	78	GLY	2.4
28	CG	82	GLY	2.4
29	DH	95	GLY	2.4
30	CJ	119	GLY	2.4
30	DJ	16	GLY	2.4
30	DJ	19	ASN	2.4
34	CN	29	GLY	2.4
35	CO	101	GLY	2.4
44	CX	28	GLY	2.4
47	C0	26	GLY	2.4
22	CA	441	U	2.4
22	CA	811	U	2.4
11	BK	18	ASP	2.4
40	CT	109	ASP	2.4
5	BE	48	PHE	2.4
11	AK	105	PHE	2.4
29	DH	47	PHE	2.4
38	DR	101	PHE	2.4
22	CA	563	A	2.4
22	CA	1366	A	2.4
2	AB	111	ILE	2.4
2	AB	181	ILE	2.4
2	AB	100	MET	2.4
2	BB	92	VAL	2.4
4	BD	53	VAL	2.4
4	BD	64	ILE	2.4
4	BD	124	MET	2.4
9	AI	116	VAL	2.4
11	AK	84	VAL	2.4
12	BL	33	VAL	2.4
5	BE	52	LYS	2.4
5	BE	126	LYS	2.4
12	BL	50	ARG	2.4
13	AM	25	VAL	2.4
15	BO	12	VAL	2.4
19	BS	62	VAL	2.4
31	CK	62	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
32	CL	95	ILE	2.4
37	CQ	28	VAL	2.4
45	DY	40	VAL	2.4
49	D2	47	VAL	2.4
52	D5	26	ILE	2.4
20	BT	74	ARG	2.4
33	CM	2	ARG	2.4
39	CS	21	ARG	2.4
39	CS	40	MET	2.4
13	BM	76	SER	2.4
25	CD	145	SER	2.4
3	BC	190	HIS	2.4
6	AF	30	THR	2.4
8	BH	12	THR	2.4
31	CK	78	THR	2.4
22	CA	257	C	2.4
22	CA	786	C	2.4
28	CG	12	PRO	2.4
4	BD	76	TYR	2.3
10	AJ	65	TYR	2.3
3	BC	113	ALA	2.3
4	AD	27	ALA	2.3
4	AD	43	ALA	2.3
4	AD	163	GLU	2.3
5	BE	17	ALA	2.3
6	AF	66	ALA	2.3
7	BG	98	ALA	2.3
9	BI	78	ALA	2.3
10	AJ	29	ALA	2.3
11	AK	41	ALA	2.3
19	BS	22	ALA	2.3
22	CA	39	G	2.3
22	CA	205	G	2.3
22	CA	625	G	2.3
22	CA	1179	G	2.3
22	CA	1300	G	2.3
22	CA	1653	G	2.3
22	CA	2228	G	2.3
22	CA	2413	G	2.3
24	CC	123	ALA	2.3
24	DC	166	ALA	2.3
27	DF	32	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
28	DG	173	GLU	2.3
29	CH	59	ALA	2.3
29	CH	74	ALA	2.3
29	DH	84	ALA	2.3
29	DH	102	ALA	2.3
36	CP	23	ALA	2.3
36	CP	46	GLU	2.3
38	CR	118	ALA	2.3
42	DV	101	GLU	2.3
53	DA	2110	G	2.3
2	AB	43	LEU	2.3
2	BB	109	GLN	2.3
5	BE	82	GLN	2.3
9	AI	52	LEU	2.3
9	AI	98	LEU	2.3
9	BI	75	GLN	2.3
10	BJ	20	GLN	2.3
2	BB	58	ASN	2.3
5	AE	19	ASN	2.3
15	BO	20	ASN	2.3
17	BQ	50	ASN	2.3
18	BR	55	LEU	2.3
25	CD	100	LEU	2.3
27	CF	16	LEU	2.3
28	CG	72	LEU	2.3
28	DG	50	LEU	2.3
29	CH	18	GLN	2.3
29	DH	90	LEU	2.3
39	CS	6	GLN	2.3
40	CT	31	GLN	2.3
22	CA	390	U	2.3
22	CA	1406	U	2.3
22	CA	2079	U	2.3
32	CL	88	ASN	2.3
53	DA	34	U	2.3
3	BC	194	GLY	2.3
7	AG	34	GLY	2.3
9	BI	77	GLY	2.3
19	BS	72	GLY	2.3
24	DC	127	GLY	2.3
28	CG	21	GLY	2.3
29	DH	107	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
45	CY	55	GLY	2.3
5	BE	41	ASP	2.3
12	BL	109	ASP	2.3
22	CA	480	A	2.3
22	CA	632	A	2.3
22	CA	1789	A	2.3
6	AF	56	LYS	2.3
7	BG	116	MET	2.3
9	BI	109	ARG	2.3
17	AQ	37	PHE	2.3
18	BR	57	ARG	2.3
19	AS	29	LYS	2.3
19	BS	81	ARG	2.3
25	CD	161	MET	2.3
28	DG	177	LYS	2.3
44	CX	68	LYS	2.3
45	CY	45	ARG	2.3
45	CY	72	ARG	2.3
47	C0	30	ARG	2.3
47	C0	54	MET	2.3
2	AB	40	ILE	2.3
2	BB	200	ILE	2.3
24	CC	74	ILE	2.3
27	DF	154	ILE	2.3
38	CR	87	SER	2.3
39	CS	98	ILE	2.3
38	CR	110	VAL	2.3
39	CS	102	SER	2.3
43	DW	70	ILE	2.3
6	BF	84	VAL	2.3
16	BP	78	VAL	2.3
25	CD	73	VAL	2.3
26	CE	14	VAL	2.3
26	DE	4	VAL	2.3
27	DF	149	VAL	2.3
22	CA	106	C	2.3
22	CA	281	C	2.3
22	CA	795	C	2.3
22	CA	1625	C	2.3
22	CA	1774	C	2.3
22	CA	1790	C	2.3
29	DH	128	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
6	BF	76	THR	2.3
11	BK	111	THR	2.3
21	BU	2	PRO	2.3
24	DC	140	THR	2.3
27	CF	158	THR	2.3
30	CJ	20	PRO	2.3
32	CL	42	THR	2.3
1	AA	5	U	2.3
1	BA	5	U	2.3
1	BA	104	G	2.3
1	BA	133	U	2.3
1	BA	260	G	2.3
22	CA	17	G	2.3
22	CA	51	G	2.3
22	CA	824	U	2.3
22	CA	1224	U	2.3
22	CA	1245	G	2.3
22	CA	1311	G	2.3
22	CA	2622	U	2.3
22	CA	2680	U	2.3
44	DX	85	GLU	2.3
53	DA	2423	U	2.3
55	DI	107	GLU	2.3
22	CA	2693	G	2.3
28	DG	116	GLN	2.3
4	BD	135	TYR	2.3
5	BE	128	TYR	2.3
7	BG	147	ALA	2.3
9	AI	44	ALA	2.3
13	AM	23	TYR	2.3
15	AO	76	ALA	2.3
18	BR	23	TYR	2.3
32	CL	13	ASN	2.3
42	DV	53	ASN	2.3
1	BA	223	A	2.3
4	AD	21	LEU	2.3
7	BG	99	LEU	2.3
8	BH	82	GLY	2.3
15	AO	81	LEU	2.3
16	AP	74	LEU	2.3
22	CA	56	A	2.3
22	CA	800	A	2.3

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Mol	Chain	Res	Type	RSRZ
22	CA	943	A	2.3
22	CA	1655	A	2.3
22	CA	1791	A	2.3
22	CA	2358	A	2.3
28	CG	53	GLY	2.3
28	CG	71	LEU	2.3
29	CH	58	LEU	2.3
29	CH	107	GLY	2.3
39	CS	67	GLY	2.3
41	DU	93	LEU	2.3
27	DF	113	ASP	2.3
28	DG	166	ASP	2.3
2	BB	225	ARG	2.3
15	AO	72	ARG	2.3
2	AB	174	LYS	2.3
2	BB	45	LYS	2.3
7	BG	56	LYS	2.3
12	BL	43	LYS	2.3
27	CF	17	MET	2.3
46	CZ	9	LYS	2.3
46	DZ	2	LYS	2.3
47	C0	21	LYS	2.3
22	CA	557	C	2.3
22	CA	823	C	2.3
22	CA	1536	C	2.3
34	CN	130	PHE	2.3
45	DY	46	PHE	2.3
3	BC	53	SER	2.3
7	BG	54	SER	2.3
14	BN	58	SER	2.3
26	CE	15	SER	2.3
35	CO	119	SER	2.3
46	DZ	10	SER	2.3
2	AB	15	HIS	2.3
2	BB	94	HIS	2.3
1	BA	1122	U	2.3
5	BE	141	ILE	2.3
6	BF	29	ILE	2.3
10	BJ	15	HIS	2.3
11	AK	110	ILE	2.3
24	CC	243	HIS	2.3
35	CO	16	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
4	BD	155	VAL	2.3
12	AL	4	VAL	2.3
13	AM	65	VAL	2.3
16	AP	47	GLU	2.3
21	AU	32	VAL	2.3
22	CA	193	U	2.3
37	CQ	26	VAL	2.3
44	CX	83	GLU	2.3
46	CZ	59	GLU	2.3
1	BA	844	G	2.3
1	BA	1253	G	2.3
2	AB	193	PRO	2.3
2	AB	227	GLN	2.3
5	BE	84	PRO	2.3
7	BG	52	GLN	2.3
8	BH	4	GLN	2.3
10	AJ	20	GLN	2.3
10	AJ	32	THR	2.3
10	AJ	39	PRO	2.3
10	AJ	99	GLN	2.3
12	BL	35	THR	2.3
17	AQ	70	THR	2.3
21	BU	42	THR	2.3
22	CA	248	G	2.3
22	CA	452	G	2.3
22	CA	778	G	2.3
22	CA	1091	G	2.3
22	CA	1190	G	2.3
22	CA	1381	G	2.3
22	CA	1659	G	2.3
28	CG	122	THR	2.3
31	CK	70	THR	2.3
31	CK	137	PRO	2.3
46	DZ	16	THR	2.3
48	D1	26	THR	2.3
53	DA	1091	G	2.3
53	DA	2116	G	2.3
1	BA	1363	A	2.3
22	CA	439	A	2.3
22	CA	833	A	2.3
22	CA	1133	A	2.3
22	CA	1679	A	2.3

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Mol	Chain	Res	Type	RSRZ
22	CA	2872	A	2.3
27	CF	23	ASN	2.3
29	CH	66	ASN	2.3
53	DA	144	A	2.3
3	BC	95	ALA	2.3
4	BD	80	ALA	2.3
5	BE	125	ALA	2.3
5	BE	127	ALA	2.3
11	AK	73	ALA	2.3
13	AM	18	ALA	2.3
18	BR	27	ALA	2.3
21	BU	50	ALA	2.3
29	CH	65	ALA	2.3
46	DZ	61	ALA	2.3
2	AB	101	LEU	2.3
2	AB	114	LEU	2.3
2	AB	205	ASP	2.3
2	BB	114	LEU	2.3
3	BC	169	ARG	2.3
6	AF	39	LEU	2.3
10	AJ	90	LEU	2.3
13	BM	79	ARG	2.3
14	BN	33	ASP	2.3
17	BQ	77	ARG	2.3
18	AR	68	LEU	2.3
24	CC	63	ARG	2.3
25	CD	153	GLY	2.3
29	CH	95	GLY	2.3
29	CH	122	LEU	2.3
30	CJ	32	GLY	2.3
34	CN	38	ARG	2.3
37	CQ	90	GLY	2.3
40	CT	88	ARG	2.3
5	BE	14	LYS	2.3
8	BH	22	LYS	2.3
8	BH	87	LYS	2.3
30	CJ	100	LYS	2.3
1	BA	1397	C	2.3
22	CA	837	C	2.3
1	AA	1017	U	2.3
1	BA	261	U	2.3
22	CA	2713	U	2.3

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Mol	Chain	Res	Type	RSRZ
2	BB	39	HIS	2.3
6	AF	37	HIS	2.3
15	BO	42	HIS	2.3
19	BS	69	HIS	2.3
25	CD	30	GLU	2.3
32	CL	110	GLU	2.3
34	CN	28	PHE	2.3
34	CN	111	GLU	2.3
37	CQ	19	SER	2.3
55	DI	16	SER	2.3
2	AB	90	PHE	2.3
7	AG	42	ILE	2.3
9	BI	50	GLN	2.3
9	BI	126	GLN	2.3
10	AJ	25	ILE	2.3
10	BJ	35	GLN	2.3
14	BN	4	GLN	2.3
22	CA	48	G	2.3
22	CA	380	G	2.3
22	CA	669	G	2.3
22	CA	940	G	2.3
22	CA	1346	G	2.3
22	CA	1374	G	2.3
22	CA	2697	G	2.3
24	CC	116	ILE	2.3
33	CM	90	VAL	2.3
39	CS	4	VAL	2.3
46	DZ	11	VAL	2.3
22	CA	429	A	2.3
22	CA	616	A	2.3
24	CC	136	PRO	2.3
26	CE	189	THR	2.3
27	DF	155	THR	2.3
29	CH	77	THR	2.3
34	CN	7	THR	2.3
36	CP	31	THR	2.3
24	CC	134	ASN	2.3
6	BF	24	ARG	2.3
10	AJ	72	ARG	2.3
13	AM	3	ARG	2.3
17	BQ	6	ARG	2.3
31	DK	96	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
43	CW	79	ARG	2.3
45	DY	37	ARG	2.3
2	AB	8	ASP	2.3
3	BC	104	ALA	2.3
4	BD	114	ALA	2.3
15	AO	9	ALA	2.3
20	BT	34	LYS	2.3
20	BT	46	ALA	2.3
26	CE	11	ALA	2.3
27	DF	107	ALA	2.3
26	CE	64	GLY	2.3
28	CG	176	LYS	2.3
34	CN	5	LYS	2.3
34	CN	100	LYS	2.3
35	DO	117	ASP	2.3
36	CP	66	GLY	2.3
36	CP	68	LYS	2.3
37	DQ	111	LYS	2.3
44	CX	15	ASP	2.3
4	BD	108	GLY	2.3
12	AL	92	GLY	2.3
19	AS	26	GLY	2.3
20	BT	42	GLY	2.3
24	CC	169	GLY	2.3
24	CC	196	GLY	2.3
47	C0	6	LYS	2.3
55	DI	97	LYS	2.3
2	BB	54	LEU	2.3
5	AE	124	LEU	2.3
12	BL	90	LEU	2.3
31	CK	36	LEU	2.3
3	AC	193	TYR	2.3
11	AK	77	TYR	2.3
12	BL	38	TYR	2.3
18	BR	70	TYR	2.3
1	AA	4	U	2.3
2	AB	96	TRP	2.3
22	CA	16	C	2.3
22	CA	264	C	2.3
22	CA	1092	C	2.3
22	CA	1278	C	2.3
22	CA	1804	C	2.3

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Mol	Chain	Res	Type	RSRZ
22	CA	2326	C	2.3
30	CJ	123	GLU	2.2
31	CK	132	HIS	2.2
33	CM	144	GLU	2.2
3	BC	100	GLN	2.2
10	BJ	99	GLN	2.2
13	BM	49	SER	2.2
14	AN	58	SER	2.2
29	DH	113	SER	2.2
34	CN	27	SER	2.2
40	CT	53	SER	2.2
40	CT	108	SER	2.2
1	AA	86	G	2.2
1	BA	1361	G	2.2
22	CA	2732	G	2.2
22	CA	2816	G	2.2
53	DA	1056	G	2.2
53	DA	1071	G	2.2
3	BC	203	PHE	2.2
22	CA	127	A	2.2
4	BD	200	ILE	2.2
9	AI	83	ILE	2.2
11	BK	31	ILE	2.2
19	AS	49	ILE	2.2
26	CE	148	ILE	2.2
4	BD	61	VAL	2.2
13	AM	28	THR	2.2
19	AS	79	THR	2.2
25	CD	121	THR	2.2
26	CE	4	VAL	2.2
27	CF	89	VAL	2.2
28	CG	126	PRO	2.2
39	CS	32	THR	2.2
39	CS	99	THR	2.2
2	AB	178	ASN	2.2
3	AC	107	ARG	2.2
3	BC	25	ASN	2.2
9	AI	122	ARG	2.2
11	BK	128	ARG	2.2
13	AM	92	ARG	2.2
13	BM	70	ARG	2.2
18	AR	57	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
24	CC	69	ARG	2.2
26	CE	117	ARG	2.2
28	DG	101	ASN	2.2
29	CH	73	ASN	2.2
29	CH	145	ASN	2.2
7	AG	131	LYS	2.2
10	AJ	82	LYS	2.2
13	AM	27	LYS	2.2
17	BQ	81	LYS	2.2
19	BS	18	LYS	2.2
24	CC	36	LYS	2.2
41	CU	26	LYS	2.2
8	AH	54	ASP	2.2
26	CE	91	ASP	2.2
1	BA	620	C	2.2
4	BD	109	ALA	2.2
5	BE	28	GLY	2.2
8	BH	123	GLY	2.2
10	AJ	21	ALA	2.2
10	AJ	23	ALA	2.2
11	BK	41	ALA	2.2
22	CA	236	C	2.2
22	CA	1326	U	2.2
22	CA	1777	U	2.2
27	CF	126	GLY	2.2
29	CH	102	ALA	2.2
33	CM	130	GLY	2.2
38	DR	118	ALA	2.2
39	CS	42	ALA	2.2
7	AG	47	LEU	2.2
14	AN	46	LEU	2.2
27	DF	170	LEU	2.2
10	BJ	81	GLU	2.2
15	AO	69	TYR	2.2
26	CE	16	GLU	2.2
12	BL	6	GLN	2.2
1	BA	1491	G	2.2
22	CA	326	G	2.2
22	CA	458	G	2.2
22	CA	776	G	2.2
22	CA	794	A	2.2
22	CA	1360	G	2.2

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Mol	Chain	Res	Type	RSRZ
22	CA	1555	G	2.2
22	CA	1637	A	2.2
22	CA	1799	G	2.2
22	CA	2227	A	2.2
53	DA	1087	G	2.2
7	BG	3	ARG	2.2
8	BH	84	ARG	2.2
11	BK	93	ARG	2.2
11	BK	105	PHE	2.2
44	CX	77	ARG	2.2
55	DI	53	ARG	2.2
2	AB	210	VAL	2.2
2	BB	37	LYS	2.2
13	AM	8	ASN	2.2
17	AQ	7	THR	2.2
21	AU	43	THR	2.2
17	AQ	22	VAL	2.2
19	BS	70	LYS	2.2
20	AT	57	ILE	2.2
13	AM	60	VAL	2.2
24	CC	75	PRO	2.2
24	DC	37	ASN	2.2
28	DG	48	ASN	2.2
29	DH	71	LYS	2.2
29	DH	79	THR	2.2
30	CJ	95	LYS	2.2
30	DJ	94	ASN	2.2
32	CL	51	LYS	2.2
33	CM	135	ILE	2.2
34	CN	132	THR	2.2
38	CR	98	ILE	2.2
39	CS	19	THR	2.2
40	CT	72	THR	2.2
3	BC	151	VAL	2.2
4	BD	143	VAL	2.2
5	AE	38	VAL	2.2
11	BK	74	VAL	2.2
32	CL	52	VAL	2.2
33	CM	127	VAL	2.2
41	CU	88	LYS	2.2
49	D2	53	LYS	2.2
22	CA	92	U	2.2

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Mol	Chain	Res	Type	RSRZ
22	CA	499	U	2.2
22	CA	2240	U	2.2
53	DA	1173	U	2.2
1	BA	183	C	2.2
1	BA	312	C	2.2
1	BA	328	C	2.2
10	BJ	19	ASP	2.2
11	BK	85	MET	2.2
22	CA	1172	C	2.2
22	CA	2830	C	2.2
27	CF	26	MET	2.2
53	DA	1178	C	2.2
11	BK	43	GLY	2.2
24	CC	193	GLY	2.2
24	DC	73	GLY	2.2
29	DH	92	GLY	2.2
30	CJ	85	GLY	2.2
3	BC	50	ALA	2.2
5	BE	113	ALA	2.2
7	AG	152	ALA	2.2
9	AI	42	GLU	2.2
12	BL	101	ALA	2.2
13	BM	47	GLU	2.2
14	BN	88	ALA	2.2
21	BU	36	GLU	2.2
24	DC	190	ALA	2.2
27	CF	165	GLU	2.2
28	CG	65	ALA	2.2
30	CJ	104	ALA	2.2
40	CT	64	ALA	2.2
41	DU	25	GLU	2.2
45	CY	21	ALA	2.2
45	DY	76	GLU	2.2
2	AB	117	LEU	2.2
4	BD	55	LEU	2.2
9	AI	87	LEU	2.2
33	DM	92	LEU	2.2
45	DY	68	LEU	2.2
10	BJ	64	GLN	2.2
34	CN	97	GLN	2.2
22	CA	1373	A	2.2
22	CA	1634	A	2.2

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Mol	Chain	Res	Type	RSRZ
22	CA	1829	A	2.2
22	CA	2705	A	2.2
53	DA	2887[A]	A	2.2
1	BA	105	G	2.2
2	AB	5	SER	2.2
7	BG	125	SER	2.2
13	BM	21	SER	2.2
22	CA	107	G	2.2
22	CA	250	G	2.2
22	CA	1137	G	2.2
22	CA	1171	G	2.2
22	CA	1266	G	2.2
22	CA	1364	G	2.2
22	CA	2686	G	2.2
45	DY	78	TYR	2.2
29	DH	93	SER	2.2
48	D1	27	SER	2.2
4	AD	170	TRP	2.2
10	AJ	16	ARG	2.2
12	BL	114	ARG	2.2
14	AN	13	ARG	2.2
24	CC	101	ARG	2.2
34	CN	59	ARG	2.2
38	DR	11	ARG	2.2
1	AA	1030	U	2.2
3	BC	150	LYS	2.2
15	BO	73	LYS	2.2
20	BT	44	LYS	2.2
21	AU	49	LYS	2.2
22	CA	100	U	2.2
22	CA	827	U	2.2
40	CT	27	LYS	2.2
45	CY	44	LYS	2.2
21	BU	9	ASN	2.2
25	CD	32	ASN	2.2
2	AB	198	PHE	2.2
2	AB	220	THR	2.2
10	BJ	13	PHE	2.2
2	AB	9	MET	2.2
11	BK	116	ILE	2.2
12	BL	42	PRO	2.2
22	CA	336	C	2.2

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Mol	Chain	Res	Type	RSRZ
24	DC	131	PRO	2.2
27	CF	139	PRO	2.2
30	DJ	46	THR	2.2
53	DA	1102	C	2.2
4	AD	50	ASP	2.2
14	AN	38	ASP	2.2
14	BN	18	ASP	2.2
17	BQ	15	ASP	2.2
19	BS	40	ILE	2.2
25	CD	18	ASP	2.2
31	CK	71	ASP	2.2
43	CW	90	ASP	2.2
9	AI	67	VAL	2.2
21	BU	3	VAL	2.2
27	CF	149	VAL	2.2
28	CG	140	VAL	2.2
4	AD	16	GLY	2.2
4	BD	202	GLU	2.2
5	BE	13	GLU	2.2
7	BG	40	GLU	2.2
8	BH	43	GLU	2.2
8	BH	53	GLY	2.2
21	AU	44	GLU	2.2
26	CE	144	GLU	2.2
3	AC	61	ALA	2.2
5	BE	58	ALA	2.2
5	BE	59	ALA	2.2
7	BG	108	ALA	2.2
10	AJ	86	ALA	2.2
17	BQ	24	ALA	2.2
20	AT	46	ALA	2.2
24	DC	92	ALA	2.2
28	CG	119	ALA	2.2
28	DG	13	ALA	2.2
29	CH	128	HIS	2.2
32	CL	93	GLN	2.2
33	CM	137	ALA	2.2
36	CP	59	ALA	2.2
1	BA	306	A	2.2
1	BA	325	A	2.2
1	BA	946	A	2.2
22	CA	428	A	2.2

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Mol	Chain	Res	Type	RSRZ
22	CA	1439	A	2.2
22	CA	1597	A	2.2
22	CA	1616	A	2.2
36	CP	29	HIS	2.2
44	CX	46	HIS	2.2
49	C2	46	HIS	2.2
9	AI	94	LEU	2.2
18	AR	29	LEU	2.2
19	AS	47	LEU	2.2
24	DC	130	LEU	2.2
1	BA	203	G	2.2
1	BA	1305	G	2.2
22	CA	86	G	2.2
22	CA	388	G	2.2
22	CA	411	G	2.2
22	CA	442	G	2.2
22	CA	729	G	2.2
22	CA	942	G	2.2
22	CA	1031	G	2.2
53	DA	2885[A]	G	2.2
3	BC	35	SER	2.2
3	BC	143	ARG	2.2
7	BG	53	ARG	2.2
14	BN	37	SER	2.2
15	AO	88	ARG	2.2
15	BO	63	ARG	2.2
19	AS	32	ARG	2.2
21	BU	34	ARG	2.2
38	CR	58	ARG	2.2
39	CS	15	SER	2.2
42	CV	86	ARG	2.2
1	BA	1049	U	2.2
22	CA	90	U	2.2
15	BO	69	TYR	2.2
36	CP	64	TYR	2.2
12	BL	111	LYS	2.2
14	BN	23	LYS	2.2
24	CC	108	LYS	2.2
25	CD	55	LYS	2.2
29	DH	112	LYS	2.2
43	CW	68	LYS	2.2
1	BA	175	C	2.2

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Mol	Chain	Res	Type	RSRZ
1	BA	1243	C	2.2
2	AB	24	ASN	2.2
22	CA	968	C	2.2
25	CD	58	ASN	2.2
7	BG	101	MET	2.2
25	CD	165	MET	2.2
28	CG	62	TRP	2.2
28	CG	75	MET	2.2
45	DY	39	TRP	2.2
5	BE	90	THR	2.2
9	AI	51	PRO	2.1
11	BK	117	PRO	2.1
24	CC	129	THR	2.2
24	CC	131	PRO	2.1
27	CF	18	THR	2.2
33	CM	5	THR	2.2
35	CO	72	ASP	2.2
37	DQ	104	THR	2.2
49	D2	22	THR	2.2
4	AD	123	ILE	2.1
7	AG	139	GLU	2.1
11	AK	97	ILE	2.1
27	DF	177	PHE	2.1
29	DH	29	PHE	2.1
39	CS	46	GLU	2.1
43	CW	4	ILE	2.1
55	DI	70	GLU	2.1
5	AE	88	VAL	2.1
5	AE	123	VAL	2.1
7	AG	75	VAL	2.1
8	AH	39	VAL	2.1
12	AL	33	VAL	2.1
14	BN	11	VAL	2.1
36	CP	78	VAL	2.1
13	AM	94	GLY	2.1
22	CA	28	A	2.1
22	CA	979	A	2.1
22	CA	1274	A	2.1
22	CA	1821	A	2.1
22	CA	2820	A	2.1
22	CA	2829	A	2.1
30	CJ	29	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
30	DJ	91	GLY	2.1
32	CL	15	GLY	2.1
32	CL	36	GLY	2.1
41	DU	90	GLY	2.1
43	CW	87	GLN	2.1
44	CX	73	GLY	2.1
47	C0	28	GLY	2.1
55	DI	78	GLY	2.1
2	AB	61	ALA	2.1
6	BF	66	ALA	2.1
7	AG	61	ALA	2.1
20	BT	81	ALA	2.1
24	CC	122	ALA	2.1
32	CL	119	ALA	2.1
1	AA	1286	U	2.1
1	BA	942	G	2.1
2	BB	7	ARG	2.1
2	BB	10	LEU	2.1
3	AC	136	ARG	2.1
4	BD	82	LEU	2.1
9	AI	12	ARG	2.1
10	AJ	9	ARG	2.1
22	CA	75	G	2.1
22	CA	234	U	2.1
22	CA	425	G	2.1
22	CA	467	G	2.1
22	CA	1368	G	2.1
22	CA	1568	G	2.1
22	CA	1975	G	2.1
22	CA	2223	G	2.1
17	AQ	8	LEU	2.1
17	AQ	11	ARG	2.1
27	CF	133	ARG	2.1
28	CG	152	ARG	2.1
29	DH	123	ARG	2.1
46	CZ	7	ARG	2.1
6	BF	87	SER	2.1
13	AM	30	SER	2.1
24	CC	118	SER	2.1
27	DF	118	SER	2.1
35	DO	119	SER	2.1
41	CU	21	SER	2.1

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Mol	Chain	Res	Type	RSRZ
50	C3	8	SER	2.1
2	AB	64	LYS	2.1
7	AG	11	LYS	2.1
8	BH	50	LYS	2.1
22	CA	1295	C	2.1
22	CA	1305	C	2.1
22	CA	2442	C	2.1
22	CA	2699	C	2.1
2	BB	154	MET	2.1
4	BD	65	TYR	2.1
7	AG	44	TYR	2.1
14	BN	62	ASN	2.1
25	CD	45	TYR	2.1
29	DH	145	ASN	2.1
33	CM	93	ASN	2.1
7	BG	63	GLU	2.1
14	AN	18	ASP	2.1
30	DJ	116	ASP	2.1
52	C5	20	ASP	2.1
2	BB	29	PRO	2.1
5	BE	57	PRO	2.1
17	AQ	41	THR	2.1
34	CN	74	THR	2.1
22	CA	91	A	2.1
22	CA	430	A	2.1
4	BD	72	PHE	2.1
4	BD	123	ILE	2.1
7	BG	29	ILE	2.1
26	CE	195	GLN	2.1
31	CK	86	GLN	2.1
2	AB	168	HIS	2.1
2	BB	107	VAL	2.1
6	AF	10	VAL	2.1
7	BG	19	GLY	2.1
9	AI	10	GLY	2.1
14	AN	14	VAL	2.1
16	AP	78	VAL	2.1
17	BQ	12	VAL	2.1
24	CC	149	GLY	2.1
28	DG	57	GLY	2.1
30	CJ	16	GLY	2.1
34	DN	80	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
48	C1	35	GLY	2.1
22	CA	1798	U	2.1
2	AB	74	ARG	2.1
2	AB	139	ARG	2.1
9	AI	124	ARG	2.1
15	BO	54	ARG	2.1
21	BU	35	ARG	2.1
22	CA	98	G	2.1
22	CA	512	G	2.1
22	CA	2027	G	2.1
22	CA	2357	G	2.1
22	CA	2363	G	2.1
2	AB	185	ALA	2.1
2	AB	206	ALA	2.1
3	BC	71	ALA	2.1
9	AI	17	ALA	2.1
16	AP	58	ALA	2.1
29	DH	140	ALA	2.1
5	AE	156	LYS	2.1
1	BA	1320	C	2.1
2	BB	86	SER	2.1
7	BG	37	SER	2.1
13	BM	46	SER	2.1
15	BO	70	LEU	2.1
27	DF	152	LEU	2.1
28	CG	177	LYS	2.1
29	CH	22	LYS	2.1
36	CP	85	LYS	2.1
19	AS	38	SER	2.1
41	DU	50	LEU	2.1
22	CA	47	C	2.1
22	CA	426	C	2.1
22	CA	1314	C	2.1
22	CA	1454	C	2.1
22	CA	1646	C	2.1
22	CA	2275	C	2.1
32	CL	21	CYS	2.1
53	DA	1092	C	2.1
4	BD	140	ASN	2.1
6	BF	21	MET	2.1
10	BJ	58	ASN	2.1
10	BJ	66	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
11	BK	81	ASN	2.1
11	BK	83	GLU	2.1
15	BO	26	GLU	2.1
33	DM	106	GLU	2.1
2	BB	88	ASP	2.1
3	BC	181	ASP	2.1
13	AM	86	TYR	2.1
16	AP	17	TYR	2.1
22	CA	42	A	2.1
22	CA	443	A	2.1
22	CA	945	A	2.1
22	CA	1029	A	2.1
22	CA	2860	A	2.1
24	DC	161	TYR	2.1
39	CS	2	TYR	2.1
1	BA	610	U	2.1
2	AB	189	THR	2.1
2	BB	89	GLN	2.1
2	BB	201	PRO	2.1
5	AE	97	GLN	2.1
8	AH	55	THR	2.1
10	AJ	22	THR	2.1
25	CD	49	GLN	2.1
22	CA	67	U	2.1
25	CD	67	HIS	2.1
2	AB	124	GLY	2.1
2	BB	99	GLY	2.1
3	BC	11	ARG	2.1
4	BD	24	GLY	2.1
4	BD	106	GLY	2.1
5	BE	69	ARG	2.1
6	BF	44	ARG	2.1
7	AG	112	GLY	2.1
9	BI	106	ARG	2.1
10	AJ	38	GLY	2.1
13	AM	93	ARG	2.1
14	BN	13	ARG	2.1
14	BN	72	GLY	2.1
16	BP	14	ARG	2.1
18	BR	44	ILE	2.1
24	DC	270	ARG	2.1
25	CD	179	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
29	CH	34	GLY	2.1
30	CJ	89	GLY	2.1
31	CK	66	GLY	2.1
33	CM	123	ARG	2.1
37	CQ	51	ARG	2.1
55	DI	125	ARG	2.1
16	AP	16	PHE	2.1
5	AE	94	VAL	2.1
22	CA	363	G	2.1
22	CA	474	G	2.1
22	CA	695	G	2.1
22	CA	785	G	2.1
22	CA	1661	G	2.1
22	CA	2035	G	2.1
27	CF	12	VAL	2.1
53	DA	2120	G	2.1
6	BF	53	LYS	2.1
7	AG	110	LYS	2.1
16	AP	76	LYS	2.1
25	CD	159	LYS	2.1
27	CF	3	LYS	2.1
27	CF	9	LYS	2.1
35	CO	56	LYS	2.1
43	CW	83	LYS	2.1
2	BB	76	ALA	2.1
3	BC	146	ALA	2.1
7	BG	24	ALA	2.1
11	AK	21	ALA	2.1
16	AP	81	ALA	2.1
20	AT	11	ALA	2.1
22	CA	179	C	2.1
22	CA	673	C	2.1
22	CA	951	C	2.1
22	CA	1611	C	2.1
22	CA	1806	C	2.1
27	DF	45	ALA	2.1
32	CL	60	ALA	2.1
49	C2	15	ALA	2.1
53	DA	1100	C	2.1
2	BB	101	LEU	2.1
12	BL	49	LEU	2.1
44	CX	35	SER	2.1

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Mol	Chain	Res	Type	RSRZ
45	DY	42	SER	2.1
4	AD	160	GLU	2.1
6	AF	102	MET	2.1
10	AJ	24	GLU	2.1
14	BN	6	MET	2.1
17	AQ	26	GLU	2.1
26	CE	100	MET	2.1
41	CU	24	MET	2.1
12	BL	46	ASN	2.1
37	CQ	3	ASN	2.1
42	CV	53	ASN	2.1
44	CX	12	ASN	2.1
2	AB	167	ASP	2.1
2	BB	8	ASP	2.1
22	CA	575	A	2.1
22	CA	1359	A	2.1
22	CA	1427	A	2.1
22	CA	1652	A	2.1
22	CA	2062	A	2.1
22	CA	2432	A	2.1
26	CE	22	ASP	2.1
34	CN	106	ASP	2.1
53	DA	1103	A	2.1
20	BT	48	GLN	2.1
22	CA	427	U	2.1
22	CA	1198	U	2.1
22	CA	1294	U	2.1
22	CA	1379	U	2.1
3	BC	40	ARG	2.1
3	BC	126	ARG	2.1
7	BG	16	PRO	2.1
8	BH	77	ARG	2.1
9	AI	84	THR	2.1
12	BL	121	ARG	2.1
13	AM	87	ARG	2.1
14	AN	59	ARG	2.1
18	BR	41	PRO	2.1
18	BR	74	HIS	2.1
27	CF	68	THR	2.1
28	CG	163	ARG	2.1
29	CH	104	THR	2.1
31	CK	88	THR	2.1

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Mol	Chain	Res	Type	RSRZ
37	CQ	113	ARG	2.1
43	CW	80	HIS	2.1
48	C1	52	ARG	2.1
1	BA	242	G	2.1
4	BD	96	GLY	2.1
4	BD	176	GLY	2.1
6	BF	20	GLY	2.1
7	BG	82	GLY	2.1
9	AI	40	GLY	2.1
11	BK	104	GLY	2.1
12	BL	85	GLY	2.1
22	CA	54	G	2.1
22	CA	124	G	2.1
22	CA	189	G	2.1
22	CA	469	G	2.1
22	CA	491	G	2.1
22	CA	500	G	2.1
22	CA	1358	G	2.1
22	CA	2201	G	2.1
22	CA	2624	G	2.1
22	CA	2894	G	2.1
24	DC	254	GLY	2.1
27	DF	41	GLY	2.1
30	DJ	99	GLY	2.1
31	CK	26	GLY	2.1
37	DQ	105	GLY	2.1
38	CR	82	GLY	2.1
1	BA	210	C	2.1
1	BA	330	C	2.1
1	BA	379	C	2.1
1	BA	1322	C	2.1
2	AB	59	LYS	2.1
6	AF	36	ILE	2.1
7	BG	131	LYS	2.1
8	AH	125	ILE	2.1
8	BH	69	LYS	2.1
10	AJ	30	LYS	2.1
12	BL	120	LYS	2.1
14	AN	82	ILE	2.1
15	BO	48	LYS	2.1
18	AR	26	ILE	2.1
2	AB	80	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
4	AD	182	PHE	2.1
22	CA	806	C	2.1
22	CA	838	C	2.1
22	CA	1656	C	2.1
22	CA	1752	C	2.1
22	CA	2066	C	2.1
22	CA	2078	C	2.1
22	CA	2874	C	2.1
26	CE	123	LYS	2.1
27	CF	60	ILE	2.1
27	DF	120	LYS	2.1
28	DG	24	ILE	2.1
29	DH	41	LYS	2.1
41	DU	68	LYS	2.1
27	DF	138	PHE	2.1
53	DA	145	C	2.1
4	BD	201	VAL	2.1
5	AE	137	VAL	2.1
11	BK	32	VAL	2.1
16	BP	71	VAL	2.1
17	AQ	13	VAL	2.1
19	AS	67	VAL	2.1
29	DH	9	VAL	2.1
2	BB	55	ALA	2.1
4	AD	88	GLU	2.0
9	AI	73	SER	2.1
14	AN	80	SER	2.1
15	AO	7	ALA	2.1
16	BP	68	SER	2.1
11	AK	85	MET	2.0
20	AT	54	MET	2.0
24	CC	82	GLU	2.0
29	CH	63	ALA	2.1
29	DH	49	ALA	2.1
29	DH	59	ALA	2.1
32	CL	121	GLU	2.0
4	BD	171	LEU	2.0
11	BK	42	LEU	2.0
19	AS	15	LEU	2.0
1	BA	1150	A	2.0
7	BG	68	ASN	2.0
22	CA	256	A	2.0

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Mol	Chain	Res	Type	RSRZ
22	CA	546	U	2.0
22	CA	573	U	2.0
22	CA	615	U	2.0
22	CA	1785	A	2.0
22	CA	1819	A	2.0
22	CA	2679	A	2.0
53	DA	547	A	2.0
53	DA	892	A	2.0
4	BD	40	GLN	2.0
14	AN	4	GLN	2.0
15	BO	40	GLN	2.0
24	DC	121	ASP	2.0
30	CJ	107	GLN	2.0
42	DV	89	ASP	2.0
4	AD	47	ARG	2.0
19	BS	55	ARG	2.0
21	BU	21	ARG	2.0
34	CN	50	ARG	2.0
44	DX	41[A]	ARG	2.0
44	DX	55	ARG	2.0
15	BO	46	HIS	2.0
1	AA	1018	G	2.0
1	BA	232	G	2.0
1	BA	799	G	2.0
1	BA	945	G	2.0
4	AD	169	THR	2.0
5	AE	103	THR	2.0
6	BF	67	PRO	2.0
12	BL	41	THR	2.0
13	BM	55	THR	2.0
22	CA	30	G	2.0
22	CA	537	G	2.0
22	CA	1356	G	2.0
22	CA	1645	G	2.0
22	CA	2061	G	2.0
22	CA	2692	G	2.0
22	CA	2822	G	2.0
26	CE	129	PRO	2.0
35	CO	37	THR	2.0
35	CO	57	THR	2.0
53	DA	2115	G	2.0
1	BA	95	C	2.0

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Mol	Chain	Res	Type	RSRZ
1	BA	1209	C	2.0
2	BB	152	LYS	2.0
6	AF	104	LYS	2.0
11	BK	14	LYS	2.0
17	BQ	71	LYS	2.0
22	CA	66	C	2.0
22	CA	228	C	2.0
22	CA	1306	C	2.0
24	CC	150	LYS	2.0
34	CN	86	LYS	2.0
51	D4	52	LYS	2.0
11	BK	88	GLY	2.0
25	CD	3	GLY	2.0
30	CJ	137	GLY	2.0
34	CN	37	GLY	2.0
9	AI	79	ILE	2.0
24	DC	267	ILE	2.0
2	BB	142	GLU	2.0
4	AD	142	VAL	2.0
4	AD	147	GLU	2.0
9	AI	103	PHE	2.0
9	BI	92	GLU	2.0
12	AL	61	PHE	2.0
15	BO	75	VAL	2.0
16	AP	71	VAL	2.0
24	DC	77	VAL	2.0
25	CD	90	PHE	2.0
27	DF	40	VAL	2.0
29	CH	61	VAL	2.0
35	CO	114	GLU	2.0
45	DY	7	VAL	2.0
46	DZ	17	GLU	2.0
47	D0	58	GLU	2.0
55	DI	98	GLU	2.0
1	BA	619	U	2.0
2	BB	100	MET	2.0
9	AI	46	MET	2.0
12	BL	47	SER	2.0
17	BQ	14	SER	2.0
22	CA	235	U	2.0
22	CA	846	U	2.0
26	CE	125	SER	2.0

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Mol	Chain	Res	Type	RSRZ
30	CJ	88	SER	2.0
53	DA	2111	U	2.0
54	DD	1	MET	2.0
22	CA	190	A	2.0
22	CA	457	A	2.0
22	CA	633	A	2.0
22	CA	1090	A	2.0
22	CA	1535	A	2.0
22	CA	1596	A	2.0
22	CA	1803	A	2.0
4	BD	43	ALA	2.0
4	BD	79	ALA	2.0
7	AG	147	ALA	2.0
7	AG	150	ALA	2.0
13	AM	61	ALA	2.0
34	CN	64	TRP	2.0
36	DP	37	ALA	2.0
36	DP	50	ALA	2.0
36	DP	57	ALA	2.0
38	CR	116	ALA	2.0
15	BO	37	ASN	2.0
35	CO	81	ASN	2.0
47	C0	49	ASN	2.0
2	AB	212	LEU	2.0
4	AD	82	LEU	2.0
15	BO	35	GLN	2.0
20	BT	82	GLN	2.0
26	CE	5	LEU	2.0
32	CL	58	LEU	2.0
42	DV	54	GLN	2.0
24	CC	72	ASP	2.0
24	CC	187	ASP	2.0
24	DC	168	ASP	2.0
30	DJ	64	ASP	2.0
39	CS	95	ASP	2.0
45	CY	65	ASP	2.0
9	AI	11	ARG	2.0
14	BN	24	ARG	2.0
20	BT	60	ARG	2.0
27	DF	133	ARG	2.0
35	CO	30	ARG	2.0
52	D5	12	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
3	BC	6	HIS	2.0
24	CC	25	HIS	2.0
1	BA	212	G	2.0
1	BA	1302	C	2.0
2	AB	28	LYS	2.0
2	BB	59	LYS	2.0
7	AG	36	LYS	2.0
8	BH	33	LYS	2.0
13	AM	44	LYS	2.0
22	CA	31	C	2.0
22	CA	302	C	2.0
22	CA	394	C	2.0
22	CA	600	G	2.0
22	CA	623	C	2.0
22	CA	628	G	2.0
22	CA	681	G	2.0
22	CA	796	C	2.0
22	CA	964	C	2.0
22	CA	1320	C	2.0
22	CA	2047	C	2.0
22	CA	2523	G	2.0
24	DC	111	LYS	2.0
25	CD	106	LYS	2.0
43	CW	34	LYS	2.0
47	D0	3[A]	LYS	2.0
5	BE	133	PRO	2.0
7	AG	71	PRO	2.0
9	BI	51	PRO	2.0
11	AK	91	PRO	2.0
12	AL	3	THR	2.0
27	DF	68	THR	2.0
28	CG	67	THR	2.0
28	CG	118	PRO	2.0
36	CP	65	THR	2.0
4	AD	127	GLY	2.0
10	BJ	33	GLY	2.0
11	BK	51	GLY	2.0
17	BQ	56	GLY	2.0
18	BR	37	GLY	2.0
47	D0	15	GLY	2.0
55	DI	21	GLY	2.0
22	CA	82	U	2.0

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Mol	Chain	Res	Type	RSRZ
22	CA	437	U	2.0
27	CF	7	TYR	2.0
27	DF	7	TYR	2.0
53	DA	2172	U	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	2MG	BA	1207	24/25	0.73	0.15	122,126,131,131	0
22	3TD	CA	1915	21/22	0.75	0.12	109,112,115,116	0
22	PSU	CA	1917	20/21	0.75	0.11	102,107,110,112	0
1	2MG	BA	966	24/25	0.76	0.15	128,136,145,147	0
22	2MA	CA	2503	23/24	0.77	0.21	87,90,92,94	0
22	PSU	CA	1911	20/21	0.79	0.10	103,108,113,116	0
22	PSU	CA	746	20/21	0.82	0.17	88,91,95,95	0
22	6MZ	CA	2030	23/24	0.83	0.20	93,99,101,102	0
22	6MZ	CA	1618	23/24	0.84	0.15	91,97,99,100	0
22	PSU	CA	955	20/21	0.85	0.17	100,105,109,110	0
1	5MC	BA	967	21/22	0.86	0.12	127,132,143,145	0
1	5MC	BA	1407	21/22	0.86	0.15	86,91,95,96	0
22	PSU	CA	2457	20/21	0.87	0.14	91,97,101,102	0
1	G7M	BA	527	24/25	0.87	0.15	63,71,78,84	0
22	1MG	CA	745	24/25	0.88	0.16	85,88,93,95	0
22	PSU	CA	2580	20/21	0.89	0.12	83,88,90,92	0
34	4D4	CN	81	12/13	0.89	0.18	94,97,99,100	0
53	3TD	DA	1915	21/22	0.89	0.09	76,81,87,94	0
1	2MG	BA	1516	24/25	0.90	0.14	67,74,79,83	0
1	MA6	BA	1518	24/25	0.90	0.14	68,73,78,85	0
22	PSU	CA	2504	20/21	0.90	0.14	83,87,90,91	0
1	PSU	BA	516	20/21	0.90	0.11	73,79,89,91	0
22	PSU	CA	2605	20/21	0.90	0.14	71,79,82,83	0
22	2MG	CA	1835	24/25	0.90	0.15	74,82,84,86	0
22	G7M	CA	2069	24/25	0.90	0.17	88,94,96,100	0
53	PSU	DA	1917	20/21	0.90	0.09	63,72,79,84	0
1	2MG	AA	1207	24/25	0.91	0.12	89,94,98,100	0
22	5MC	CA	1962	21/22	0.91	0.13	73,78,80,83	0
1	UR3	BA	1498	21/22	0.91	0.13	69,76,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	5MU	CA	747	21/22	0.91	0.14	82,91,96,97	0
22	OMG	CA	2251	24/25	0.91	0.17	85,92,95,98	0
1	MA6	BA	1519	24/25	0.91	0.15	67,73,79,81	0
22	OMC	CA	2498	21/22	0.91	0.18	90,97,99,102	0
22	OMU	CA	2552	21/22	0.92	0.15	80,85,87,87	0
22	2MG	CA	2445	24/25	0.92	0.14	88,92,96,99	0
1	4OC	BA	1402	22/23	0.92	0.14	82,86,90,90	0
1	2MG	AA	966	24/25	0.92	0.13	69,75,80,83	0
12	D2T	BL	89	10/11	0.92	0.13	64,74,78,93	0
22	5MU	CA	1939	21/22	0.92	0.13	70,78,83,83	0
1	PSU	AA	516	20/21	0.93	0.09	68,75,81,81	0
53	PSU	DA	1911	20/21	0.93	0.08	69,74,80,80	0
1	G7M	AA	527	24/25	0.94	0.11	64,66,70,75	0
54	MEQ	DD	150[A]	10/11	0.94	0.10	23,32,39,40	10
54	MEQ	DD	150[B]	10/11	0.94	0.10	28,32,38,39	10
1	5MC	AA	967	21/22	0.95	0.10	70,76,83,84	0
12	D2T	AL	89	10/11	0.95	0.10	59,65,70,77	0
53	2MG	DA	1835	24/25	0.96	0.09	45,50,57,57	0
53	5MC	DA	1962	21/22	0.96	0.10	38,48,55,59	0
53	PSU	DA	2604	20/21	0.96	0.08	33,44,54,57	0
1	UR3	AA	1498	21/22	0.96	0.09	50,58,65,69	0
1	MA6	AA	1519	24/25	0.96	0.10	51,56,63,67	0
34	4D4	DN	81[A]	12/13	0.96	0.09	33,38,42,43	9
34	4D4	DN	81[B]	12/13	0.96	0.09	33,36,40,41	9
1	MA6	AA	1518	24/25	0.97	0.08	45,54,59,64	0
1	5MC	AA	1407	21/22	0.97	0.07	51,59,62,63	0
53	1MG	DA	745	24/25	0.97	0.07	25,34,41,44	0
53	6MZ	DA	2030	23/24	0.97	0.07	22,30,36,42	0
53	2MA	DA	2503	23/24	0.97	0.07	21,37,44,48	0
53	OMU	DA	2552	21/22	0.97	0.09	35,42,46,49	0
53	PSU	DA	2580	20/21	0.97	0.07	27,32,38,42	0
53	PSU	DA	746	20/21	0.97	0.07	28,37,43,44	0
53	5MU	DA	747	21/22	0.97	0.07	27,36,43,46	0
53	6MZ	DA	1618	23/24	0.97	0.07	29,36,44,47	0
1	4OC	AA	1402	22/23	0.97	0.08	59,62,68,70	0
1	2MG	AA	1516	24/25	0.97	0.07	47,53,60,67	0
53	PSU	DA	955	20/21	0.98	0.05	28,33,40,40	0
53	PSU	DA	2504	20/21	0.98	0.05	28,36,44,45	0
53	5MU	DA	1939	21/22	0.98	0.07	36,42,45,50	0
53	G7M	DA	2069	24/25	0.98	0.06	34,38,43,43	0
53	OMG	DA	2251	24/25	0.98	0.06	23,34,41,43	0
53	PSU	DA	2605	20/21	0.98	0.06	38,45,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	2MG	DA	2445	24/25	0.98	0.06	23,32,38,40	0
53	H2U	DA	2449	20/21	0.98	0.06	26,32,38,42	0
53	PSU	DA	2457	20/21	0.98	0.05	31,36,43,45	0
53	OMC	DA	2498	21/22	0.98	0.06	28,33,38,40	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3036	1/1	0.45	0.24	94,94,94,94	0
56	MG	CA	3073	1/1	0.54	0.19	93,93,93,93	0
56	MG	CA	3074	1/1	0.54	0.24	91,91,91,91	0
56	MG	CA	3145	1/1	0.54	0.15	90,90,90,90	0
56	MG	CA	3093	1/1	0.58	0.20	91,91,91,91	0
58	MPD	DE	301	8/8	0.59	0.25	57,67,76,80	0
56	MG	CA	3059	1/1	0.62	0.24	91,91,91,91	0
66	EDO	DB	211	4/4	0.62	0.24	68,70,71,73	0
56	MG	CA	3006	1/1	0.63	0.26	100,100,100,100	0
56	MG	CA	3155	1/1	0.63	0.21	93,93,93,93	0
56	MG	CA	3079	1/1	0.66	0.22	94,94,94,94	0
56	MG	CA	3146	1/1	0.67	0.29	60,60,60,60	1
56	MG	CA	3062	1/1	0.67	0.20	90,90,90,90	0
56	MG	CA	3122	1/1	0.68	0.17	85,85,85,85	0
56	MG	AA	1628	1/1	0.69	0.17	80,80,80,80	0
56	MG	CA	3083	1/1	0.69	0.16	93,93,93,93	0
56	MG	CA	3153	1/1	0.69	0.17	86,86,86,86	0
56	MG	CA	3121	1/1	0.70	0.18	86,86,86,86	0
56	MG	DA	3109	1/1	0.70	0.26	88,88,88,88	0
56	MG	CA	3035	1/1	0.71	0.20	81,81,81,81	0
59	PUT	AA	1675	6/6	0.71	0.22	65,66,71,72	0
56	MG	CA	3075	1/1	0.71	0.15	92,92,92,92	0
56	MG	AA	1610	1/1	0.72	0.28	85,85,85,85	0
56	MG	CA	3030	1/1	0.72	0.14	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3131	1/1	0.73	0.25	79,79,79,79	0
56	MG	CA	3086	1/1	0.73	0.18	78,78,78,78	0
56	MG	CA	3031	1/1	0.73	0.22	90,90,90,90	0
56	MG	CA	3096	1/1	0.74	0.16	92,92,92,92	0
56	MG	CA	3070	1/1	0.74	0.14	90,90,90,90	0
56	MG	BA	1609	1/1	0.74	0.25	89,89,89,89	0
58	MPD	DA	3205	8/8	0.75	0.19	58,63,68,70	0
56	MG	CA	3089	1/1	0.75	0.17	80,80,80,80	0
56	MG	CA	3112	1/1	0.75	0.30	81,81,81,81	0
56	MG	DA	3137	1/1	0.75	0.43	56,56,56,56	1
56	MG	CA	3154	1/1	0.76	0.16	90,90,90,90	0
56	MG	CA	3080	1/1	0.77	0.17	88,88,88,88	0
58	MPD	DT	201	8/8	0.77	0.30	55,63,66,73	0
56	MG	BA	1639	1/1	0.77	0.18	78,78,78,78	0
65	ACY	DA	3196	4/4	0.77	0.25	59,65,67,71	0
56	MG	BA	1640	1/1	0.77	0.19	79,79,79,79	0
58	MPD	DK	201	8/8	0.78	0.21	60,66,71,73	0
56	MG	DA	3128	1/1	0.78	0.29	74,74,74,74	0
56	MG	CA	3037	1/1	0.78	0.17	102,102,102,102	0
61	PEG	DQ	201	7/7	0.78	0.17	63,70,74,76	0
56	MG	AA	1617	1/1	0.78	0.15	82,82,82,82	0
56	MG	BA	1601	1/1	0.78	0.18	78,78,78,78	0
68	TRS	DA	3221	8/8	0.78	0.20	65,69,75,77	0
56	MG	BA	1627	1/1	0.79	0.20	83,83,83,83	0
56	MG	CA	3140	1/1	0.79	0.19	76,76,76,76	0
67	GUN	DA	3212	11/11	0.79	0.16	52,58,63,69	0
56	MG	DA	3182	1/1	0.79	0.29	86,86,86,86	0
56	MG	DA	3181	1/1	0.80	0.18	79,79,79,79	0
56	MG	AA	1654	1/1	0.80	0.27	91,91,91,91	0
59	PUT	DA	3195	6/6	0.80	0.20	39,46,50,57	0
56	MG	DB	206	1/1	0.80	0.20	82,82,82,82	0
62	SPD	DA	3207	10/10	0.80	0.28	57,63,68,70	0
56	MG	BA	1637	1/1	0.80	0.20	80,80,80,80	0
56	MG	AA	1664	1/1	0.80	0.13	78,78,78,78	0
58	MPD	DE	302	8/8	0.80	0.27	60,65,67,67	0
56	MG	DA	3177	1/1	0.80	0.24	75,75,75,75	0
56	MG	C3	101	1/1	0.81	0.14	97,97,97,97	0
56	MG	DA	3041	1/1	0.81	0.16	50,50,50,50	0
56	MG	CA	3123	1/1	0.81	0.11	75,75,75,75	0
58	MPD	DA	3208	8/8	0.81	0.19	56,62,70,74	0
56	MG	CA	3018	1/1	0.81	0.15	79,79,79,79	0
56	MG	CA	3084	1/1	0.81	0.15	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1623	1/1	0.81	0.18	71,71,71,71	0
56	MG	CB	202	1/1	0.81	0.12	86,86,86,86	0
56	MG	BA	1631	1/1	0.82	0.16	76,76,76,76	0
59	PUT	AA	1674	6/6	0.82	0.18	61,62,67,69	0
56	MG	DA	3118	1/1	0.82	0.27	79,79,79,79	0
56	MG	DA	3119	1/1	0.82	0.25	66,66,66,66	0
60	ZN	AB	301	1/1	0.82	0.23	140,140,140,140	0
56	MG	CA	3090	1/1	0.82	0.14	80,80,80,80	0
56	MG	DA	3129	1/1	0.82	0.14	70,70,70,70	0
64	PGE	D1	102	10/10	0.82	0.21	61,66,71,74	0
56	MG	DA	3132	1/1	0.82	0.18	71,71,71,71	0
56	MG	CA	3116	1/1	0.82	0.32	75,75,75,75	0
56	MG	CA	3025	1/1	0.82	0.23	92,92,92,92	0
58	MPD	DN	201	8/8	0.82	0.17	57,63,66,71	0
56	MG	AA	1603	1/1	0.83	0.18	82,82,82,82	0
56	MG	CA	3124	1/1	0.83	0.17	87,87,87,87	0
56	MG	DA	3141	1/1	0.83	0.22	73,73,73,73	0
56	MG	DA	3168	1/1	0.83	0.14	77,77,77,77	0
56	MG	DA	3171	1/1	0.83	0.21	76,76,76,76	0
56	MG	CA	3019	1/1	0.83	0.14	81,81,81,81	0
59	PUT	DA	3223	6/6	0.83	0.21	46,49,51,53	0
56	MG	CA	3133	1/1	0.83	0.16	75,75,75,75	0
56	MG	CA	3020	1/1	0.83	0.29	83,83,83,83	0
56	MG	AA	1658	1/1	0.83	0.13	70,70,70,70	0
58	MPD	DA	3192	8/8	0.83	0.23	56,60,64,66	0
56	MG	BA	1641	1/1	0.83	0.17	86,86,86,86	0
56	MG	CA	3002	1/1	0.83	0.30	91,91,91,91	0
56	MG	AA	1661	1/1	0.83	0.14	79,79,79,79	0
56	MG	DA	3130	1/1	0.83	0.26	77,77,77,77	0
56	MG	BA	1632	1/1	0.84	0.20	68,68,68,68	0
56	MG	CA	3021	1/1	0.84	0.24	93,93,93,93	0
56	MG	CA	3129	1/1	0.84	0.25	84,84,84,84	0
56	MG	CA	3066	1/1	0.84	0.23	85,85,85,85	0
58	MPD	DT	202	8/8	0.84	0.29	65,66,75,75	0
56	MG	DA	3003	1/1	0.84	0.12	75,75,75,75	0
56	MG	CA	3109	1/1	0.84	0.21	72,72,72,72	0
56	MG	DA	3179	1/1	0.84	0.12	76,76,76,76	0
56	MG	CA	3137	1/1	0.84	0.16	78,78,78,78	0
56	MG	AA	1613	1/1	0.84	0.27	80,80,80,80	0
56	MG	DB	205	1/1	0.84	0.16	74,74,74,74	0
56	MG	CA	3072	1/1	0.84	0.16	92,92,92,92	0
58	MPD	DA	3190	8/8	0.84	0.18	55,64,69,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3122	1/1	0.84	0.27	77,77,77,77	0
56	MG	AA	1609	1/1	0.84	0.30	79,79,79,79	0
56	MG	CA	3147	1/1	0.84	0.21	55,55,55,55	1
56	MG	CA	3058	1/1	0.84	0.16	76,76,76,76	0
56	MG	BA	1605	1/1	0.85	0.14	81,81,81,81	0
56	MG	CA	3135	1/1	0.85	0.20	83,83,83,83	0
56	MG	AA	1606	1/1	0.85	0.27	83,83,83,83	0
56	MG	DA	3138	1/1	0.85	0.16	60,60,60,60	0
56	MG	CA	3138	1/1	0.85	0.13	80,80,80,80	0
56	MG	DA	3163	1/1	0.85	0.14	73,73,73,73	0
56	MG	AA	1627	1/1	0.85	0.24	80,80,80,80	0
56	MG	CA	3144	1/1	0.85	0.26	73,73,73,73	0
56	MG	DA	3175	1/1	0.85	0.19	72,72,72,72	0
56	MG	CA	3034	1/1	0.85	0.11	82,82,82,82	0
56	MG	CA	3063	1/1	0.85	0.23	93,93,93,93	0
59	PUT	DA	3206	6/6	0.85	0.21	58,61,62,63	0
59	PUT	DA	3222	6/6	0.85	0.20	62,64,65,68	0
56	MG	DA	3121	1/1	0.85	0.27	85,85,85,85	0
56	MG	AA	1608	1/1	0.85	0.26	76,76,76,76	0
61	PEG	DA	3200	7/7	0.85	0.19	52,54,67,67	0
56	MG	DA	3125	1/1	0.85	0.29	69,69,69,69	0
56	MG	DA	3126	1/1	0.85	0.25	75,75,75,75	0
56	MG	DB	207	1/1	0.85	0.19	75,75,75,75	0
57	PG4	BA	1642	13/13	0.85	0.15	52,61,66,69	0
57	PG4	DR	202	13/13	0.85	0.17	47,56,62,65	0
56	MG	CA	3098	1/1	0.85	0.11	89,89,89,89	0
56	MG	AA	1619	1/1	0.85	0.14	81,81,81,81	0
56	MG	DA	3169	1/1	0.86	0.23	77,77,77,77	0
58	MPD	AA	1671	8/8	0.86	0.18	63,65,70,73	0
56	MG	CA	3060	1/1	0.86	0.21	93,93,93,93	0
56	MG	CA	3118	1/1	0.86	0.17	87,87,87,87	0
56	MG	DA	3115	1/1	0.86	0.13	56,56,56,56	0
56	MG	AA	1602	1/1	0.86	0.15	79,79,79,79	0
61	PEG	DA	3199	7/7	0.86	0.18	49,56,67,67	0
56	MG	AA	1663	1/1	0.86	0.13	79,79,79,79	0
61	PEG	DA	3219	7/7	0.86	0.24	61,66,70,73	0
61	PEG	DA	3227	7/7	0.86	0.22	57,59,71,73	0
61	PEG	DP	201	7/7	0.86	0.14	61,65,67,67	0
56	MG	AA	1615	1/1	0.86	0.18	74,74,74,74	0
56	MG	CA	3087	1/1	0.86	0.13	83,83,83,83	0
56	MG	DA	3146	1/1	0.86	0.13	77,77,77,77	0
56	MG	CA	3125	1/1	0.86	0.15	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DB	208	1/1	0.86	0.24	79,79,79,79	0
66	EDO	D0	101	4/4	0.86	0.23	61,63,66,68	0
59	PUT	AA	1672	6/6	0.86	0.20	63,63,66,70	0
56	MG	AA	1601	1/1	0.86	0.25	66,66,66,66	0
56	MG	DA	3133	1/1	0.87	0.17	67,67,67,67	0
56	MG	CA	3141	1/1	0.87	0.21	77,77,77,77	0
56	MG	DA	3042	1/1	0.87	0.09	75,75,75,75	0
56	MG	CA	3014	1/1	0.87	0.11	78,78,78,78	0
56	MG	DA	3144	1/1	0.87	0.11	69,69,69,69	0
56	MG	CA	3071	1/1	0.87	0.22	95,95,95,95	0
56	MG	DA	3161	1/1	0.87	0.16	71,71,71,71	0
56	MG	CA	3111	1/1	0.87	0.18	77,77,77,77	0
56	MG	CA	3130	1/1	0.87	0.13	78,78,78,78	0
56	MG	CA	3150	1/1	0.87	0.23	85,85,85,85	0
56	MG	BA	1617	1/1	0.87	0.11	82,82,82,82	0
56	MG	DA	3173	1/1	0.87	0.22	77,77,77,77	0
56	MG	AA	1644	1/1	0.87	0.11	76,76,76,76	0
56	MG	CA	3061	1/1	0.87	0.14	86,86,86,86	0
64	PGE	D3	101	10/10	0.87	0.18	58,65,67,68	0
56	MG	BA	1633	1/1	0.87	0.25	85,85,85,85	0
66	EDO	DB	210	4/4	0.87	0.22	65,67,68,69	0
56	MG	BA	1636	1/1	0.87	0.25	83,83,83,83	0
56	MG	BA	1630	1/1	0.87	0.10	98,98,98,98	0
59	PUT	AA	1673	6/6	0.87	0.16	63,64,68,69	0
56	MG	DA	3008	1/1	0.87	0.14	55,55,55,55	0
56	MG	CA	3047	1/1	0.88	0.10	77,77,77,77	0
56	MG	DA	3035	1/1	0.88	0.17	38,38,38,38	0
56	MG	CA	3119	1/1	0.88	0.08	83,83,83,83	0
56	MG	CA	3120	1/1	0.88	0.21	74,74,74,74	0
59	PUT	DA	3213	6/6	0.88	0.18	49,55,55,58	0
56	MG	DA	3140	1/1	0.88	0.16	65,65,65,65	0
56	MG	BA	1620	1/1	0.88	0.11	78,78,78,78	0
56	MG	BA	1625	1/1	0.88	0.17	89,89,89,89	0
56	MG	AA	1616	1/1	0.88	0.42	83,83,83,83	0
56	MG	DA	3152	1/1	0.88	0.33	65,65,65,65	0
61	PEG	DA	3201	7/7	0.88	0.19	53,56,63,66	0
58	MPD	AA	1676	8/8	0.88	0.20	60,66,72,76	0
56	MG	BA	1638	1/1	0.88	0.17	75,75,75,75	0
56	MG	DA	3162	1/1	0.88	0.13	69,69,69,69	0
56	MG	CA	3076	1/1	0.88	0.18	83,83,83,83	0
56	MG	AA	1625	1/1	0.88	0.18	70,70,70,70	0
56	MG	AA	1651	1/1	0.88	0.11	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3170	1/1	0.88	0.15	66,66,66,66	0
56	MG	AA	1621	1/1	0.88	0.28	79,79,79,79	0
66	EDO	DA	3209	4/4	0.88	0.28	55,59,62,67	0
56	MG	DA	3172	1/1	0.88	0.19	73,73,73,73	0
56	MG	CA	3045	1/1	0.88	0.10	80,80,80,80	0
56	MG	CA	3115	1/1	0.88	0.28	73,73,73,73	0
56	MG	CA	3085	1/1	0.88	0.12	78,78,78,78	0
56	MG	DA	3131	1/1	0.88	0.19	70,70,70,70	0
56	MG	CA	3055	1/1	0.89	0.20	78,78,78,78	0
59	PUT	DA	3189	6/6	0.89	0.16	44,48,51,54	0
56	MG	DA	3147	1/1	0.89	0.29	73,73,73,73	0
56	MG	DA	3149	1/1	0.89	0.10	62,62,62,62	0
56	MG	AA	1612	1/1	0.89	0.18	70,70,70,70	0
56	MG	DA	3153	1/1	0.89	0.19	67,67,67,67	0
57	PG4	DA	3193	13/13	0.89	0.18	52,56,66,66	0
57	PG4	DA	3217	13/13	0.89	0.15	57,66,72,75	0
61	PEG	AL	201	7/7	0.89	0.12	57,64,71,73	0
57	PG4	DQ	202	13/13	0.89	0.13	50,58,66,66	0
56	MG	DA	3160	1/1	0.89	0.23	71,71,71,71	0
56	MG	CA	3097	1/1	0.89	0.10	83,83,83,83	0
56	MG	CA	3126	1/1	0.89	0.23	74,74,74,74	0
56	MG	CA	3127	1/1	0.89	0.14	84,84,84,84	0
56	MG	CA	3128	1/1	0.89	0.27	82,82,82,82	0
56	MG	DA	3016	1/1	0.89	0.14	63,63,63,63	0
61	PEG	D3	102	7/7	0.89	0.19	50,54,70,71	0
56	MG	BA	1611	1/1	0.89	0.12	64,64,64,64	0
56	MG	CA	3024	1/1	0.89	0.17	75,75,75,75	0
56	MG	AA	1620	1/1	0.89	0.19	72,72,72,72	0
56	MG	DA	3065	1/1	0.89	0.11	70,70,70,70	0
56	MG	CA	3148	1/1	0.89	0.19	73,73,73,73	0
56	MG	CA	3051	1/1	0.89	0.10	71,71,71,71	0
56	MG	CA	3151	1/1	0.89	0.10	82,82,82,82	0
66	EDO	DB	212	4/4	0.89	0.23	59,60,64,64	0
66	EDO	DR	203	4/4	0.89	0.26	53,54,57,60	0
56	MG	DA	3180	1/1	0.89	0.22	78,78,78,78	0
56	MG	DA	3143	1/1	0.89	0.14	77,77,77,77	0
56	MG	CA	3134	1/1	0.89	0.15	79,79,79,79	0
56	MG	AA	1626	1/1	0.90	0.15	84,84,84,84	0
56	MG	CA	3007	1/1	0.90	0.16	82,82,82,82	0
56	MG	DA	3145	1/1	0.90	0.11	69,69,69,69	0
56	MG	DA	3174	1/1	0.90	0.13	77,77,77,77	0
56	MG	DA	3021	1/1	0.90	0.09	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3127	1/1	0.90	0.34	65,65,65,65	0
56	MG	DA	3178	1/1	0.90	0.12	79,79,79,79	0
58	MPD	DA	3211	8/8	0.90	0.17	54,57,64,66	0
56	MG	CA	3038	1/1	0.90	0.18	78,78,78,78	0
56	MG	CA	3039	1/1	0.90	0.10	81,81,81,81	0
56	MG	CA	3081	1/1	0.90	0.09	83,83,83,83	0
56	MG	DA	3156	1/1	0.90	0.30	74,74,74,74	0
56	MG	DA	3158	1/1	0.90	0.11	63,63,63,63	0
64	PGE	DA	3226	10/10	0.90	0.18	59,63,67,69	0
64	PGE	DU	101	10/10	0.90	0.14	44,60,69,71	0
56	MG	CA	3010	1/1	0.90	0.10	77,77,77,77	0
56	MG	DA	3103	1/1	0.90	0.12	44,44,44,44	0
56	MG	BA	1623	1/1	0.90	0.25	86,86,86,86	0
56	MG	DB	209	1/1	0.90	0.17	69,69,69,69	0
57	PG4	AA	1670	13/13	0.90	0.14	52,62,68,68	0
59	PUT	DA	3188	6/6	0.90	0.12	32,39,44,48	0
56	MG	AA	1624	1/1	0.90	0.18	80,80,80,80	0
56	MG	CA	3033	1/1	0.90	0.19	90,90,90,90	0
56	MG	AA	1605	1/1	0.90	0.35	76,76,76,76	0
56	MG	AA	1630	1/1	0.90	0.16	86,86,86,86	0
59	PUT	DA	3214	6/6	0.90	0.21	49,52,56,57	0
56	MG	CA	3026	1/1	0.91	0.08	75,75,75,75	0
56	MG	CA	3041	1/1	0.91	0.09	72,72,72,72	0
56	MG	CA	3149	1/1	0.91	0.12	69,69,69,69	0
59	PUT	DA	3184	6/6	0.91	0.17	45,52,53,56	0
56	MG	CA	3068	1/1	0.91	0.10	85,85,85,85	0
56	MG	CA	3029	1/1	0.91	0.08	79,79,79,79	0
56	MG	CA	3046	1/1	0.91	0.20	85,85,85,85	0
56	MG	CA	3091	1/1	0.91	0.20	77,77,77,77	0
56	MG	CA	3092	1/1	0.91	0.10	83,83,83,83	0
56	MG	AA	1669	1/1	0.91	0.18	76,76,76,76	0
59	PUT	DA	3220	6/6	0.91	0.19	56,58,62,67	0
56	MG	CA	3048	1/1	0.91	0.09	74,74,74,74	0
56	MG	AA	1642	1/1	0.91	0.17	88,88,88,88	0
56	MG	DA	3005	1/1	0.91	0.10	72,72,72,72	0
56	MG	CA	3052	1/1	0.91	0.10	79,79,79,79	0
56	MG	CA	3103	1/1	0.91	0.14	86,86,86,86	0
56	MG	CA	3104	1/1	0.91	0.24	83,83,83,83	0
56	MG	DA	3028	1/1	0.91	0.08	49,49,49,49	0
56	MG	AA	1614	1/1	0.91	0.20	75,75,75,75	0
56	MG	CA	3001	1/1	0.91	0.10	80,80,80,80	0
61	PEG	DL	201	7/7	0.91	0.12	55,58,62,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	1632	1/1	0.91	0.10	79,79,79,79	0
56	MG	CA	3113	1/1	0.91	0.16	63,63,63,63	0
56	MG	DA	3151	1/1	0.91	0.26	80,80,80,80	0
62	SPD	DA	3183	10/10	0.91	0.12	42,51,57,57	0
56	MG	DA	3070	1/1	0.91	0.10	52,52,52,52	0
63	1PE	DA	3185	16/16	0.91	0.15	39,51,68,74	0
64	PGE	DA	3204	10/10	0.91	0.16	53,61,69,70	0
64	PGE	DA	3215	10/10	0.91	0.15	56,62,66,70	0
64	PGE	DA	3218	10/10	0.91	0.13	50,55,64,68	0
56	MG	DA	3072	1/1	0.91	0.10	53,53,53,53	0
64	PGE	DS	201	10/10	0.91	0.13	50,56,66,68	0
56	MG	DA	3085	1/1	0.91	0.10	44,44,44,44	0
56	MG	DA	3087	1/1	0.91	0.10	31,31,31,31	0
56	MG	DA	3092	1/1	0.91	0.11	39,39,39,39	0
56	MG	DA	3097	1/1	0.91	0.10	37,37,37,37	0
65	ACY	DA	3202	4/4	0.91	0.20	53,59,61,64	0
56	MG	CA	3139	1/1	0.91	0.15	71,71,71,71	0
66	EDO	DA	3216	4/4	0.91	0.17	60,61,62,67	0
56	MG	CA	3005	1/1	0.91	0.10	96,96,96,96	0
56	MG	DA	3165	1/1	0.91	0.28	70,70,70,70	0
56	MG	DA	3167	1/1	0.91	0.17	64,64,64,64	0
56	MG	CA	3082	1/1	0.91	0.12	79,79,79,79	0
56	MG	CA	3117	1/1	0.91	0.27	79,79,79,79	0
56	MG	AA	1641	1/1	0.91	0.10	71,71,71,71	0
56	MG	BA	1613	1/1	0.91	0.08	65,65,65,65	0
56	MG	CA	3078	1/1	0.92	0.16	85,85,85,85	0
56	MG	CA	3132	1/1	0.92	0.11	80,80,80,80	0
56	MG	BA	1626	1/1	0.92	0.15	80,80,80,80	0
56	MG	DA	3040	1/1	0.92	0.10	48,48,48,48	0
56	MG	DA	3154	1/1	0.92	0.17	68,68,68,68	0
56	MG	CA	3107	1/1	0.92	0.16	70,70,70,70	0
62	SPD	DA	3225	10/10	0.92	0.13	34,45,52,63	0
56	MG	AA	1655	1/1	0.92	0.11	77,77,77,77	0
56	MG	DA	3055	1/1	0.92	0.07	36,36,36,36	0
56	MG	DA	3060	1/1	0.92	0.10	77,77,77,77	0
56	MG	CA	3152	1/1	0.92	0.14	77,77,77,77	0
56	MG	DA	3066	1/1	0.92	0.09	44,44,44,44	0
56	MG	CA	3110	1/1	0.92	0.15	70,70,70,70	0
56	MG	CA	3003	1/1	0.92	0.07	80,80,80,80	0
56	MG	DA	3079	1/1	0.92	0.08	55,55,55,55	0
56	MG	CA	3008	1/1	0.92	0.08	79,79,79,79	0
57	PG4	DS	202	13/13	0.92	0.10	42,48,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	CA	3042	1/1	0.92	0.07	70,70,70,70	0
66	EDO	DA	3198	4/4	0.92	0.32	49,53,54,55	0
56	MG	CA	3004	1/1	0.92	0.18	95,95,95,95	0
66	EDO	DA	3210	4/4	0.92	0.21	62,65,69,73	0
56	MG	DA	3093	1/1	0.92	0.11	57,57,57,57	0
56	MG	CA	3142	1/1	0.92	0.10	69,69,69,69	0
56	MG	DA	3100	1/1	0.92	0.09	46,46,46,46	0
56	MG	CA	3065	1/1	0.92	0.10	73,73,73,73	0
56	MG	DA	3176	1/1	0.92	0.14	70,70,70,70	0
56	MG	CA	3057	1/1	0.92	0.09	82,82,82,82	0
56	MG	CA	3102	1/1	0.92	0.11	78,78,78,78	0
61	PEG	DA	3228	7/7	0.92	0.15	55,58,61,64	0
56	MG	BA	1602	1/1	0.93	0.09	76,76,76,76	0
56	MG	DA	3004	1/1	0.93	0.10	66,66,66,66	0
56	MG	BA	1621	1/1	0.93	0.12	54,54,54,54	0
56	MG	DA	3104	1/1	0.93	0.12	44,44,44,44	0
56	MG	DA	3106	1/1	0.93	0.10	44,44,44,44	0
56	MG	CA	3101	1/1	0.93	0.12	82,82,82,82	0
56	MG	DA	3012	1/1	0.93	0.08	56,56,56,56	0
56	MG	BA	1603	1/1	0.93	0.14	83,83,83,83	0
56	MG	CA	3028	1/1	0.93	0.08	69,69,69,69	0
56	MG	DA	3120	1/1	0.93	0.23	75,75,75,75	0
56	MG	DA	3022	1/1	0.93	0.09	40,40,40,40	0
56	MG	AA	1645	1/1	0.93	0.13	67,67,67,67	0
56	MG	DA	3029	1/1	0.93	0.08	41,41,41,41	0
56	MG	DA	3033	1/1	0.93	0.10	47,47,47,47	0
63	1PE	DA	3203	16/16	0.93	0.14	50,55,64,65	0
56	MG	BA	1606	1/1	0.93	0.11	85,85,85,85	0
56	MG	CA	3108	1/1	0.93	0.16	65,65,65,65	0
56	MG	CA	3011	1/1	0.93	0.12	78,78,78,78	0
56	MG	AA	1646	1/1	0.93	0.08	59,59,59,59	0
56	MG	CA	3016	1/1	0.93	0.08	71,71,71,71	0
56	MG	DA	3058	1/1	0.93	0.12	38,38,38,38	0
56	MG	AA	1640	1/1	0.93	0.12	65,65,65,65	0
56	MG	DA	3136	1/1	0.93	0.22	74,74,74,74	0
56	MG	AA	1659	1/1	0.93	0.08	68,68,68,68	0
56	MG	CA	3114	1/1	0.93	0.22	68,68,68,68	0
66	EDO	DA	3194	4/4	0.93	0.25	52,52,52,58	0
56	MG	DA	3069	1/1	0.93	0.14	53,53,53,53	0
56	MG	BA	1614	1/1	0.93	0.11	77,77,77,77	0
56	MG	DA	3142	1/1	0.93	0.12	64,64,64,64	0
56	MG	DA	3229	1/1	0.93	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DB	201	1/1	0.93	0.07	62,62,62,62	0
56	MG	AA	1660	1/1	0.93	0.21	86,86,86,86	0
56	MG	CA	3094	1/1	0.93	0.12	68,68,68,68	0
56	MG	CB	201	1/1	0.93	0.10	91,91,91,91	0
56	MG	CA	3136	1/1	0.93	0.09	87,87,87,87	0
66	EDO	D1	101	4/4	0.93	0.15	47,52,57,63	0
56	MG	CA	3022	1/1	0.93	0.19	78,78,78,78	0
56	MG	DA	3002	1/1	0.93	0.10	66,66,66,66	0
56	MG	CB	203	1/1	0.94	0.08	90,90,90,90	0
56	MG	DA	3094	1/1	0.94	0.08	38,38,38,38	0
56	MG	DA	3095	1/1	0.94	0.07	49,49,49,49	0
59	PUT	DA	3224	6/6	0.94	0.12	43,45,54,60	0
56	MG	CA	3100	1/1	0.94	0.07	78,78,78,78	0
56	MG	AA	1647	1/1	0.94	0.12	82,82,82,82	0
56	MG	DA	3047	1/1	0.94	0.07	54,54,54,54	0
56	MG	DA	3053	1/1	0.94	0.07	38,38,38,38	0
56	MG	AA	1607	1/1	0.94	0.21	76,76,76,76	0
56	MG	DA	3139	1/1	0.94	0.08	57,57,57,57	0
56	MG	CA	3064	1/1	0.94	0.13	75,75,75,75	0
56	MG	AA	1604	1/1	0.94	0.21	73,73,73,73	0
56	MG	CA	3106	1/1	0.94	0.20	67,67,67,67	0
56	MG	AA	1611	1/1	0.94	0.10	63,63,63,63	0
56	MG	BA	1607	1/1	0.94	0.11	84,84,84,84	0
56	MG	CA	3069	1/1	0.94	0.07	80,80,80,80	0
56	MG	CA	3043	1/1	0.94	0.14	67,67,67,67	0
56	MG	CA	3095	1/1	0.94	0.09	71,71,71,71	0
56	MG	DA	3148	1/1	0.94	0.07	66,66,66,66	0
56	MG	AA	1636	1/1	0.94	0.10	81,81,81,81	0
56	MG	BA	1624	1/1	0.94	0.23	86,86,86,86	0
56	MG	AA	1618	1/1	0.94	0.28	78,78,78,78	0
56	MG	DA	3090	1/1	0.95	0.11	42,42,42,42	0
56	MG	CA	3013	1/1	0.95	0.21	89,89,89,89	0
56	MG	DA	3038	1/1	0.95	0.07	44,44,44,44	0
56	MG	AA	1653	1/1	0.95	0.06	63,63,63,63	0
56	MG	DA	3164	1/1	0.95	0.13	70,70,70,70	0
56	MG	CA	3044	1/1	0.95	0.14	73,73,73,73	0
56	MG	DA	3166	1/1	0.95	0.18	73,73,73,73	0
56	MG	CA	3077	1/1	0.95	0.07	83,83,83,83	0
56	MG	DA	3099	1/1	0.95	0.08	60,60,60,60	0
56	MG	AA	1657	1/1	0.95	0.14	77,77,77,77	0
56	MG	BA	1604	1/1	0.95	0.17	75,75,75,75	0
56	MG	AA	1667	1/1	0.95	0.09	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3057	1/1	0.95	0.09	40,40,40,40	0
59	PUT	DM	201	6/6	0.95	0.10	46,49,53,54	0
56	MG	BA	1616	1/1	0.95	0.07	86,86,86,86	0
56	MG	CA	3067	1/1	0.95	0.16	84,84,84,84	0
56	MG	AA	1622	1/1	0.95	0.20	74,74,74,74	0
56	MG	BA	1628	1/1	0.95	0.06	74,74,74,74	0
56	MG	CA	3009	1/1	0.95	0.19	78,78,78,78	0
56	MG	BA	1619	1/1	0.95	0.11	66,66,66,66	0
56	MG	DA	3025	1/1	0.95	0.06	41,41,41,41	0
56	MG	DA	3124	1/1	0.95	0.23	72,72,72,72	0
56	MG	DA	3076	1/1	0.95	0.07	67,67,67,67	0
56	MG	AA	1662	1/1	0.95	0.08	74,74,74,74	0
56	MG	CA	3105	1/1	0.95	0.17	68,68,68,68	0
56	MG	CA	3027	1/1	0.95	0.12	97,97,97,97	0
56	MG	DA	3088	1/1	0.95	0.08	32,32,32,32	0
56	MG	CA	3054	1/1	0.96	0.09	83,83,83,83	0
56	MG	DA	3043	1/1	0.96	0.06	49,49,49,49	0
56	MG	DA	3135	1/1	0.96	0.09	56,56,56,56	0
56	MG	AA	1635	1/1	0.96	0.07	74,74,74,74	0
56	MG	DA	3096	1/1	0.96	0.16	69,69,69,69	0
56	MG	DA	3049	1/1	0.96	0.05	45,45,45,45	0
56	MG	DA	3051	1/1	0.96	0.07	53,53,53,53	0
62	SPD	DA	3187	10/10	0.96	0.09	36,43,46,47	0
56	MG	CA	3056	1/1	0.96	0.14	75,75,75,75	0
56	MG	DA	3054	1/1	0.96	0.06	35,35,35,35	0
58	MPD	DS	203	8/8	0.96	0.10	41,45,50,53	0
56	MG	DA	3010	1/1	0.96	0.08	37,37,37,37	0
64	PGE	DA	3186	10/10	0.96	0.09	37,42,58,59	0
56	MG	BA	1622	1/1	0.96	0.09	70,70,70,70	0
56	MG	AA	1631	1/1	0.96	0.08	54,54,54,54	0
56	MG	DA	3110	1/1	0.96	0.04	33,33,33,33	0
56	MG	DA	3111	1/1	0.96	0.09	61,61,61,61	0
56	MG	DA	3017	1/1	0.96	0.12	36,36,36,36	0
56	MG	DA	3116	1/1	0.96	0.05	57,57,57,57	0
56	MG	DA	3117	1/1	0.96	0.07	54,54,54,54	0
56	MG	AA	1656	1/1	0.96	0.11	67,67,67,67	0
65	ACY	DA	3191	4/4	0.96	0.10	48,50,52,53	0
56	MG	DB	203	1/1	0.96	0.05	51,51,51,51	0
56	MG	BA	1634	1/1	0.96	0.06	76,76,76,76	0
56	MG	CA	3017	1/1	0.96	0.10	82,82,82,82	0
56	MG	DA	3027	1/1	0.96	0.14	42,42,42,42	0
56	MG	DA	3155	1/1	0.96	0.10	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	1608	1/1	0.96	0.06	78,78,78,78	0
56	MG	DA	3157	1/1	0.96	0.16	65,65,65,65	0
56	MG	DA	3074	1/1	0.96	0.12	42,42,42,42	0
56	MG	BA	1618	1/1	0.96	0.15	74,74,74,74	0
56	MG	CA	3032	1/1	0.96	0.06	71,71,71,71	0
56	MG	AA	1666	1/1	0.96	0.06	73,73,73,73	0
56	MG	DA	3036	1/1	0.96	0.07	43,43,43,43	0
56	MG	AA	1638	1/1	0.96	0.09	86,86,86,86	0
56	MG	BA	1629	1/1	0.96	0.14	77,77,77,77	0
56	MG	CA	3023	1/1	0.96	0.09	75,75,75,75	0
56	MG	AA	1677	1/1	0.97	0.07	79,79,79,79	0
56	MG	DA	3082	1/1	0.97	0.08	49,49,49,49	0
56	MG	DA	3083	1/1	0.97	0.06	50,50,50,50	0
56	MG	CA	3053	1/1	0.97	0.14	80,80,80,80	0
56	MG	AA	1643	1/1	0.97	0.06	66,66,66,66	0
56	MG	DA	3006	1/1	0.97	0.08	43,43,43,43	0
56	MG	DA	3007	1/1	0.97	0.05	40,40,40,40	0
56	MG	AA	1639	1/1	0.97	0.07	79,79,79,79	0
56	MG	DA	3044	1/1	0.97	0.06	41,41,41,41	0
56	MG	DA	3046	1/1	0.97	0.07	33,33,33,33	0
56	MG	DA	3009	1/1	0.97	0.07	59,59,59,59	0
56	MG	CA	3012	1/1	0.97	0.05	69,69,69,69	0
56	MG	DA	3050	1/1	0.97	0.11	55,55,55,55	0
56	MG	DA	3098	1/1	0.97	0.04	37,37,37,37	0
56	MG	AA	1648	1/1	0.97	0.06	56,56,56,56	0
56	MG	BA	1612	1/1	0.97	0.06	77,77,77,77	0
56	MG	DA	3101	1/1	0.97	0.06	51,51,51,51	0
56	MG	CA	3015	1/1	0.97	0.14	76,76,76,76	0
56	MG	AA	1629	1/1	0.97	0.07	67,67,67,67	0
56	MG	AA	1668	1/1	0.97	0.14	60,60,60,60	0
56	MG	CA	3099	1/1	0.97	0.06	69,69,69,69	0
56	MG	CA	3049	1/1	0.97	0.06	64,64,64,64	0
56	MG	DA	3062	1/1	0.97	0.06	50,50,50,50	0
56	MG	DA	3150	1/1	0.97	0.11	49,49,49,49	0
66	EDO	DA	3197	4/4	0.97	0.12	56,58,62,65	0
56	MG	DA	3113	1/1	0.97	0.04	38,38,38,38	0
56	MG	DA	3063	1/1	0.97	0.07	42,42,42,42	0
56	MG	CA	3143	1/1	0.97	0.05	74,74,74,74	0
56	MG	AA	1652	1/1	0.97	0.10	49,49,49,49	0
56	MG	DA	3030	1/1	0.97	0.11	34,34,34,34	0
56	MG	DA	3031	1/1	0.97	0.04	34,34,34,34	0
56	MG	DA	3001	1/1	0.97	0.06	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3073	1/1	0.97	0.05	38,38,38,38	0
56	MG	DA	3159	1/1	0.97	0.10	62,62,62,62	0
56	MG	DA	3034	1/1	0.97	0.04	33,33,33,33	0
56	MG	CA	3088	1/1	0.97	0.13	68,68,68,68	0
56	MG	DA	3077	1/1	0.97	0.05	70,70,70,70	0
56	MG	DA	3105	1/1	0.98	0.04	41,41,41,41	0
56	MG	DA	3080	1/1	0.98	0.04	61,61,61,61	0
56	MG	CA	3040	1/1	0.98	0.06	59,59,59,59	0
56	MG	DA	3061	1/1	0.98	0.05	60,60,60,60	0
56	MG	DA	3024	1/1	0.98	0.05	64,64,64,64	0
56	MG	DA	3048	1/1	0.98	0.06	35,35,35,35	0
60	ZN	C5	101	1/1	0.98	0.07	117,117,117,117	0
56	MG	DA	3064	1/1	0.98	0.07	41,41,41,41	0
56	MG	AA	1634	1/1	0.98	0.10	78,78,78,78	0
56	MG	DB	202	1/1	0.98	0.04	40,40,40,40	0
56	MG	DA	3091	1/1	0.98	0.12	36,36,36,36	0
56	MG	AA	1637	1/1	0.98	0.08	57,57,57,57	0
56	MG	DA	3068	1/1	0.98	0.05	70,70,70,70	0
56	MG	DA	3039	1/1	0.98	0.04	39,39,39,39	0
56	MG	DA	3052	1/1	0.98	0.11	41,41,41,41	0
56	MG	BA	1635	1/1	0.98	0.09	72,72,72,72	0
56	MG	DR	201	1/1	0.98	0.27	66,66,66,66	0
56	MG	BA	1615	1/1	0.98	0.06	62,62,62,62	0
56	MG	AA	1633	1/1	0.98	0.10	72,72,72,72	0
56	MG	DA	3075	1/1	0.98	0.04	48,48,48,48	0
56	MG	DA	3019	1/1	0.98	0.04	34,34,34,34	0
56	MG	AA	1665	1/1	0.98	0.10	78,78,78,78	0
56	MG	DA	3102	1/1	0.98	0.07	35,35,35,35	0
56	MG	DA	3078	1/1	0.98	0.09	72,72,72,72	0
56	MG	DA	3059	1/1	0.98	0.05	42,42,42,42	0
56	MG	DA	3023	1/1	0.99	0.03	41,41,41,41	0
56	MG	DA	3037	1/1	0.99	0.07	37,37,37,37	0
56	MG	DA	3013	1/1	0.99	0.04	52,52,52,52	0
56	MG	DA	3071	1/1	0.99	0.08	37,37,37,37	0
56	MG	DA	3014	1/1	0.99	0.07	36,36,36,36	0
56	MG	DA	3026	1/1	0.99	0.04	50,50,50,50	0
56	MG	DA	3056	1/1	0.99	0.08	44,44,44,44	0
56	MG	DA	3015	1/1	0.99	0.07	54,54,54,54	0
56	MG	DA	3123	1/1	0.99	0.05	43,43,43,43	0
56	MG	BA	1610	1/1	0.99	0.05	69,69,69,69	0
56	MG	AA	1650	1/1	0.99	0.04	63,63,63,63	0
56	MG	DA	3018	1/1	0.99	0.04	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	ZN	D5	101	1/1	0.99	0.03	63,63,63,63	0
56	MG	DA	3045	1/1	0.99	0.06	44,44,44,44	0
56	MG	AA	1649	1/1	0.99	0.04	64,64,64,64	0
56	MG	DA	3081	1/1	0.99	0.03	52,52,52,52	0
56	MG	DA	3032	1/1	0.99	0.05	31,31,31,31	0
56	MG	DA	3020	1/1	0.99	0.03	30,30,30,30	0
56	MG	DA	3084	1/1	0.99	0.06	48,48,48,48	0
56	MG	DA	3107	1/1	0.99	0.03	33,33,33,33	0
56	MG	DA	3134	1/1	0.99	0.08	65,65,65,65	0
56	MG	DB	204	1/1	0.99	0.07	57,57,57,57	0
56	MG	DA	3108	1/1	0.99	0.08	38,38,38,38	0
56	MG	DA	3011	1/1	0.99	0.10	33,33,33,33	0
56	MG	CA	3050	1/1	0.99	0.04	65,65,65,65	0
56	MG	DA	3067	1/1	0.99	0.05	50,50,50,50	0
56	MG	DA	3112	1/1	0.99	0.10	44,44,44,44	0
56	MG	DA	3089	1/1	0.99	0.09	32,32,32,32	0
56	MG	DA	3086	1/1	1.00	0.05	40,40,40,40	0
56	MG	DA	3114	1/1	1.00	0.01	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.