



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2017 – 10:03 PM EDT

PDB ID : 4YBB
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

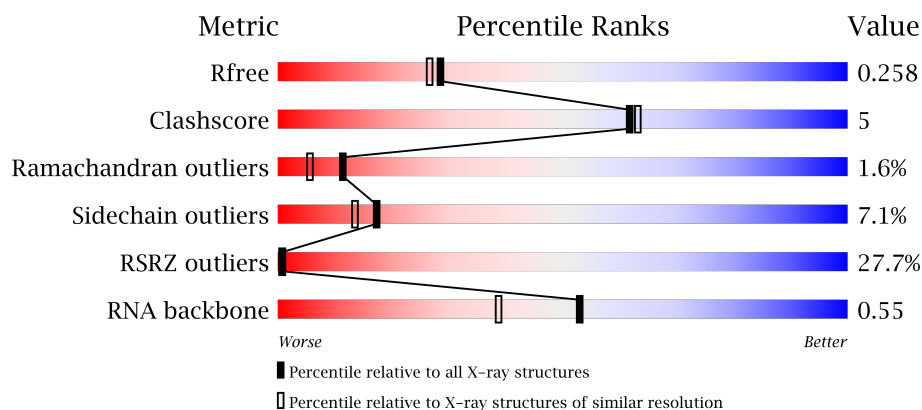
1 Overall quality at a glance

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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)
RNA backbone	2435	1063 (2.70-1.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>5%</div> </div> </div>
1	BA	1534	<div> <div>11%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>5%</div> </div> </div>
2	AB	224	<div> <div>60%</div> <div> <div></div> <div>82%</div> <div>16%</div> </div> </div>
2	BB	224	<div> <div>71%</div> <div> <div></div> <div>79%</div> <div>19%</div> </div> </div>

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

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Mol	Chain	Length	Quality of chain
15	BO	88	
16	AP	82	
16	BP	82	
17	AQ	80	
17	BQ	80	
18	AR	55	
18	BR	55	
19	AS	79	
19	BS	79	
20	AT	86	
20	BT	86	
21	AU	56	
21	BU	56	
22	CA	2904	
23	CB	120	
23	DB	120	
24	CC	271	
24	DC	271	
25	CD	209	
26	CE	201	
26	DE	201	
27	CF	177	
27	DF	177	
28	CG	176	
28	DG	176	

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Mol	Chain	Length	Quality of chain
29	CH	149	
29	DH	149	
30	CJ	134	
30	DJ	134	
31	CK	142	
31	DK	142	
32	CL	123	
32	DL	123	
33	CM	144	
33	DM	144	
34	CN	136	
34	DN	136	
35	CO	125	
35	DO	125	
36	CP	117	
36	DP	117	
37	CQ	114	
37	DQ	114	
38	CR	117	
38	DR	117	
39	CS	103	
39	DS	103	
40	CT	110	
40	DT	110	
41	CU	93	


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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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	1603	-	-	-	X
56	MG	AA	1608	-	-	-	X
56	MG	AA	1611	-	-	-	X
56	MG	AA	1612	-	-	-	X
56	MG	AA	1631	-	-	-	X
56	MG	AA	1642	-	-	-	X
56	MG	AA	1661	-	-	-	X
56	MG	BA	1605	-	-	-	X
56	MG	BA	1624	-	-	-	X
56	MG	BA	1632	-	-	-	X
56	MG	CA	3002	-	-	-	X
56	MG	CA	3005	-	-	-	X
56	MG	CA	3025	-	-	-	X
56	MG	CA	3036	-	-	-	X
56	MG	CA	3132	-	-	-	X
56	MG	CA	3150	-	-	-	X
56	MG	CB	202	-	-	-	X
56	MG	DA	3006	-	-	-	X
56	MG	DA	3011	-	-	-	X
56	MG	DA	3015	-	-	-	X
56	MG	DA	3022	-	-	-	X
56	MG	DA	3027	-	-	-	X
56	MG	DA	3033	-	-	-	X
56	MG	DA	3035	-	-	-	X
56	MG	DA	3044	-	-	-	X
56	MG	DA	3045	-	-	-	X
56	MG	DA	3048	-	-	-	X
56	MG	DA	3057	-	-	-	X
56	MG	DA	3064	-	-	-	X
56	MG	DA	3069	-	-	-	X
56	MG	DA	3088	-	-	-	X
56	MG	DA	3090	-	-	-	X
56	MG	DA	3091	-	-	-	X
56	MG	DA	3108	-	-	-	X
56	MG	DA	3119	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	DA	3122	-	-	-	X
56	MG	DA	3125	-	-	-	X
56	MG	DA	3126	-	-	-	X
56	MG	DA	3172	-	-	-	X
56	MG	DA	3177	-	-	-	X
57	PG4	DA	3193	-	-	X	X
57	PG4	DR	202	-	-	X	X
58	MPD	AA	1671	-	-	-	X
58	MPD	AA	1676	-	-	-	X
58	MPD	DA	3192	-	-	-	X
58	MPD	DA	3205	-	-	-	X
58	MPD	DA	3208	-	-	-	X
58	MPD	DE	301	-	-	-	X
58	MPD	DN	201	-	-	X	-
59	PUT	AA	1672	-	-	-	X
59	PUT	DA	3184	-	-	-	X
59	PUT	DA	3189	-	-	-	X
59	PUT	DA	3214	-	-	-	X
59	PUT	DA	3220	-	-	-	X
59	PUT	DA	3222	-	-	-	X
59	PUT	DA	3223	-	-	X	X
59	PUT	DM	201	-	-	-	X
60	ZN	AB	301	-	-	-	X
61	PEG	D3	102	-	-	X	X
61	PEG	DA	3200	-	-	-	X
61	PEG	DA	3219	-	-	-	X
61	PEG	DP	201	-	-	X	-
62	SPD	DA	3187	-	-	-	X
62	SPD	DA	3225	-	-	-	X
64	PGE	D1	102	-	-	-	X
64	PGE	DA	3186	-	-	-	X
65	ACY	DA	3202	-	-	-	X
66	EDO	D0	101	-	-	-	X
66	EDO	DA	3198	-	-	-	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		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 (three-letter code: MG) (formula: Mg).

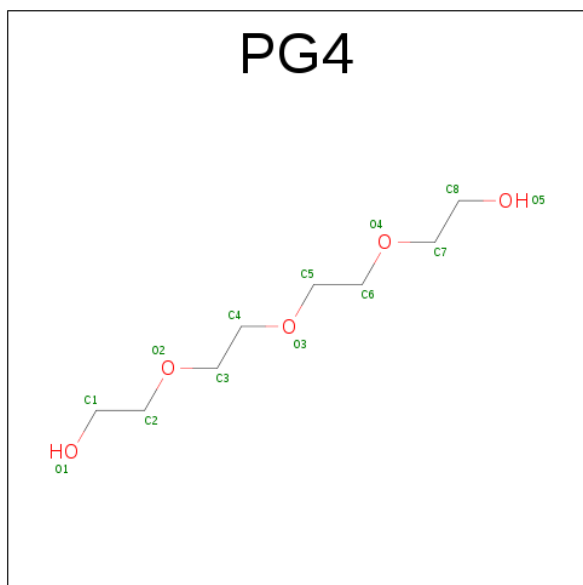
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BA	41	Total	Mg	0	0
			41	41		
56	CA	155	Total	Mg	0	0
			155	155		
56	CB	3	Total	Mg	0	0
			3	3		
56	DR	1	Total	Mg	0	0
			1	1		
56	AA	70	Total	Mg	0	0
			70	70		

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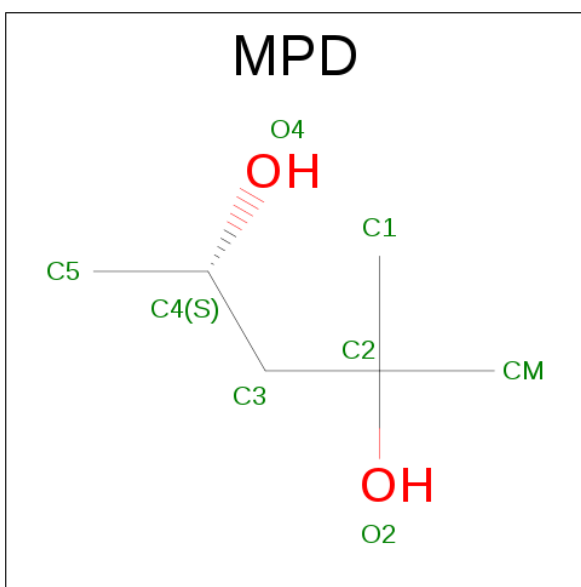
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DA	183	Total	Mg	0	0
			183	183		
56	C3	1	Total	Mg	0	0
			1	1		
56	DB	9	Total	Mg	0	0
			9	9		

- Molecule 57 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



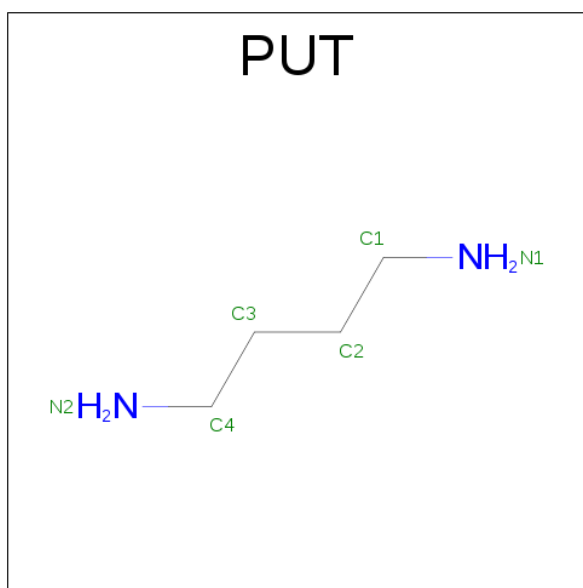
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			13	8	5		
57	BA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DQ	1	Total	C	O	0	0
			13	8	5		
57	DR	1	Total	C	O	0	0
			13	8	5		
57	DS	1	Total	C	O	0	0
			13	8	5		

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: 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	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-DIAMINOBTANE (three-letter code: PUT) (formula: C₄H₁₂N₂).



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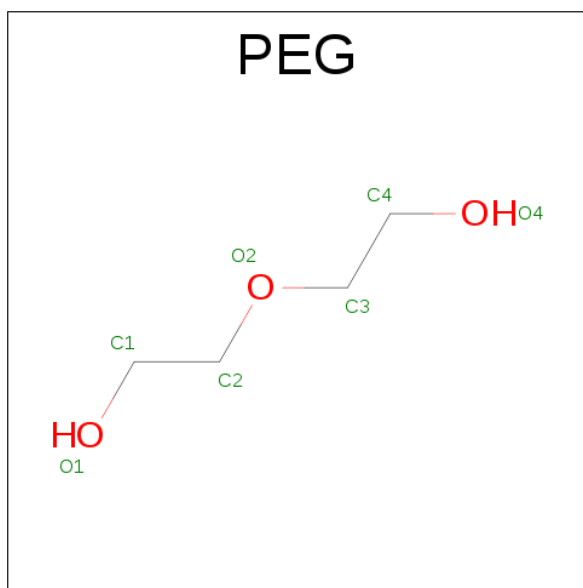
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DM	1	Total	C	N	0	0
			6	4	2		

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

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

- Molecule 61 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



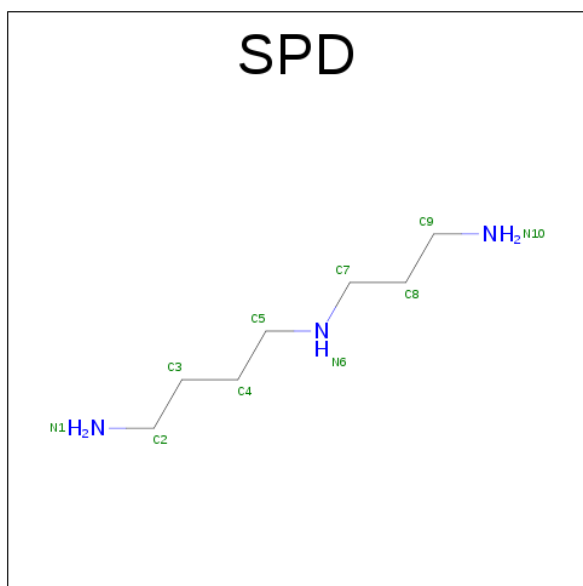
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		

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



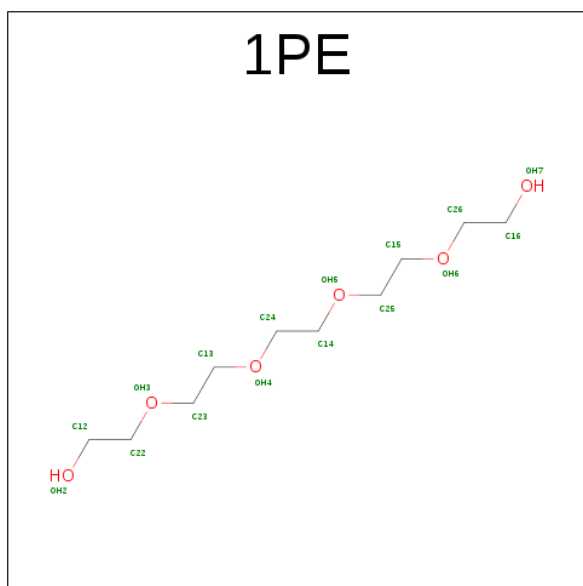
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	DA	1	Total C N 10 7 3	0	0
62	DA	1	Total C N 10 7 3	0	0
62	DA	1	Total C N 10 7 3	0	0

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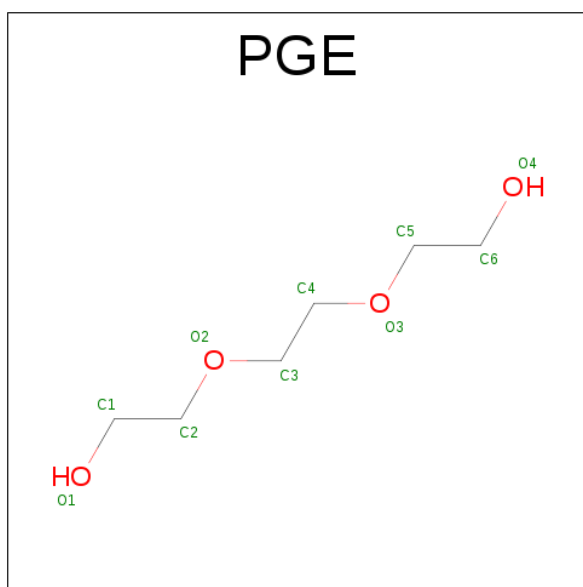
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	DA	1	Total	C	N	0	0
			10	7	3		

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



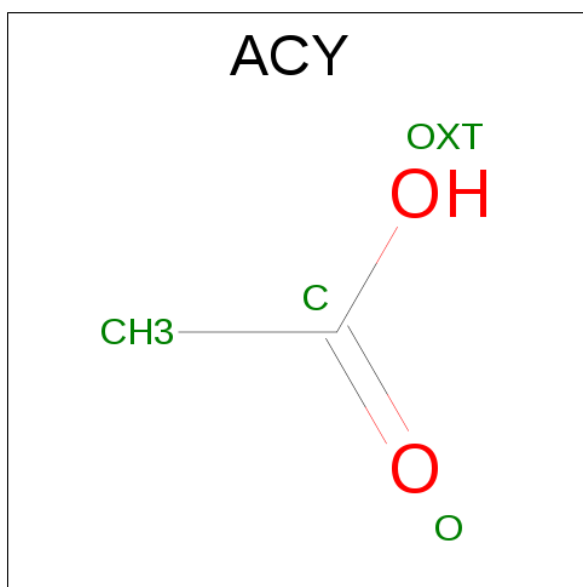
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	DA	1	Total	C	O	0	0
			16	10	6		
63	DA	1	Total	C	O	0	0
			16	10	6		

- Molecule 64 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



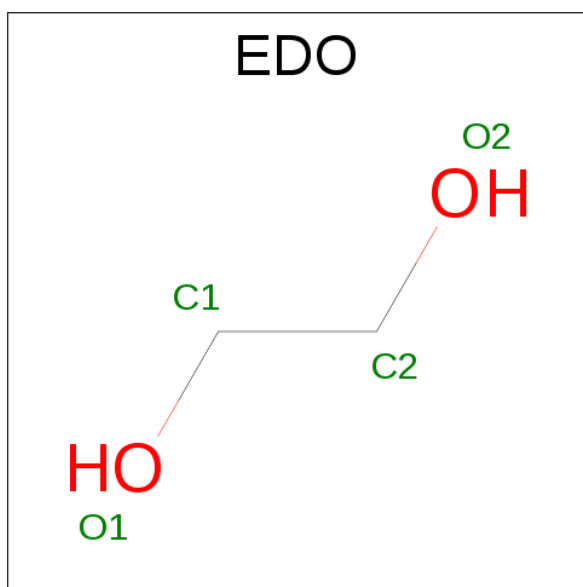
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DS	1	Total	C	O	0	0
			10	6	4		
64	DU	1	Total	C	O	0	0
			10	6	4		
64	D1	1	Total	C	O	0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

- Molecule 65 is ACETIC ACID (three-letter code: 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 (three-letter code: EDO) (formula: C₂H₆O₂).



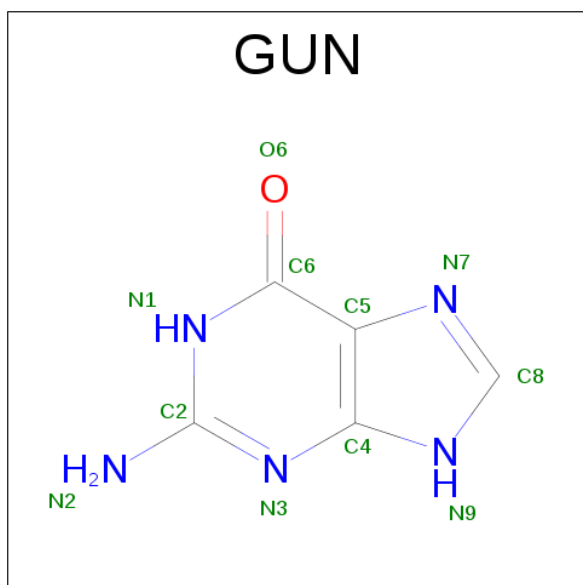
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		

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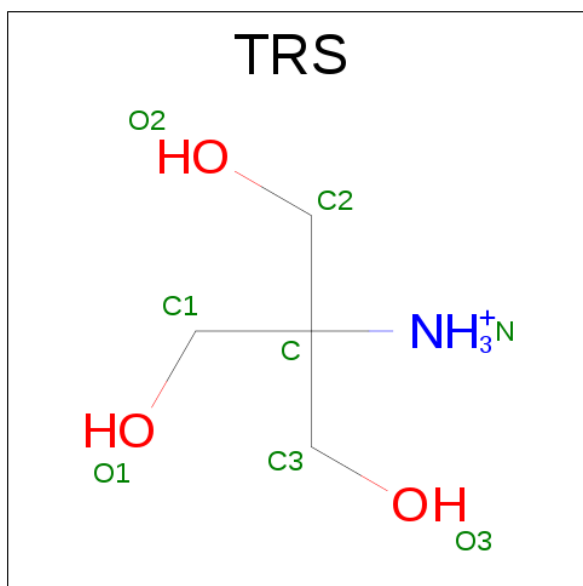
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DB	1	Total	C	O	0	0
			4	2	2		
66	DB	1	Total	C	O	0	0
			4	2	2		
66	DB	1	Total	C	O	0	0
			4	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 (three-letter code: 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 (three-letter code: 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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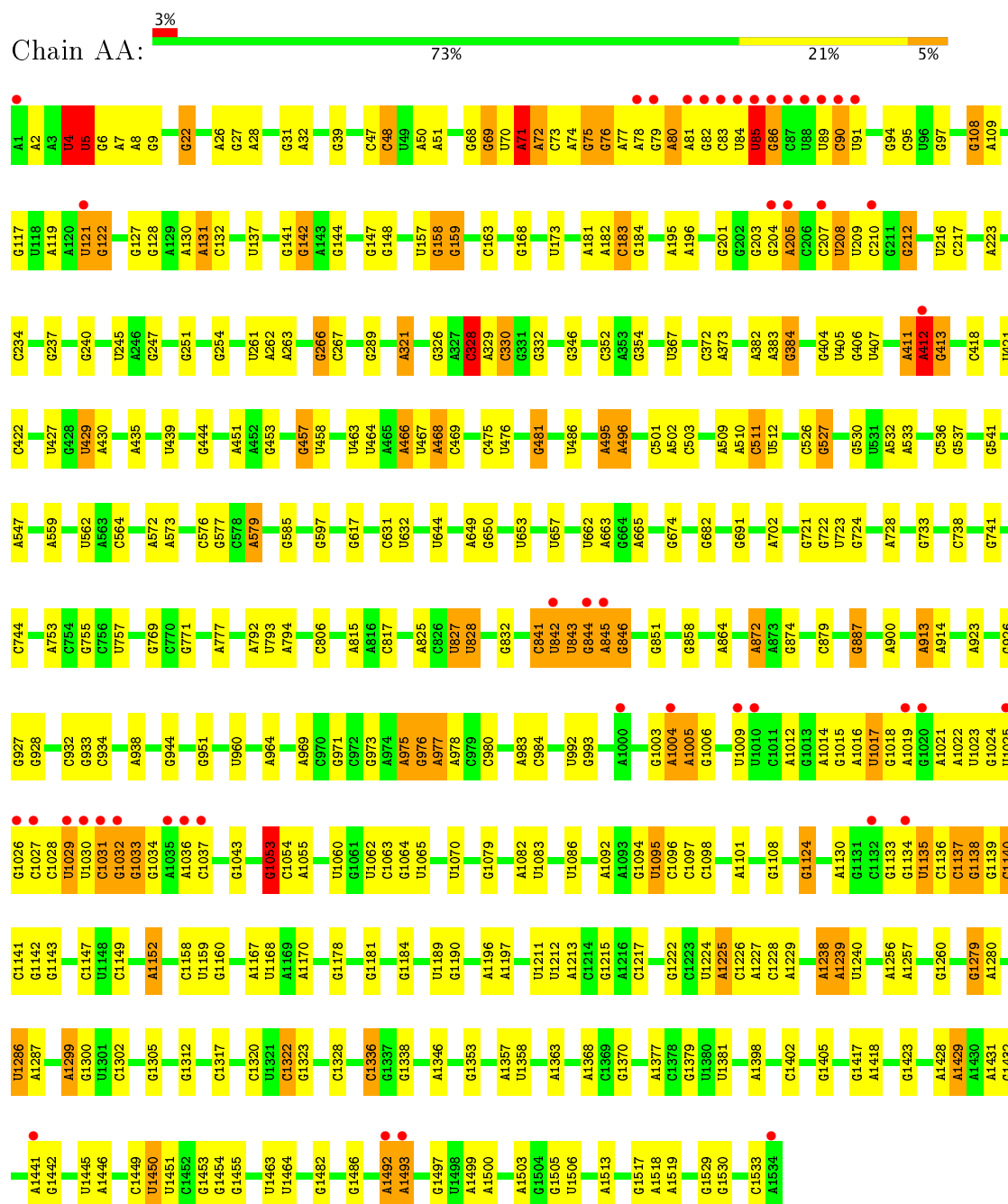
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	D3	25	Total 25	O 25	0	0
69	D4	38	Total 38	O 38	0	0
69	D5	14	Total 14	O 14	0	0

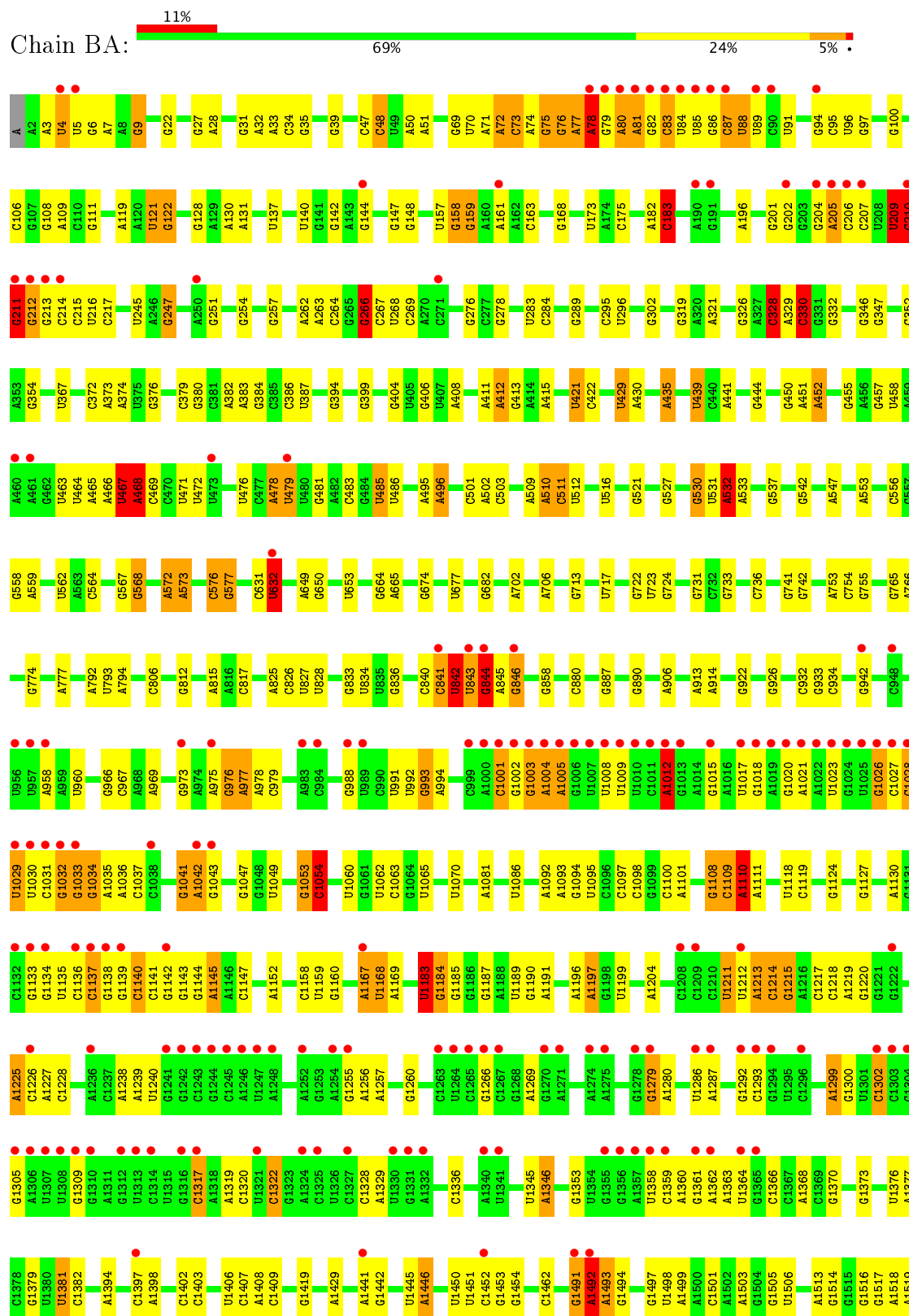
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

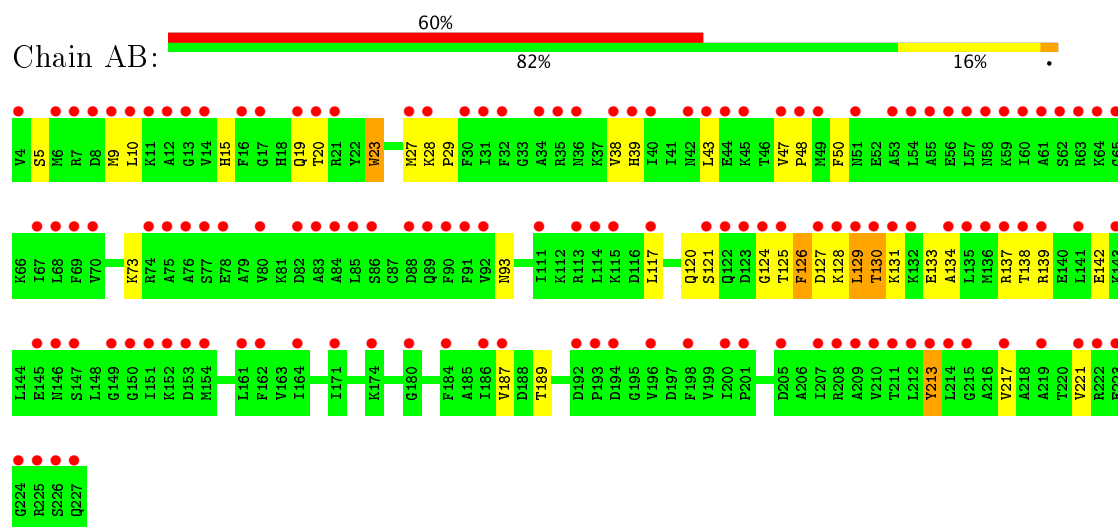
• Molecule 1: 16S rRNA



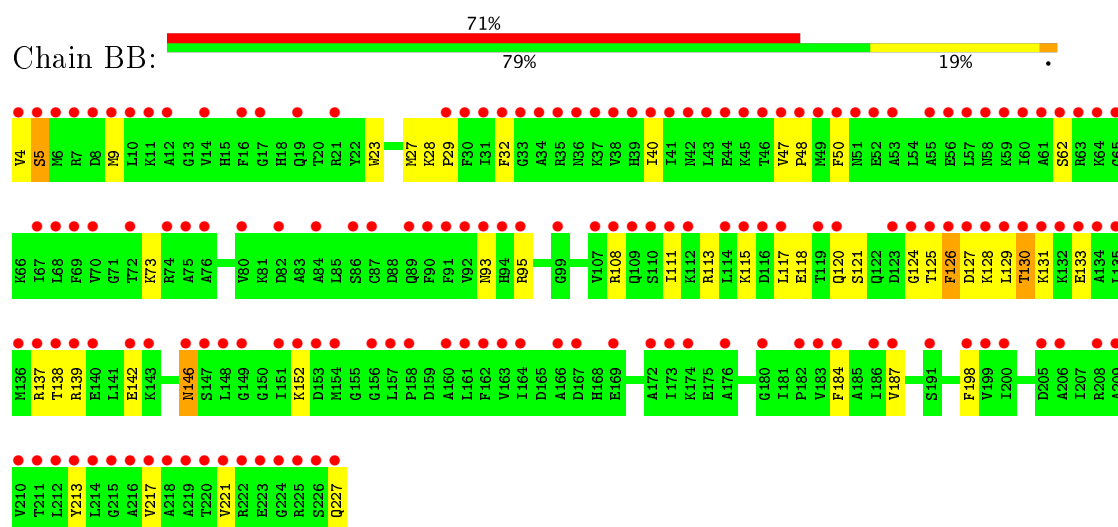
• Molecule 1: 16S rRNA



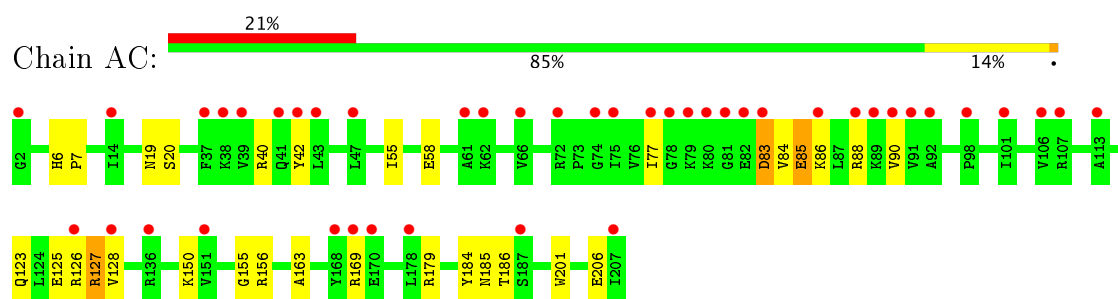
• Molecule 2: 30S ribosomal protein S2



• Molecule 2: 30S ribosomal protein S2

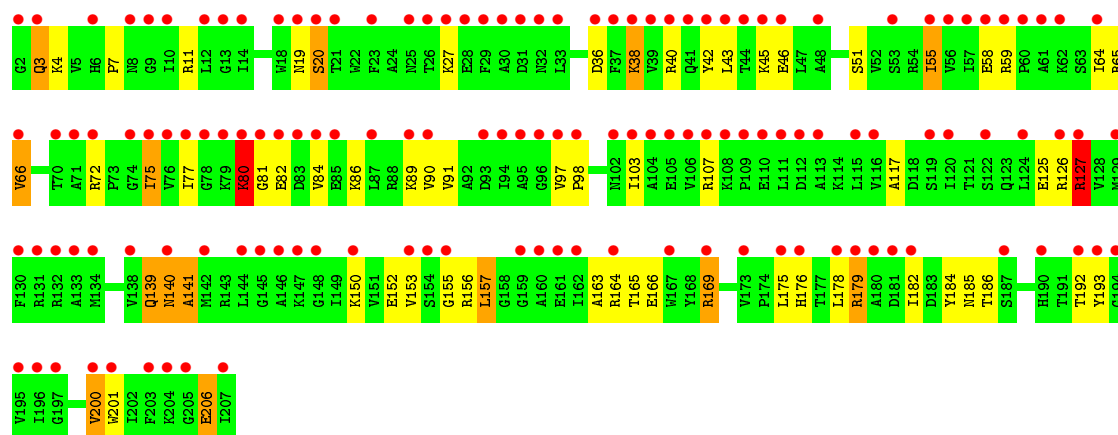


• Molecule 3: 30S ribosomal protein S3

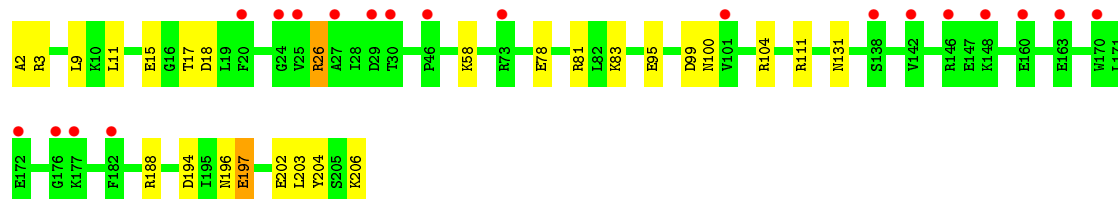
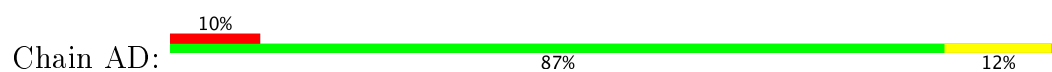


• Molecule 3: 30S ribosomal protein S3

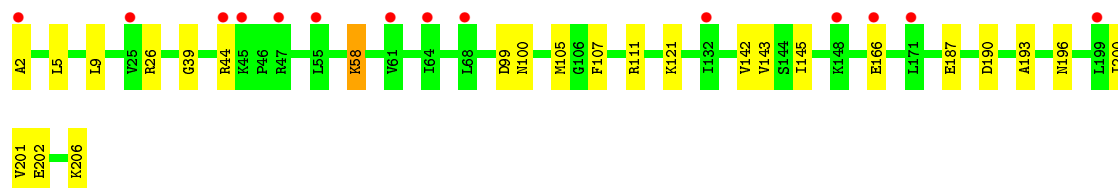
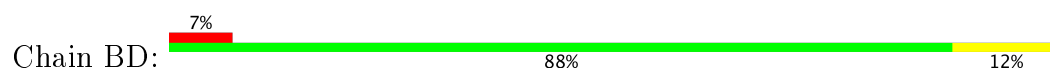




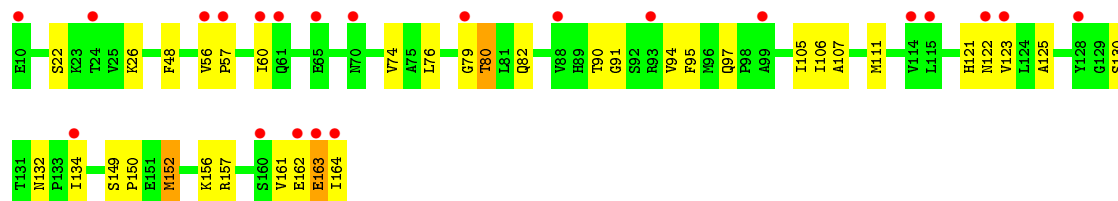
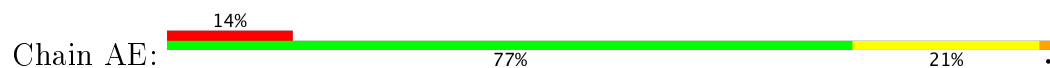
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4

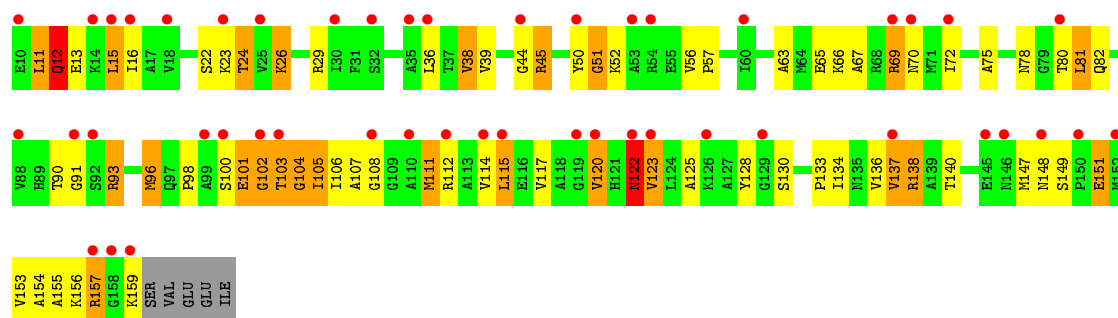


• Molecule 5: 30S ribosomal protein S5

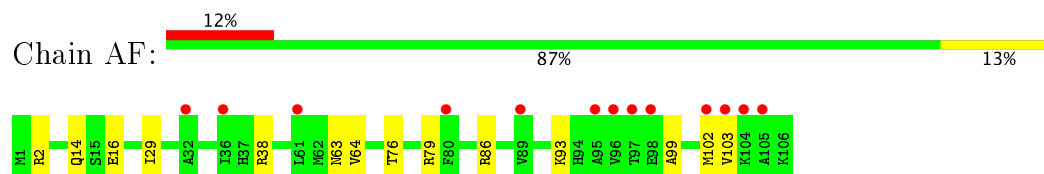


• Molecule 5: 30S ribosomal protein S5

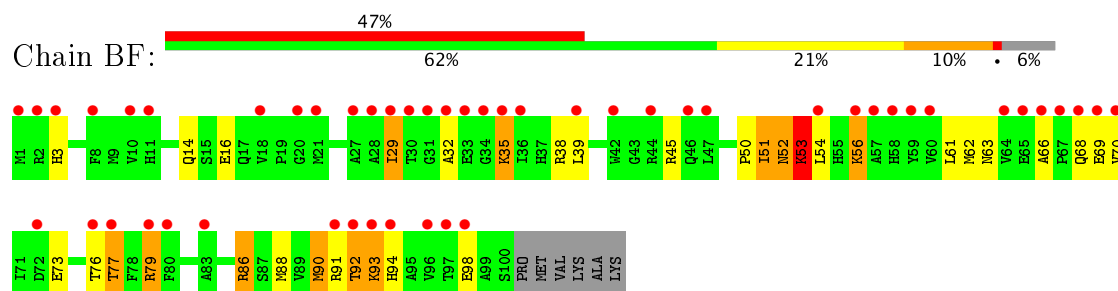




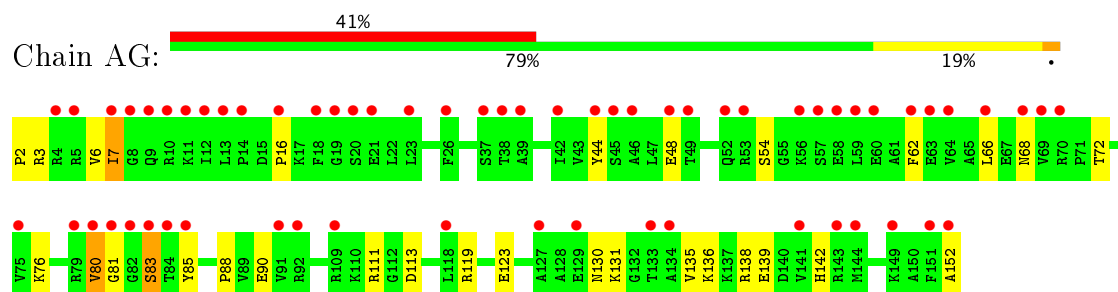
- Molecule 6: 30S ribosomal protein S6



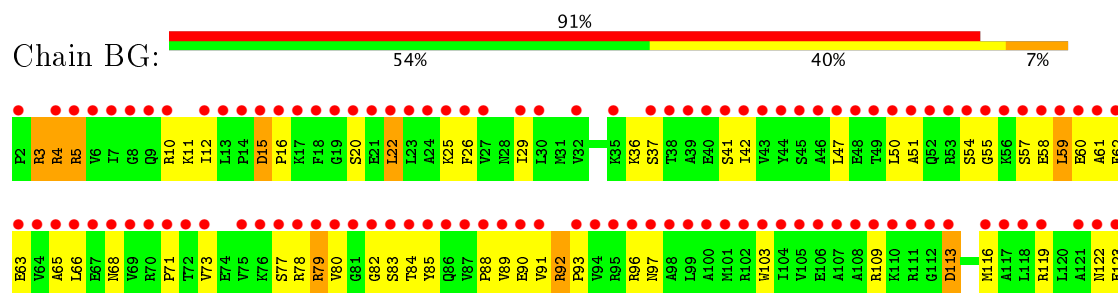
- Molecule 6: 30S ribosomal protein S6

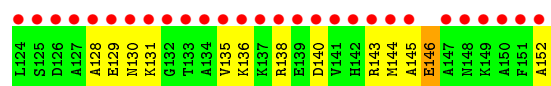


- Molecule 7: 30S ribosomal protein S7

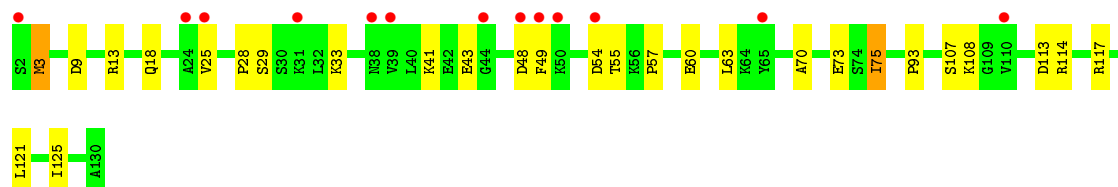
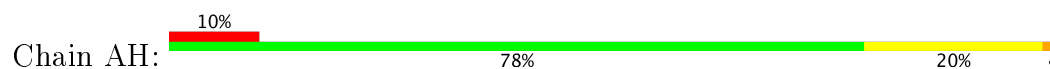


- Molecule 7: 30S ribosomal protein S7

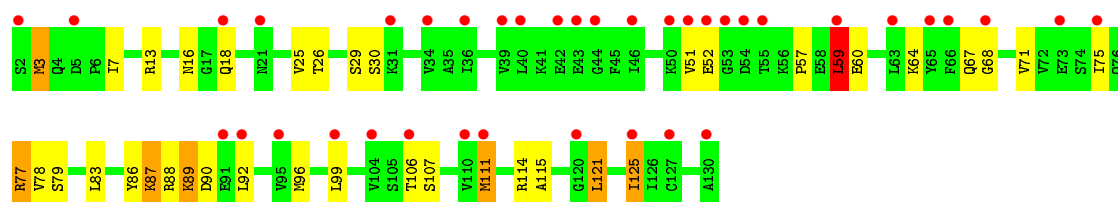
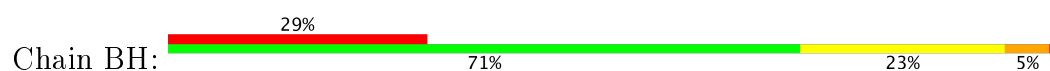




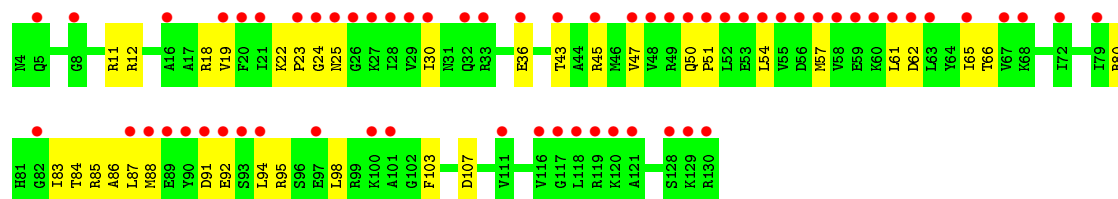
• Molecule 8: 30S ribosomal protein S8



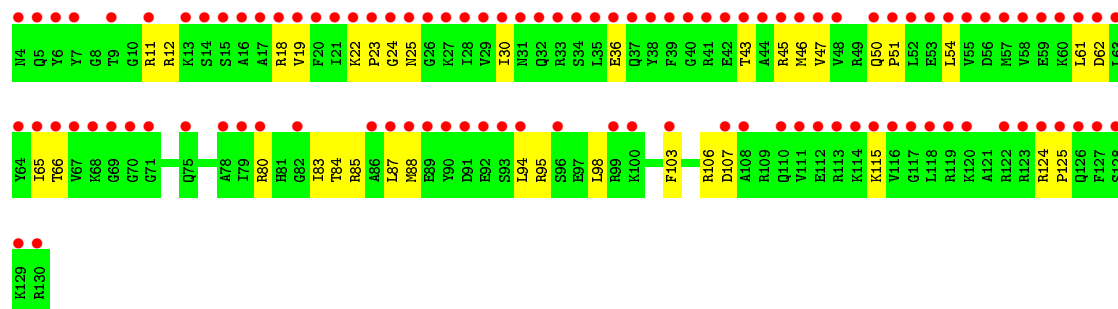
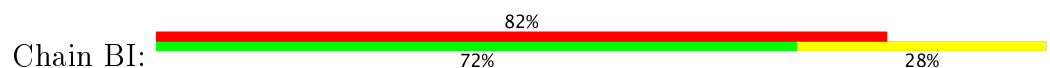
• Molecule 8: 30S ribosomal protein S8



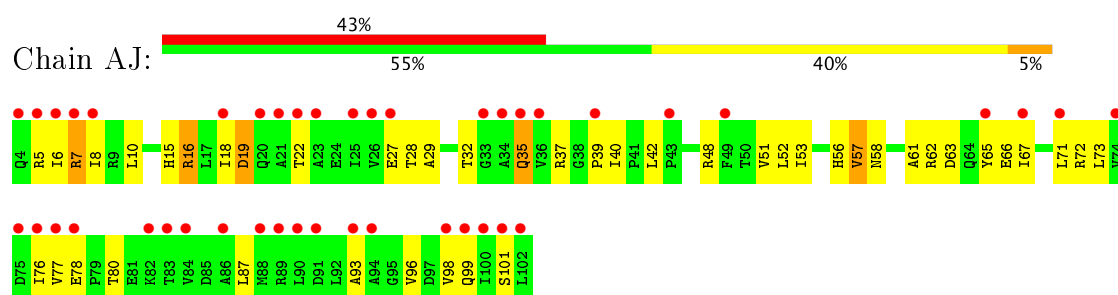
• Molecule 9: 30S ribosomal protein S9



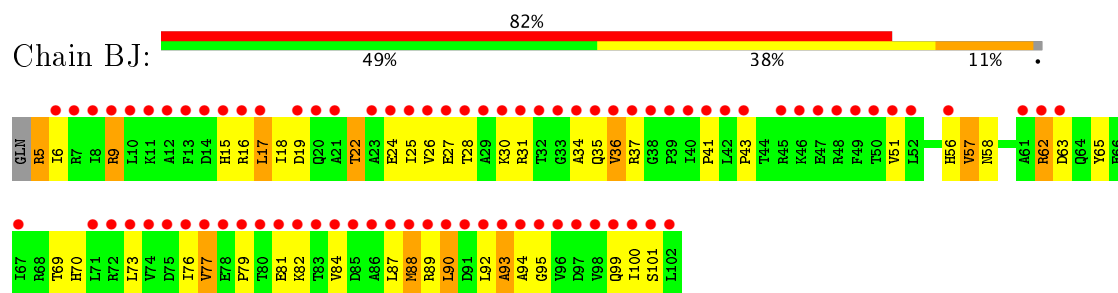
• Molecule 9: 30S ribosomal protein S9



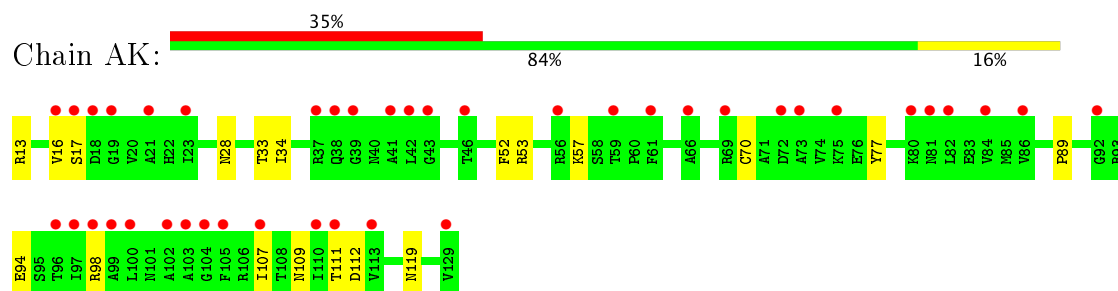
• Molecule 10: 30S ribosomal protein S10



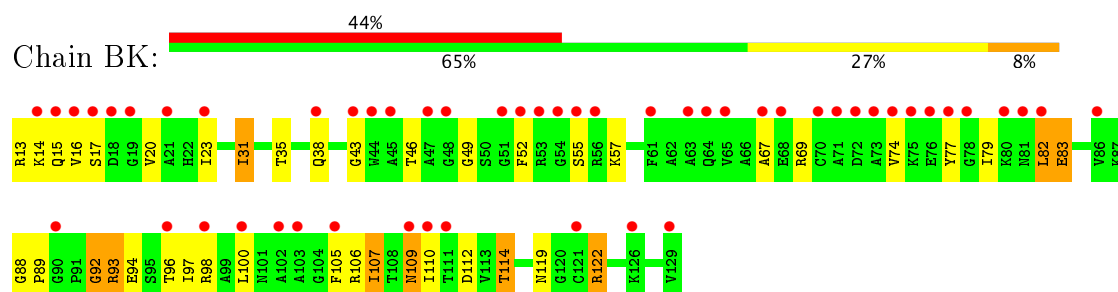
- Molecule 10: 30S ribosomal protein S10



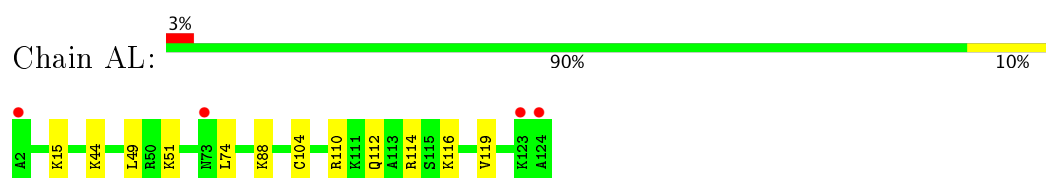
- Molecule 11: 30S ribosomal protein S11



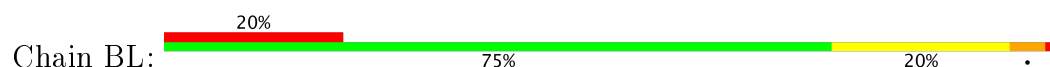
- Molecule 11: 30S ribosomal protein S11

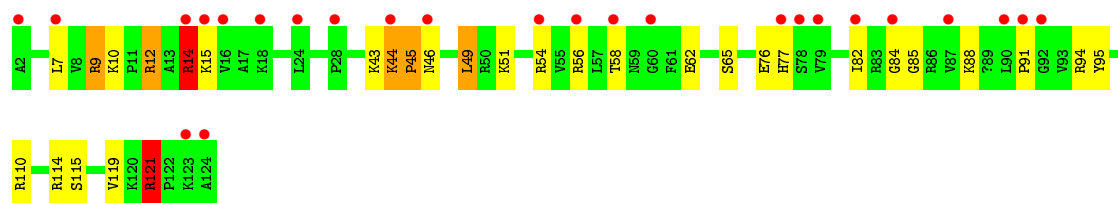


- Molecule 12: 30S ribosomal protein S12

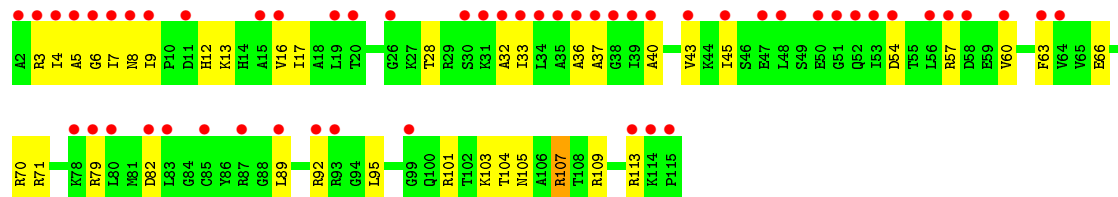


- Molecule 12: 30S ribosomal protein S12

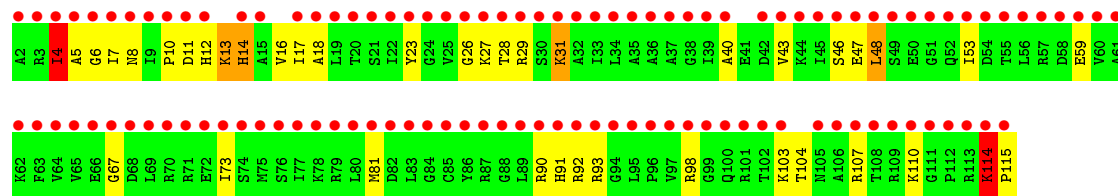




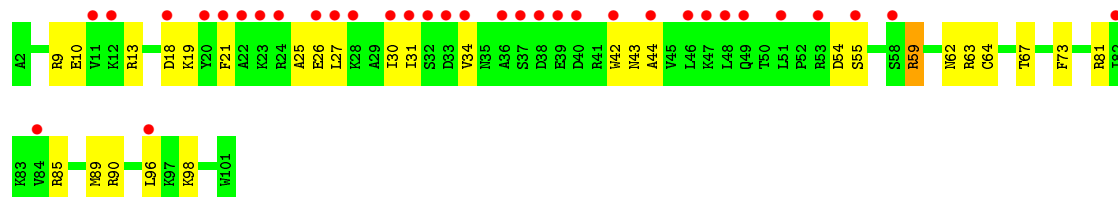
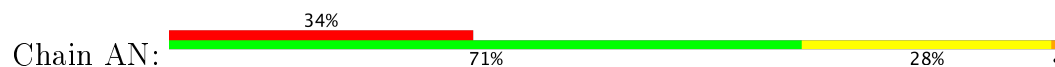
• Molecule 13: 30S ribosomal protein S13



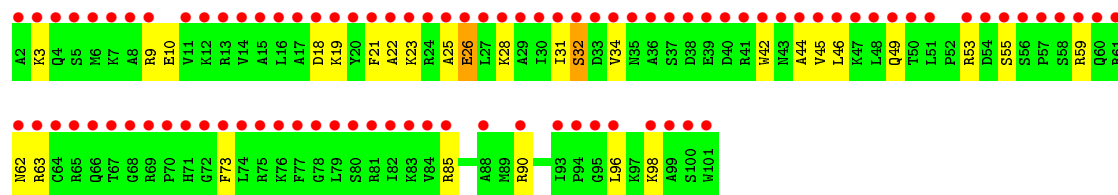
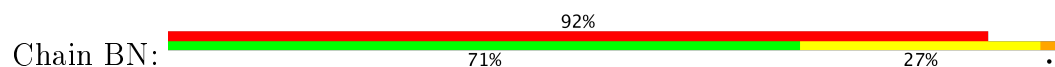
• Molecule 13: 30S ribosomal protein S13



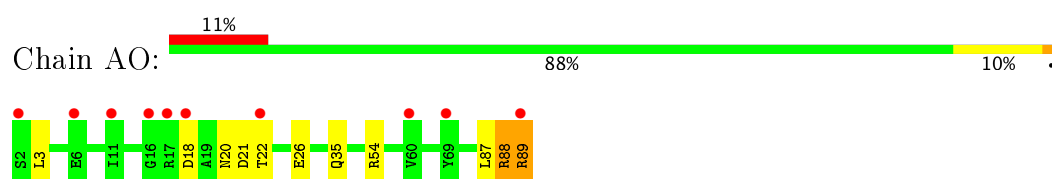
• Molecule 14: 30S ribosomal protein S14



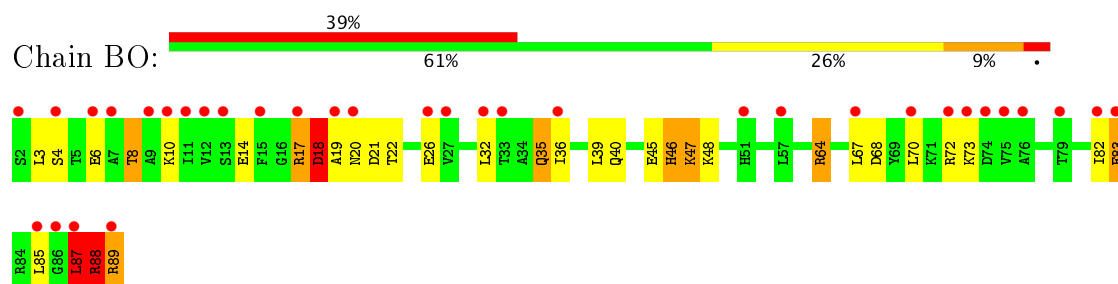
• Molecule 14: 30S ribosomal protein S14



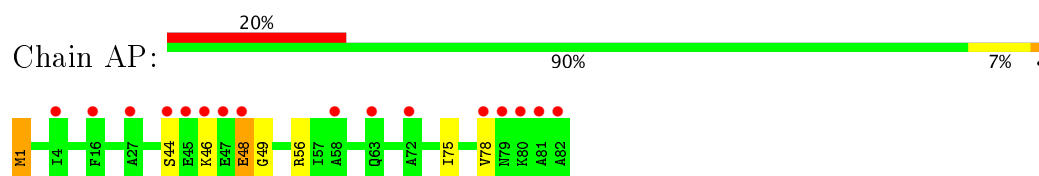
• Molecule 15: 30S ribosomal protein S15



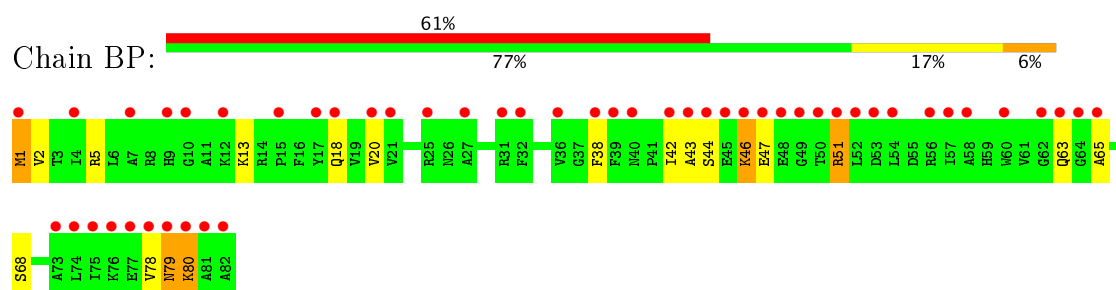
- Molecule 15: 30S ribosomal protein S15



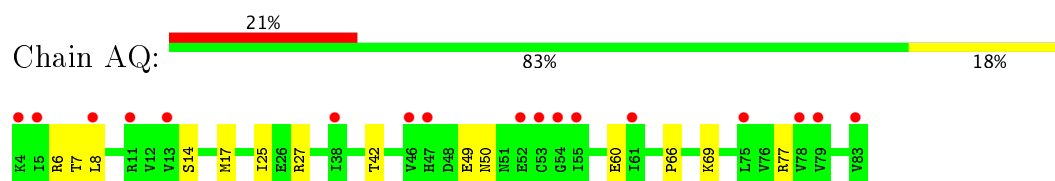
- Molecule 16: 30S ribosomal protein S16



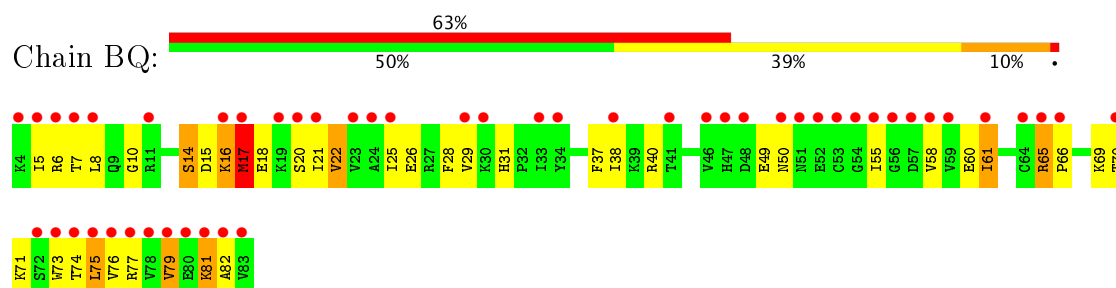
- Molecule 16: 30S ribosomal protein S16



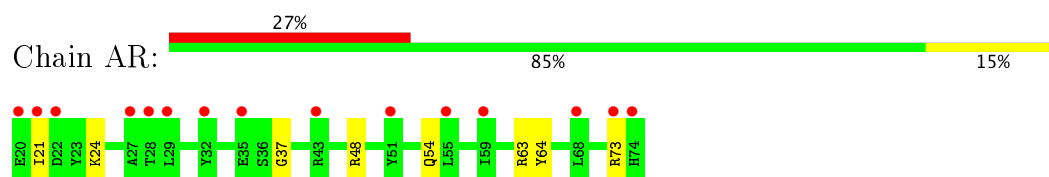
- Molecule 17: 30S ribosomal protein S17



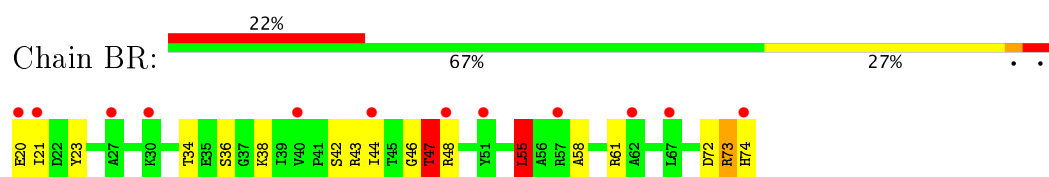
- Molecule 17: 30S ribosomal protein S17



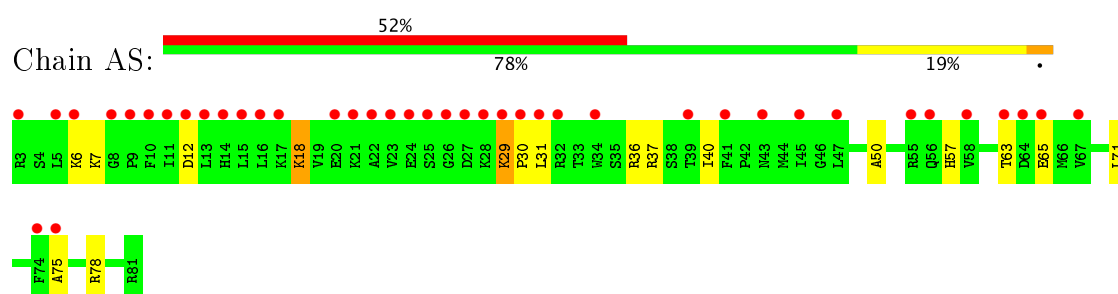
- Molecule 18: 30S ribosomal protein S18



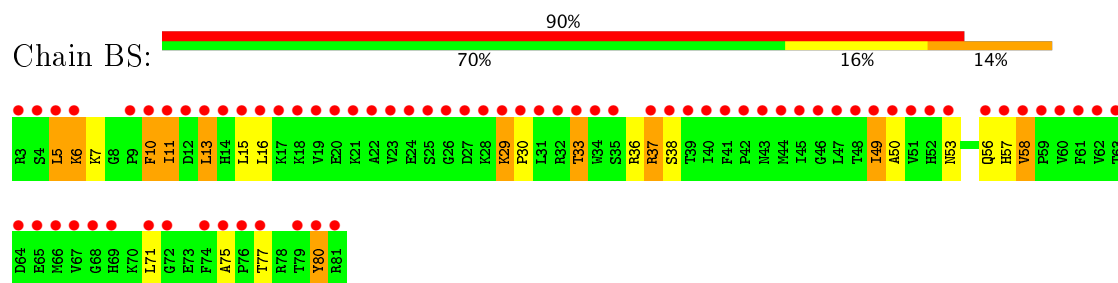
- Molecule 18: 30S ribosomal protein S18



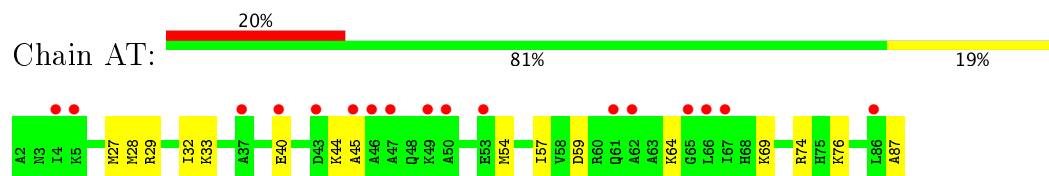
- Molecule 19: 30S ribosomal protein S19



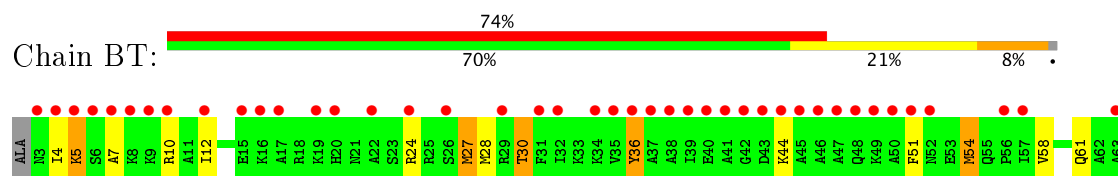
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

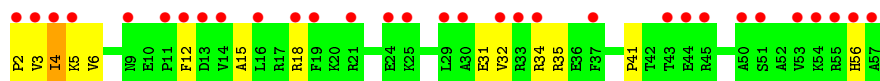
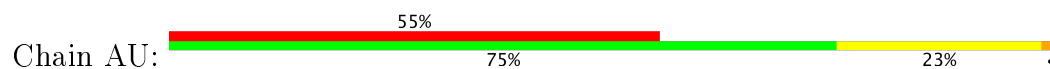


- Molecule 20: 30S ribosomal protein S20

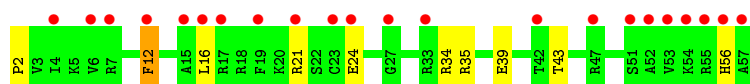
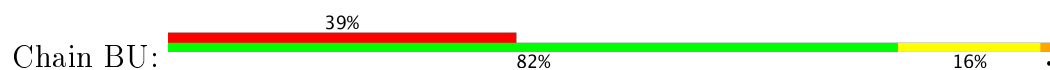




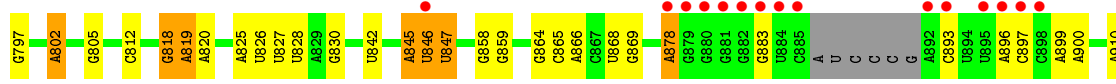
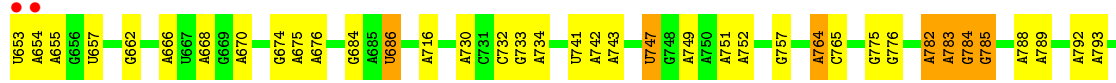
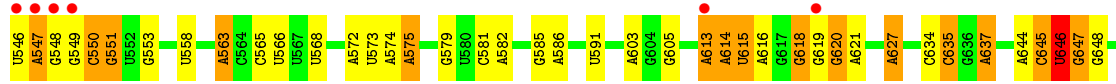
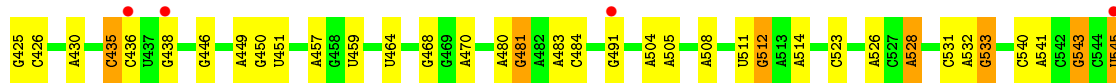
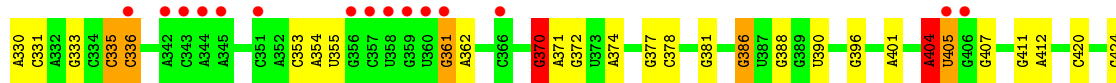
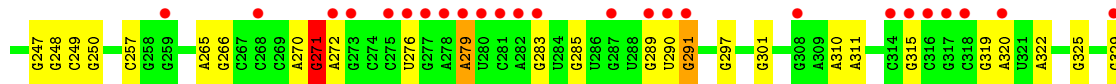
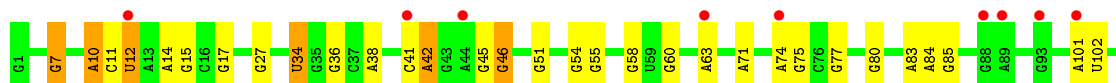
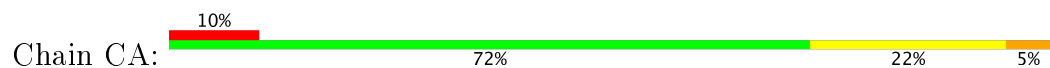
- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21



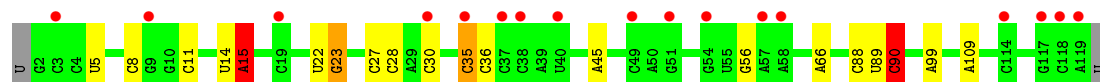
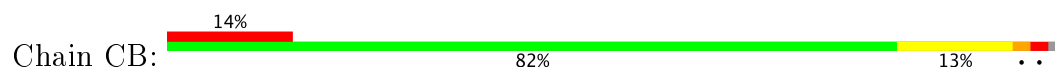
- Molecule 22: 23S rRNA



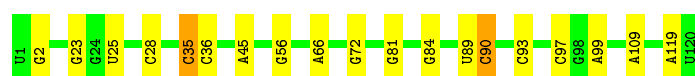
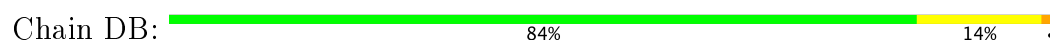




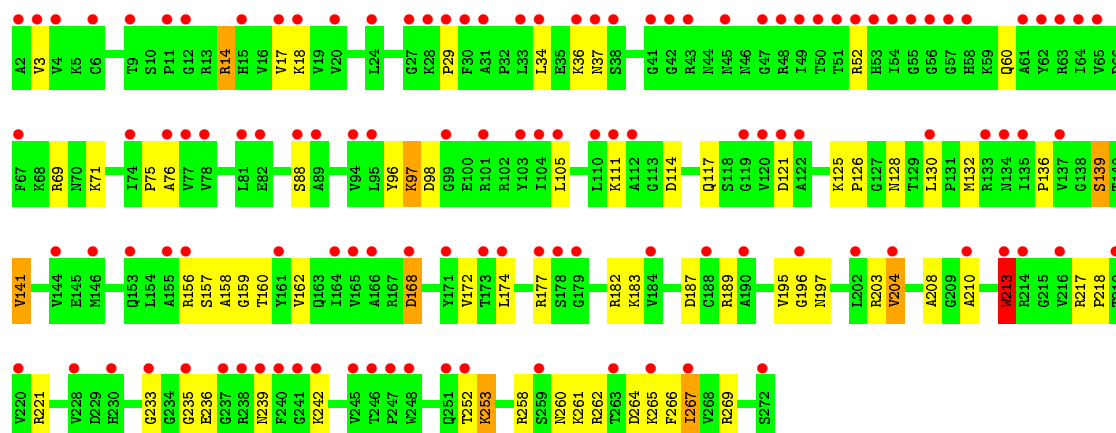
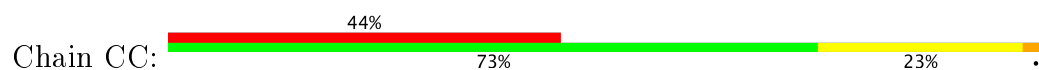
- Molecule 23: 5S rRNA



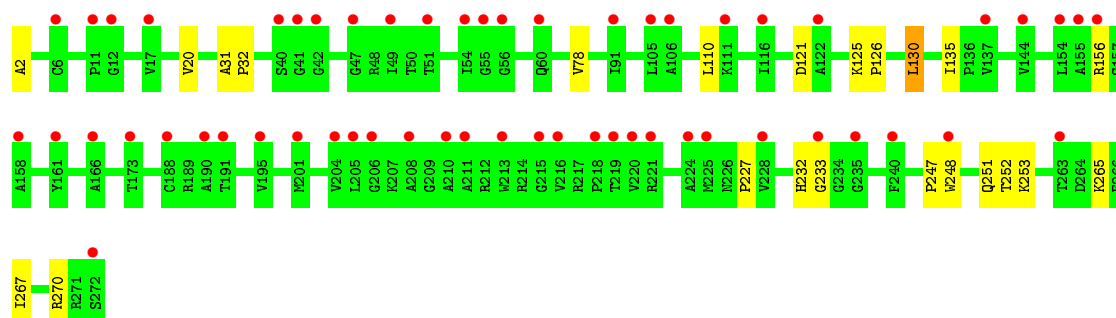
- Molecule 23: 5S rRNA



- Molecule 24: 50S ribosomal protein L2

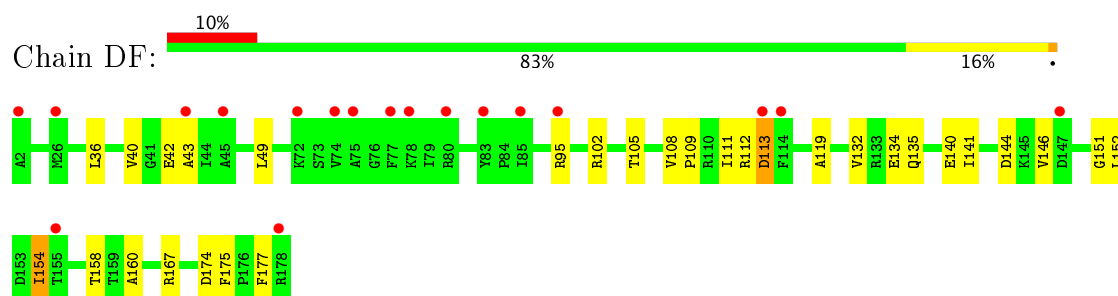


- Molecule 24: 50S ribosomal protein L2

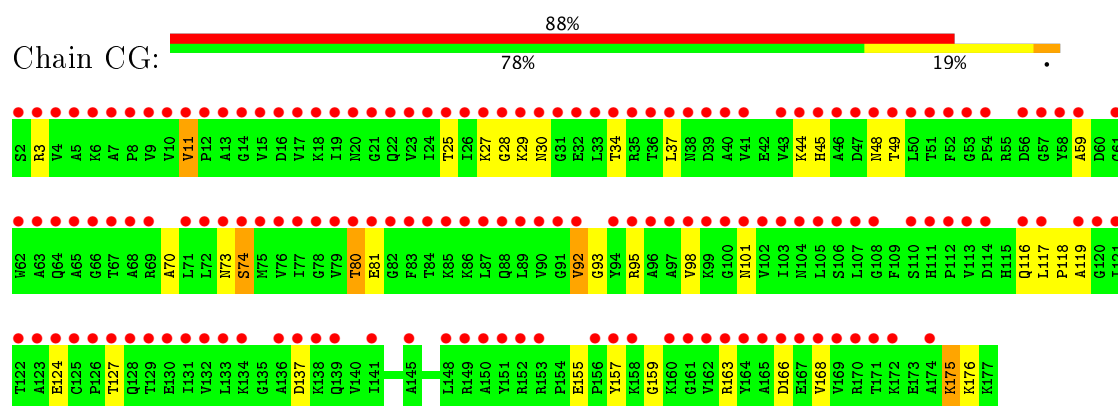


- Molecule 25: 50S ribosomal protein L3

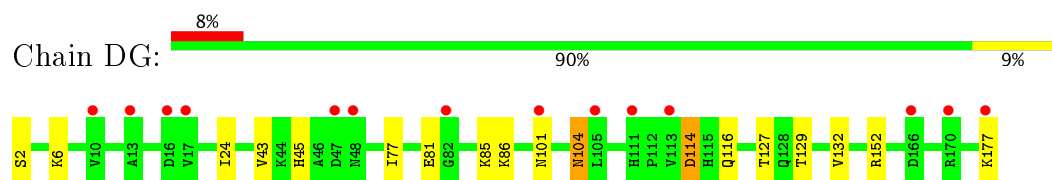
- Molecule 27: 50S ribosomal protein L5



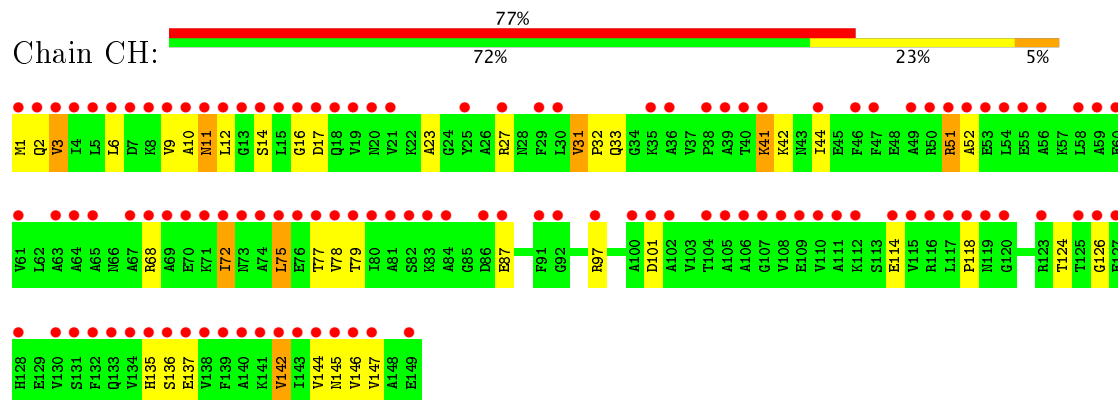
- Molecule 28: 50S ribosomal protein L6



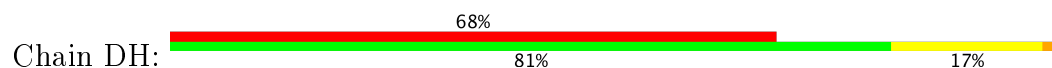
- Molecule 28: 50S ribosomal protein L6

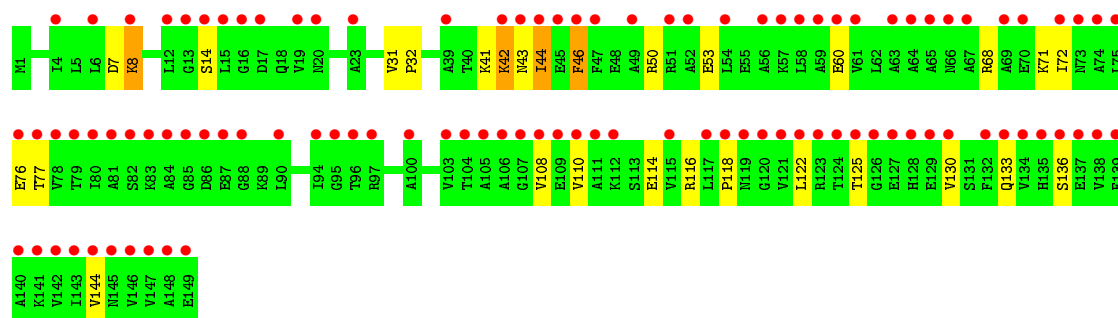


- Molecule 29: 50S ribosomal protein L9

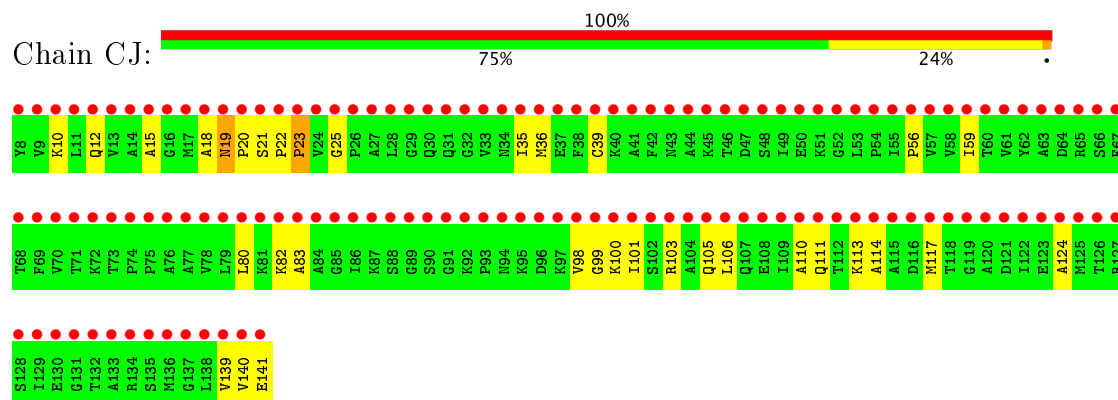


- Molecule 29: 50S ribosomal protein L9

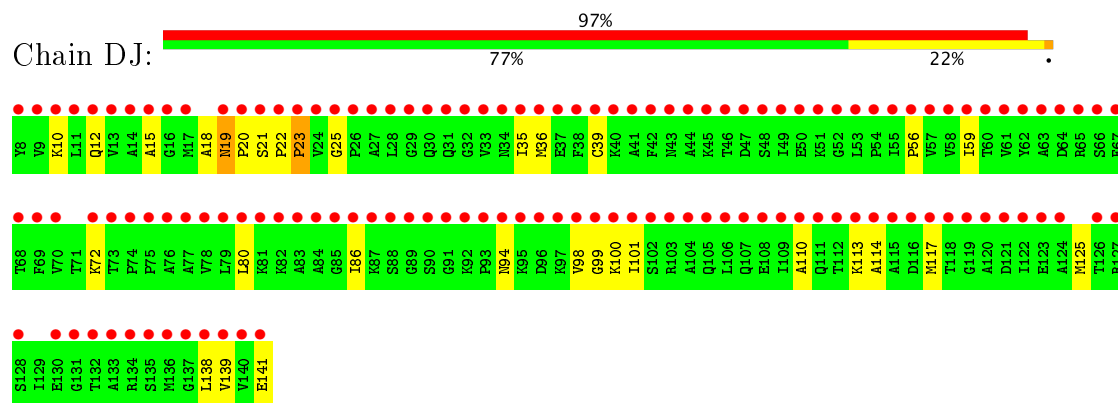




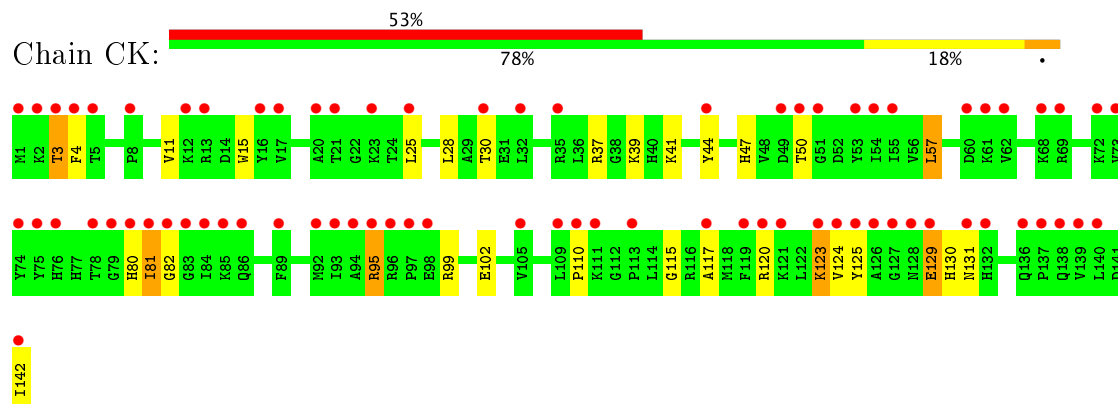
- Molecule 30: 50S ribosomal protein L11



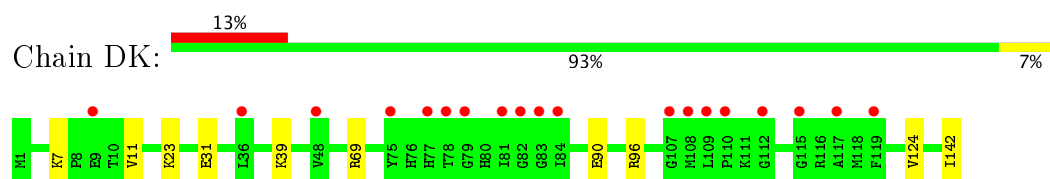
- Molecule 30: 50S ribosomal protein L11



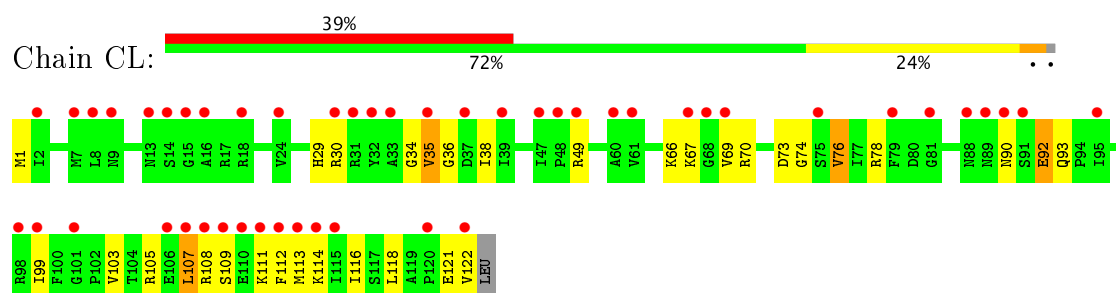
- Molecule 31: 50S ribosomal protein L13



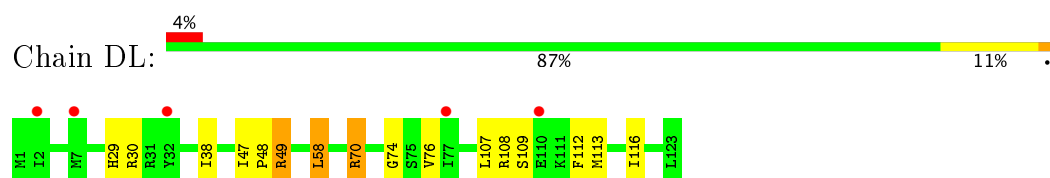
- Molecule 31: 50S ribosomal protein L13



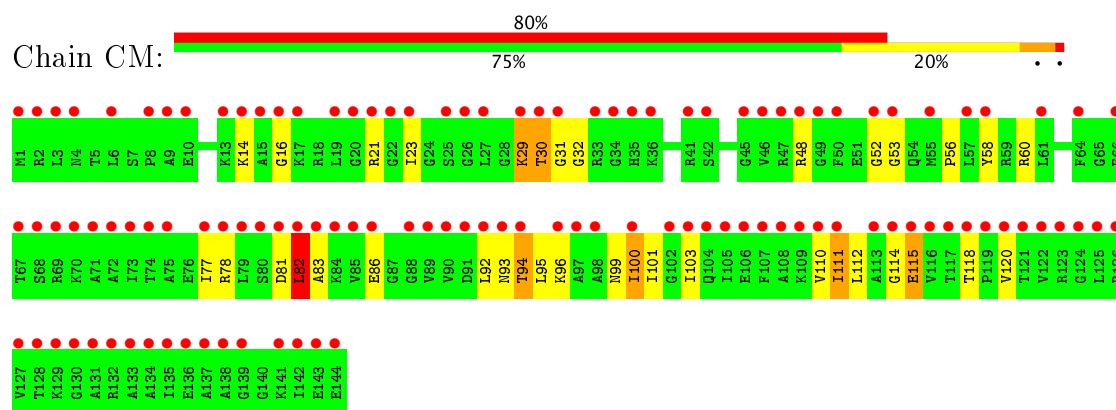
- Molecule 32: 50S ribosomal protein L14



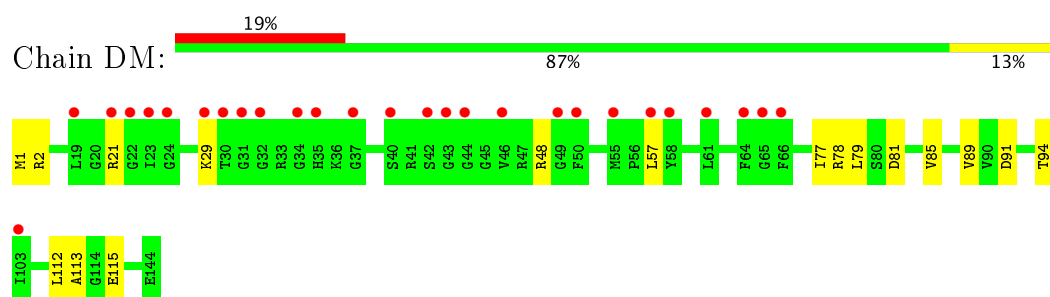
- Molecule 32: 50S ribosomal protein L14



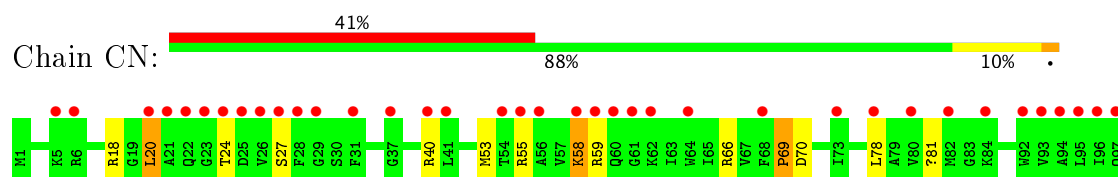
- Molecule 33: 50S ribosomal protein L15



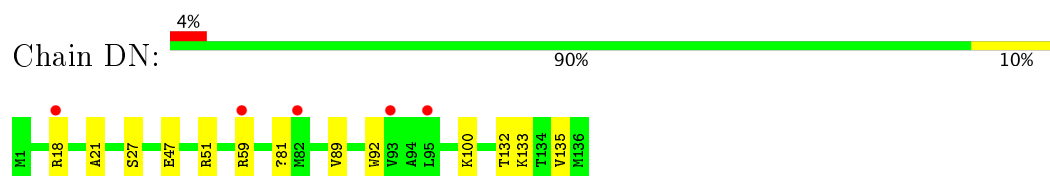
- Molecule 33: 50S ribosomal protein L15



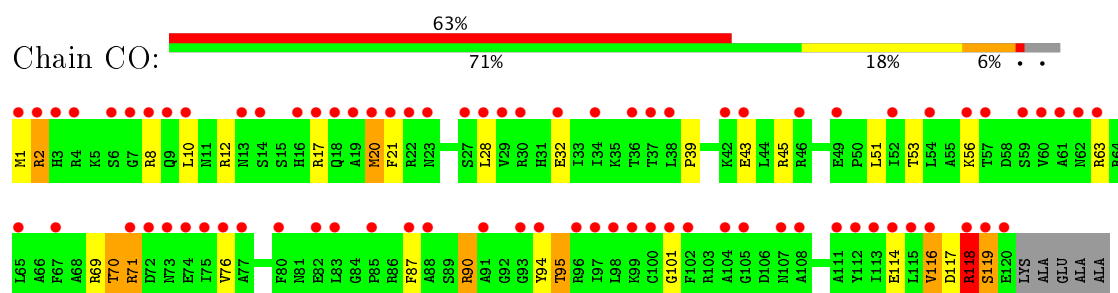
- Molecule 34: 50S ribosomal protein L16



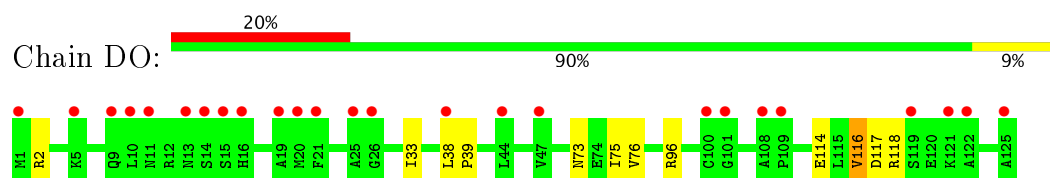
- Molecule 34: 50S ribosomal protein L16



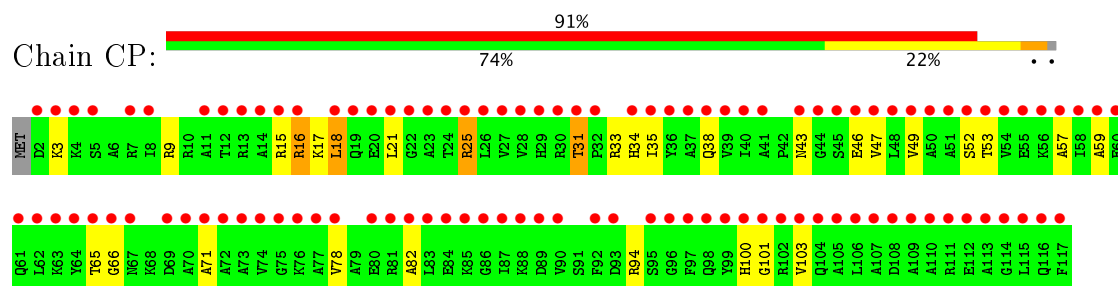
- Molecule 35: 50S ribosomal protein L17



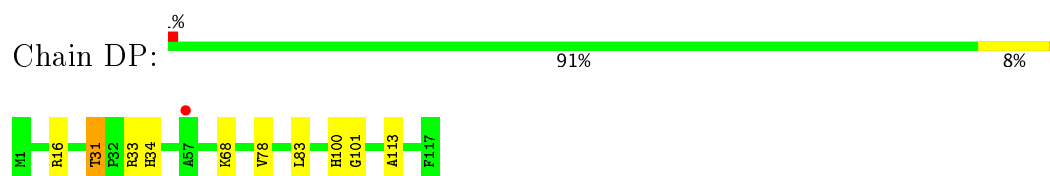
- Molecule 35: 50S ribosomal protein L17



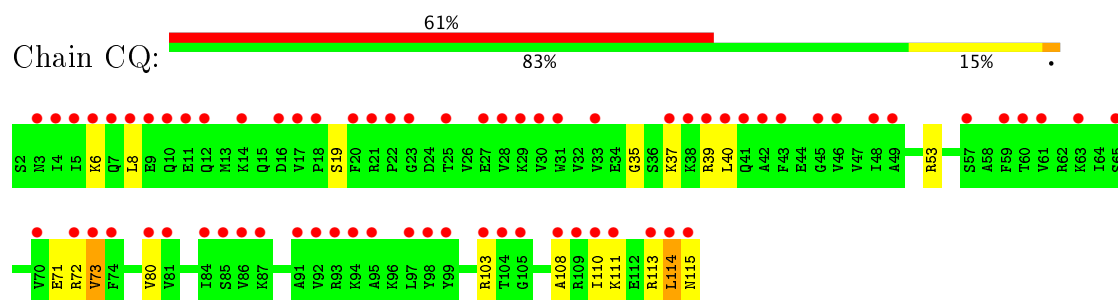
- Molecule 36: 50S ribosomal protein L18



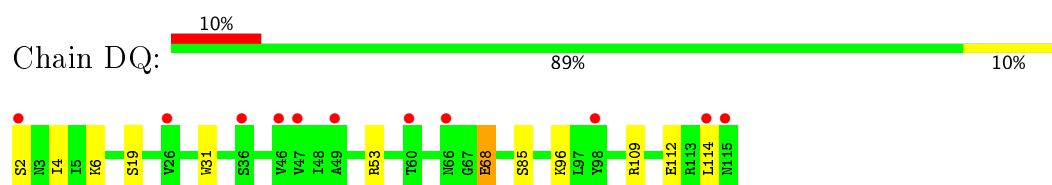
- Molecule 36: 50S ribosomal protein L18



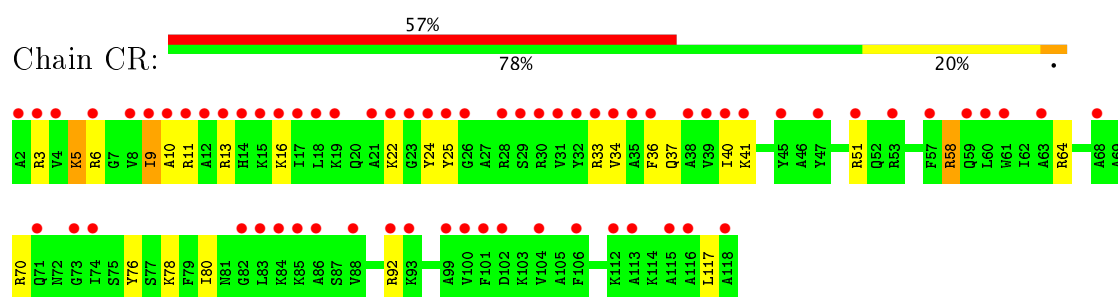
- Molecule 37: 50S ribosomal protein L19



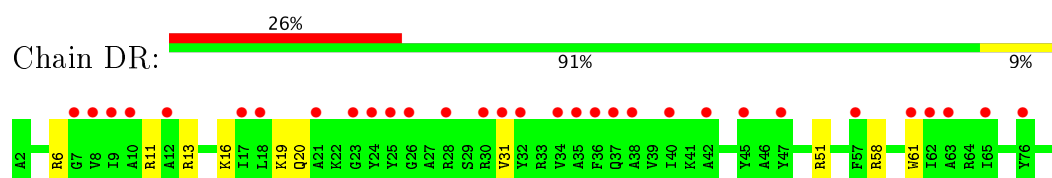
- Molecule 37: 50S ribosomal protein L19



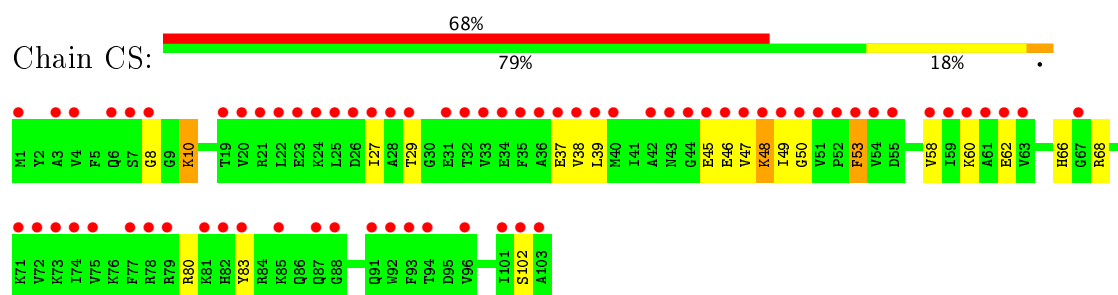
- Molecule 38: 50S ribosomal protein L20



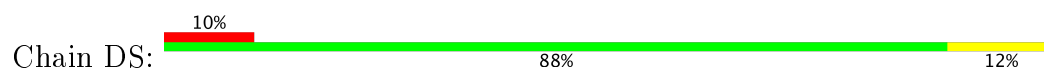
- Molecule 38: 50S ribosomal protein L20

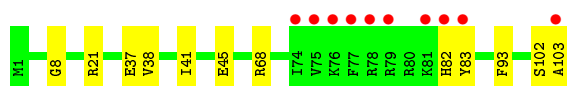


- Molecule 39: 50S ribosomal protein L21

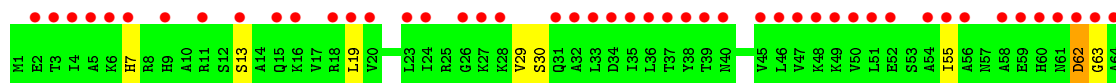
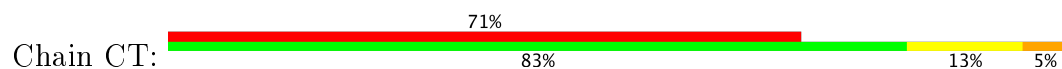


- Molecule 39: 50S ribosomal protein L21

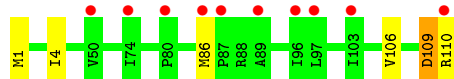




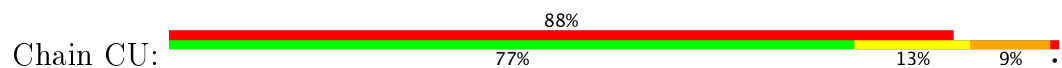
- Molecule 40: 50S ribosomal protein L22



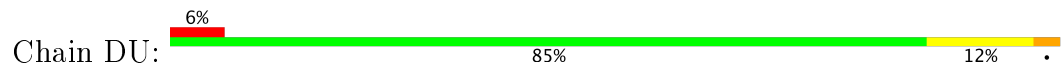
- Molecule 40: 50S ribosomal protein L22



- Molecule 41: 50S ribosomal protein L23



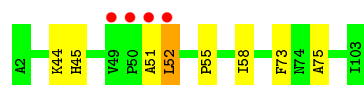
- Molecule 41: 50S ribosomal protein L23



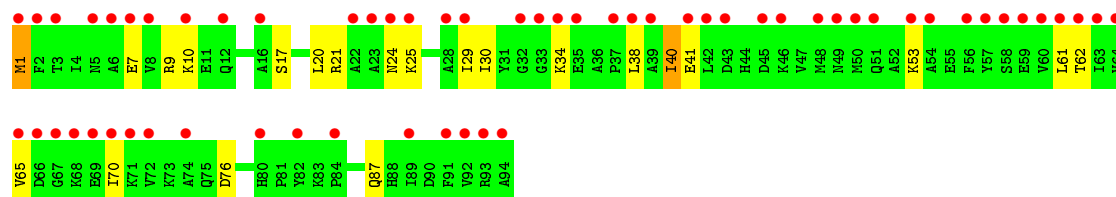
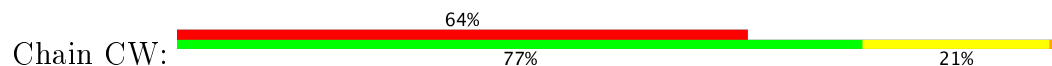
- Molecule 42: 50S ribosomal protein L24



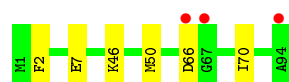
- Molecule 42: 50S ribosomal protein L24



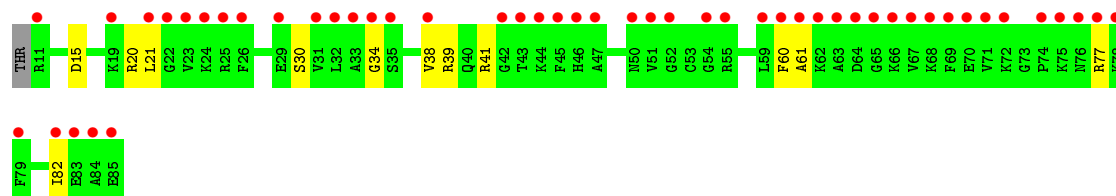
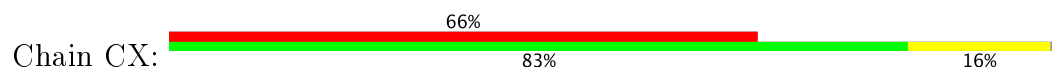
- Molecule 43: 50S ribosomal protein L25



- Molecule 43: 50S ribosomal protein L25



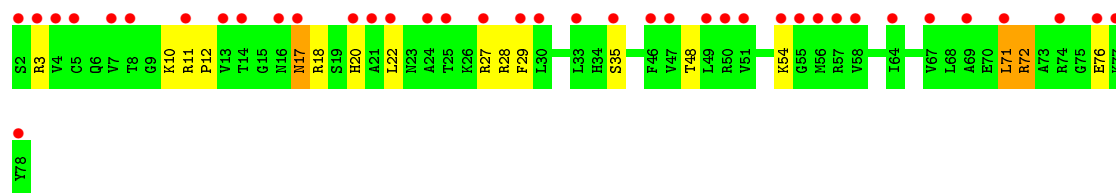
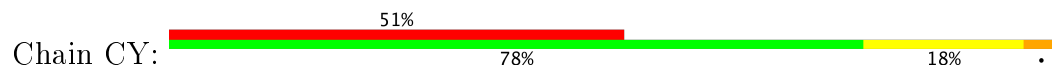
- Molecule 44: 50S ribosomal protein L27



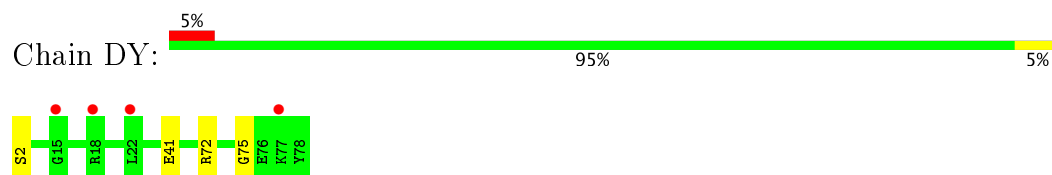
- Molecule 44: 50S ribosomal protein L27



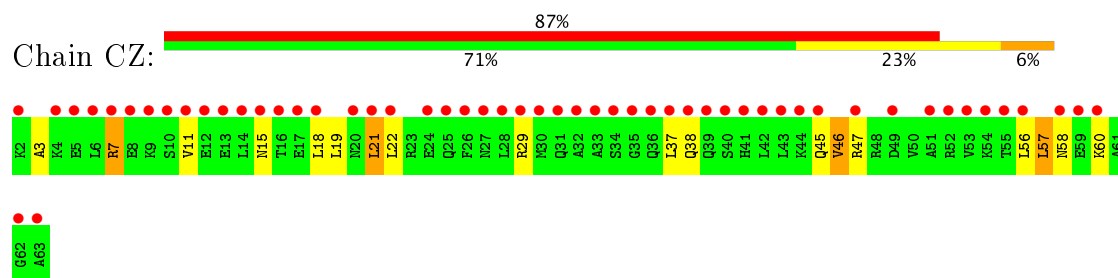
- Molecule 45: 50S ribosomal protein L28



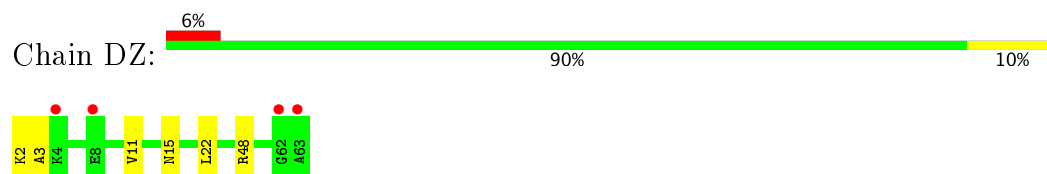
- Molecule 45: 50S ribosomal protein L28



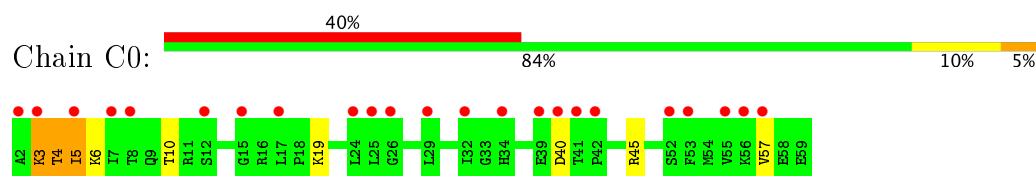
- Molecule 46: 50S ribosomal protein L29



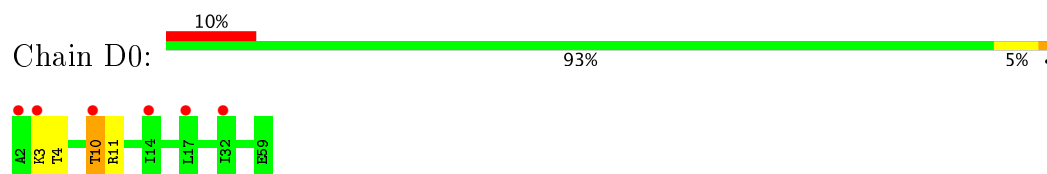
- Molecule 46: 50S ribosomal protein L29



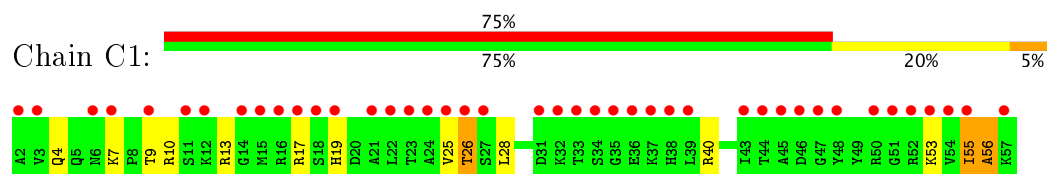
- Molecule 47: 50S ribosomal protein L30



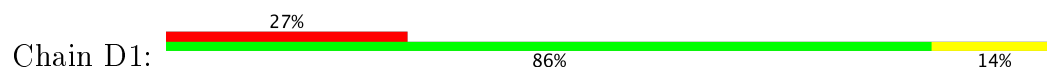
- Molecule 47: 50S ribosomal protein L30

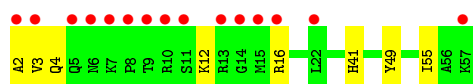


- Molecule 48: 50S ribosomal protein L32

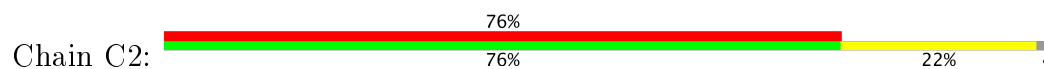


- Molecule 48: 50S ribosomal protein L32

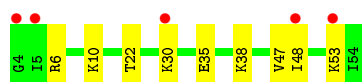
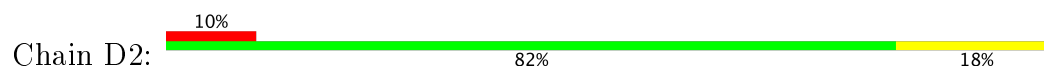




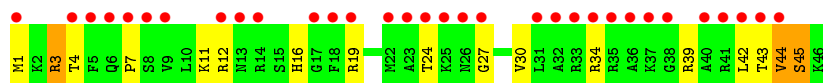
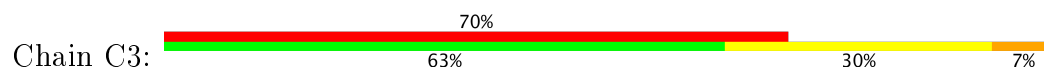
- Molecule 49: 50S ribosomal protein L33



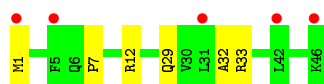
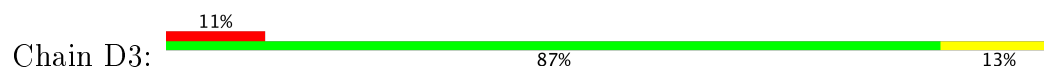
- Molecule 49: 50S ribosomal protein L33



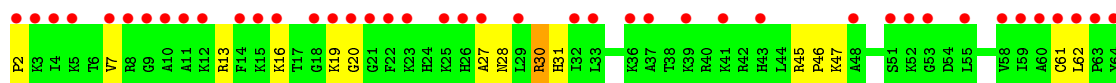
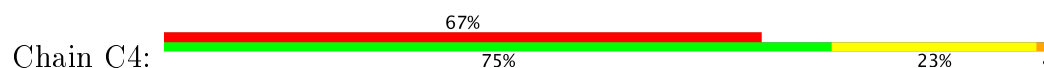
- Molecule 50: 50S ribosomal protein L34



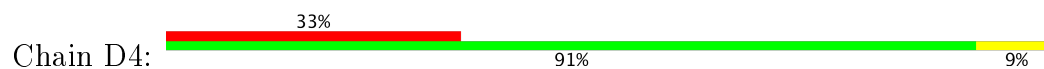
- Molecule 50: 50S ribosomal protein L34



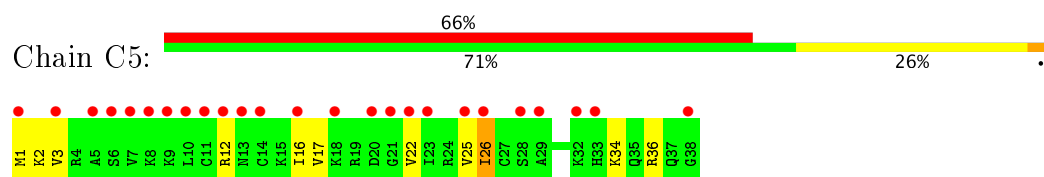
- Molecule 51: 50S ribosomal protein L35



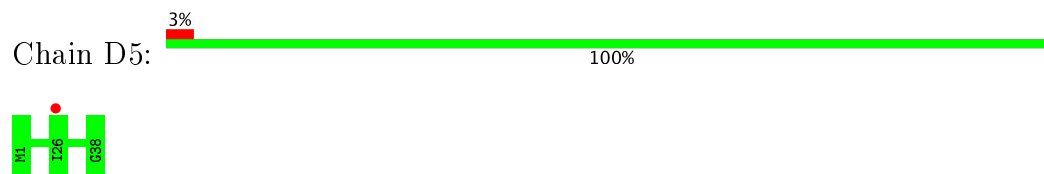
- Molecule 51: 50S ribosomal protein L35



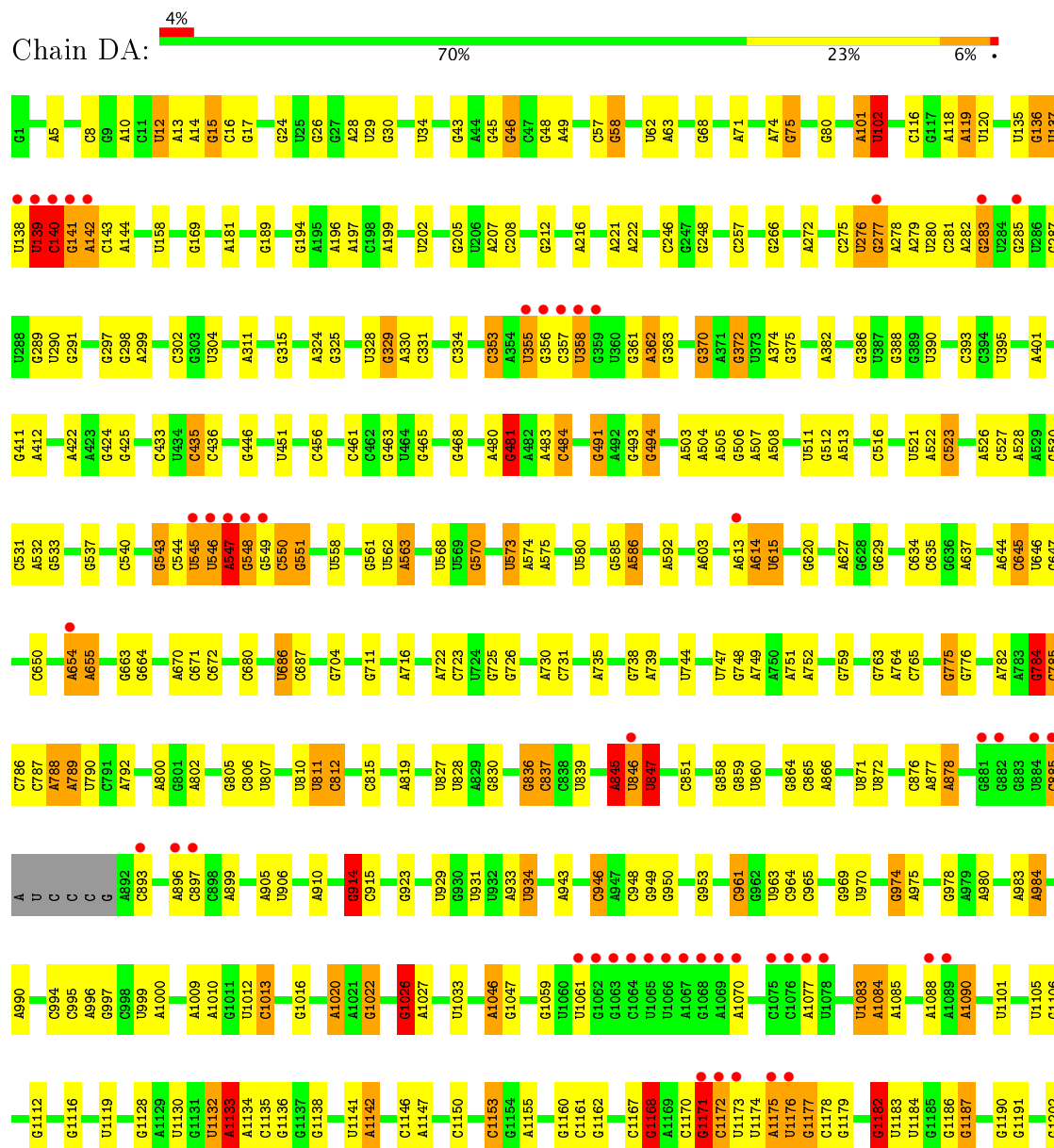
- Molecule 52: 50S ribosomal protein L36

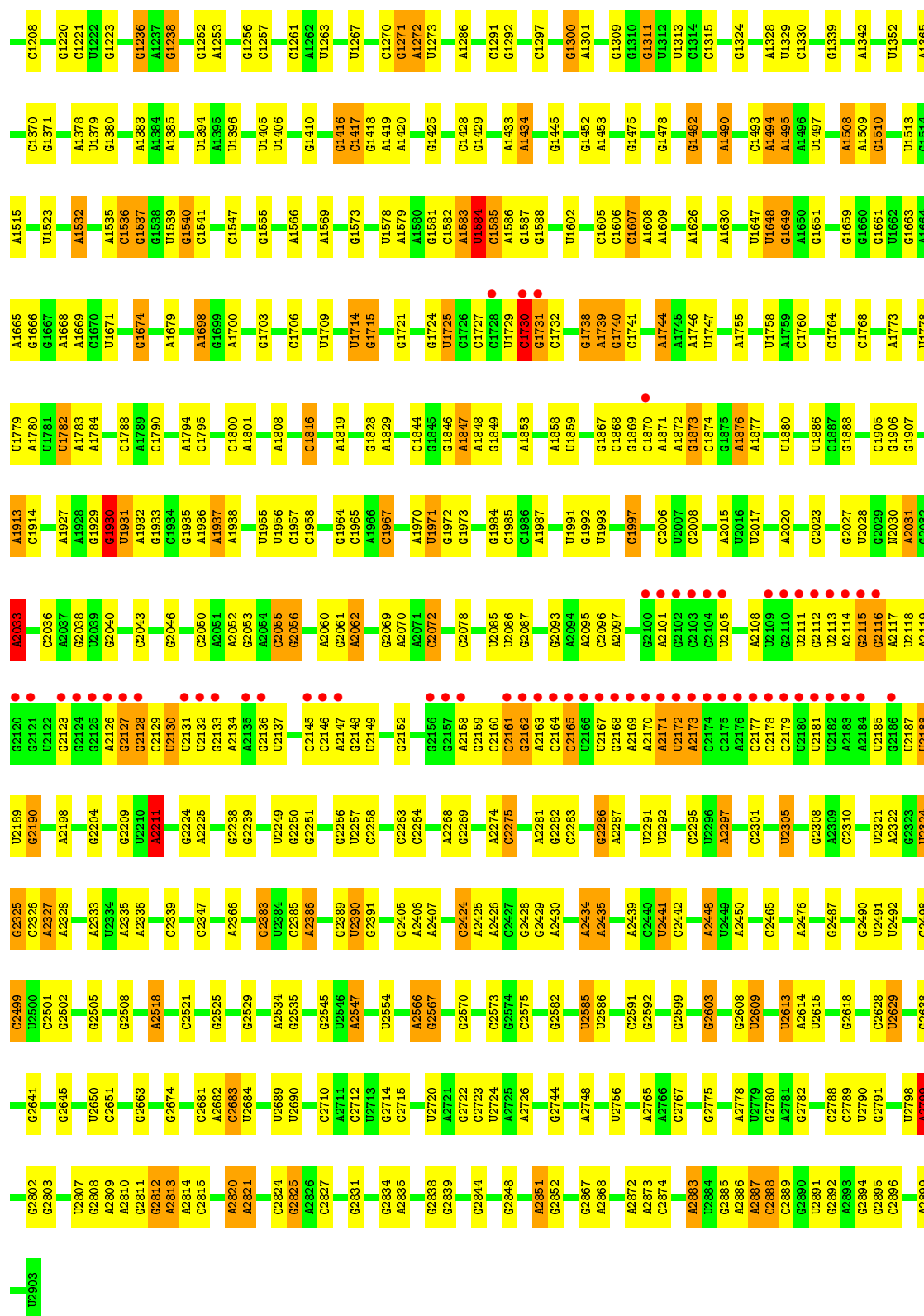


- Molecule 52: 50S ribosomal protein L36

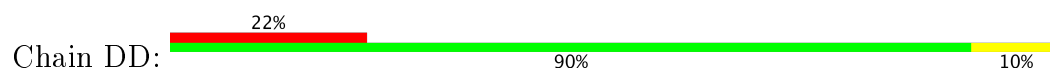


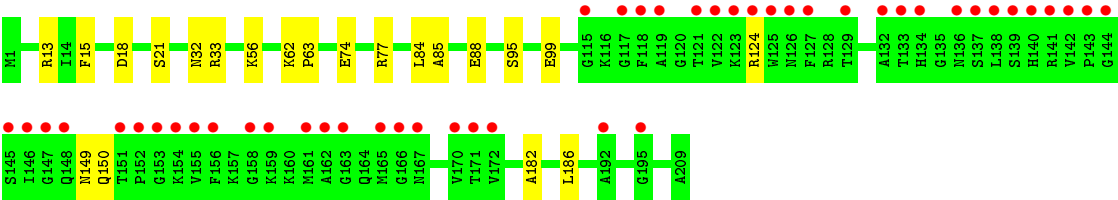
- Molecule 53: 23S rRNA



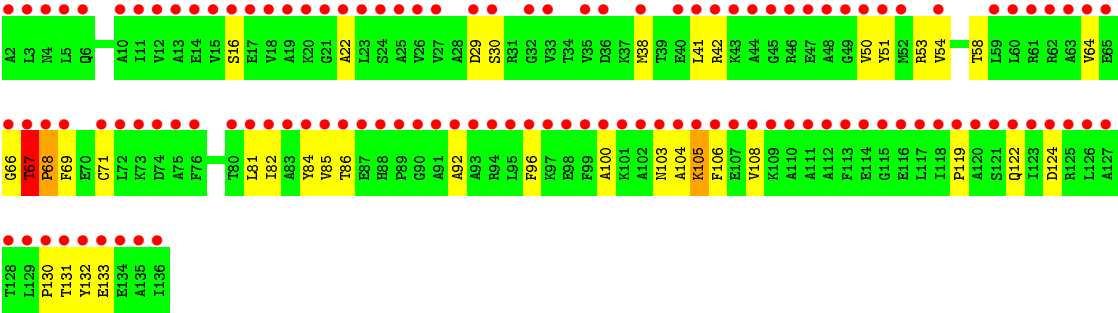
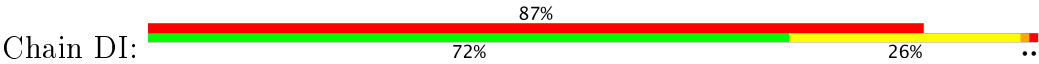


- Molecule 54: 50S ribosomal protein L3





• 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 0.242 , 0.258	Depositor DCC
R_{free} test set	10048 reflections (0.33%)	DCC
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 51.8	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: MA6, GUN, 1PE, 2MA, 2MG, ACY, PEG, 1MG, 3TD, PGE, G7M, D2T, UR3, SPD, 4D4, 5MU, ZN, 5MC, MPD, PG4, 6MZ, TRS, OMC, MG, OMG, H2U, EDO, MEQ, OMU, PUT, 4OC, PSU

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	0.58	0/36593	0.98	33/57081 (0.1%)
1	BA	0.52	0/36568	1.03	90/57042 (0.2%)
2	AB	0.36	0/1784	0.55	0/2403
2	BB	0.39	0/1784	0.59	0/2403
3	AC	0.39	0/1652	0.55	0/2225
3	BC	0.42	0/1652	0.76	0/2225
4	AD	0.37	0/1665	0.53	0/2227
4	BD	0.43	0/1665	0.57	0/2227
5	AE	0.48	0/1157	0.61	0/1557
5	BE	0.56	0/1118	1.07	4/1504 (0.3%)
6	AF	0.43	0/881	0.56	0/1189
6	BF	0.47	0/835	0.90	2/1128 (0.2%)
7	AG	0.35	0/1196	0.51	0/1602
7	BG	0.41	0/1196	0.83	1/1602 (0.1%)
8	AH	0.43	0/989	0.58	0/1326
8	BH	0.38	0/989	0.82	3/1326 (0.2%)
9	AI	0.37	0/1034	0.60	0/1375
9	BI	0.33	0/1034	0.60	0/1375
10	AJ	0.57	0/806	0.68	0/1089
10	BJ	0.73	0/797	0.66	0/1077
11	AK	0.39	0/893	0.54	0/1205
11	BK	0.45	0/893	0.86	0/1205
12	AL	0.49	0/960	0.65	0/1286
12	BL	0.53	0/960	0.93	3/1286 (0.2%)
13	AM	0.38	0/893	0.63	0/1193
13	BM	0.35	0/893	0.90	0/1193
14	AN	0.40	0/817	0.60	0/1088
14	BN	0.49	0/817	0.70	0/1088
15	AO	0.42	0/722	0.52	0/964
15	BO	0.43	0/722	0.88	1/964 (0.1%)
16	AP	0.40	0/659	0.59	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BP	0.48	0/659	0.89	0/884
17	AQ	0.44	0/658	0.61	0/881
17	BQ	0.43	0/658	0.82	0/881
18	AR	0.41	0/463	0.55	0/621
18	BR	0.45	0/463	0.98	1/621 (0.2%)
19	AS	0.37	0/653	0.56	0/877
19	BS	0.43	0/653	0.85	1/877 (0.1%)
20	AT	0.40	0/676	0.53	0/895
20	BT	0.40	0/671	0.82	1/888 (0.1%)
21	AU	0.53	0/472	0.57	0/627
21	BU	0.46	0/472	0.60	0/627
22	CA	0.51	3/69165 (0.0%)	1.00	108/107896 (0.1%)
23	CB	0.41	0/2828	0.90	2/4410 (0.0%)
23	DB	0.79	0/2872	1.12	7/4478 (0.2%)
24	CC	0.40	0/2122	0.76	2/2852 (0.1%)
24	DC	0.57	0/2122	0.71	0/2852
25	CD	0.40	0/1586	0.71	0/2134
26	CE	0.37	0/1571	0.71	2/2113 (0.1%)
26	DE	0.58	0/1571	0.66	0/2113
27	CF	0.33	0/1435	0.75	0/1926
27	DF	0.46	0/1435	0.63	0/1926
28	CG	0.39	0/1343	0.50	0/1816
28	DG	0.53	0/1343	0.61	0/1816
29	CH	0.38	0/1121	0.56	0/1515
29	DH	0.39	0/1121	0.54	0/1515
30	CJ	0.44	0/993	0.63	0/1341
30	DJ	0.48	0/993	0.66	0/1341
31	CK	0.35	0/1152	0.50	0/1551
31	DK	0.69	0/1152	0.75	0/1551
32	CL	0.39	0/947	0.73	0/1268
32	DL	0.64	0/955	0.79	2/1279 (0.2%)
33	CM	0.40	0/1062	0.89	2/1413 (0.1%)
33	DM	0.64	0/1062	0.71	0/1413
34	CN	0.34	0/1081	0.64	0/1443
34	DN	0.64	0/1092	0.73	0/1457
35	CO	0.40	0/973	0.74	1/1301 (0.1%)
35	DO	0.69	0/1006	0.79	1/1345 (0.1%)
36	CP	0.33	0/902	0.68	0/1209
36	DP	0.50	0/910	0.62	0/1219
37	CQ	0.37	0/929	0.71	1/1242 (0.1%)
37	DQ	0.65	0/929	0.68	0/1242
38	CR	0.39	0/960	0.68	0/1278
38	DR	0.74	0/960	0.75	0/1278

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	CS	0.37	0/829	0.73	0/1107
39	DS	0.77	0/829	0.76	1/1107 (0.1%)
40	CT	0.40	0/864	0.75	0/1156
40	DT	0.72	0/864	0.75	0/1156
41	CU	0.39	0/745	0.94	5/994 (0.5%)
41	DU	0.59	0/745	0.72	0/994
42	CV	0.40	0/788	0.87	0/1051
42	DV	0.55	0/788	0.70	0/1051
43	CW	0.29	0/766	0.61	0/1025
43	DW	0.64	0/766	0.67	0/1025
44	CX	0.38	0/576	0.68	0/762
44	DX	0.68	0/598	0.78	2/790 (0.3%)
45	CY	0.36	0/635	0.67	0/848
45	DY	0.58	0/635	0.70	0/848
46	CZ	0.34	0/502	0.77	0/667
46	DZ	0.54	0/502	0.58	0/667
47	C0	0.34	0/453	0.69	0/605
47	D0	0.65	0/467	0.71	0/623
48	C1	0.42	0/450	0.73	0/599
48	D1	0.65	0/450	0.73	0/599
49	C2	0.43	0/416	0.71	0/554
49	D2	0.60	0/421	0.66	0/561
50	C3	0.46	0/380	0.81	0/498
50	D3	0.66	0/380	0.84	0/498
51	C4	0.37	0/513	0.70	0/676
51	D4	0.56	0/513	0.64	0/676
52	C5	0.38	0/303	0.98	1/397 (0.3%)
52	D5	0.62	0/303	0.81	0/397
53	DA	1.00	34/69295 (0.0%)	1.31	473/108100 (0.4%)
54	DD	0.72	0/1576	0.76	2/2119 (0.1%)
55	DI	0.42	0/1037	0.60	0/1402
All	All	0.65	37/309204 (0.0%)	1.02	752/462103 (0.2%)

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 (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CA	1936	A	N9-C4	-9.34	1.32	1.37
53	DA	463	G	C8-N7	6.92	1.35	1.30
53	DA	1330	C	C4-C5	-6.51	1.37	1.43
53	DA	465	G	C6-N1	-6.50	1.35	1.39
53	DA	1679	A	N7-C5	-6.28	1.35	1.39
53	DA	2269	G	C8-N7	6.27	1.34	1.30
53	DA	800	A	C5-C4	-6.17	1.34	1.38
53	DA	680	C	N1-C6	-5.92	1.33	1.37
53	DA	654	A	N9-C4	5.83	1.41	1.37
53	DA	788	A	N3-C4	-5.74	1.31	1.34
53	DA	516	C	P-OP2	-5.69	1.39	1.49
53	DA	1607	C	P-O5'	-5.63	1.54	1.59
53	DA	1847	A	N9-C4	5.57	1.41	1.37
53	DA	573	U	P-OP2	-5.56	1.39	1.49
53	DA	2641	G	C8-N7	5.55	1.34	1.30
53	DA	527	C	N1-C6	-5.49	1.33	1.37
53	DA	2892	G	P-O5'	-5.43	1.54	1.59
22	CA	528	A	N9-C4	-5.35	1.34	1.37
53	DA	1147	A	C6-N1	-5.32	1.31	1.35
53	DA	819	A	C6-N1	-5.29	1.31	1.35
53	DA	2641	G	N3-C4	-5.26	1.31	1.35
53	DA	2040	G	C6-N1	-5.25	1.35	1.39
53	DA	2052	A	N9-C4	-5.25	1.34	1.37
22	CA	1132	U	O3'-P	5.24	1.67	1.61
53	DA	2249	U	C2-N3	-5.24	1.34	1.37
53	DA	586	A	N3-C4	-5.23	1.31	1.34
53	DA	2499	C	P-OP1	-5.22	1.40	1.49
53	DA	2336	A	N3-C4	-5.19	1.31	1.34
53	DA	30	G	N3-C4	-5.18	1.31	1.35
53	DA	1671	U	C2-N3	-5.16	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	DA	2442	C	C4-C5	-5.12	1.38	1.43
53	DA	2053	G	O3'-P	-5.12	1.55	1.61
53	DA	1666	G	N9-C4	5.10	1.42	1.38
53	DA	1263	U	C2-N3	-5.09	1.34	1.37
53	DA	1937	A	N3-C4	-5.08	1.31	1.34
53	DA	1844	C	N1-C6	-5.07	1.34	1.37
53	DA	1992	G	N7-C5	-5.04	1.36	1.39

All (752) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	1997	C	O5'-P-OP2	-13.03	93.98	105.70
53	DA	574	A	O5'-P-OP1	-12.59	94.37	105.70
53	DA	914	G	N1-C6-O6	12.55	127.43	119.90
22	CA	963	U	O5'-P-OP2	-12.45	94.50	105.70
22	CA	948	C	O5'-P-OP1	-11.07	95.74	105.70
53	DA	2499	C	N1-C2-O2	-10.91	112.35	118.90
53	DA	751	A	O5'-P-OP1	-10.83	95.95	105.70
53	DA	570	G	C5-C6-O6	-10.70	122.18	128.60
53	DA	512	G	O4'-C1'-N9	10.69	116.75	108.20
1	BA	330	C	O4'-C1'-N1	10.34	116.47	108.20
22	CA	2250	G	O4'-C1'-N9	-10.33	99.94	108.20
53	DA	570	G	C4-C5-N7	10.17	114.87	110.80
22	CA	1936	A	C2-N3-C4	-10.09	105.55	110.60
53	DA	2813	A	N1-C6-N6	10.06	124.64	118.60
53	DA	847	U	O5'-P-OP2	-9.90	96.79	105.70
1	BA	412	A	O4'-C1'-N9	9.85	116.08	108.20
53	DA	2448	A	O5'-P-OP2	-9.79	96.89	105.70
5	BE	104	GLY	N-CA-C	9.67	137.28	113.10
53	DA	1987	A	O5'-P-OP2	-9.66	97.01	105.70
53	DA	963	U	O5'-P-OP2	-9.57	97.08	105.70
53	DA	1663	G	O5'-P-OP2	-9.54	97.12	105.70
1	AA	117	G	O5'-P-OP2	-9.50	97.15	105.70
1	BA	558	G	O5'-P-OP1	-9.50	97.15	105.70
53	DA	29	U	O5'-P-OP2	-9.44	97.21	105.70
53	DA	574	A	O5'-P-OP2	9.36	121.94	110.70
53	DA	1648	U	O5'-P-OP1	-9.10	97.51	105.70
53	DA	2450	A	O5'-P-OP2	-9.06	97.55	105.70
53	DA	1935	G	O5'-P-OP2	-8.98	97.61	105.70
22	CA	1936	A	N3-C4-N9	-8.96	120.23	127.40
53	DA	802	A	O5'-P-OP1	-8.93	97.67	105.70
22	CA	1272	A	O5'-P-OP1	-8.89	97.70	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	914	G	C5-C6-O6	-8.88	123.27	128.60
53	DA	738	G	O5'-P-OP2	-8.85	97.74	105.70
53	DA	329	G	O5'-P-OP2	-8.72	97.85	105.70
1	BA	632	U	N3-C2-O2	-8.67	116.13	122.20
53	DA	1134	A	O5'-P-OP1	-8.67	97.90	105.70
22	CA	1936	A	N3-C4-C5	8.57	132.80	126.80
53	DA	465	G	N3-C2-N2	8.57	125.90	119.90
53	DA	1010	A	O5'-P-OP2	-8.57	97.99	105.70
53	DA	2848	G	O4'-C1'-N9	8.53	115.02	108.20
53	DA	1965	C	O5'-P-OP2	-8.45	98.09	105.70
53	DA	1026	G	O5'-P-OP1	-8.40	98.14	105.70
53	DA	1605	C	N1-C2-O2	-8.38	113.88	118.90
22	CA	752	A	O4'-C1'-N9	8.30	114.84	108.20
22	CA	2250	G	C4-N9-C1'	8.27	137.25	126.50
53	DA	2275	C	O5'-P-OP2	-8.24	98.29	105.70
1	BA	209	U	C2-N1-C1'	8.23	127.58	117.70
53	DA	1272	A	O5'-P-OP1	-8.23	98.29	105.70
41	CU	3	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	BA	632	U	N1-C2-O2	8.15	128.50	122.80
53	DA	2645	G	O4'-C1'-N9	8.14	114.72	108.20
1	BA	1397	C	C2-N1-C1'	8.12	127.73	118.80
53	DA	1779	U	N1-C2-O2	-8.11	117.12	122.80
53	DA	974	G	C5-C6-O6	8.08	133.45	128.60
1	BA	330	C	C2-N1-C1'	-8.07	109.92	118.80
12	BL	14	ARG	CG-CD-NE	8.06	128.73	111.80
53	DA	570	G	C6-C5-N7	-8.05	125.57	130.40
53	DA	465	G	C5-C6-O6	8.04	133.42	128.60
22	CA	2326	C	P-O3'-C3'	8.02	129.33	119.70
53	DA	914	G	C6-C5-N7	-8.01	125.59	130.40
53	DA	2868	A	O5'-P-OP2	-7.99	98.51	105.70
53	DA	463	G	N9-C4-C5	7.91	108.56	105.40
53	DA	570	G	N1-C6-O6	7.91	124.64	119.90
53	DA	763	G	O5'-P-OP1	-7.86	98.63	105.70
53	DA	1434	A	O4'-C1'-N9	7.84	114.47	108.20
1	BA	1110	A	O4'-C1'-N9	-7.83	101.94	108.20
53	DA	739	A	N1-C6-N6	7.78	123.27	118.60
53	DA	672	C	N3-C4-C5	7.75	125.00	121.90
1	BA	452	A	O4'-C1'-N9	-7.75	102.00	108.20
53	DA	1847	A	N7-C8-N9	7.74	117.67	113.80
53	DA	570	G	C5-N7-C8	-7.68	100.46	104.30
12	BL	85	GLY	N-CA-C	-7.66	93.95	113.10
53	DA	1134	A	OP1-P-OP2	7.64	131.06	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	207	C	C6-N1-C2	-7.63	117.25	120.30
53	DA	1997	C	O5'-P-OP1	7.63	119.86	110.70
53	DA	1630	A	O5'-P-OP2	-7.62	98.84	105.70
22	CA	1171	G	O4'-C1'-N9	7.62	114.29	108.20
41	CU	3	ARG	N-CA-C	-7.59	90.52	111.00
1	BA	330	C	C6-N1-C1'	7.51	129.81	120.80
53	DA	1328	A	O5'-P-OP2	-7.51	98.94	105.70
1	BA	1042	A	O5'-P-OP2	-7.50	98.95	105.70
1	BA	1001	C	C6-N1-C2	-7.48	117.31	120.30
53	DA	704	G	O4'-C1'-N9	7.48	114.18	108.20
22	CA	481	G	O4'-C1'-N9	7.47	114.17	108.20
53	DA	2820	A	C8-N9-C4	7.45	108.78	105.80
22	CA	528	A	C2-N3-C4	-7.45	106.88	110.60
22	CA	2425	A	P-O3'-C3'	7.42	128.60	119.70
44	DX	39	ARG	NE-CZ-NH1	7.42	124.01	120.30
53	DA	12	U	C2-N1-C1'	7.42	126.60	117.70
53	DA	1584	U	N1-C2-O2	7.40	127.98	122.80
53	DA	481	G	O4'-C1'-N9	7.40	114.12	108.20
53	DA	807	U	N3-C4-O4	7.36	124.55	119.40
53	DA	465	G	N1-C2-N2	-7.35	109.58	116.20
53	DA	1584	U	C2-N1-C1'	7.35	126.52	117.70
1	BA	211	G	C4-N9-C1'	7.34	136.04	126.50
22	CA	943	A	O5'-P-OP2	-7.34	99.10	105.70
39	DS	68	ARG	NE-CZ-NH1	-7.33	116.63	120.30
22	CA	995	C	O4'-C1'-N1	-7.33	102.34	108.20
1	BA	183	C	C2-N1-C1'	7.32	126.85	118.80
53	DA	1784	A	N1-C6-N6	7.32	122.99	118.60
1	BA	467	U	C2-N1-C1'	7.30	126.47	117.70
53	DA	1271	G	OP1-P-OP2	-7.30	108.64	119.60
53	DA	116	C	N3-C4-N4	-7.29	112.90	118.00
53	DA	2813	A	C5-C6-N6	-7.28	117.88	123.70
22	CA	511	U	O5'-P-OP2	-7.27	99.16	105.70
33	CM	52	GLY	N-CA-C	-7.25	94.98	113.10
53	DA	140	C	C6-N1-C2	-7.24	117.41	120.30
53	DA	2046	G	C2-N3-C4	-7.23	108.29	111.90
53	DA	731	C	O5'-P-OP2	-7.20	99.22	105.70
53	DA	2036	C	O5'-P-OP2	-7.19	99.23	105.70
1	BA	576	C	O5'-P-OP2	-7.18	99.23	105.70
53	DA	1220	G	N1-C2-N2	-7.18	109.74	116.20
1	BA	532	A	N1-C6-N6	7.17	122.90	118.60
22	CA	2072	C	O5'-P-OP2	-7.17	99.25	105.70
53	DA	12	U	C6-N1-C2	-7.17	116.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	2490	G	O5'-P-OP2	-7.15	99.26	105.70
53	DA	463	G	C8-N9-C4	-7.14	103.54	106.40
53	DA	946	C	N1-C2-O2	-7.12	114.63	118.90
53	DA	181	A	N9-C4-C5	7.12	108.65	105.80
53	DA	2575	C	N1-C2-O2	7.10	123.16	118.90
53	DA	1937	A	O4'-C1'-N9	7.08	113.86	108.20
1	BA	632	U	C2-N1-C1'	7.08	126.19	117.70
53	DA	102	U	C2-N1-C1'	7.08	126.19	117.70
1	BA	4	U	C2-N1-C1'	7.06	126.17	117.70
22	CA	900	A	O4'-C1'-N9	7.04	113.83	108.20
53	DA	139	U	N1-C2-O2	7.03	127.72	122.80
53	DA	2263	C	N3-C4-C5	7.02	124.71	121.90
53	DA	2883	A	O5'-P-OP2	-7.02	99.38	105.70
53	DA	2641	G	C5-C6-O6	7.00	132.80	128.60
22	CA	1378	A	P-O3'-C3'	6.99	128.09	119.70
53	DA	2641	G	N3-C4-N9	-6.98	121.81	126.00
53	DA	1286	A	O5'-P-OP2	-6.98	99.42	105.70
53	DA	2407	A	O5'-P-OP1	-6.98	99.42	105.70
53	DA	1668	A	O5'-P-OP2	-6.97	99.43	105.70
53	DA	1768	C	O5'-P-OP2	-6.97	99.43	105.70
53	DA	1706	C	O4'-C1'-N1	6.96	113.77	108.20
22	CA	2225	A	P-O3'-C3'	6.96	128.06	119.70
53	DA	208	C	O5'-P-OP2	-6.96	99.44	105.70
53	DA	672	C	C5-C4-N4	-6.94	115.34	120.20
1	BA	792	A	O4'-C1'-N9	6.92	113.74	108.20
53	DA	570	G	N9-C4-C5	-6.91	102.64	105.40
53	DA	2820	A	N1-C6-N6	6.91	122.74	118.60
22	CA	757	G	N3-C4-C5	6.89	132.04	128.60
53	DA	1602	U	N3-C4-O4	-6.89	114.58	119.40
1	AA	4	U	C2-N1-C1'	6.88	125.95	117.70
1	AA	1279	G	C4-N9-C1'	6.87	135.43	126.50
53	DA	1297	C	N3-C2-O2	-6.87	117.09	121.90
53	DA	671	C	C6-N1-C2	-6.87	117.55	120.30
8	BH	68	GLY	N-CA-C	-6.86	95.95	113.10
53	DA	1171	G	C8-N9-C4	-6.85	103.66	106.40
1	BA	1109	C	P-O3'-C3'	6.84	127.91	119.70
53	DA	950	G	O5'-P-OP2	-6.83	99.55	105.70
22	CA	34	U	C5'-C4'-O4'	-6.81	100.93	109.10
53	DA	1155	A	N1-C6-N6	-6.81	114.51	118.60
20	BT	66	LEU	CA-CB-CG	6.81	130.95	115.30
53	DA	2056	G	O4'-C1'-N9	-6.78	102.78	108.20
1	AA	887	G	O5'-P-OP2	-6.78	99.60	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	1270	C	O5'-P-OP2	-6.74	99.63	105.70
53	DA	2808	G	O5'-P-OP2	-6.74	99.64	105.70
53	DA	2681	C	O5'-P-OP2	-6.73	99.64	105.70
1	AA	330	C	C2-N3-C4	6.72	123.26	119.90
53	DA	1162	G	O5'-P-OP2	-6.67	99.69	105.70
1	BA	573	A	O4'-C1'-N9	-6.67	102.86	108.20
1	BA	842	U	C5-C6-N1	6.67	126.03	122.70
53	DA	101	A	O4'-C1'-N9	6.66	113.53	108.20
1	BA	1012	A	N3-C4-N9	-6.66	122.08	127.40
22	CA	140	C	N1-C2-O2	6.65	122.89	118.90
53	DA	2033	A	O5'-P-OP1	-6.65	99.71	105.70
53	DA	2638	G	O4'-C1'-N9	6.65	113.52	108.20
53	DA	1819	A	N1-C6-N6	6.64	122.58	118.60
53	DA	984	A	O4'-C1'-N9	6.64	113.51	108.20
1	BA	1167	A	C8-N9-C4	-6.61	103.15	105.80
53	DA	830	G	O5'-P-OP1	-6.61	99.75	105.70
1	BA	573	A	O5'-P-OP1	-6.60	99.76	105.70
53	DA	2889	C	N1-C2-O2	-6.58	114.95	118.90
53	DA	2618	G	N3-C2-N2	-6.58	115.29	119.90
53	DA	2712	C	N3-C4-C5	6.58	124.53	121.90
22	CA	2884	U	N3-C2-O2	-6.57	117.60	122.20
53	DA	26	G	C2-N3-C4	-6.57	108.61	111.90
53	DA	2815	C	N1-C2-O2	-6.57	114.96	118.90
22	CA	545	U	N3-C2-O2	-6.56	117.61	122.20
22	CA	646	U	P-O3'-C3'	6.54	127.55	119.70
53	DA	751	A	O5'-P-OP2	6.54	118.55	110.70
53	DA	1967	C	N3-C4-C5	-6.54	119.29	121.90
15	BO	87	LEU	CA-CB-CG	6.53	130.33	115.30
53	DA	116	C	C5-C4-N4	6.53	124.77	120.20
53	DA	2390	U	O5'-P-OP2	-6.53	99.82	105.70
1	AA	330	C	C5-C6-N1	6.53	124.26	121.00
32	DL	70	ARG	NE-CZ-NH2	-6.52	117.04	120.30
53	DA	807	U	C5-C4-O4	-6.51	121.99	125.90
53	DA	181	A	C8-N9-C4	-6.50	103.20	105.80
53	DA	1847	A	C8-N9-C4	-6.49	103.20	105.80
53	DA	1311	G	O4'-C1'-N9	6.48	113.39	108.20
22	CA	2250	G	C8-N9-C1'	-6.48	118.58	127.00
53	DA	2249	U	C4-C5-C6	-6.48	115.81	119.70
53	DA	1788	C	C5-C4-N4	-6.48	115.67	120.20
6	BF	92	THR	N-CA-C	6.46	128.46	111.00
22	CA	2585	U	C5'-C4'-O4'	-6.46	101.34	109.10
53	DA	1779	U	N3-C2-O2	6.46	126.72	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	12	U	N3-C2-O2	-6.46	117.68	122.20
53	DA	1020	A	N1-C6-N6	6.45	122.47	118.60
53	DA	978	G	N3-C2-N2	6.45	124.42	119.90
53	DA	1300	G	O5'-P-OP2	-6.44	99.90	105.70
53	DA	1171	G	C4-N9-C1'	6.44	134.87	126.50
1	BA	328	C	C2-N1-C1'	6.43	125.88	118.80
22	CA	2250	G	N7-C8-N9	6.42	116.31	113.10
53	DA	1261	C	O5'-P-OP2	-6.42	99.92	105.70
53	DA	2008	C	O5'-P-OP2	-6.42	99.92	105.70
53	DA	2424	C	N3-C4-N4	-6.42	113.51	118.00
23	DB	97	C	N1-C2-O2	-6.40	115.06	118.90
53	DA	1009	A	OP1-P-OP2	-6.40	110.00	119.60
53	DA	2027	G	N1-C6-O6	-6.39	116.06	119.90
23	DB	81	G	C5-C6-O6	-6.39	124.76	128.60
53	DA	139	U	N3-C2-O2	-6.39	117.73	122.20
53	DA	1257	C	C6-N1-C2	6.38	122.85	120.30
53	DA	202	U	N3-C2-O2	-6.37	117.74	122.20
53	DA	1313	U	C2-N1-C1'	6.37	125.34	117.70
53	DA	299	A	O5'-P-OP2	-6.35	99.98	105.70
1	BA	183	C	N1-C2-O2	6.35	122.71	118.90
53	DA	2518	A	OP2-P-O3'	6.34	119.15	105.20
1	BA	532	A	C5-C6-N6	-6.33	118.64	123.70
1	AA	1053	G	OP2-P-O3'	6.32	119.11	105.20
53	DA	181	A	N1-C6-N6	-6.31	114.81	118.60
1	BA	328	C	C6-N1-C2	-6.29	117.78	120.30
53	DA	914	G	C4-C5-N7	6.29	113.32	110.80
53	DA	1311	G	N1-C6-O6	6.29	123.67	119.90
22	CA	2250	G	C6-C5-N7	-6.28	126.63	130.40
1	BA	1397	C	N1-C2-O2	6.27	122.66	118.90
22	CA	2566	A	O4'-C1'-N9	6.27	113.21	108.20
19	BS	10	PHE	CB-CG-CD1	-6.26	116.42	120.80
53	DA	748	G	O4'-C1'-N9	6.25	113.20	108.20
53	DA	1190	G	N3-C4-C5	6.24	131.72	128.60
53	DA	670	A	O4'-C1'-N9	-6.24	103.21	108.20
22	CA	1174	U	N3-C2-O2	-6.24	117.83	122.20
1	AA	579	A	O5'-P-OP2	-6.23	100.09	105.70
53	DA	1709	U	C5-C4-O4	-6.23	122.16	125.90
22	CA	1584	U	C2-N1-C1'	6.22	125.17	117.70
53	DA	1784	A	C5-C6-N6	-6.22	118.72	123.70
1	BA	78	A	C8-N9-C4	-6.22	103.31	105.80
53	DA	2614	A	N1-C6-N6	6.21	122.33	118.60
22	CA	783	A	N1-C6-N6	6.21	122.33	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	BG	54	SER	N-CA-C	-6.20	94.25	111.00
53	DA	1330	C	N3-C4-N4	6.20	122.34	118.00
22	CA	2585	U	N1-C1'-C2'	-6.19	105.19	112.00
53	DA	997	G	C5-C6-O6	6.19	132.31	128.60
53	DA	1297	C	N1-C2-O2	6.18	122.61	118.90
53	DA	1709	U	N3-C4-O4	6.18	123.73	119.40
1	BA	553	A	O5'-P-OP2	-6.18	100.14	105.70
22	CA	140	C	P-O3'-C3'	6.17	127.10	119.70
41	CU	3	ARG	NE-CZ-NH2	-6.17	117.22	120.30
22	CA	2689	U	O4'-C1'-N1	-6.16	103.28	108.20
23	CB	15	A	P-O3'-C3'	6.16	127.09	119.70
53	DA	1828	G	O5'-P-OP2	-6.16	100.16	105.70
53	DA	1208	C	N3-C2-O2	-6.15	117.59	121.90
22	CA	528	A	C5-C6-N1	-6.15	114.63	117.70
53	DA	2820	A	C2-N3-C4	-6.14	107.53	110.60
53	DA	2715	C	C6-N1-C2	-6.13	117.85	120.30
53	DA	17	G	N3-C4-C5	6.12	131.66	128.60
52	C5	12	ARG	CG-CD-NE	-6.12	98.95	111.80
22	CA	1943	U	C2-N3-C4	6.11	130.67	127.00
1	AA	330	C	C6-N1-C2	-6.11	117.86	120.30
53	DA	2050	C	N3-C4-C5	6.11	124.34	121.90
53	DA	528	A	O5'-P-OP1	6.10	118.02	110.70
22	CA	2430	A	O4'-C1'-N9	6.10	113.08	108.20
53	DA	334	C	C6-N1-C2	6.09	122.74	120.30
53	DA	2448	A	O5'-P-OP1	-6.09	100.22	105.70
1	AA	971	G	O4'-C1'-N9	6.09	113.07	108.20
53	DA	2301	C	C6-N1-C2	-6.08	117.87	120.30
53	DA	370	G	O5'-P-OP2	-6.08	100.23	105.70
53	DA	1116	G	N1-C6-O6	-6.06	116.26	119.90
53	DA	687	C	O5'-P-OP2	-6.06	100.25	105.70
1	AA	321	A	O5'-P-OP2	-6.05	100.25	105.70
53	DA	752	A	N9-C4-C5	6.05	108.22	105.80
22	CA	793	A	O5'-P-OP2	-6.04	100.26	105.70
53	DA	1985	C	O5'-P-OP2	-6.04	100.26	105.70
53	DA	194	G	N3-C4-C5	6.03	131.62	128.60
53	DA	2835	A	O4'-C1'-N9	-6.03	103.37	108.20
22	CA	1607	C	O4'-C1'-N1	-6.03	103.38	108.20
53	DA	140	C	N3-C2-O2	-6.03	117.68	121.90
53	DA	2813	A	C5-N7-C8	-6.03	100.89	103.90
1	AA	328	C	N1-C2-O2	6.03	122.52	118.90
53	DA	1153	C	N1-C2-O2	6.03	122.52	118.90
1	AA	844	G	C2-N3-C4	6.01	114.91	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	2028	U	C5-C4-O4	-6.00	122.30	125.90
1	AA	330	C	C2-N1-C1'	6.00	125.40	118.80
53	DA	328	U	OP1-P-O3'	6.00	118.41	105.20
1	BA	211	G	C8-N9-C1'	-6.00	119.20	127.00
53	DA	2006	C	N1-C2-O2	6.00	122.50	118.90
22	CA	1914	C	N1-C2-O2	5.99	122.50	118.90
53	DA	1666	G	N1-C6-O6	-5.99	116.31	119.90
53	DA	1116	G	C5-C6-O6	5.98	132.19	128.60
53	DA	246	C	O5'-P-OP2	-5.98	100.32	105.70
22	CA	2308	G	O4'-C1'-N9	5.98	112.98	108.20
53	DA	2824	C	C6-N1-C2	-5.97	117.91	120.30
22	CA	1584	U	N3-C2-O2	-5.97	118.02	122.20
22	CA	1828	G	O5'-P-OP2	-5.97	100.33	105.70
35	DO	2	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	BA	576	C	O5'-P-OP1	5.96	117.85	110.70
53	DA	2641	G	N1-C6-O6	-5.96	116.32	119.90
1	BA	1003	G	C4-N9-C1'	5.95	134.24	126.50
53	DA	465	G	N1-C6-O6	-5.95	116.33	119.90
22	CA	783	A	N7-C8-N9	5.95	116.78	113.80
22	CA	12	U	N3-C2-O2	-5.95	118.03	122.20
22	CA	793	A	C8-N9-C4	5.95	108.18	105.80
22	CA	1807	G	O4'-C1'-N9	5.94	112.95	108.20
22	CA	135	U	C2-N1-C1'	5.94	124.83	117.70
53	DA	1223	G	C8-N9-C4	5.94	108.78	106.40
53	DA	2820	A	OP1-P-O3'	5.92	118.23	105.20
1	AA	872	A	O4'-C1'-N9	5.92	112.94	108.20
22	CA	635	C	C6-N1-C2	-5.92	117.93	120.30
53	DA	2821	A	N9-C4-C5	-5.92	103.43	105.80
22	CA	783	A	C8-N9-C4	-5.91	103.44	105.80
53	DA	744	U	N3-C4-O4	5.91	123.53	119.40
53	DA	1630	A	N1-C6-N6	-5.90	115.06	118.60
1	BA	496	A	O4'-C1'-N9	5.90	112.92	108.20
22	CA	1584	U	N1-C2-O2	5.89	126.93	122.80
53	DA	1236	G	O4'-C1'-N9	5.89	112.91	108.20
1	BA	573	A	P-O3'-C3'	5.89	126.76	119.70
1	BA	1054	C	C6-N1-C2	-5.88	117.95	120.30
53	DA	1339	G	C5-C6-O6	-5.88	125.07	128.60
1	BA	27	G	N1-C6-O6	5.88	123.42	119.90
22	CA	38	A	O5'-P-OP2	-5.87	100.42	105.70
22	CA	528	A	O4'-C1'-N9	-5.86	103.51	108.20
53	DA	1429	G	C5-C6-O6	5.86	132.12	128.60
22	CA	2585	U	O4'-C1'-N1	-5.86	103.51	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	1238	G	O5'-P-OP2	-5.86	100.43	105.70
53	DA	923	G	N1-C6-O6	-5.85	116.39	119.90
53	DA	2629	U	O5'-P-OP2	-5.85	100.44	105.70
1	AA	328	C	N3-C2-O2	-5.84	117.81	121.90
53	DA	1190	G	C2-N3-C4	-5.84	108.98	111.90
22	CA	1943	U	C5-C4-O4	5.84	129.40	125.90
1	BA	1397	C	C6-N1-C2	-5.83	117.97	120.30
53	DA	140	C	N1-C2-O2	5.83	122.40	118.90
53	DA	999	U	C5-C4-O4	5.83	129.40	125.90
53	DA	2027	G	C5-C6-N1	5.83	114.41	111.50
53	DA	592	A	C6-N1-C2	-5.82	115.11	118.60
24	CC	213	TRP	CA-CB-CG	5.82	124.76	113.70
22	CA	140	C	N3-C2-O2	-5.82	117.83	121.90
1	BA	183	C	C6-N1-C1'	-5.82	113.82	120.80
53	DA	484	C	N1-C2-O2	5.81	122.39	118.90
53	DA	1394	U	O4'-C1'-N1	-5.81	103.55	108.20
53	DA	1425	G	C8-N9-C4	-5.81	104.08	106.40
53	DA	102	U	N3-C2-O2	-5.81	118.14	122.20
53	DA	521	U	C6-N1-C2	-5.80	117.52	121.00
53	DA	1133	A	O4'-C1'-N9	5.80	112.84	108.20
18	BR	55	LEU	CA-CB-CG	5.79	128.63	115.30
53	DA	784	G	OP1-P-O3'	5.79	117.95	105.20
53	DA	1584	U	C6-N1-C1'	-5.79	113.09	121.20
53	DA	2282	G	O4'-C1'-N9	5.79	112.83	108.20
1	BA	209	U	N1-C2-O2	5.79	126.85	122.80
53	DA	1187	G	N1-C6-O6	-5.79	116.43	119.90
1	BA	485	U	C2-N1-C1'	5.79	124.64	117.70
1	BA	530	G	C4-N9-C1'	5.79	134.02	126.50
22	CA	545	U	C2-N1-C1'	5.77	124.63	117.70
53	DA	1679	A	O5'-P-OP2	-5.77	100.51	105.70
53	DA	1984	G	O5'-P-OP2	-5.76	100.52	105.70
1	BA	468	A	N7-C8-N9	5.75	116.68	113.80
53	DA	212	G	N9-C4-C5	5.75	107.70	105.40
53	DA	2813	A	C4-C5-N7	5.75	113.58	110.70
1	BA	1001	C	C5-C6-N1	5.75	123.88	121.00
1	AA	1279	G	N7-C8-N9	5.74	115.97	113.10
1	AA	330	C	N1-C2-O2	5.74	122.34	118.90
53	DA	655	A	N1-C6-N6	-5.74	115.16	118.60
53	DA	1329	U	N3-C4-O4	5.74	123.42	119.40
53	DA	1780	A	OP1-P-OP2	-5.74	111.00	119.60
53	DA	914	G	OP2-P-O3'	5.73	117.81	105.20
6	BF	35	LYS	CA-CB-CG	5.73	126.00	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CA	2585	U	N3-C2-O2	-5.72	118.19	122.20
53	DA	13	A	OP1-P-O3'	5.72	117.79	105.20
22	CA	12	U	C6-N1-C2	-5.72	117.57	121.00
53	DA	181	A	C5-C6-N6	5.71	128.27	123.70
53	DA	446	G	N1-C6-O6	5.71	123.33	119.90
53	DA	8	C	N1-C2-O2	-5.71	115.47	118.90
1	BA	1012	A	C8-N9-C4	-5.71	103.52	105.80
22	CA	818	G	P-O3'-C3'	5.71	126.55	119.70
53	DA	395	U	O4'-C1'-N1	5.71	112.76	108.20
22	CA	1368	G	C8-N9-C4	-5.70	104.12	106.40
53	DA	205	G	O4'-C1'-N9	5.70	112.76	108.20
53	DA	1671	U	N3-C4-O4	-5.70	115.41	119.40
53	DA	1220	G	C2-N3-C4	-5.70	109.05	111.90
1	AA	412	A	N9-C1'-C2'	5.69	121.40	114.00
22	CA	2250	G	C8-N9-C4	-5.69	104.12	106.40
53	DA	1965	C	O5'-P-OP1	5.69	117.53	110.70
53	DA	547	A	C8-N9-C4	-5.69	103.53	105.80
22	CA	613	A	O4'-C1'-N9	-5.69	103.65	108.20
53	DA	2465	C	O5'-P-OP2	-5.68	100.58	105.70
53	DA	1182	G	N3-C4-C5	-5.68	125.76	128.60
22	CA	1265	A	O5'-P-OP2	-5.68	100.59	105.70
53	DA	914	G	C5-N7-C8	-5.68	101.46	104.30
53	DA	2258	C	N1-C2-O2	5.68	122.31	118.90
22	CA	1174	U	N1-C2-O2	5.67	126.77	122.80
24	CC	196	GLY	N-CA-C	5.67	127.29	113.10
22	CA	764	A	N1-C6-N6	-5.67	115.20	118.60
23	DB	81	G	C4-C5-N7	5.67	113.07	110.80
37	CQ	114	LEU	CA-CB-CG	5.67	128.34	115.30
53	DA	13	A	C6-N1-C2	-5.67	115.20	118.60
53	DA	102	U	N1-C2-O2	5.67	126.77	122.80
53	DA	2336	A	C6-N1-C2	-5.67	115.20	118.60
53	DA	1936	A	C8-N9-C4	5.66	108.07	105.80
53	DA	2027	G	C2-N3-C4	5.66	114.73	111.90
53	DA	1171	G	N3-C4-C5	-5.66	125.77	128.60
53	DA	1221	C	N3-C4-C5	5.66	124.16	121.90
22	CA	2848	G	N1-C6-O6	-5.65	116.51	119.90
53	DA	2815	C	N3-C2-O2	5.65	125.86	121.90
53	DA	511	U	O5'-P-OP2	-5.64	100.62	105.70
53	DA	2211	A	N1-C6-N6	5.64	121.98	118.60
53	DA	775	G	O4'-C1'-N9	5.64	112.71	108.20
1	AA	1279	G	C8-N9-C1'	-5.63	119.68	127.00
22	CA	802	A	O5'-P-OP1	-5.63	100.64	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	1531	A	N1-C6-N6	5.62	121.97	118.60
1	AA	85	U	C2-N1-C1'	5.61	124.43	117.70
53	DA	923	G	C5-C6-O6	5.61	131.97	128.60
53	DA	975	A	N1-C6-N6	-5.61	115.23	118.60
53	DA	997	G	N3-C4-N9	-5.60	122.64	126.00
22	CA	2723	C	C6-N1-C2	-5.60	118.06	120.30
53	DA	851	C	O5'-P-OP2	-5.60	100.66	105.70
53	DA	1649	G	O5'-P-OP1	-5.59	100.67	105.70
1	BA	209	U	C6-N1-C1'	-5.59	113.37	121.20
53	DA	2072	C	N1-C2-O2	5.59	122.25	118.90
1	BA	1110	A	O5'-C5'-C4'	5.58	122.31	111.70
53	DA	463	G	N3-C4-N9	-5.58	122.65	126.00
53	DA	789	A	C6-N1-C2	-5.58	115.25	118.60
5	BE	123	VAL	CB-CA-C	-5.58	100.80	111.40
53	DA	2825	G	C4-N9-C1'	5.58	133.75	126.50
53	DA	2439	A	N1-C6-N6	5.57	121.94	118.60
53	DA	491	G	N9-C4-C5	5.56	107.63	105.40
53	DA	461	C	C6-N1-C2	-5.56	118.08	120.30
53	DA	1573	G	C2-N3-C4	-5.56	109.12	111.90
53	DA	2405	G	O4'-C1'-N9	5.56	112.65	108.20
1	BA	441	A	O5'-P-OP2	5.56	117.37	110.70
53	DA	1936	A	N9-C4-C5	-5.55	103.58	105.80
22	CA	2680	U	P-O3'-C3'	5.55	126.36	119.70
26	CE	40	ARG	CG-CD-NE	5.55	123.45	111.80
53	DA	2508	G	O5'-P-OP2	-5.55	100.71	105.70
53	DA	2834	G	N1-C6-O6	-5.55	116.57	119.90
1	BA	573	A	OP2-P-O3'	5.55	117.41	105.20
53	DA	2888[A]	C	C6-N1-C2	-5.54	118.08	120.30
53	DA	2888[B]	C	C6-N1-C2	-5.54	118.08	120.30
53	DA	2250	G	C8-N9-C4	-5.54	104.18	106.40
53	DA	974	G	N1-C6-O6	-5.54	116.58	119.90
22	CA	1352	U	O4'-C1'-N1	5.53	112.63	108.20
53	DA	1958	C	N3-C4-N4	5.53	121.87	118.00
53	DA	1153	C	N3-C2-O2	-5.53	118.03	121.90
53	DA	2799	A	C5-C6-N6	-5.52	119.28	123.70
53	DA	2807	U	O5'-P-OP2	-5.52	100.73	105.70
53	DA	837	C	N3-C4-C5	5.52	124.11	121.90
53	DA	1730	C	C6-N1-C2	-5.52	118.09	120.30
44	DX	39	ARG	NE-CZ-NH2	-5.52	117.54	120.30
53	DA	1730	C	N3-C2-O2	-5.51	118.04	121.90
53	DA	494	G	N3-C4-C5	5.51	131.36	128.60
53	DA	800	A	O4'-C1'-N9	-5.51	103.79	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	2615	U	O5'-P-OP1	-5.51	100.74	105.70
33	CM	114	GLY	N-CA-C	5.51	126.88	113.10
53	DA	786	C	N3-C4-C5	5.50	124.10	121.90
53	DA	526	A	OP2-P-O3'	5.50	117.29	105.20
1	BA	1110	A	C4-N9-C1'	5.50	136.19	126.30
53	DA	2386	A	N9-C4-C5	5.49	108.00	105.80
53	DA	2297	A	O5'-P-OP1	-5.49	100.76	105.70
53	DA	1370	C	O5'-P-OP2	-5.49	100.76	105.70
32	DL	58	LEU	CA-CB-CG	5.49	127.92	115.30
1	BA	1032	G	C4-N9-C1'	5.49	133.63	126.50
53	DA	1022	G	C4-C5-N7	-5.49	108.61	110.80
53	DA	2038	G	O5'-P-OP2	-5.49	100.76	105.70
53	DA	1171	G	N7-C8-N9	5.48	115.84	113.10
53	DA	1371	G	C8-N9-C4	5.48	108.59	106.40
53	DA	1626	A	C8-N9-C4	-5.48	103.61	105.80
53	DA	2448	A	OP1-P-OP2	5.47	127.81	119.60
23	DB	81	G	C6-C5-N7	-5.47	127.11	130.40
53	DA	1291	C	O5'-P-OP2	-5.47	100.78	105.70
53	DA	1958	C	C5-C4-N4	-5.47	116.37	120.20
1	BA	399	G	C8-N9-C4	-5.47	104.21	106.40
53	DA	836	G	OP2-P-O3'	5.47	117.23	105.20
53	DA	2426	A	N9-C4-C5	-5.47	103.61	105.80
53	DA	978	G	C4-C5-N7	5.46	112.98	110.80
53	DA	545	U	C5-C6-N1	5.46	125.43	122.70
53	DA	2683	C	N1-C2-O2	-5.46	115.62	118.90
53	DA	2807	U	OP1-P-OP2	5.46	127.79	119.60
1	AA	183	C	C6-N1-C2	-5.46	118.12	120.30
22	CA	757	G	N3-C4-N9	-5.46	122.72	126.00
53	DA	16	C	O5'-P-OP2	-5.46	100.79	105.70
53	DA	1160	G	N3-C4-N9	-5.46	122.72	126.00
22	CA	1648	U	O5'-P-OP1	-5.46	100.79	105.70
53	DA	1671	U	N3-C2-O2	-5.46	118.38	122.20
22	CA	2884	U	N1-C2-O2	5.45	126.62	122.80
22	CA	1937	A	O4'-C1'-N9	5.45	112.56	108.20
22	CA	2714	G	O5'-P-OP2	-5.45	100.79	105.70
53	DA	1150	C	C6-N1-C2	5.45	122.48	120.30
53	DA	2070	A	N1-C6-N6	-5.45	115.33	118.60
53	DA	994	C	N3-C4-N4	-5.45	114.19	118.00
53	DA	1182	G	C8-N9-C4	-5.45	104.22	106.40
23	CB	90	C	C6-N1-C2	-5.45	118.12	120.30
53	DA	2585	U	OP1-P-O3'	5.43	117.16	105.20
53	DA	2501	C	C5-C6-N1	5.43	123.72	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DD	77	ARG	NE-CZ-NH1	-5.43	117.58	120.30
53	DA	2281	A	N1-C6-N6	5.43	121.86	118.60
22	CA	370	G	O5'-P-OP2	-5.42	100.82	105.70
53	DA	2844	G	C2-N3-C4	-5.42	109.19	111.90
1	BA	1397	C	C6-N1-C1'	-5.42	114.30	120.80
53	DA	1147	A	N1-C6-N6	-5.41	115.35	118.60
53	DA	1602	U	N1-C2-O2	5.41	126.59	122.80
53	DA	2715	C	O5'-P-OP2	-5.41	100.83	105.70
53	DA	2767	C	C6-N1-C2	-5.40	118.14	120.30
1	AA	1418	A	C8-N9-C4	-5.40	103.64	105.80
53	DA	1971	U	O5'-P-OP1	5.40	117.18	110.70
1	BA	205	A	C8-N9-C4	-5.40	103.64	105.80
1	BA	922	G	C8-N9-C4	-5.40	104.24	106.40
1	AA	412	A	O4'-C1'-N9	5.40	112.52	108.20
1	AA	22	G	O5'-P-OP2	-5.39	100.85	105.70
1	BA	1183	U	C5'-C4'-C3'	-5.39	107.37	116.00
53	DA	1602	U	C5-C4-O4	5.39	129.13	125.90
53	DA	2790	U	O5'-P-OP2	-5.39	100.85	105.70
53	DA	1022	G	C5-C6-O6	5.39	131.83	128.60
53	DA	759	G	C4-C5-N7	5.39	112.95	110.80
53	DA	1778	U	OP1-P-OP2	5.39	127.68	119.60
22	CA	545	U	P-O3'-C3'	5.38	126.16	119.70
53	DA	212	G	C8-N9-C4	-5.38	104.25	106.40
53	DA	1324	G	O4'-C1'-N9	5.38	112.51	108.20
53	DA	1659	G	N3-C4-N9	-5.38	122.77	126.00
53	DA	2799	A	N1-C6-N6	5.38	121.83	118.60
53	DA	810	U	N1-C2-O2	5.38	126.56	122.80
53	DA	324	A	O5'-P-OP2	-5.37	100.86	105.70
53	DA	670	A	O5'-P-OP2	-5.37	100.86	105.70
53	DA	744	U	C5-C6-N1	5.37	125.39	122.70
53	DA	2599	G	C4-C5-N7	5.37	112.95	110.80
53	DA	1973	G	O5'-P-OP2	-5.37	100.87	105.70
1	AA	71	A	N1-C6-N6	5.37	121.82	118.60
53	DA	788	A	C8-N9-C4	-5.37	103.65	105.80
1	BA	1279	G	C4-N9-C1'	5.36	133.47	126.50
53	DA	1508	A	C5-N7-C8	-5.36	101.22	103.90
53	DA	1782	U	O5'-P-OP1	-5.36	100.88	105.70
53	DA	43	G	N3-C2-N2	-5.36	116.15	119.90
53	DA	1329	U	N1-C2-O2	-5.35	119.05	122.80
22	CA	135	U	O4'-C1'-N1	-5.35	103.92	108.20
22	CA	545	U	N1-C2-O2	5.35	126.54	122.80
53	DA	1679	A	C4-C5-C6	5.34	119.67	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	2780	G	C2-N3-C4	-5.34	109.23	111.90
22	CA	2395	C	C6-N1-C2	-5.34	118.16	120.30
53	DA	663	G	N1-C2-N2	5.34	121.00	116.20
53	DA	2250	G	N7-C8-N9	5.33	115.77	113.10
53	DA	523	C	O5'-P-OP2	-5.33	100.90	105.70
53	DA	1584	U	N3-C2-O2	-5.33	118.47	122.20
53	DA	1016	G	C5-C6-O6	5.33	131.80	128.60
22	CA	1914	C	N3-C2-O2	-5.33	118.17	121.90
53	DA	2789	C	OP2-P-O3'	5.33	116.92	105.20
53	DA	735	A	C5-C6-N6	-5.32	119.44	123.70
53	DA	537	G	C4-C5-N7	5.32	112.93	110.80
53	DA	806	C	N3-C2-O2	-5.32	118.18	121.90
53	DA	2839	G	O5'-P-OP2	-5.32	100.91	105.70
53	DA	1315	C	N1-C2-O2	5.32	122.09	118.90
22	CA	961	C	O4'-C1'-N1	-5.31	103.95	108.20
53	DA	304	U	O5'-P-OP2	-5.31	100.92	105.70
53	DA	2614	A	C5-C6-N6	-5.31	119.45	123.70
22	CA	1606	C	O4'-C1'-N1	5.31	112.45	108.20
53	DA	2710	C	C5-C4-N4	5.31	123.92	120.20
53	DA	24	G	O5'-P-OP2	-5.31	100.92	105.70
53	DA	68	G	C5-C6-O6	-5.31	125.42	128.60
53	DA	1329	U	C5-C4-O4	-5.31	122.72	125.90
53	DA	2430[A]	A	O5'-P-OP2	-5.29	100.93	105.70
53	DA	2430[B]	A	O5'-P-OP2	-5.29	100.93	105.70
8	BH	67	GLN	N-CA-C	-5.29	96.71	111.00
53	DA	2820	A	N9-C4-C5	-5.29	103.68	105.80
53	DA	815	C	O5'-P-OP2	-5.29	100.94	105.70
22	CA	995	C	C2-N1-C1'	5.29	124.62	118.80
1	BA	844	G	O4'-C1'-N9	-5.29	103.97	108.20
22	CA	1936	A	N1-C2-N3	5.29	131.94	129.30
53	DA	2046	G	N1-C2-N2	-5.29	111.44	116.20
1	BA	210	C	C6-N1-C2	-5.29	118.19	120.30
22	CA	1272	A	O4'-C1'-N9	-5.28	103.97	108.20
53	DA	1330	C	C5-C4-N4	-5.28	116.50	120.20
1	BA	209	U	N3-C2-O2	-5.28	118.50	122.20
53	DA	885	C	C6-N1-C2	-5.28	118.19	120.30
53	DA	2264	C	N3-C4-N4	-5.28	114.30	118.00
1	BA	1012	A	O4'-C1'-N9	5.28	112.42	108.20
53	DA	1602	U	O4'-C1'-N1	5.28	112.42	108.20
53	DA	2825	G	N3-C4-C5	-5.28	125.96	128.60
53	DA	2366	A	O5'-P-OP2	-5.27	100.95	105.70
53	DA	2820	A	N3-C4-C5	5.27	130.49	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	570	G	OP2-P-O3'	5.27	116.79	105.20
53	DA	949	G	OP1-P-OP2	5.27	127.50	119.60
1	BA	1364	U	C2-N1-C1'	5.26	124.01	117.70
1	BA	266	G	O4'-C1'-N9	-5.26	103.99	108.20
1	BA	577	G	OP1-P-O3'	5.26	116.76	105.20
1	BA	1397	C	N3-C2-O2	-5.26	118.22	121.90
53	DA	964	C	C2-N3-C4	5.26	122.53	119.90
53	DA	513	A	OP2-P-O3'	5.25	116.76	105.20
26	CE	88	ARG	CA-CB-CG	5.25	124.95	113.40
53	DA	997	G	N1-C6-O6	-5.25	116.75	119.90
41	CU	3	ARG	CB-CA-C	5.24	120.88	110.40
53	DA	990	A	OP1-P-OP2	-5.24	111.74	119.60
54	DD	124	ARG	NE-CZ-NH2	-5.24	117.68	120.30
53	DA	2613	U	N3-C2-O2	-5.24	118.53	122.20
53	DA	2263	C	N3-C4-N4	-5.23	114.34	118.00
53	DA	208	C	N1-C2-O2	5.23	122.04	118.90
53	DA	26	G	N3-C4-C5	5.23	131.22	128.60
53	DA	2723	C	C6-N1-C2	-5.23	118.21	120.30
1	BA	1211	U	P-O3'-C3'	5.23	125.97	119.70
22	CA	512	G	O4'-C1'-N9	5.23	112.38	108.20
5	BE	15	LEU	CA-CB-CG	5.23	127.32	115.30
53	DA	1000	A	C8-N9-C4	5.22	107.89	105.80
53	DA	2274	A	OP2-P-O3'	5.22	116.69	105.20
53	DA	586	A	N9-C4-C5	5.22	107.89	105.80
53	DA	2295	C	O5'-P-OP2	-5.22	101.00	105.70
53	DA	2570	G	N1-C6-O6	-5.22	116.77	119.90
53	DA	1661	G	N9-C4-C5	5.21	107.49	105.40
53	DA	2851	A	O5'-P-OP2	-5.21	101.01	105.70
53	DA	207	A	OP2-P-O3'	5.21	116.67	105.20
1	BA	330	C	N3-C2-O2	-5.21	118.25	121.90
53	DA	1026	G	O5'-P-OP2	5.21	116.95	110.70
53	DA	2802	G	N3-C4-N9	-5.21	122.87	126.00
53	DA	1022	G	N9-C4-C5	5.21	107.48	105.40
53	DA	1202	G	N1-C6-O6	-5.20	116.78	119.90
41	CU	3	ARG	CA-CB-CG	5.20	124.84	113.40
53	DA	2756	U	C5-C4-O4	5.20	129.02	125.90
53	DA	422	A	O5'-P-OP2	5.20	116.94	110.70
53	DA	570	G	N3-C4-N9	5.19	129.12	126.00
53	DA	1146	C	O5'-P-OP2	-5.19	101.03	105.70
53	DA	522	A	C5-N7-C8	-5.19	101.30	103.90
53	DA	2582	G	N3-C2-N2	5.19	123.53	119.90
22	CA	1779	U	N1-C2-N3	5.19	118.02	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	965	C	N3-C4-C5	5.19	123.98	121.90
53	DA	1669	A	C6-N1-C2	-5.19	115.48	118.60
1	AA	792	A	O4'-C1'-N9	5.19	112.35	108.20
53	DA	980	A	O5'-P-OP1	-5.19	101.03	105.70
53	DA	1020	A	N9-C4-C5	-5.19	103.72	105.80
23	DB	99	A	C2-N3-C4	-5.19	108.00	110.60
53	DA	563	A	O5'-P-OP1	-5.19	101.03	105.70
53	DA	946	C	C6-N1-C2	-5.19	118.22	120.30
53	DA	562	U	N3-C2-O2	-5.18	118.57	122.20
22	CA	818	G	O3'-P-O5'	5.18	113.85	104.00
53	DA	28	A	OP2-P-O3'	5.18	116.60	105.20
53	DA	995	C	O4'-C1'-N1	-5.18	104.06	108.20
53	DA	784	G	P-O3'-C3'	5.18	125.91	119.70
53	DA	1698	A	C6-C5-N7	-5.18	128.68	132.30
53	DA	2810	A	O5'-P-OP2	-5.18	101.04	105.70
53	DA	1760	C	C6-N1-C2	5.18	122.37	120.30
53	DA	2499	C	N1-C2-N3	5.18	122.82	119.20
53	DA	1888	G	O5'-P-OP2	-5.17	101.04	105.70
1	AA	328	C	C2-N1-C1'	5.17	124.49	118.80
53	DA	2814	A	OP1-P-OP2	5.17	127.36	119.60
1	BA	330	C	N3-C4-N4	-5.17	114.38	118.00
1	BA	73	C	O4'-C1'-N1	5.17	112.33	108.20
53	DA	1168	G	C2-N3-C4	-5.16	109.32	111.90
53	DA	1252	G	O5'-P-OP1	-5.16	101.05	105.70
53	DA	1930	G	N3-C4-N9	-5.16	122.90	126.00
1	BA	1492	A	P-O3'-C3'	5.16	125.89	119.70
1	BA	452	A	C5-N7-C8	-5.16	101.32	103.90
22	CA	404	A	P-O3'-C3'	5.16	125.89	119.70
22	CA	2585	U	N1-C2-O2	5.16	126.41	122.80
53	DA	2724	U	O5'-P-OP2	-5.16	101.06	105.70
5	BE	122	ASN	N-CA-C	5.16	124.92	111.00
22	CA	271	G	P-O3'-C3'	5.16	125.89	119.70
22	CA	1730	C	C6-N1-C2	-5.16	118.24	120.30
53	DA	2062	A	OP2-P-O3'	5.16	116.54	105.20
53	DA	2756	U	N3-C2-O2	-5.16	118.59	122.20
53	DA	1927	A	N1-C6-N6	-5.15	115.51	118.60
1	BA	842	U	C6-N1-C2	-5.15	117.91	121.00
53	DA	494	G	C8-N9-C4	5.15	108.46	106.40
1	AA	1286	U	C2-N1-C1'	5.14	123.87	117.70
1	BA	328	C	N3-C2-O2	-5.14	118.30	121.90
53	DA	1220	G	N3-C2-N2	5.14	123.50	119.90
1	BA	1168	U	C5-C6-N1	5.14	125.27	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	970	U	O5'-P-OP2	-5.14	101.07	105.70
53	DA	2435	A	O5'-P-OP1	-5.14	101.07	105.70
12	BL	121	ARG	NE-CZ-NH1	5.14	122.87	120.30
53	DA	1659	G	C8-N9-C1'	5.14	133.68	127.00
1	BA	1003	G	C8-N9-C1'	-5.13	120.33	127.00
1	BA	1322	C	C2-N1-C1'	5.13	124.45	118.80
22	CA	653	U	C5-C6-N1	5.13	125.27	122.70
1	BA	1322	C	N1-C2-O2	5.13	121.98	118.90
53	DA	2020	A	OP2-P-O3'	5.13	116.49	105.20
53	DA	929	U	N1-C2-O2	-5.13	119.21	122.80
53	DA	845	A	N1-C6-N6	5.12	121.67	118.60
53	DA	2812	G	N3-C4-C5	5.12	131.16	128.60
53	DA	1788	C	N3-C4-N4	5.12	121.58	118.00
53	DA	1849	G	N3-C2-N2	-5.11	116.32	119.90
53	DA	2838	G	OP2-P-O3'	5.11	116.45	105.20
53	DA	433	C	N1-C2-O2	-5.11	115.83	118.90
53	DA	298	G	C5-C6-O6	-5.11	125.54	128.60
53	DA	503	A	C8-N9-C4	-5.11	103.76	105.80
53	DA	2487	G	OP2-P-O3'	5.11	116.43	105.20
53	DA	2439	A	C4-C5-C6	5.10	119.55	117.00
53	DA	465	G	C6-N1-C2	5.10	128.16	125.10
53	DA	752	A	N1-C6-N6	-5.10	115.54	118.60
1	AA	5	U	C5-C6-N1	5.09	125.25	122.70
53	DA	202	U	C5-C4-O4	5.09	128.95	125.90
53	DA	372	G	O5'-P-OP2	5.09	116.81	110.70
22	CA	140	C	C2-N1-C1'	5.09	124.40	118.80
22	CA	2071	A	O3'-P-O5'	-5.09	94.33	104.00
53	DA	561	G	C5-N7-C8	-5.09	101.76	104.30
53	DA	1160	G	N9-C4-C5	5.09	107.44	105.40
53	DA	2775	G	OP2-P-O3'	5.09	116.39	105.20
53	DA	8	C	C6-N1-C2	-5.08	118.27	120.30
22	CA	185	G	C8-N9-C4	-5.08	104.37	106.40
53	DA	969	G	N9-C4-C5	-5.08	103.37	105.40
53	DA	1429	G	N1-C6-O6	-5.08	116.85	119.90
53	DA	1936	A	O4'-C1'-N9	5.08	112.26	108.20
8	BH	59	LEU	CA-CB-CG	5.08	126.97	115.30
53	DA	2391	G	O4'-C1'-N9	5.08	112.26	108.20
53	DA	2448	A	N9-C4-C5	5.08	107.83	105.80
35	CO	101	GLY	N-CA-C	5.07	125.78	113.10
53	DA	943	A	C2-N3-C4	-5.07	108.06	110.60
53	DA	1651	G	C8-N9-C4	-5.07	104.37	106.40
53	DA	2429[A]	G	C4-N9-C1'	-5.07	119.91	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	2429[B]	G	C4-N9-C1'	-5.07	119.91	126.50
53	DA	2492	U	C5-C6-N1	5.07	125.24	122.70
1	AA	858	G	N3-C4-N9	5.07	129.04	126.00
1	BA	530	G	C8-N9-C1'	-5.07	120.41	127.00
22	CA	60	G	C4-N9-C1'	-5.07	119.91	126.50
53	DA	811	U	C5-C4-O4	5.07	128.94	125.90
1	BA	572	A	O3'-P-O5'	5.06	113.61	104.00
22	CA	757	G	N1-C6-O6	5.06	122.94	119.90
53	DA	837	C	C2-N3-C4	-5.06	117.37	119.90
53	DA	969	G	C4-C5-N7	5.06	112.82	110.80
53	DA	2887[A]	A	N1-C6-N6	5.06	121.63	118.60
53	DA	2887[B]	A	N1-C6-N6	5.06	121.63	118.60
22	CA	1340	U	C2-N1-C1'	5.05	123.76	117.70
22	CA	974	G	C4-C5-N7	5.05	112.82	110.80
53	DA	1328	A	OP2-P-O3'	5.05	116.31	105.20
53	DA	2684	U	C6-N1-C2	-5.05	117.97	121.00
53	DA	1674	G	O4'-C1'-N9	-5.05	104.16	108.20
1	AA	1222	G	C5-C6-O6	-5.05	125.57	128.60
53	DA	102	U	C6-N1-C1'	-5.05	114.13	121.20
23	DB	93	C	N3-C4-C5	5.05	123.92	121.90
53	DA	506	G	C2-N3-C4	-5.04	109.38	111.90
53	DA	468	G	C2-N3-C4	-5.04	109.38	111.90
1	AA	1279	G	C6-C5-N7	-5.04	127.38	130.40
53	DA	1267	U	N1-C2-O2	-5.04	119.28	122.80
1	BA	27	G	C5-C6-O6	-5.03	125.58	128.60
1	BA	468	A	C8-N9-C4	-5.03	103.79	105.80
53	DA	1698	A	N1-C6-N6	5.03	121.62	118.60
53	DA	749	A	O5'-P-OP2	-5.03	101.17	105.70
53	DA	1930	G	N3-C2-N2	-5.03	116.38	119.90
1	BA	211	G	N3-C4-C5	-5.03	126.09	128.60
53	DA	1816	C	N1-C2-O2	-5.03	115.88	118.90
22	CA	135	U	C5-C6-N1	5.02	125.21	122.70
53	DA	2684	U	O5'-P-OP2	-5.02	101.18	105.70
53	DA	663	G	N3-C2-N2	-5.02	116.38	119.90
22	CA	741	U	N3-C2-O2	5.02	125.72	122.20
53	DA	1605	C	N3-C2-O2	5.02	125.41	121.90
53	DA	2810	A	OP1-P-OP2	5.02	127.13	119.60
1	BA	479	U	C5-C6-N1	5.02	125.21	122.70
53	DA	1905	C	N3-C4-N4	-5.02	114.49	118.00
53	DA	2782	G	C4-N9-C1'	5.02	133.02	126.50
53	DA	2008	C	N3-C4-N4	5.01	121.51	118.00
53	DA	2055	C	N1-C2-O2	-5.01	115.89	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	1964	G	O4'-C1'-N9	-5.01	104.19	108.20
53	DA	1208	C	N1-C2-O2	5.01	121.91	118.90
1	BA	1499	A	N1-C6-N6	5.01	121.60	118.60
23	DB	72	G	C2-N3-C4	-5.00	109.40	111.90
53	DA	530	G	N1-C6-O6	5.00	122.90	119.90
53	DA	1790	C	N3-C4-N4	5.00	121.50	118.00
53	DA	2722	G	N3-C2-N2	-5.00	116.40	119.90

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

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	191	0
1	BA	32908	0	16580	233	0
2	AB	1753	0	1780	26	0
2	BB	1753	0	1780	28	0
3	AC	1625	0	1696	15	0
3	BC	1625	0	1696	35	0
4	AD	1643	0	1707	20	0
4	BD	1643	0	1707	17	0
5	AE	1144	0	1185	28	0
5	BE	1105	0	1148	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AF	862	0	864	9	0
6	BF	817	0	808	22	0
7	AG	1182	0	1238	21	0
7	BG	1182	0	1238	33	0
8	AH	979	0	1031	18	0
8	BH	979	0	1031	18	0
9	AI	1022	0	1070	27	0
9	BI	1022	0	1070	24	0
10	AJ	796	0	836	40	0
10	BJ	787	0	828	20	0
11	AK	877	0	887	14	0
11	BK	877	0	887	28	0
12	AL	957	0	1017	9	0
12	BL	957	0	1017	21	0
13	AM	884	0	941	33	0
13	BM	884	0	941	24	0
14	AN	805	0	844	28	0
14	BN	805	0	844	40	0
15	AO	714	0	734	8	0
15	BO	714	0	734	23	0
16	AP	649	0	666	5	0
16	BP	649	0	666	10	0
17	AQ	649	0	691	9	0
17	BQ	649	0	691	21	0
18	AR	456	0	478	6	0
18	BR	456	0	478	13	0
19	AS	638	0	665	15	0
19	BS	638	0	665	28	0
20	AT	670	0	719	12	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	410	0
23	CB	2529	0	1281	12	0
23	DB	2569	0	1301	9	0
24	CC	2083	0	2154	37	0
24	DC	2083	0	2154	15	0
25	CD	1565	0	1616	30	0
26	CE	1552	0	1619	26	0
26	DE	1552	0	1619	3	0
27	CF	1411	0	1444	22	0
27	DF	1411	0	1444	19	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	6	0
29	CH	1110	0	1148	13	0
29	DH	1110	0	1148	13	0
30	CJ	979	0	1028	24	0
30	DJ	979	0	1028	28	0
31	CK	1129	0	1162	16	0
31	DK	1129	0	1162	5	0
32	CL	938	0	1012	21	0
32	DL	946	0	1023	11	0
33	CM	1053	0	1129	31	0
33	DM	1053	0	1129	11	0
34	CN	1075	0	1155	6	0
34	DN	1092	0	1179	10	0
35	CO	960	0	1000	17	0
35	DO	993	0	1034	6	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	23	0
38	DR	947	0	1019	12	0
39	CS	816	0	839	9	0
39	DS	816	0	839	7	0
40	CT	857	0	922	6	0
40	DT	857	0	922	3	0
41	CU	739	0	807	18	0
41	DU	739	0	807	12	0
42	CV	780	0	831	26	0
42	DV	780	0	831	4	0
43	CW	753	0	780	7	0
43	DW	753	0	780	2	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	2	0
46	CZ	501	0	531	10	0
46	DZ	501	0	531	4	0
47	C0	449	0	488	2	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	6	0
49	D2	414	0	442	8	0
50	C3	377	0	418	14	0
50	D3	377	0	418	7	0
51	C4	504	0	572	10	0
51	D4	504	0	572	5	0
52	C5	302	0	340	7	0
52	D5	302	0	340	0	0
53	DA	62361	0	31381	308	0
54	DD	1576	0	1627	14	0
55	DI	1023	0	1052	20	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	1	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	0	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	2	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	1	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	2370	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 (2370) 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:N	14:BN:26:GLU:OE2	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
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
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:H92	62:DA:3225:SPD:H52	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BN:26:GLU:H	14:BN:26:GLU:CD	1.84	0.81
13:BM:11:ASP:OD1	13:BM:12:HIS:N	2.14	0.81
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:N	16:BP:1:MET:SD	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
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
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
1:BA:319:G:N7	69:BA:1722:HOH:O	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
8:BH:77:ARG:NE	8:BH:79:SER:O	2.24	0.71
1:BA:1279:G:OP1	10:BJ:9:ARG:NH2	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:2495:G:N7	69:CA:3681:HOH:O	2.23	0.70
22:CA:616:A:OP2	69:CA:3263:HOH:O	2.08	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
19:BS:36:ARG:NH2	19:BS:75:ALA:O	2.25	0.70
22:CA:686:U:OP2	69:CA:3607:HOH:O	2.08	0.69
22:CA:581:C:OP2	38:CR:33:ARG:NE	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
22:CA:1962:5MC:HM53	69:CA:3753:HOH:O	1.93	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
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
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
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
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:806:C:H4'	57:AA:1670:PG4:H11	1.76	0.66
1:AA:412:A:H1'	1:AA:413:G:H5'	1.75	0.66
53:DA:2799:A:N7	69:DA:5142:HOH:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:19:ASN:ND2	14:AN:90:ARG:O	2.28	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
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: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
22:CA:733:G:OP1	69:CA:3711:HOH:O	2.14	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:1378:A:O2'	22:CA:1380:G:N7	2.23	0.66
22:CA:998:C:OP2	38:CR:58:ARG:NH2	2.28	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:2127:G:O2'	53:DA:2128:G:O4'	2.13	0.65
53:DA:788:A:OP1	59:DA:3223:PUT:H42	1.97	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:1361:G:N2	1:BA:1362:A:N7	2.45	0.65
1:BA:450:G:O5'	69:BA:1918:HOH:O	2.14	0.65
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
50:C3:11:LYS:NZ	69:C3:201:HOH:O	2.29	0.65
22:CA:85:G:OP1	42:CV:7:ARG:N	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
41:DU:1:MET:HE3	41:DU:1:MET:H1	1.64	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
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
1:AA:1225:A:H2'	1:AA:1226:C:C5	2.35	0.61
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
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:HH11	41:CU:3:ARG:HG2	1.66	0.60
53:DA:545:U:H2'	53:DA:546:U:O3'	2.01	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
11:BK:92:GLY:O	11:BK:94:GLU:N	2.32	0.60
7:AG:90:GLU:OE2	7:AG:90:GLU:N	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N3	1:AA:844:G:H2'	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
52:C5:26:ILE:HD13	52:C5:26:ILE:H	1.66	0.60
22:CA:2131:U:H5'	22:CA:2132:U:H5''	1.84	0.60
36:CP:17:LYS:HE2	36:CP:17:LYS:HA	1.84	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
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:1228:C:P	13:AM:107:ARG:HH22	2.26	0.59
1:AA:427:U:O2'	1:AA:541:G:OP1	2.21	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
25:CD:149:ASN:OD1	25:CD:150:GLN:N	2.35	0.59
23:CB:30:C:OP1	36:CP:3:LYS:NZ	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
22:CA:1368:G:N7	69:CA:3533:HOH:O	2.31	0.59
1:BA:1492:A:H2'	22:CA:1913:A:C6	2.38	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
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
1:AA:80:A:C2	1:AA:90:C:N3	2.71	0.59
5:BE:154:ALA:C	5:BE:156:LYS:H	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DA:787:C:OP1	59:DA:3223:PUT:N1	2.36	0.58
53:DA:711:G:OP1	69:DA:5064:HOH:O	2.16	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
29:DH:41:LYS:HA	29:DH:44:ILE:HG23	1.84	0.58
3:BC:126:ARG:O	3:BC:127:ARG:HB2	2.03	0.58
47:D0:10:THR:HG22	47:D0:11:ARG:HG3	1.85	0.58
53:DA:1119:U:OP2	69:DA:5002:HOH:O	2.16	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
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:HD3	15:BO:17:ARG:N	2.19	0.58
51:D4:63:PRO:O	69:D4:128:HOH:O	2.17	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
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
22:CA:666:A:H4'	33:CM:48:ARG:HD2	1.86	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
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:2872:A:N7	69:DA:4918:HOH:O	2.32	0.58
7:BG:92:ARG:HB3	7:BG:93:PRO:HD2	1.86	0.57
53:DA:1171:G:H2'	53:DA:1172:C:C4	2.39	0.57
53:DA:948:C:O2'	63:DA:3203:1PE:H241	2.04	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
53:DA:2831:G:OP1	54:DD:56:LYS:NZ	2.36	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
22:CA:396:G:H1'	45:CY:29:PHE:HB3	1.84	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: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
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
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
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:1172:C:C4	53:DA:1173:U:H1'	2.39	0.57
53:DA:142:A:H2'	53:DA:143:C:C6	2.40	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
14:BN:21:PHE:C	14:BN:26:GLU:OE1	2.44	0.56
1:BA:483:C:O2	16:BP:13:LYS:NZ	2.38	0.56
53:DA:1020:A:C2	53:DA:1141:U:C2	2.93	0.56
53:DA:357:C:H2'	53:DA:358:U:C6	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1317:C:H2'	14:BN:49:GLN:HE21	1.70	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:1478:G:H1	53:DA:1513:U:H3	1.54	0.56
53:DA:544:C:H3'	53:DA:545:U:C2	2.41	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
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
42:CV:74:ASN:C	42:CV:76:ALA:H	2.10	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
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
39:DS:21:ARG:HH21	57:DS:202:PG4:H71	1.71	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:HE3	5:BE:26:LYS:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
38:CR:9:ILE:HD12	38:CR:9:ILE:C	2.27	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:976:G:OP2	1:AA:1358:U:O2'	2.25	0.55
1:AA:842:U:H3'	1:AA:843:U:C5'	2.37	0.55
1:BA:394:G:OP2	69:BA:1887:HOH:O	2.18	0.55
6:AF:16:GLU:HG2	4:BD:193:ALA:HA	1.87	0.55
32:CL:70:ARG:NH1	32:CL:74:GLY:O	2.40	0.55
33:CM:111:ILE:HG22	33:CM:112:LEU:N	2.21	0.55
35:CO:56:LYS:NZ	35:CO:87:PHE:O	2.39	0.55
48:D1:12:LYS:NZ	69:D1:240:HOH:O	2.38	0.55
53:DA:1847:A:H8	53:DA:1847:A:P	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:2031:A:C6	53:DA:2498:OMC:H1'	2.42	0.55
53:DA:282:A:H2'	53:DA:283:G:C8	2.42	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:1394:U:H4'	22:CA:1603:A:H4'	1.89	0.54
22:CA:301:G:OP2	42:CV:82:ARG:NH1	2.40	0.54
53:DA:1171:G:N3	53:DA:1179:G:N2	2.56	0.54
53:DA:189:G:N7	66:DA:3197:EDO:H21	2.22	0.54
2:AB:27:MET:HE1	2:AB:187:VAL:HG12	1.88	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
1:AA:1217:C:P	14:AN:9:ARG:HH21	2.29	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
26:CE:98:LYS:NZ	69:CE:303:HOH:O	2.40	0.54
22:CA:2360:G:H1'	33:CM:60:ARG:HD3	1.88	0.54
22:CA:2334:U:O4	36:CP:16:ARG:NH2	2.40	0.54
33:DM:85:VAL:HB	33:DM:94:THR:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:C3:44:VAL:HG13	50:C3:45:SER:H	1.72	0.54
29:CH:79:THR:HA	29:CH:145:ASN:HB2	1.88	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:HB3	41:CU:69:ARG:NH1	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
55:DI:131:THR:OG1	55:DI:133:GLU:O	2.19	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:H5''	23:CB:90:C:H6	1.72	0.54
50:D3:29:GLN:HG2	61:D3:102:PEG:H21	1.91	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
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:1170:C:H2'	22:CA:1171:G:C8	2.42	0.53
22:CA:582:A:N7	69:CA:3262:HOH:O	2.34	0.53
53:DA:2172:U:H4'	53:DA:2173:A:H5'	1.90	0.53
53:DA:551:G:H8	53:DA:551:G:H5'	1.73	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AM:79:ARG:NH1	27:DF:113:ASP:OD1	2.41	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
9:AI:85:ARG:HA	9:AI:88:MET:HE3	1.90	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
48:C1:55:ILE:HG22	48:C1:56:ALA:N	2.23	0.53
23:CB:35:C:C2'	23:CB:36:C:H5'	2.38	0.53
22:CA:1993:U:H4'	25:CD:133:THR:CG2	2.38	0.53
53:DA:2383:G:O6	69:DA:4990:HOH:O	2.18	0.53
1:AA:617:G:O2'	69:AA:1936: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: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:1419:A:O2'	22:CA:1421:G:N7	2.32	0.53
22:CA:528:A:C2	22:CA:2042:A:H2'	2.43	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
1:AA:1379:G:N7	7:AG:2:PRO:HB2	2.24	0.53
49:C2:25:LYS:NZ	49:C2:32:GLU:O	2.36	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
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
15:AO:20:ASN:O	15:AO:22:THR:N	2.41	0.52
2:BB:126:PHE:C	2:BB:128:LYS:H	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:BA:264:C:O2'	17:BQ:66:PRO:O	2.26	0.52
20:BT:44:LYS:HD3	20:BT:87:ALA:HA	1.90	0.52
22:CA:2526:G:O2'	52:C5:1:MET:HB3	2.09	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:1170:C:H2'	53:DA:1171:G:C8	2.44	0.52
53:DA:141:G:H3'	53:DA:142:A:C5	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
6:BF:51:ILE:C	6:BF:53:LYS:H	2.12	0.52
11:BK:112:ASP:HB3	21:BU:2:PRO:HG2	1.90	0.52
52:C5:22:VAL:HG11	52:C5:36:ARG:HG3	1.90	0.52
22:CA:1869:G:H3'	22:CA:1870:C:H5'	1.92	0.52
22:CA:797:G:N7	69:CA:3296:HOH:O	2.34	0.52
41:CU:60:THR:O	69:CU:102:HOH:O	2.19	0.52
53:DA:1536:C:H4'	53:DA:1537:G:H5''	1.91	0.52
53:DA:543:G:H5''	53:DA:543:G:H8	1.74	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
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
5:BE:101:GLU:O	5:BE:102:GLY:C	2.48	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
53:DA:1869:G:C2	53:DA:1873:G:C6	2.98	0.52
63:DA:3185:1PE:H222	69:DA:6271:HOH:O	2.09	0.52
53:DA:2256:G:N2	57:DA:3193:PG4:H61	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	7:BG:59:LEU:HD23	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:O4	58:DN:201:MPD:HM2	2.08	0.52
39:DS:82:HIS:NE2	69:DS:341:HOH:O	2.33	0.52
1:AA:1428:A:H2'	1:AA:1429:A:O4'	2.10	0.52
15:AO:26:GLU:N	15:AO:26:GLU:OE1	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:139:U:HO2'	22:CA:141:G:H1	1.55	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:1060:U:H4'	10:AJ:53:ILE:HG23	1.91	0.52
1:AA:412:A:H1'	1:AA:413:G:C5'	2.39	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
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
50:D3:32:ALA:HB2	61:D3:102:PEG:H12	1.91	0.52
53:DA:62:U:O4'	58:DA:3205:MPD:H31	2.10	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
22:CA:2061:G:H5''	22:CA:2503:2MA:HM22	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:126:PHE:C	2:AB:128:LYS:H	2.13	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: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:1900:A:O2'	69:CA:3824:HOH:O	2.19	0.51
24:CC:111:LYS:NZ	24:CC:114:ASP:OD1	2.41	0.51
22:CA:2081:U:OP1	45:CY:17:ASN:ND2	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: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
1:BA:1226:C:N4	13:BM:103:LYS:HE3	2.25	0.51
5:BE:93:ARG:HG3	5:BE:128:TYR:HB2	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: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
22:CA:381:G:OP1	45:CY:18:ARG:NH2	2.37	0.51
57:DA:3193:PG4:H12	69:DA:6907:HOH:O	2.10	0.51
1:BA:467:U:H3'	1:BA:468:A:H5''	1.93	0.51
1:BA:31:G:O2'	1:BA:48:C:N4	2.43	0.51
24:CC:210:ALA:HA	24:CC:213:TRP:CE2	2.45	0.51
22:CA:2264:C:N4	44:CX:15:ASP:OD2	2.43	0.51
58:DA:3211:MPD:O4	58:DA:3211:MPD:O2	2.28	0.51
1:AA:1016:A:N3	1:AA:1016:A:H2'	2.26	0.51
1:AA:121:U:H5''	1:AA:122:G:OP2	2.11	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
48:C1:53:LYS:HE3	48:C1:56:ALA:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
47:C0:5:ILE:HG13	47:C0:6:LYS:N	2.25	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
27:DF:102:ARG:NH1	69:DF:206:HOH:O	2.43	0.51
1:AA:1299:A:H2'	1:AA:1299:A:N3	2.26	0.51
1:AA:411:A:P	4:AD:26:ARG:HH22	2.33	0.51
1:BA:966:2MG:H2'	1:BA:967:5MC:C6	2.45	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
1:AA:722:G:N3	1:AA:722:G:H3'	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
48:C1:55:ILE:HG22	48:C1:56:ALA:H	1.75	0.51
35:CO:90:ARG:CZ	35:CO:116:VAL:HG11	2.41	0.51
53:DA:1171:G:C2	53:DA:1179:G:C2	2.99	0.51
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
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
1:BA:1406:U:C2'	1:BA:1407:5MC:H5'	2.42	0.50
1:BA:257:G:O6	69:BA:1714:HOH:O	2.19	0.50
1:BA:202:G:HO2'	1:BA:468:A:H8	1.59	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
26:CE:41:GLN:C	26:CE:43:THR:H	2.15	0.50
22:CA:2496:C:OP2	34:CN:81:4D4:H8	2.10	0.50
39:CS:49:ILE:HG22	39:CS:53:PHE:C	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:CL:1:MET:HB2	32:CL:67:LYS:HG3	1.93	0.50
53:DA:1913:A:H4'	53:DA:1913:A:OP1	2.12	0.50
4:AD:99:ASP:OD1	4:AD:100:ASN:N	2.45	0.50
1:BA:1462:C:O2'	37:CQ:111:LYS:NZ	2.44	0.50
1:BA:991:U:H4'	1:BA:992:U:C5'	2.41	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:1059:G:H4'	30:DJ:117:MET:HE2	1.93	0.50
53:DA:2116:G:N7	53:DA:2165:C:N4	2.57	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
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
20:BT:27:MET:HG3	20:BT:28:MET:N	2.27	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
7:BG:51:ALA:O	7:BG:55:GLY:N	2.36	0.50
22:CA:1390:U:H2'	22:CA:1391:U:H5'	1.94	0.50
22:CA:971:G:OP2	22:CA:974:G:N2	2.44	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
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
66:DA:3210:EDO:H21	38:DR:16:LYS:HG3	1.94	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
1:BA:276:G:OP1	17:BQ:14:SER:OG	2.21	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:1422:G:N2	22:CA:1577:C:H1'	2.27	0.50
22:CA:662:G:O3'	33:CM:16:GLY:HA2	2.11	0.50
25:CD:112:THR:O	25:CD:195:GLY:HA2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:CR:9:ILE:HD12	38:CR:10:ALA:N	2.27	0.50
50:D3:12:ARG:HH21	50:D3:12:ARG:HG2	1.77	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
53:DA:664:G:OP2	69:DA:5108: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
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
1:BA:1047:G:HO2'	1:BA:1215:G:HO2'	1.56	0.50
3:BC:3:GLN:N	3:BC:3:GLN:OE1	2.45	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
13:AM:95:LEU:C	13:AM:109:ARG:HG2	2.32	0.49
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
53:DA:142:A:H1'	41:DU:1:MET:HE1	1.92	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:1016:A:N1	1:AA:1017:U:O2'	2.44	0.49
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	1.95	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
32:DL:113:MET:CE	32:DL:116:ILE:HD11	2.41	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
15:BO:45:GLU:O	15:BO:47:LYS:N	2.44	0.49
17:BQ:81:LYS:N	17:BQ:81:LYS:HD3	2.27	0.49
22:CA:1340:U:C5	22:CA:1603:A:C8	3.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:842:U:C2	1:BA:844:G:H5'	2.48	0.49
1:BA:79:G:N2	1:BA:91:U:N3	2.59	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
36:DP:31:THR:HG22	36:DP:34:HIS:H	1.77	0.49
12:BL:121:ARG:HH11	12:BL:121:ARG:HG2	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
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:1381:U:C5	1:BA:1382:C:C5	3.01	0.49
1:BA:842:U:H3'	1:BA:843:U:H5''	1.95	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: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
53:DA:933:A:H5'	53:DA:934:U:OP2	2.12	0.49
61:DQ:201:PEG:H22	69:DQ:313:HOH:O	2.12	0.49
1:AA:526:C:H2'	1:AA:527:G7M:H5'	1.93	0.49
1:AA:71:A:O2'	1:AA:72:A:OP2	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:184:G:O2'	20:AT:69:LYS:NZ	2.36	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: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:1516:2MG:N2	1:BA:1519:MA6:OP2	2.43	0.48
1:BA:958:A:N6	19:BS:77:THR:O	2.46	0.48
51:C4:62:LEU:HB3	51:C4:65:ALA:HB2	1.95	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
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:AA:975:A:H8	1:AA:1357:A:HO2'	1.61	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:107:ILE:HD11	11:BK:110:ILE:HG12	1.95	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
13:BM:31:LYS:HA	13:BM:31:LYS:HE3	1.93	0.48
14:BN:32:SER:HA	14:BN:42:TRP:CZ2	2.48	0.48
14:BN:10:GLU:HG3	14:BN:63:ARG:HD2	1.95	0.48
15:BO:18:ASP:OD1	15:BO:20:ASN:N	2.28	0.48
15:BO:4:SER:O	15:BO:8:THR:HG23	2.13	0.48
22:CA:377:G:C6	22:CA:378:C:C4	3.00	0.48
35:CO:53:THR:HG1	35:CO:94:TYR:HH	1.61	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
1:AA:131:A:H2'	1:AA:132:C:C6	2.49	0.48
2:AB:120:GLN:HG3	2:AB:121:SER:N	2.29	0.48
2:AB:15:HIS:HB3	2:AB:43:LEU:HD11	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
51:C4:45:ARG:N	51:C4:46:PRO:HD2	2.29	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
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
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
1:BA:1302:C:C5	13:BM:17:ILE:HD11	2.49	0.48
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	1.96	0.48
22:CA:1638:C:O2	22:CA:2698:U:O2'	2.24	0.48
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
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
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:2489:U:HO2'	22:CA:2491:U:H5	1.61	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:1137:C:H1'	1:AA:1138:G:N2	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
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:CA	12:BL:14:ARG:HH11	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
2:AB:133:GLU:OE2	2:AB:137:ARG:NH1	2.39	0.48
14:BN:31:ILE:HA	14:BN:34:VAL:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BN:45:VAL:HG12	19:BS:10:PHE:HE1	1.79	0.48
1:BA:376:G:H5''	16:BP:5:ARG:HB2	1.96	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: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
1:AA:1003:G:N2	1:AA:1004:A:O2'	2.46	0.48
5:AE:162:GLU:HG3	5:AE:163:GLU:N	2.28	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:CG	6:BF:86:ARG:HH11	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:1342:A:OP1	41:DU:40:LYS:NZ	2.40	0.48
53:DA:137:U:H2'	53:DA:140:C:C1'	2.44	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:2020:A:H5'	48:C1:9:THR:CG2	2.44	0.48
22:CA:563:A:N3	38:CR:37:GLN:NE2	2.61	0.48
22:CA:818:G:O2'	22:CA:819:A:O4'	2.27	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
5:AE:94:VAL:HG22	5:AE:111:MET:CE	2.44	0.47
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: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
22:CA:17:G:H4'	38:CR:25:TYR:CE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:CR:78:LYS:HE2	38:CR:117:LEU:HD21	1.95	0.47
42:CV:74:ASN:ND2	42:CV:74:ASN:O	2.44	0.47
53:DA:1105:U:H2'	53:DA:1106:G:C8	2.49	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
53:DA:811:U:H2'	33:DM:21:ARG:HA	1.96	0.47
53:DA:2305:U:C2	27:DF:151:GLY:HA3	2.48	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
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:2200:C:O2	22:CA:2226:C:N4	2.47	0.47
22:CA:249:C:H5'	22:CA:2394:C:O2'	2.13	0.47
22:CA:223:A:O2'	22:CA:420:C:O2	2.30	0.47
31:CK:37:ARG:NH2	31:CK:44:TYR:OH	2.47	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:H5''	1:AA:159:G:H8	1.79	0.47
14:AN:42:TRP:CD1	14:AN:43:ASN:N	2.83	0.47
10:AJ:51:VAL:HB	14:AN:81:ARG:HB2	1.96	0.47
5:BE:26:LYS:CA	5:BE:26:LYS:HE3	2.44	0.47
5:BE:81:LEU:HB3	5:BE:147:MET:SD	2.54	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:CZ	45:CY:72:ARG:HB2	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
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:455:G:C2	1:BA:478:A:C2	3.02	0.47
1:BA:411:A:P	4:BD:26:ARG:HH12	2.38	0.47
22:CA:558:U:H1'	31:CK:47:HIS:HB3	1.96	0.47
33:CM:29:LYS:C	33:CM:31:GLY:H	2.17	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:H4'	53:DA:1971:U:OP2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
55:DI:68:PRO:HD2	55:DI:69:PHE:CE2	2.49	0.47
9:BI:36:GLU:HA	9:BI:45:ARG:HE	1.79	0.47
22:CA:1178:C:C2	22:CA:1179:G:N7	2.82	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
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
59:DA:3222:PUT:H11	59:DA:3222:PUT:H41	1.47	0.47
53:DA:871:U:H2'	53:DA:872:U:C6	2.50	0.47
24:DC:125:LYS:HB2	24:DC:126:PRO:HD2	1.96	0.47
1:AA:944:G:N1	1:AA:1338:G:OP2	2.41	0.47
5:AE:80:THR:OG1	5:AE:122:ASN:O	2.32	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
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
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
22:CA:2674:G:H4'	32:CL:30:ARG:HD2	1.97	0.47
53:DA:2286:G:OP1	49:D2:30:LYS:NZ	2.37	0.47
59:DA:3222:PUT:H42	69:DL:343:HOH:O	2.13	0.47
53:DA:493:G:H2'	53:DA:494:G:O4'	2.14	0.47
30:DJ:19:ASN:N	30:DJ:20:PRO:HD2	2.29	0.47
1:AA:207:C:H2'	1:AA:208:U:C2	2.49	0.47
2:AB:20:THR:HG22	2:AB:39:HIS:CE1	2.50	0.47
6:AF:14:GLN:NE2	4:BD:166:GLU:OE1	2.48	0.47
1:AA:1228:C:P	13:AM:107:ARG:NH2	2.88	0.47
15:AO:89:ARG:NH1	53:DA:716:A:OP1	2.48	0.47
7:BG:42:ILE:HG21	7:BG:116:MET:HG3	1.96	0.47
7:BG:4:ARG:HG3	7:BG:5:ARG:N	2.29	0.47
22:CA:818:G:H2'	22:CA:819:A:H5''	1.97	0.47
35:CO:8:ARG:HB3	35:CO:10:LEU:HG	1.95	0.47
22:CA:2379:G:H4'	36:CP:21:LEU:HD11	1.97	0.47
36:CP:34:HIS:N	36:CP:65:THR:O	2.47	0.47
22:CA:2019:A:H4'	38:CR:34:VAL:HG21	1.96	0.47
53:DA:1171:G:H3'	53:DA:1172:C:C5	2.50	0.47
53:DA:1171:G:N3	53:DA:1179:G:C2	2.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DA:2498:OMC:HM22	53:DA:2499:C:O4'	2.15	0.47
53:DA:281:C:H2'	53:DA:282:A:C8	2.50	0.47
15:AO:89:ARG:NH1	53:DA:716:A:P	2.88	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
49:C2:11:LEU:HA	49:C2:50:LYS:O	2.15	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
24:CC:260:ASN:C	24:CC:262:ARG:H	2.18	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:O	42:CV:39:ILE:HG22	2.14	0.47
53:DA:1309:G:H4'	50:D3:7:PRO:HB2	1.96	0.47
53:DA:1133:A:N3	59:DA:3214:PUT:H22	2.30	0.47
55:DI:29:ASP:OD1	55:DI:30:SER:N	2.48	0.47
30:DJ:113:LYS:O	30:DJ:117:MET:HG2	2.15	0.47
30:DJ:12:GLN:HA	30:DJ:56:PRO:HA	1.97	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
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
11:BK:97:ILE:HD11	21:BU:16:LEU:HG	1.96	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
53:DA:1555:G:OP1	59:DA:3220:PUT:H41	2.13	0.47
1:AA:451:A:H61	1:AA:481:G:H5'	1.80	0.47
1:AA:75:G:C2	1:AA:76:G:H1'	2.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:BC:19:ASN:ND2	14:BN:90:ARG:O	2.47	0.47
22:CA:135:U:H3	22:CA:144:A:H61	1.61	0.47
22:CA:514:A:N3	22:CA:581:C:O2'	2.41	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
29:CH:135:HIS:CG	29:CH:136:SER:H	2.32	0.47
22:CA:1061:U:OP2	30:CJ:10:LYS:NZ	2.48	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
6:AF:102:MET:CE	18:AR:24:LYS:HB3	2.45	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
51:D4:42:ARG:NH2	69:D4:113:HOH:O	2.48	0.46
53:DA:137:U:C6	53:DA:140:C:H1'	2.51	0.46
1:AA:1464:U:P	37:DQ:109:ARG:HH12	2.38	0.46
1:AA:1229:A:OP2	13:AM:113:ARG:NH1	2.48	0.46
8:AH:3:MET:N	8:AH:3:MET:SD	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:HD2	19:AS:7:LYS:H	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
53:DA:1700:A:N1	69:DA:6711:HOH:O	2.36	0.46
53:DA:545:U:H6	53:DA:548:G:P	2.38	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
22:CA:223:A:N1	22:CA:407:G:O2'	2.41	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
48:D1:2:ALA:N	69:D1:204:HOH:O	2.48	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
1:AA:1018:G:N3	1:AA:1018:G:H2'	2.30	0.46
1:AA:468:A:C8	1:AA:469:C:C6	3.03	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: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
22:CA:846:U:O2'	22:CA:847:U:P	2.74	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
49:D2:22:THR:OG1	51:D4:34:THR:OG1	2.26	0.46
53:DA:2256:G:N3	57:DA:3193:PG4:H31	2.29	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
54:DD:99:GLU:HG2	54:DD:182:ALA:HB2	1.98	0.46
1:AA:1152:A:H5''	10:AJ:15:HIS:HB2	1.97	0.46
9:AI:19:VAL:HG11	9:AI:83:ILE:HA	1.98	0.46
1:AA:1492:A:H4'	12:AL:44:LYS:HE2	1.97	0.46
13:AM:54:ASP:HA	13:AM:57:ARG:HD2	1.98	0.46
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.97	0.46
1:BA:1299:A:N3	1:BA:1299:A:H2'	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
50:C3:43:THR:OG1	50:C3:44:VAL:N	2.48	0.46
22:CA:1808:A:N1	45:CY:28:ARG:HD2	2.31	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)
25:CD:121:THR:HB	25:CD:127:PHE:CD2	2.51	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
14:BN:22:ALA:C	14:BN:26:GLU:OE1	2.53	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
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
23:CB:8:C:O3'	36:CP:25:ARG:NH1	2.48	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
1:AA:254:G:H4'	17:AQ:17:MET:HE2	1.98	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
50:C3:30:VAL:O	50:C3:34:ARG:HG3	2.15	0.46
42:CV:51:ALA:O	42:CV:52:LEU:HB2	2.16	0.46
53:DA:1738:G:HO2'	53:DA:1739:A:H8	1.63	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:1004:A:C2	1:BA:1026:G:C2	3.04	0.46
1:BA:532:A:N3	1:BA:532:A:H2'	2.30	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:1274:A:N3	22:CA:1297:C:H1'	2.30	0.46
22:CA:1783:A:H5'	22:CA:2608:G:H4'	1.97	0.46
25:CD:149:ASN:O	25:CD:151:THR:O	2.33	0.46
25:CD:97:SER:OG	25:CD:98:VAL:N	2.49	0.46
27:CF:40:VAL:HG11	27:CF:50:LEU:HD13	1.98	0.46
22:CA:533:G:H5'	38:CR:24:TYR:CE1	2.51	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
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
14:BN:23:LYS:C	14:BN:26:GLU:OE2	2.54	0.46
18:BR:34:THR:CG2	18:BR:38:LYS:HB2	2.45	0.46
50:C3:3:ARG:NE	50:C3:3:ARG:HA	2.31	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
15:BO:89:ARG:HH12	22:CA:716:A:P	2.39	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
5:AE:94:VAL:HG22	5:AE:111:MET:HE3	1.98	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:ND2	7:BG:130:ASN:O	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:N	15:BO:26:GLU:OE1	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
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:1110:A:H8	1:BA:1110:A:H5'	1.81	0.45
1:BA:1119:C:OP2	9:BI:11:ARG:NH1	2.48	0.45
1:BA:157:U:C2'	1:BA:158:G:H5'	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
51:C4:27:ALA:O	51:C4:28:ASN:HB2	2.16	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
37:DQ:2:SER:O	37:DQ:6:LYS:HB2	2.16	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:1363:C:O2'	22:CA:1809:A:N3	2.40	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
53:DA:142:A:C5	53:DA:143:C:N4	2.84	0.45
53:DA:1583:A:O2'	53:DA:1584:U:O5'	2.30	0.45
53:DA:2224:G:P	24:DC:265:LYS:NZ	2.89	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:1003:G:H21	1:BA:1005:A:H5'	1.81	0.45
1:BA:840:C:H2'	1:BA:841:C:C5'	2.46	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: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
22:CA:846:U:H1'	22:CA:847:U:C5	2.51	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:2189:U:H2'	53:DA:2190:G:O4'	2.16	0.45
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
53:DA:846:U:O2'	53:DA:847:U:P	2.74	0.45
27:DF:140:GLU:OE1	27:DF:140:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DQ:4:ILE:H	37:DQ:4:ILE:HD12	1.82	0.45
1:AA:1423:G:OP1	32:DL:49:ARG:NH2	2.49	0.45
1:AA:657:U:O2	15:AO:22:THR:HG23	2.16	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: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
22:CA:637:A:P	33:CM:112:LEU:HB3	2.56	0.45
53:DA:2886[A]:A:H2'	53:DA:2887[A]:A:H8	1.81	0.45
58:DA:3205:MPD:H52	58:DA:3205:MPD:HM2	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:1041:G:H2'	1:BA:1042:A:C8	2.51	0.45
1:BA:77:A:H2'	1:BA:78:A:C8	2.52	0.45
6:BF:88:MET:SD	6:BF:90:MET:HE2	2.56	0.45
1:BA:501:C:OP1	12:BL:114:ARG:NH2	2.50	0.45
13:BM:48:LEU:HD22	13:BM:53:ILE:HG12	1.99	0.45
22:CA:1906:G:C8	22:CA:1929:G:H2'	2.52	0.45
22:CA:27:G:C2	22:CA:512:G:N3	2.85	0.45
22:CA:2807:U:C4	22:CA:2808:G:N7	2.84	0.45
22:CA:644:A:H2'	22:CA:645:C:O4'	2.16	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:H1'	2.31	0.45
55:DI:119:PRO:HG2	55:DI:122:GLN:HB2	1.98	0.45
55:DI:85:VAL:HG22	55:DI:92:ALA: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:1309:G:H1'	13:BM:73:ILE:HG23	1.99	0.45
1:BA:464:U:N3	1:BA:467:U:OP2	2.37	0.45
1:BA:96:U:O2'	1:BA:97:G:H5'	2.17	0.45
1:BA:542:G:H5'	4:BD:39:GLY:HA3	1.98	0.45
5:BE:134:ILE:H	5:BE:134:ILE:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:AA:1031:C:O2'	1:AA:1032:G:OP2	2.26	0.45
1:AA:5:U:H6	1:AA:5:U:H3'	1.81	0.45
1:AA:1097:C:H4'	2:AB:139:ARG:HH21	1.81	0.45
1:AA:1079:G:H5'	5:AE:134:ILE:CD1	2.46	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:1402:4OC:HM22	1:BA:1403:C:H5'	1.98	0.45
1:BA:247:G:C6	1:BA:278:G:C2	3.05	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
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:H6	1:BA:842:U:O5'	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
11:BK:23:ILE:HD11	11:BK:93:ARG:HA	1.98	0.45
42:CV:5:ILE:HD12	42:CV:67:VAL:HG12	1.98	0.45
32:DL:113:MET:HE1	32:DL:116:ILE:HD11	1.99	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:31:G:O2'	1:AA:48:C:N4	2.50	0.45
1:AA:7:A:O2'	5:AE:106:ILE:HD11	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2046:G:H1'	48:C1:19:HIS:CD2	2.52	0.45
51:C4:7:VAL:HB	51:C4:61:CYS:HB3	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:193:U:H5	69:CA:3617:HOH:O	1.99	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:2584:U:H2'	22:CA:2585:U:H5'	1.99	0.45
22:CA:2572:A:C8	25:CD:150:GLN:HB3	2.52	0.45
27:CF:40:VAL:HG13	27:CF:41:GLY:N	2.32	0.45
30:CJ:18:ALA:C	30:CJ:20:PRO:HD2	2.38	0.45
22:CA:17:G:H4'	38:CR:25:TYR:HE2	1.81	0.45
53:DA:1932:A:H2'	53:DA:1933:G:O4'	2.17	0.45
62:DA:3225:SPD:C9	62:DA:3225:SPD:C5	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
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
8:BH:86:TYR:C	8:BH:87:LYS:HD2	2.37	0.44
10:BJ:15:HIS:HB3	10:BJ:70:HIS:NE2	2.31	0.44
50:C3:44:VAL:HG22	50:C3:45:SER:N	2.32	0.44
25:CD:133:THR:HG23	25:CD:134:HIS:N	2.32	0.44
22:CA:1248:G:C2	38:CR:3:ARG:HD2	2.52	0.44
38:CR:58:ARG:HG3	38:CR:92:ARG:HD2	1.98	0.44
43:CW:29:ILE:HG12	43:CW:30:ILE:N	2.31	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
53:DA:629:G:H4'	53:DA:650:C:O2	2.17	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:105:ILE:HG23	5:AE:123:VAL:HG23	2.00	0.44
5:AE:74:VAL:HG22	5:AE:76:LEU:HD23	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:C3:12:ARG:HG2	50:C3:12:ARG:HH21	1.82	0.44
22:CA:1937:A:O2'	22:CA:1939:5MU:H71	2.18	0.44
22:CA:2502:G:C5'	22:CA:2503:2MA:H5''	2.47	0.44
22:CA:543:G:H8	22:CA:543:G:H5''	1.82	0.44
24:CC:141:VAL:O	24:CC:162:VAL:N	2.43	0.44
24:CC:37:ASN:HB3	24:CC:60:GLN:O	2.17	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
49:D2:47:VAL:CG1	49:D2:48:ILE:N	2.80	0.44
53:DA:57:C:H2'	53:DA:58:G:O4'	2.18	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
1:AA:158:G:H2'	1:AA:159:G:H5''	1.99	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: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:225:C:H2'	22:CA:226:A:O4'	2.17	0.44
22:CA:2619:C:OP1	25:CD:157:LYS:NZ	2.44	0.44
22:CA:320:A:H4'	22:CA:322:A:N7	2.33	0.44
22:CA:247:G:H4'	22:CA:386:G:C5	2.52	0.44
22:CA:449:A:OP2	69:CA:3239:HOH:O	2.20	0.44
33:CM:100:ILE:HG12	33:CM:101:ILE:HG23	2.00	0.44
33:CM:81:ASP:O	33:CM:83:ALA:N	2.50	0.44
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
53:DA:481:G:C4	53:DA:507:A:C2	3.06	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:DJ:18:ALA:C	30:DJ:20:PRO:HD2	2.37	0.44
41:DU:67:VAL:HG22	41:DU:76:ARG:HG3	1.99	0.44
53:DA:2386:A:N3	44:DX:41[A]:ARG:HG3	2.32	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
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
1:BA:1219:A:OP1	14:BN:53:ARG:HD2	2.18	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
22:CA:674:G:H1'	26:CE:69:ARG:CD	2.48	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
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:155:GLY:HA2	3:BC:163:ALA:HB1	2.00	0.44
3:BC:65:ARG:O	3:BC:66:VAL:O	2.34	0.44
11:BK:13:ARG:NH1	11:BK:77:TYR:OH	2.51	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
40:DT:110:ARG:CG	40:DT:110:ARG:OXT	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1225:A:H2'	1:BA:1226:C:C5	2.52	0.44
1:AA:843:U:H3	2:BB:115:LYS:HD3	1.82	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:1847:A:HO2'	53:DA:1848:A:H8	1.63	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
1:AA:1463:U:H2'	1:AA:1464:U:C6	2.53	0.44
1:AA:85:U:H6	1:AA:86:G:N1	2.15	0.44
10:AJ:29:ALA:HA	10:AJ:32:THR:HG22	2.00	0.44
3:AC:6:HIS:CG	14:AN:89:MET:HB3	2.52	0.44
17:AQ:49:GLU:O	17:AQ:50:ASN:HB2	2.18	0.44
1:AA:1322:C:P	19:AS:78:ARG:HH22	2.40	0.44
6:BF:53:LYS:NZ	6:BF:53:LYS:HA	2.33	0.44
22:CA:118:A:C8	22:CA:119:A:C8	3.06	0.44
22:CA:12:U:H2'	22:CA:12:U:O2	2.18	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
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:1450:U:O2'	1:BA:1451:U:H2'	2.17	0.44
3:BC:38:LYS:N	3:BC:38:LYS:HD3	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
1:BA:1217:C:P	14:BN:9:ARG:HH21	2.38	0.44
14:BN:46:LEU:HD22	19:BS:13:LEU:HD23	2.00	0.44
1:BA:263:A:P	20:BT:74:ARG:NH1	2.91	0.44
24:CC:182:ARG:NH2	24:CC:183:LYS:O	2.51	0.44
22:CA:2683:C:H4'	25:CD:13:ARG:NH1	2.33	0.44
22:CA:396:G:C1'	45:CY:29:PHE:HB3	2.47	0.44
53:DA:1494:A:C2	53:DA:1495:A:C4	3.05	0.44
53:DA:1494:A:HO2'	53:DA:1495:A:P	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DR:20:GLN:HG3	57:DR:202:PG4:H31	1.98	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
6:BF:88:MET:SD	6:BF:90:MET:CE	3.06	0.43
6:BF:91:ARG:CG	6:BF:93:LYS:NZ	2.80	0.43
52:C5:1:MET:HB3	52:C5:34:LYS:HE2	2.00	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
22:CA:468:G:N7	50:C3:39:ARG:NH2	2.63	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
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
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
8:AH:41:LYS:HD2	8:AH:48:ASP:HA	2.00	0.43
1:AA:1014:A:OP1	19:AS:18:LYS:NZ	2.51	0.43
1:BA:1127:G:H1	1:BA:1145:A:H61	1.65	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
12:BL:45:PRO:HD2	12:BL:46:ASN:H	1.84	0.43
14:BN:26:GLU:N	14:BN:26:GLU:CD	2.61	0.43
48:C1:25:VAL:HG13	48:C1:26:THR:N	2.33	0.43
27:CF:126:GLY:O	27:CF:158:THR:HG21	2.17	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
53:DA:5:A:C2	53:DA:2899:A:C2	3.06	0.43
1:AA:464:U:C2	1:AA:466:A:H5''	2.53	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:1359:C:O2'	1:BA:1361:G:N7	2.52	0.43
1:BA:268:U:H2'	1:BA:269:C:C6	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BJ:19:ASP:HA	10:BJ:22:THR:HB	2.00	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:H42	61:DP:201:PEG:H22	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:27:MET:HE2	2:AB:189:THR:HA	2.01	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
12:AL:116:LYS:NZ	69:AL:304:HOH:O	2.45	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
2:BB:32:PHE:N	2:BB:40:ILE:O	2.52	0.43
1:BA:532:A:H61	3:BC:193:TYR:HD2	1.66	0.43
11:BK:106:ARG:HG2	11:BK:106:ARG:HH11	1.84	0.43
12:BL:51:LYS:N	12:BL:51:LYS:HD2	2.33	0.43
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: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:125:A:OP2	50:C3:19:ARG:NH2	2.44	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:2751:G:C2	28:CG:3:ARG:NH1	2.87	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
53:DA:2886[A]:A:C6	53:DA:2887[A]:A:C5	3.06	0.43
53:DA:388:G:N7	53:DA:390:U:H2'	2.33	0.43
1:BA:1408:A:C2	1:BA:1494:G:C4	3.07	0.43
1:BA:302:G:N3	1:BA:556:C:H4'	2.34	0.43
50:C3:24:THR:HG23	50:C3:27:GLY:H	1.83	0.43
22:CA:2889:C:N4	22:CA:2890:G:C6	2.87	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
31:CK:57:LEU:HD23	31:CK:129:GLU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:CO:20:MET:HG3	35:CO:21:PHE:N	2.32	0.43
49:D2:35:GLU:OE2	49:D2:48:ILE:HD11	2.18	0.43
53:DA:1183:U:H2'	53:DA:1184:U:C6	2.54	0.43
53:DA:1847:A:C8	53:DA:1847:A:P	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
5:AE:90:THR:HG22	5:AE:91:GLY:N	2.34	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:844:G:N3	1:BA:844:G:H3'	2.33	0.43
1:BA:81:A:C2	1:BA:89:U:O2	2.72	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
9:BI:85:ARG:HA	9:BI:88:MET:HE3	2.01	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:2086:U:H2'	22:CA:2087:G:C8	2.53	0.43
22:CA:2716:C:O2'	22:CA:2717:C:H5'	2.19	0.43
22:CA:55:G:C2	22:CA:116:C:C2	3.06	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:1385:A:O2'	53:DA:1396:U:O2	2.33	0.43
53:DA:141:G:H3'	53:DA:142:A:C4	2.54	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
53:DA:876:C:H2'	53:DA:877:A:O4'	2.19	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:HG23	8:AH:75:ILE:O	2.19	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
1:BA:429:U:H5'	4:BD:9:LEU:HD12	2.00	0.43
5:BE:75:ALA:O	5:BE:82:GLN:NE2	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
48:D1:3:VAL:HG22	48:D1:4:GLN:N	2.34	0.43
53:DA:2116:G:C6	53:DA:2171:A:N6	2.84	0.43
53:DA:570:G:H2'	53:DA:2030:6MZ:N7	2.34	0.43
53:DA:914:G:H3'	53:DA:914:G:C8	2.53	0.43
30:DJ:56:PRO:HG2	30:DJ:72:LYS:HB2	2.01	0.43
1:AA:1464:U:OP2	37:DQ:109:ARG:NH1	2.52	0.43
13:AM:107:ARG:HH11	13:AM:107:ARG:HG2	1.83	0.43
11:AK:107:ILE:HG13	21:AU:12:PHE:CE2	2.54	0.43
1:BA:1144:G:H5''	1:BA:1145:A:OP2	2.19	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
1:BA:86:G:H1'	1:BA:87:C:C6	2.54	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:2419:U:H5''	49:C2:22:THR:HG21	2.01	0.43
22:CA:1390:U:C2'	22:CA:1391:U:H5'	2.49	0.43
22:CA:1915:3TD:H10A	22:CA:1916:A:C4	2.53	0.43
22:CA:2680:U:HO2'	22:CA:2681:C:C5'	2.32	0.43
22:CA:335:C:HO2'	22:CA:336:C:P	2.41	0.43
22:CA:36:G:N3	22:CA:450:G:O2'	2.51	0.43
22:CA:619:G:OP2	22:CA:620:G:N2	2.49	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: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
7:AG:135:VAL:HG23	7:AG:136:LYS:N	2.33	0.43
7:AG:80:VAL:HG12	7:AG:81:GLY:N	2.34	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:1498:UR3:O4'	1:BA:1519:MA6:H2	2.19	0.43
1:BA:209:U:H4'	1:BA:210:C:OP2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	24:CC:97:LYS:HD3	2.34	0.43
25:CD:151:THR:C	25:CD:153:GLY:N	2.71	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
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
2:AB:129:LEU:O	2:AB:130:THR:CB	2.67	0.43
2:AB:19:GLN:HA	2:AB:38:VAL:HA	2.01	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
22:CA:1027:A:N7	22:CA:1126:A:C2	2.86	0.43
22:CA:51:G:N3	22:CA:119: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
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
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
50:D3:29:GLN:HG2	61:D3:102:PEG:H32	2.01	0.43
53:DA:1141:U:H4'	53:DA:1142:A:O4'	2.19	0.43
53:DA:864:G:C6	53:DA:865:C:N4	2.87	0.43
30:DJ:114:ALA:CB	30:DJ:125:MET:SD	3.07	0.43
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
1:AA:501:C:OP1	12:AL:114:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BE:154:ALA:C	5:BE:156:LYS:N	2.73	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
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
22:CA:166:U:OP2	69:CA:3785:HOH:O	2.22	0.42
22:CA:2304:G:O2'	27:CF:130:MET:O	2.37	0.42
22:CA:446:G:OP1	38:CR:5:LYS:NZ	2.52	0.42
24:CC:17:VAL:HB	24:CC:204:VAL:CG1	2.49	0.42
22:CA:1790:C:O2'	24:CC:208:ALA:HB2	2.18	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
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
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
22:CA:1009:A:N3	22:CA:1153:C:O2'	2.44	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: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
22:CA:2032:G:N3	25:CD:150:GLN:HG2	2.33	0.42
26:CE:75:SER:OG	26:CE:77:ILE:HG12	2.18	0.42
22:CA:1338:G:H5''	41:CU:17:SER:HB2	2.00	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
1:AA:1405:G:O4'	1:AA:1519:MA6:H4'	2.20	0.42
1:AA:157:U:H2'	1:AA:158:G:H5'	2.01	0.42
1:AA:196:A:OP1	20:AT:64:LYS:NZ	2.47	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
48:C1:13:ARG:HD2	48:C1:17:ARG:NH2	2.35	0.42
22:CA:124:G:C5	50:C3:19:ARG:NH1	2.87	0.42
22:CA:1341:G:OP1	22:CA:1397:U:N3	2.47	0.42
22:CA:191:A:H2'	22:CA:192:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CA:2788:C:H2'	22:CA:2789:C:C6	2.55	0.42
22:CA:846:U:H1'	22:CA:847:U:H5	1.84	0.42
26:CE:77:ILE:HG13	26:CE:78:TRP:HE3	1.84	0.42
22:CA:2531:A:H5'	28:CG:157:TYR:CZ	2.54	0.42
41:CU:69:ARG:NE	41:CU:69:ARG:O	2.52	0.42
50:D3:33:ARG:HG2	61:D3:102:PEG:H42	2.01	0.42
53:DA:914:G:C3'	53:DA:914:G:C8	3.02	0.42
27:DF:141:ILE:HG23	27:DF:146:VAL:CG1	2.50	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
10:AJ:65:TYR:CB	14:AN:96:LEU:HD11	2.50	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
1:BA:213:G:N7	1:BA:214:C:C4	2.87	0.42
6:BF:38:ARG:NH1	6:BF:61:LEU:HD21	2.34	0.42
11:BK:82:LEU:N	11:BK:82:LEU:CD2	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:1867:G:O6	22:CA:1875:G:N2	2.52	0.42
22:CA:1867:G:O2'	22:CA:1868:C:H5'	2.19	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
30:CJ:12:GLN:HA	30:CJ:56:PRO:HA	2.02	0.42
32:CL:35:VAL:HG12	32:CL:36:GLY:N	2.35	0.42
53:DA:1172:C:N4	53:DA:1173:U:C2	2.87	0.42
53:DA:158:U:H1'	53:DA:169:G:N2	2.33	0.42
53:DA:1609:A:N6	69:DA:5835:HOH:O	2.52	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
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
1:BA:511:C:H5'	4:BD:44:ARG:NH1	2.35	0.42
11:BK:20:VAL:N	11:BK:35:THR:O	2.52	0.42
18:BR:20:GLU:HA	18:BR:55:LEU:HD13	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
22:CA:2547:A:H4'	32:CL:29:HIS:NE2	2.35	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
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
42:DV:51:ALA:O	42:DV:52:LEU:CB	2.68	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
14:BN:31:ILE:HG23	14:BN:42:TRP:CH2	2.55	0.42
11:BK:97:ILE:HD11	21:BU:16:LEU:CG	2.50	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: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:1638:C:H4'	22:CA:2710:C:O2	2.20	0.42
22:CA:2824:C:C4	22:CA:2825:G:C5	3.08	0.42
24:CC:168:ASP:N	24:CC:168:ASP:OD1	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
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:1405:U:H2'	53:DA:1406:U:C6	2.54	0.42
53:DA:1416:G:HO2'	53:DA:1417:C:P	2.42	0.42
53:DA:1482:G:H1'	53:DA:1509:A:H61	1.83	0.42
53:DA:1583:A:HO2'	53:DA:1584:U:P	2.42	0.42
53:DA:382:A:C2	53:DA:393:C:C2	3.07	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
43:DW:46:LYS:NZ	69:DW:124:HOH:O	2.52	0.42
1:AA:1064:G:H1'	1:AA:1190:G:N2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
22:CA:526:A:N6	22:CA:2626:C:H4'	2.34	0.42
22:CA:289:G:H2'	22:CA:290:U:O4'	2.19	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: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:483:A:C2'	53:DA:484:C:H5'	2.50	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
1:BA:1118:U:H5''	9:BI:106:ARG:HG3	2.02	0.42
1:BA:632:U:O2	1:BA:632:U:H2'	2.20	0.42
2:BB:27:MET:HE1	2:BB:187:VAL:O	2.20	0.42
5:BE:115:LEU:HB3	5:BE:120:VAL:HG23	2.00	0.42
5:BE:65:GLU:OE1	5:BE:69:ARG:NH2	2.50	0.42
7:BG:145:ALA:O	7:BG:146:GLU:CG	2.68	0.42
7:BG:22:LEU:HA	7:BG:25:LYS:HE2	2.01	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
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: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
24:CC:76:ALA:HB2	24:CC:96:TYR:CD1	2.55	0.42
40:CT:69:LEU:HB3	40:CT:107:VAL:HG22	2.00	0.42
22:CA:2232:C:P	45:CY:27:ARG:HH12	2.42	0.42
46:CZ:11:VAL:HG13	46:CZ:57:LEU:HD11	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DA:1956:U:H2'	53:DA:1957:C:H5'	2.01	0.42
53:DA:277:G:O2'	53:DA:278:A:OP2	2.37	0.42
1:AA:1377:A:N3	7:AG:2:PRO:HG3	2.35	0.42
1:AA:923:A:OP1	5:AE:26:LYS:HG2	2.20	0.42
9:AI:30:ILE:HA	9:AI:65:ILE:HG13	2.02	0.42
9:AI:19:VAL:HA	9:AI:65:ILE:HG22	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: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
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
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
48:D1:41:HIS:HA	48:D1:49:TYR:OH	2.20	0.42
53:DA:2095:A:H2'	53:DA:2096:C:O4'	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: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:HD22	3:BC:178:LEU:H	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
1:BA:1049:U:H2'	14:BN:3:LYS:HE3	2.00	0.42
49:C2:48:ILE:H	49:C2:48:ILE:HD12	1.84	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
22:CA:335:C:H5''	42:CV:82:ARG:HD3	2.01	0.42
22:CA:335:C:O2'	22:CA:336:C:P	2.77	0.42
24:CC:75:PRO:HB2	24:CC:97:LYS:CE	2.50	0.42
26:CE:42:GLY:HA3	26:CE:90:GLN:O	2.19	0.42
27:CF:122:PHE:C	27:CF:124:GLY:H	2.23	0.42
53:DA:141:G:H2'	53:DA:142:A:N3	2.33	0.42
53:DA:2188:U:H2'	53:DA:2189:U:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DA:860:U:OP1	62:DA:3187:SPD:H92	2.20	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:1152:A:H5'	10:AJ:72:ARG:HH22	1.85	0.41
1:AA:933:G:O6	7:AG:3:ARG:NH1	2.49	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
18:BR:43:ARG:HG2	18:BR:44:ILE:H	1.85	0.41
22:CA:2615:U:C2	48:C1:4:GLN:HA	2.55	0.41
52:C5:17:VAL:CG1	52:C5:26:ILE:HD12	2.50	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
31:CK:125:TYR:CE2	31:CK:130:HIS:HA	2.55	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
53:DA:1175:A:H2'	53:DA:1175:A:N3	2.35	0.41
53:DA:1876:A:H2'	53:DA:1877:A:O4'	2.20	0.41
58:DA:3190:MPD:C1	58:DA:3190:MPD:H52	2.50	0.41
53:DA:75:G:H4'	46:DZ:48:ARG:NH2	2.35	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:1402:4OC:HM42	1:AA:1500:A:H61	1.85	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
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
20:AT:28:MET:HE2	20:AT:32:ILE:HD11	2.02	0.41
1:BA:374:A:OP1	1:BA:452:A:N1	2.53	0.41
6:BF:92:THR:HG22	6:BF:93:LYS:N	2.35	0.41
15:BO:45:GLU:HG2	15:BO:46:HIS:N	2.35	0.41
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:1059:G:H4'	30:CJ:117:MET:HE2	2.02	0.41
22:CA:2445:2MG:HM21	22:CA:2449:U:O4	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
53:DA:523:C:H4'	53:DA:540:C:O2	2.20	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
1:AA:68:G:C5	1:AA:69:G:H1'	2.55	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
13:AM:107:ARG:NH2	13:AM:113:ARG:HB3	2.35	0.41
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	2.02	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
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:2747:G:O6	22:CA:2755:C:H5''	2.20	0.41
22:CA:279:A:H61	22:CA:361:G:H1'	1.85	0.41
25:CD:104:VAL:O	25:CD:105:LYS:HB3	2.20	0.41
26:CE:7:ASP:OD1	26:CE:7:ASP:N	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
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: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
53:DA:846:U:HO2'	53:DA:847:U:P	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1417:G:C6	1:AA:1482:G:C6	3.08	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
14:AN:54:ASP:OD1	14:AN:59:ARG:NE	2.47	0.41
1:BA:1012:A:N1	1:BA:1018:G:O6	2.53	0.41
1:BA:33:A:H2'	1:BA:34:C:C6	2.55	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:296:U:O2'	1:BA:556:C:O2	2.34	0.41
4:BD:105:MET:SD	4:BD:143:VAL:CG1	3.09	0.41
15:BO:40:GLN:NE2	15:BO:40:GLN:HA	2.36	0.41
1:BA:254:G:H4'	17:BQ:20:SER:HB2	2.01	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:HA	42:CV:52:LEU:HD23	1.92	0.41
44:CX:61:ALA:CB	44:CX:82:ILE:HD12	2.50	0.41
53:DA:1794:A:H2'	53:DA:1795:C:C6	2.55	0.41
53:DA:275:C:H3'	53:DA:276:U:H5''	2.02	0.41
53:DA:2886[A]:A:C4	53:DA:2887[A]:A:C8	3.09	0.41
53:DA:547:A:H3'	53:DA:547:A:C8	2.54	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:O2	1:BA:209:U:H2'	2.20	0.41
5:BE:156:LYS:O	5:BE:159:LYS:NZ	2.53	0.41
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:54:MET:HE3	20:BT:58:VAL:HB	2.02	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:N	29:CH:11:ASN:OD1	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
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
53:DA:1153:C:OP2	69:DA:3826:HOH:O	2.20	0.41
53:DA:141:G:C2'	53:DA:142:A:C4	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:DA:3202:ACY:H1	69:DA:7057:HOH:O	2.21	0.41
53:DA:435:C:C2'	53:DA:436:C:H5'	2.50	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
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:1255:G:C6	1:BA:1279:G:C8	3.08	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
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:2394:C:OP2	51:C4:30:ARG:HD3	2.21	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: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
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
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
30:DJ:117:MET:CE	30:DJ:117:MET:HA	2.51	0.41
1:AA:1224:U:H3'	1:AA:1225:A:H5'	2.03	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
5:AE:57:PRO:HA	5:AE:60:ILE:CG1	2.51	0.41
9:AI:54:LEU:N	9:AI:54:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	2.03	0.41
50:C3:44:VAL:O	50:C3:45:SER:CB	2.69	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
22:CA:42:A:C2	22:CA:438:G:C2	3.09	0.41
22:CA:7:G:H4'	31:CK:15:TRP:CH2	2.56	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:HD3	34:CN:58:LYS:N	2.35	0.41
41:CU:50:LEU:N	41:CU:50:LEU:HD13	2.36	0.41
53:DA:1509:A:O2'	53:DA:1510:G:P	2.79	0.41
1:AA:1449:C:C2	1:AA:1455:G:C2	3.08	0.41
1:AA:328:C:H2'	1:AA:328:C:O2	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
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:115:LEU:CA	5:BE:120:VAL:HG23	2.50	0.41
5:BE:50:TYR:O	5:BE:51:GLY:O	2.38	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
22:CA:2796:U:H3	22:CA:2799:A:N6	2.19	0.41
22:CA:742:A:H2'	22:CA:743:A:C8	2.55	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:116:VAL:HG12	35:CO:117:ASP:N	2.35	0.41
35:CO:43:GLU:OE1	35:CO:43:GLU:HA	2.21	0.41
42:CV:16:GLY:O	42:CV:18:ASP:N	2.49	0.41
53:DA:102:U:H2'	53:DA:102:U:O2	2.20	0.41
53:DA:1178:C:C2'	53:DA:1179:G:H5'	2.51	0.41
53:DA:1417:C:H2'	53:DA:1418:G:O4'	2.20	0.41
53:DA:2162:G:OP1	53:DA:2171:A:H2'	2.20	0.41
53:DA:2015:A:H1'	61:DA:3227:PEG:H42	2.03	0.41
54:DD:62:LYS:N	54:DD:63:PRO:CD	2.83	0.41
29:DH:130:VAL:HG21	29:DH:144:VAL:HG21	2.02	0.41
1:AA:108:G:C5'	1:AA:108:G:N3	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1095:U:H2'	1:AA:1096:C:C6	2.56	0.41
1:AA:864:A:H4'	5:AE:90:THR:HG23	2.03	0.41
7:AG:131:LYS:HA	7:AG:135:VAL:HG21	2.02	0.41
5:AE:162:GLU:HG2	8:AH:114:ARG:NH2	2.36	0.41
19:AS:12:ASP:OD1	19:AS:37:ARG:NH2	2.54	0.41
1:AA:1312:G:H5'	19:AS:6:LYS:CE	2.51	0.41
20:AT:59:ASP:OD1	20:AT:76:LYS:NZ	2.47	0.41
1:BA:1062:U:H2'	1:BA:1063:C:C6	2.56	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:826:C:O2	8:BH:16:ASN:ND2	2.54	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
10:BJ:18:ILE:HD12	10:BJ:70:HIS:HB2	2.03	0.41
1:BA:502:A:OP1	12:BL:115:SER:HB3	2.21	0.41
12:BL:76:GLU:O	12:BL:77:HIS:HB2	2.21	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
17:BQ:6:ARG:HB3	17:BQ:6:ARG:CZ	2.51	0.41
19:BS:80:TYR:CG	19:BS:80:TYR:O	2.74	0.41
49:C2:15:ALA:C	49:C2:17:THR:H	2.24	0.41
22:CA:1379:U:H4'	22:CA:1380:G:OP1	2.21	0.41
22:CA:1847:A:O2'	22:CA:1848:A:H8	2.03	0.41
22:CA:2053:G:N2	22:CA:2054:A:H1'	2.36	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:2061:G:H5''	22:CA:2503:2MA:CM2	2.50	0.41
28:CG:175:LYS:HG2	28:CG:176:LYS:H	1.85	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:1607:C:OP1	69:DA:5123:HOH:O	2.22	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
58:DN:201:MPD:O4	58:DN:201:MPD:CM	2.69	0.41
13:AM:6:GLY:HA2	13:AM:66:GLU:HG3	2.01	0.41
16:AP:48:GLU:HG2	16:AP:49:GLY:H	1.85	0.41
19:AS:31:LEU:HD12	19:AS:31:LEU:N	2.36	0.41
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.51	0.41
6:BF:53:LYS:HZ2	6:BF:53:LYS:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BG:65:ALA:HA	7:BG:128:ALA:HA	2.03	0.41
10:BJ:87:LEU:HD13	10:BJ:88:MET:N	2.35	0.41
12:BL:110:ARG:HB2	12:BL:119:VAL:HG21	2.03	0.41
15:BO:3:LEU:HD13	15:BO:35:GLN:HE21	1.86	0.41
15:BO:87:LEU:O	15:BO:88:ARG:CB	2.69	0.41
20:BT:36:TYR:CD1	20:BT:36:TYR:C	2.93	0.41
22:CA:1693:U:O2'	24:CC:14:ARG:NH2	2.54	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
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:2032:G:C2	25:CD:150:GLN:HG2	2.56	0.41
26:CE:108:ILE:HG13	26:CE:109:LEU:N	2.36	0.41
27:CF:36:LEU:HD13	27:CF:36:LEU:N	2.35	0.41
31:CK:41:LYS:NZ	31:CK:50:THR:O	2.50	0.41
22:CA:1187:G:H5''	39:CS:83:TYR:CE2	2.56	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
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
15:AO:87:LEU:O	15:AO:88:ARG:CB	2.68	0.41
1:AA:263:A:P	20:AT:74:ARG:HH11	2.43	0.41
1:BA:106:C:O2	1:BA:379:C:H4'	2.21	0.41
1:BA:1409:C:H5''	22:CA:1915:3TD:H10B	2.03	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:N	9:BI:54:LEU:HD12	2.36	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:113:LYS:O	30:CJ:117:MET:HG2	2.21	0.41
30:CJ:20:PRO:HB2	30:CJ:23:PRO:HD2	2.03	0.41
38:CR:76:TYR:CZ	38:CR:80:ILE:HG13	2.56	0.41
22:CA:1223:G:P	39:CS:68:ARG:HH12	2.43	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:H5'	1:AA:108:G:N3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:AE:82:GLN:CD	5:AE:150:PRO:HD3	2.41	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: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
1:BA:75:G:C6	1:BA:76:G:C5	3.09	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
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:14:SER:C	17:BQ:17:MET:HE1	2.42	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:1857:G:O2'	22:CA:1884:G:N2	2.53	0.40
22:CA:2796:U:H3	22:CA:2799:A:H61	1.68	0.40
22:CA:565:C:H2'	22:CA:566:U:O4'	2.21	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:806:C:O4'	57:BA:1642:PG4:H72	2.21	0.40
1:BA:328:C:O2	1:BA:328:C:H2'	2.21	0.40
1:BA:450:G:P	69:BA:1918:HOH:O	2.77	0.40
17:BQ:8:LEU:HD13	17:BQ:73:TRP:CZ3	2.56	0.40
22:CA:1468:U:H2'	22:CA:1522:A:N6	2.36	0.40
22:CA:541:A:C2	22:CA:553:G:C2	3.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
9:AI:83:ILE:HG22	9:AI:87:LEU:HD13	2.04	0.40
1:BA:1402:4OC:H2'	1:BA:1402:4OC:O2	2.22	0.40
5:BE:102:GLY:C	5:BE:104:GLY:N	2.70	0.40
1:BA:1081:A:H5'	5:BE:23:LYS:HG3	2.03	0.40
6:BF:45:ARG:O	6:BF:56:LYS:HA	2.21	0.40
8:BH:96:MET:HE2	8:BH:96:MET:HB3	1.93	0.40
18:BR:23:TYR:HA	18:BR:58:ALA:HB1	2.03	0.40
48:C1:25:VAL:HG13	48:C1:26:THR:H	1.86	0.40
22:CA:1170:C:C2	22:CA:1171:G:N7	2.89	0.40
22:CA:2636:C:H4'	25:CD:81:GLU:CD	2.41	0.40
25:CD:104:VAL:CG2	25:CD:105:LYS:N	2.84	0.40
26:CE:31:VAL:HG21	26:CE:104:ALA:CB	2.51	0.40
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
22:CA:1190:G:OP1	33:CM:32:GLY:HA2	2.21	0.40
34:CN:20:LEU:N	34:CN:20:LEU:HD22	2.35	0.40
38:CR:36:PHE:CE1	38:CR:40:ILE:HD11	2.56	0.40
22:CA:310:A:H5''	42:CV:15:THR:HG22	2.03	0.40
53:DA:2534:A:C2'	53:DA:2535:G:O5'	2.70	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
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
43:DW:2:PHE:HB3	43:DW:50:MET:HE1	2.03	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
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:124:ARG:HG3	9:BI:125:PRO:HD2	2.02	0.40
9:BI:83:ILE:O	9:BI:87:LEU:HD13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BO:10:LYS:O	15:BO:14:GLU:HG3	2.21	0.40
1:BA:736:C:OP1	18:BR:61:ARG:HD2	2.21	0.40
19:BS:13:LEU:HD22	19:BS:16:LEU:HD23	2.03	0.40
22:CA:1914:C:H2'	22:CA:1915:3TD:H5'A	2.02	0.40
22:CA:2627:G:O2'	22:CA:2781:A:N1	2.41	0.40
22:CA:662:G:O2'	33:CM:14:LYS:HD3	2.22	0.40
25:CD:19:GLY:O	32:CL:73:ASP:HB3	2.22	0.40
22:CA:1651:G:H4'	35:CO:39:PRO:HG2	2.03	0.40
22:CA:2365:G:H4'	44:CX:60:PHE:CE2	2.57	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:H32	61:DA:3200:PEG:H11	1.70	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
1:AA:1449:C:H2'	1:AA:1450:U:H5'	2.03	0.40
1:AA:182:A:N1	1:AA:223:A:O2'	2.53	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
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:AA:234:C:H4'	17:AQ:66:PRO:HG3	2.03	0.40
1:BA:1111:A:H8	1:BA:1111:A:O5'	2.04	0.40
1:BA:111:G:O6	1:BA:330:C:N4	2.55	0.40
1:BA:1492:A:C5	1:BA:1493:A:C2	3.10	0.40
1:BA:283:U:C4	1:BA:284:C:C4	3.09	0.40
3:BC:11:ARG:HH21	3:BC:182:ILE:HG13	1.87	0.40
10:BJ:28:THR:HG23	10:BJ:31:ARG:NH2	2.36	0.40
1:BA:706:A:H1'	11:BK:31:ILE:HD11	2.04	0.40
15:BO:67:LEU:CD2	15:BO:88:ARG:HH22	2.35	0.40
49:C2:50:LYS:O	49:C2:51:GLU:HB3	2.22	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
22:CA:523:C:H4'	22:CA:540:C:O2	2.21	0.40
27:CF:21:ASN:ND2	27:CF:21:ASN:O	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
53:DA:1167:C:H2'	53:DA:1168:G:H5''	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:DA:1730:C:O2'	53:DA:1731:G:O5'	2.40	0.40
53:DA:2851:A:H2'	53:DA:2852:G:O4'	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
27:DF:158:THR:HG22	27:DF:160:ALA:N	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	209 (94%)	11 (5%)	2 (1%)	20	14
2	BB	222/224 (99%)	209 (94%)	11 (5%)	2 (1%)	20	14
3	AC	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	32	28
3	BC	204/206 (99%)	186 (91%)	10 (5%)	8 (4%)	3	1
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%)	5	1
7	AG	149/151 (99%)	138 (93%)	10 (7%)	1 (1%)	25	20
7	BG	149/151 (99%)	131 (88%)	15 (10%)	3 (2%)	9	4
8	AH	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
8	BH	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	22	17
9	AI	125/127 (98%)	111 (89%)	13 (10%)	1 (1%)	22	17
9	BI	125/127 (98%)	111 (89%)	13 (10%)	1 (1%)	22	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AJ	97/99 (98%)	88 (91%)	8 (8%)	1 (1%)	18	12
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%)	4	1
12	AL	120/123 (98%)	111 (92%)	9 (8%)	0	100	100
12	BL	120/123 (98%)	110 (92%)	8 (7%)	2 (2%)	11	5
13	AM	112/114 (98%)	101 (90%)	8 (7%)	3 (3%)	6	2
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%)	4	1
15	BO	86/88 (98%)	79 (92%)	2 (2%)	5 (6%)	2	0
16	AP	80/82 (98%)	73 (91%)	6 (8%)	1 (1%)	14	8
16	BP	80/82 (98%)	66 (82%)	11 (14%)	3 (4%)	4	1
17	AQ	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
17	BQ	78/80 (98%)	64 (82%)	10 (13%)	4 (5%)	2	0
18	AR	53/55 (96%)	51 (96%)	1 (2%)	1 (2%)	9	4
18	BR	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	9	4
19	AS	77/79 (98%)	69 (90%)	7 (9%)	1 (1%)	14	8
19	BS	77/79 (98%)	65 (84%)	9 (12%)	3 (4%)	3	1
20	AT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
20	BT	83/86 (96%)	77 (93%)	3 (4%)	3 (4%)	4	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%)	17	11
24	DC	269/271 (99%)	253 (94%)	15 (6%)	1 (0%)	38	35
25	CD	207/209 (99%)	193 (93%)	11 (5%)	3 (1%)	13	7
26	CE	199/201 (99%)	186 (94%)	9 (4%)	4 (2%)	9	4
26	DE	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
27	CF	175/177 (99%)	155 (89%)	14 (8%)	6 (3%)	4	1
27	DF	175/177 (99%)	165 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	CG	174/176 (99%)	135 (78%)	33 (19%)	6 (3%)	4	1
28	DG	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
29	CH	147/149 (99%)	116 (79%)	22 (15%)	9 (6%)	2	0
29	DH	147/149 (99%)	129 (88%)	16 (11%)	2 (1%)	13	7
30	CJ	132/134 (98%)	117 (89%)	11 (8%)	4 (3%)	5	1
30	DJ	132/134 (98%)	117 (89%)	11 (8%)	4 (3%)	5	1
31	CK	140/142 (99%)	127 (91%)	11 (8%)	2 (1%)	13	7
31	DK	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
32	CL	120/123 (98%)	112 (93%)	7 (6%)	1 (1%)	22	17
32	DL	121/123 (98%)	116 (96%)	4 (3%)	1 (1%)	22	17
33	CM	142/144 (99%)	128 (90%)	8 (6%)	6 (4%)	3	1
33	DM	142/144 (99%)	138 (97%)	3 (2%)	1 (1%)	25	20
34	CN	133/136 (98%)	125 (94%)	7 (5%)	1 (1%)	22	17
34	DN	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
35	CO	118/125 (94%)	110 (93%)	5 (4%)	3 (2%)	6	2
35	DO	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
36	CP	114/117 (97%)	105 (92%)	4 (4%)	5 (4%)	3	1
36	DP	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
37	CQ	112/114 (98%)	104 (93%)	7 (6%)	1 (1%)	20	14
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%)	5	1
39	DS	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
40	CT	108/110 (98%)	101 (94%)	4 (4%)	3 (3%)	6	2
40	DT	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
41	CU	91/93 (98%)	81 (89%)	7 (8%)	3 (3%)	4	1
41	DU	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	17	11
42	CV	100/102 (98%)	81 (81%)	11 (11%)	8 (8%)	1	0
42	DV	100/102 (98%)	96 (96%)	3 (3%)	1 (1%)	18	12
43	CW	92/94 (98%)	86 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	2	0
46	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
47	C0	56/58 (97%)	51 (91%)	4 (7%)	1 (2%)	10	4
47	D0	57/58 (98%)	54 (95%)	2 (4%)	1 (2%)	10	4
48	C1	54/56 (96%)	48 (89%)	4 (7%)	2 (4%)	4	1
48	D1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
49	C2	48/51 (94%)	41 (85%)	6 (12%)	1 (2%)	8	3
49	D2	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
50	C3	44/46 (96%)	40 (91%)	2 (4%)	2 (4%)	3	1
50	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
51	C4	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
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%)	2	0
All	All	11407/11629 (98%)	10507 (92%)	713 (6%)	187 (2%)	11	5

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/186 (100%)	180 (97%)	6 (3%)	44	46
2	BB	186/186 (100%)	179 (96%)	7 (4%)	38	38
3	AC	170/170 (100%)	164 (96%)	6 (4%)	41	42
3	BC	170/170 (100%)	142 (84%)	28 (16%)	2	1
4	AD	172/172 (100%)	167 (97%)	5 (3%)	48	51
4	BD	172/172 (100%)	167 (97%)	5 (3%)	48	51
5	AE	118/118 (100%)	112 (95%)	6 (5%)	28	25
5	BE	113/118 (96%)	92 (81%)	21 (19%)	2	1
6	AF	92/92 (100%)	91 (99%)	1 (1%)	78	83
6	BF	87/92 (95%)	73 (84%)	14 (16%)	3	1
7	AG	124/124 (100%)	121 (98%)	3 (2%)	54	59
7	BG	124/124 (100%)	97 (78%)	27 (22%)	1	0
8	AH	104/104 (100%)	100 (96%)	4 (4%)	38	38
8	BH	104/104 (100%)	87 (84%)	17 (16%)	3	1
9	AI	105/105 (100%)	102 (97%)	3 (3%)	48	51
9	BI	105/105 (100%)	102 (97%)	3 (3%)	48	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AJ	87/87 (100%)	81 (93%)	6 (7%)	18	14
10	BJ	86/87 (99%)	68 (79%)	18 (21%)	1	0
11	AK	90/90 (100%)	89 (99%)	1 (1%)	78	83
11	BK	90/90 (100%)	78 (87%)	12 (13%)	4	2
12	AL	102/102 (100%)	101 (99%)	1 (1%)	80	85
12	BL	102/102 (100%)	91 (89%)	11 (11%)	7	4
13	AM	92/92 (100%)	90 (98%)	2 (2%)	57	62
13	BM	92/92 (100%)	79 (86%)	13 (14%)	4	2
14	AN	83/83 (100%)	82 (99%)	1 (1%)	75	81
14	BN	83/83 (100%)	80 (96%)	3 (4%)	40	41
15	AO	76/76 (100%)	74 (97%)	2 (3%)	51	55
15	BO	76/76 (100%)	62 (82%)	14 (18%)	2	1
16	AP	65/65 (100%)	63 (97%)	2 (3%)	45	48
16	BP	65/65 (100%)	58 (89%)	7 (11%)	7	4
17	AQ	74/74 (100%)	72 (97%)	2 (3%)	50	54
17	BQ	74/74 (100%)	58 (78%)	16 (22%)	1	0
18	AR	48/48 (100%)	48 (100%)	0	100	100
18	BR	48/48 (100%)	44 (92%)	4 (8%)	13	9
19	AS	70/70 (100%)	69 (99%)	1 (1%)	71	78
19	BS	70/70 (100%)	61 (87%)	9 (13%)	5	2
20	AT	65/65 (100%)	63 (97%)	2 (3%)	45	48
20	BT	65/65 (100%)	53 (82%)	12 (18%)	2	1
21	AU	48/48 (100%)	45 (94%)	3 (6%)	21	17
21	BU	48/48 (100%)	45 (94%)	3 (6%)	21	17
24	CC	216/216 (100%)	194 (90%)	22 (10%)	8	5
24	DC	216/216 (100%)	214 (99%)	2 (1%)	82	87
25	CD	164/164 (100%)	151 (92%)	13 (8%)	14	10
26	CE	165/165 (100%)	144 (87%)	21 (13%)	5	2
26	DE	165/165 (100%)	163 (99%)	2 (1%)	75	81
27	CF	148/148 (100%)	127 (86%)	21 (14%)	4	2
27	DF	148/148 (100%)	142 (96%)	6 (4%)	35	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	CG	137/137 (100%)	115 (84%)	22 (16%)	3	1
28	DG	137/137 (100%)	129 (94%)	8 (6%)	23	20
29	CH	114/114 (100%)	96 (84%)	18 (16%)	3	1
29	DH	114/114 (100%)	103 (90%)	11 (10%)	10	6
30	CJ	104/104 (100%)	101 (97%)	3 (3%)	48	51
30	DJ	104/104 (100%)	103 (99%)	1 (1%)	80	85
31	CK	116/116 (100%)	105 (90%)	11 (10%)	10	6
31	DK	116/116 (100%)	114 (98%)	2 (2%)	66	72
32	CL	103/104 (99%)	96 (93%)	7 (7%)	18	15
32	DL	104/104 (100%)	102 (98%)	2 (2%)	62	68
33	CM	103/103 (100%)	97 (94%)	6 (6%)	23	20
33	DM	103/103 (100%)	102 (99%)	1 (1%)	80	85
34	CN	108/108 (100%)	97 (90%)	11 (10%)	8	5
34	DN	109/108 (101%)	106 (97%)	3 (3%)	49	52
35	CO	100/102 (98%)	87 (87%)	13 (13%)	5	2
35	DO	102/102 (100%)	100 (98%)	2 (2%)	60	66
36	CP	86/87 (99%)	76 (88%)	10 (12%)	6	3
36	DP	87/87 (100%)	85 (98%)	2 (2%)	56	60
37	CQ	99/99 (100%)	89 (90%)	10 (10%)	9	5
37	DQ	99/99 (100%)	95 (96%)	4 (4%)	36	36
38	CR	89/89 (100%)	81 (91%)	8 (9%)	11	7
38	DR	89/89 (100%)	87 (98%)	2 (2%)	57	62
39	CS	84/84 (100%)	74 (88%)	10 (12%)	6	3
39	DS	84/84 (100%)	81 (96%)	3 (4%)	40	41
40	CT	93/93 (100%)	79 (85%)	14 (15%)	3	1
40	DT	93/93 (100%)	91 (98%)	2 (2%)	57	62
41	CU	80/80 (100%)	66 (82%)	14 (18%)	2	1
41	DU	80/80 (100%)	77 (96%)	3 (4%)	38	38
42	CV	83/83 (100%)	71 (86%)	12 (14%)	4	2
42	DV	83/83 (100%)	82 (99%)	1 (1%)	75	81
43	CW	78/78 (100%)	65 (83%)	13 (17%)	2	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	DW	78/78 (100%)	75 (96%)	3 (4%)	38	38
44	CX	56/58 (97%)	53 (95%)	3 (5%)	26	23
44	DX	58/58 (100%)	57 (98%)	1 (2%)	66	72
45	CY	67/67 (100%)	60 (90%)	7 (10%)	8	5
45	DY	67/67 (100%)	66 (98%)	1 (2%)	70	76
46	CZ	54/54 (100%)	47 (87%)	7 (13%)	5	2
46	DZ	54/54 (100%)	54 (100%)	0	100	100
47	C0	48/48 (100%)	42 (88%)	6 (12%)	5	3
47	D0	49/48 (102%)	48 (98%)	1 (2%)	60	66
48	C1	47/47 (100%)	43 (92%)	4 (8%)	12	8
48	D1	47/47 (100%)	47 (100%)	0	100	100
49	C2	45/46 (98%)	44 (98%)	1 (2%)	57	62
49	D2	45/46 (98%)	45 (100%)	0	100	100
50	C3	38/38 (100%)	34 (90%)	4 (10%)	8	4
50	D3	38/38 (100%)	37 (97%)	1 (3%)	51	55
51	C4	51/51 (100%)	47 (92%)	4 (8%)	15	11
51	D4	51/51 (100%)	50 (98%)	1 (2%)	60	66
52	C5	34/34 (100%)	32 (94%)	2 (6%)	23	19
52	D5	34/34 (100%)	34 (100%)	0	100	100
54	DD	163/163 (100%)	161 (99%)	2 (1%)	75	81
55	DI	103/103 (100%)	100 (97%)	3 (3%)	48	51
All	All	9461/9478 (100%)	8793 (93%)	668 (7%)	17	13

All (668) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	5	SER
2	AB	23	TRP
2	AB	73	LYS
2	AB	93	ASN
2	AB	129	LEU
2	AB	213	TYR
3	AC	20	SER
3	AC	58	GLU
3	AC	83	ASP

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Mol	Chain	Res	Type
3	AC	85	GLU
3	AC	125	GLU
3	AC	201	TRP
4	AD	26	ARG
4	AD	131	ASN
4	AD	194	ASP
4	AD	196	ASN
4	AD	197	GLU
5	AE	22	SER
5	AE	48	PHE
5	AE	80	THR
5	AE	130	SER
5	AE	152	MET
5	AE	163	GLU
6	AF	93	LYS
7	AG	7	ILE
7	AG	54	SER
7	AG	83	SER
8	AH	3	MET
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	16	ARG
10	AJ	19	ASP
10	AJ	27	GLU
10	AJ	35	GLN
10	AJ	80	THR
11	AK	33	THR
12	AL	15	LYS
13	AM	71	ARG
13	AM	107	ARG
14	AN	59	ARG
15	AO	3	LEU
15	AO	89	ARG
16	AP	1	MET
16	AP	44	SER
17	AQ	14	SER
17	AQ	27	ARG

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Mol	Chain	Res	Type
19	AS	18	LYS
20	AT	40	GLU
20	AT	54	MET
21	AU	4	ILE
21	AU	41	PRO
21	AU	56	HIS
2	BB	5	SER
2	BB	23	TRP
2	BB	73	LYS
2	BB	93	ASN
2	BB	129	LEU
2	BB	146	ASN
2	BB	213	TYR
3	BC	3	GLN
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	89	LYS
3	BC	103	ILE
3	BC	107	ARG
3	BC	125	GLU
3	BC	127	ARG
3	BC	140	ASN
3	BC	152	GLU
3	BC	157	LEU
3	BC	165	THR
3	BC	169	ARG
3	BC	175	LEU
3	BC	179	ARG
3	BC	192	THR
3	BC	200	VAL
3	BC	201	TRP
3	BC	206	GLU
4	BD	5	LEU

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Mol	Chain	Res	Type
4	BD	58	LYS
4	BD	142	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	52	LYS
5	BE	69	ARG
5	BE	78	ASN
5	BE	80	THR
5	BE	81	LEU
5	BE	93	ARG
5	BE	96	MET
5	BE	101	GLU
5	BE	105	ILE
5	BE	115	LEU
5	BE	120	VAL
5	BE	122	ASN
5	BE	130	SER
5	BE	149	SER
5	BE	151	GLU
6	BF	14	GLN
6	BF	16	GLU
6	BF	29	ILE
6	BF	35	LYS
6	BF	51	ILE
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	79	ARG
6	BF	86	ARG
6	BF	93	LYS
7	BG	3	ARG
7	BG	4	ARG
7	BG	5	ARG

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Mol	Chain	Res	Type
7	BG	11	LYS
7	BG	12	ILE
7	BG	15	ASP
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	73	VAL
7	BG	77	SER
7	BG	78	ARG
7	BG	79	ARG
7	BG	89	VAL
7	BG	92	ARG
7	BG	97	ASN
7	BG	113	ASP
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	52	GLU
8	BH	59	LEU
8	BH	75	ILE
8	BH	77	ARG
8	BH	83	LEU
8	BH	87	LYS
8	BH	90	ASP
8	BH	107	SER
8	BH	111	MET
8	BH	114	ARG
8	BH	121	LEU
8	BH	125	ILE
9	BI	47	VAL

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Mol	Chain	Res	Type
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	62	ARG
10	BJ	63	ASP
10	BJ	69	THR
10	BJ	73	LEU
10	BJ	77	VAL
10	BJ	82	LYS
10	BJ	88	MET
10	BJ	90	LEU
10	BJ	99	GLN
10	BJ	100	ILE
11	BK	31	ILE
11	BK	38	GLN
11	BK	55	SER
11	BK	57	LYS
11	BK	82	LEU
11	BK	83	GLU
11	BK	100	LEU
11	BK	105	PHE
11	BK	107	ILE
11	BK	109	ASN
11	BK	114	THR
11	BK	122	ARG
12	BL	9	ARG
12	BL	10	LYS
12	BL	12	ARG
12	BL	14	ARG
12	BL	44	LYS
12	BL	49	LEU
12	BL	54	ARG
12	BL	58	THR
12	BL	88	LYS
12	BL	94	ARG

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Mol	Chain	Res	Type
12	BL	121	ARG
13	BM	4	ILE
13	BM	16	VAL
13	BM	23	TYR
13	BM	27	LYS
13	BM	29	ARG
13	BM	31	LYS
13	BM	48	LEU
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
14	BN	59	ARG
15	BO	6	GLU
15	BO	8	THR
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	73	LYS
15	BO	83	GLU
15	BO	85	LEU
15	BO	87	LEU
15	BO	88	ARG
15	BO	89	ARG
16	BP	1	MET
16	BP	18	GLN
16	BP	20	VAL
16	BP	46	LYS
16	BP	51	ARG
16	BP	63	GLN
16	BP	68	SER
17	BQ	5	ILE
17	BQ	7	THR
17	BQ	14	SER
17	BQ	16	LYS

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Mol	Chain	Res	Type
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	61	ILE
17	BQ	65	ARG
17	BQ	75	LEU
17	BQ	76	VAL
17	BQ	79	VAL
17	BQ	81	LYS
18	BR	21	ILE
18	BR	47	THR
18	BR	55	LEU
18	BR	73	ARG
19	BS	6	LYS
19	BS	7	LYS
19	BS	11	ILE
19	BS	13	LEU
19	BS	33	THR
19	BS	37	ARG
19	BS	49	ILE
19	BS	58	VAL
19	BS	80	TYR
20	BT	10	ARG
20	BT	12	ILE
20	BT	24	ARG
20	BT	27	MET
20	BT	30	THR
20	BT	36	TYR
20	BT	54	MET
20	BT	64	LYS
20	BT	66	LEU
20	BT	69	LYS
20	BT	84	ASN
20	BT	86	LEU
21	BU	12	PHE
21	BU	34	ARG
21	BU	56	HIS
24	CC	14	ARG
24	CC	18	LYS

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Mol	Chain	Res	Type
24	CC	36	LYS
24	CC	52	ARG
24	CC	88	SER
24	CC	97	LYS
24	CC	105	LEU
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	213	TRP
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	46	ARG
25	CD	73	VAL
25	CD	91	THR
25	CD	95	SER
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	44	ARG
26	CE	57	LYS
26	CE	65	THR
26	CE	67	ARG
26	CE	69	ARG
26	CE	72	SER
26	CE	78	TRP

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Mol	Chain	Res	Type
26	CE	88	ARG
26	CE	93	SER
26	CE	116	ASP
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	5	HIS
27	CF	7	TYR
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	80	ARG
27	CF	95	ARG
27	CF	104	ILE
27	CF	117	LEU
27	CF	141	ILE
27	CF	148	ARG
27	CF	149	VAL
27	CF	154	ILE
27	CF	174	ASP
28	CG	11	VAL
28	CG	25	THR
28	CG	27	LYS
28	CG	29	LYS
28	CG	30	ASN
28	CG	34	THR
28	CG	37	LEU
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	124	GLU
28	CG	127	THR
28	CG	137	ASP
28	CG	155	GLU
28	CG	166	ASP
28	CG	168	VAL
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	41	LYS
29	CH	42	LYS
29	CH	51	ARG
29	CH	72	ILE
29	CH	75	LEU
29	CH	78	VAL
29	CH	87	GLU
29	CH	97	ARG
29	CH	101	ASP
29	CH	124	THR
29	CH	142	VAL
29	CH	144	VAL
30	CJ	59	ILE
30	CJ	82	LYS
30	CJ	103	ARG
31	CK	3	THR
31	CK	28	LEU
31	CK	30	THR
31	CK	39	LYS
31	CK	57	LEU
31	CK	95	ARG
31	CK	123	LYS
31	CK	124	VAL

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Mol	Chain	Res	Type
31	CK	129	GLU
31	CK	131	ASN
31	CK	142	ILE
32	CL	49	ARG
32	CL	76	VAL
32	CL	90	ASN
32	CL	92	GLU
32	CL	105	ARG
32	CL	107	LEU
32	CL	114	LYS
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	53	MET
34	CN	58	LYS
34	CN	59	ARG
34	CN	78	LEU
34	CN	100	LYS
34	CN	111	GLU
35	CO	1	MET
35	CO	2	ARG
35	CO	20	MET
35	CO	51	LEU
35	CO	63	ARG
35	CO	70	THR
35	CO	71	ARG
35	CO	76	VAL
35	CO	90	ARG
35	CO	95	THR
35	CO	116	VAL
35	CO	118	ARG
35	CO	119	SER
36	CP	9	ARG
36	CP	16	ARG

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Mol	Chain	Res	Type
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	94	ARG
36	CP	103	VAL
37	CQ	6	LYS
37	CQ	8	LEU
37	CQ	19	SER
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
38	CR	16	LYS
38	CR	41	LYS
38	CR	51	ARG
38	CR	58	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	7	HIS
40	CT	13	SER
40	CT	19	LEU
40	CT	30	SER
40	CT	65	ASP
40	CT	66	ILE

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Mol	Chain	Res	Type
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	18	GLU
41	CU	22	THR
41	CU	30	ILE
41	CU	49	LYS
41	CU	50	LEU
41	CU	56	GLU
41	CU	68	LYS
41	CU	69	ARG
41	CU	70	HIS
41	CU	73	ARG
41	CU	77	ARG
42	CV	7	ARG
42	CV	19	LYS
42	CV	29	LEU
42	CV	35	ILE
42	CV	37	GLU
42	CV	41	LEU
42	CV	53	ASN
42	CV	61	LYS
42	CV	68	SER
42	CV	72	ILE
42	CV	74	ASN
42	CV	101	GLU
43	CW	1	MET
43	CW	7	GLU
43	CW	10	LYS
43	CW	20	LEU
43	CW	34	LYS
43	CW	40	ILE
43	CW	41	GLU
43	CW	53	LYS

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Mol	Chain	Res	Type
43	CW	61	LEU
43	CW	62	THR
43	CW	65	VAL
43	CW	70	ILE
43	CW	76	ASP
44	CX	30	SER
44	CX	38	VAL
44	CX	77	ARG
45	CY	17	ASN
45	CY	20	HIS
45	CY	22	LEU
45	CY	35	SER
45	CY	48	THR
45	CY	71	LEU
45	CY	72	ARG
46	CZ	7	ARG
46	CZ	18	LEU
46	CZ	19	LEU
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	57	VAL
48	C1	10	ARG
48	C1	26	THR
48	C1	28	LEU
48	C1	40	ARG
49	C2	47	VAL
50	C3	1	MET
50	C3	3	ARG
50	C3	4	THR
50	C3	42	LEU
51	C4	19	LYS
51	C4	30	ARG
51	C4	31	HIS
51	C4	47	LYS
52	C5	3	VAL

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Mol	Chain	Res	Type
52	C5	26	ILE
24	DC	130	LEU
24	DC	252	THR
54	DD	32	ASN
54	DD	95	SER
26	DE	7	ASP
26	DE	116	ASP
27	DF	95	ARG
27	DF	105	THR
27	DF	113	ASP
27	DF	144	ASP
27	DF	154	ILE
27	DF	174	ASP
28	DG	45	HIS
28	DG	77	ILE
28	DG	81	GLU
28	DG	85	LYS
28	DG	104	ASN
28	DG	114	ASP
28	DG	152	ARG
28	DG	177	LYS
29	DH	8	LYS
29	DH	14	SER
29	DH	42	LYS
29	DH	44	ILE
29	DH	46	PHE
29	DH	50	ARG
29	DH	53	GLU
29	DH	60	GLU
29	DH	76	GLU
29	DH	77	THR
29	DH	125	THR
55	DI	16	SER
55	DI	71	CYS
55	DI	105	LYS
30	DJ	59	ILE
31	DK	39	LYS
31	DK	124	VAL
32	DL	49	ARG
32	DL	58	LEU
33	DM	115	GLU
34	DN	27	SER

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Mol	Chain	Res	Type
34	DN	59	ARG
34	DN	135	VAL
35	DO	75	ILE
35	DO	116	VAL
36	DP	31	THR
36	DP	78	VAL
37	DQ	19	SER
37	DQ	68	GLU
37	DQ	85	SER
37	DQ	96	LYS
38	DR	11	ARG
38	DR	51	ARG
39	DS	38	VAL
39	DS	45	GLU
39	DS	102	SER
40	DT	86	MET
40	DT	109	ASP
41	DU	5	GLU
41	DU	92	ASN
41	DU	93	LEU
42	DV	55	PRO
43	DW	7	GLU
43	DW	66	ASP
43	DW	70	ILE
44	DX	11	ARG
45	DY	2	SER
47	D0	10	THR
50	D3	1	MET
51	D4	31	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
7	AG	52	GLN
26	CE	115	GLN
30	CJ	31	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	258 (16%)	9 (0%)
1	BA	1529/1534 (99%)	267 (17%)	10 (0%)
22	CA	2892/2904 (99%)	414 (14%)	32 (1%)
23	CB	117/120 (97%)	11 (9%)	0
23	DB	119/120 (99%)	8 (6%)	0
53	DA	2883/2903 (99%)	377 (13%)	26 (0%)
All	All	9070/9115 (99%)	1335 (14%)	77 (0%)

All (1335) 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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	AA	649	A
1	AA	650	G
1	AA	653	U
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
1	BA	653	U
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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	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

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Mol	Chain	Res	Type
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
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	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

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Mol	Chain	Res	Type
22	CA	362	A
22	CA	370	G
22	CA	371	A
22	CA	372	G
22	CA	386	G
22	CA	404	A
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

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Mol	Chain	Res	Type
22	CA	645	C
22	CA	646	U
22	CA	647	G
22	CA	648	G
22	CA	654	A
22	CA	655	A
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

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Mol	Chain	Res	Type
22	CA	983	A
22	CA	995	C
22	CA	996	A
22	CA	1012	U
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	1132	U
22	CA	1133	A
22	CA	1135	C
22	CA	1136	G
22	CA	1138	G
22	CA	1142	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

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Mol	Chain	Res	Type
22	CA	1253	A
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

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Mol	Chain	Res	Type
22	CA	1581	G
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

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Mol	Chain	Res	Type
22	CA	1874	C
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

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Mol	Chain	Res	Type
22	CA	2123	G
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	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	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
22	CA	2689	U

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Mol	Chain	Res	Type
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	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
53	DA	34	U
53	DA	46	G

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Mol	Chain	Res	Type
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
53	DA	355	U
53	DA	358	U

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Mol	Chain	Res	Type
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
53	DA	654	A
53	DA	655	A

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Mol	Chain	Res	Type
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	996	A
53	DA	1012	U
53	DA	1013	C
53	DA	1022	G
53	DA	1026	G
53	DA	1033	U

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Mol	Chain	Res	Type
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	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
53	DA	1417	C
53	DA	1419	A
53	DA	1428	C
53	DA	1452	G
53	DA	1453	A

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Mol	Chain	Res	Type
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
53	DA	1740	G
53	DA	1744	A
53	DA	1755	A
53	DA	1764	C
53	DA	1773	A

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Mol	Chain	Res	Type
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
53	DA	2056	G
53	DA	2060	A
53	DA	2061	G
53	DA	2062	A
53	DA	2069	G7M

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Mol	Chain	Res	Type
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
53	DA	2168	G
53	DA	2169	A
53	DA	2170	A
53	DA	2171	A
53	DA	2172	U

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Mol	Chain	Res	Type
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	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	2424	C
53	DA	2425	A
53	DA	2434	A
53	DA	2435	A
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

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Mol	Chain	Res	Type
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	2874	C
53	DA	2883	A
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	2MG	AA	1207	1	19,26,27	1.25	3 (15%)	20,38,41	2.39	8 (40%)
1	4OC	AA	1402	1	16,23,24	0.78	0	19,32,35	1.56	1 (5%)
1	5MC	AA	1407	1	15,22,23	1.59	1 (6%)	17,32,35	1.12	2 (11%)
1	UR3	AA	1498	1	14,22,23	0.72	0	16,32,35	0.61	0
1	2MG	AA	1516	1	19,26,27	1.14	2 (10%)	20,38,41	2.09	7 (35%)
1	MA6	AA	1518	1	16,26,27	1.00	1 (6%)	18,38,41	1.88	4 (22%)
1	MA6	AA	1519	1	16,26,27	0.97	1 (6%)	18,38,41	2.23	5 (27%)
1	PSU	AA	516	1,56	16,21,22	1.17	1 (6%)	20,30,33	3.36	6 (30%)
1	G7M	AA	527	1	19,26,27	1.25	2 (10%)	19,39,42	2.32	6 (31%)
1	2MG	AA	966	1	19,26,27	1.36	2 (10%)	20,38,41	2.30	7 (35%)
1	5MC	AA	967	1	15,22,23	1.31	1 (6%)	17,32,35	1.32	2 (11%)
12	D2T	AL	89	12	5,9,10	1.96	1 (20%)	3,11,13	0.60	0
1	2MG	BA	1207	1	19,26,27	1.35	3 (15%)	20,38,41	2.48	9 (45%)
1	4OC	BA	1402	1	16,23,24	0.72	0	19,32,35	1.13	2 (10%)
1	5MC	BA	1407	1	15,22,23	1.57	2 (13%)	17,32,35	1.06	2 (11%)
1	UR3	BA	1498	1	14,22,23	0.85	1 (7%)	16,32,35	0.71	0
1	2MG	BA	1516	1	19,26,27	1.34	2 (10%)	20,38,41	2.34	6 (30%)
1	MA6	BA	1518	1	16,26,27	1.00	1 (6%)	18,38,41	2.11	3 (16%)
1	MA6	BA	1519	1	16,26,27	0.98	1 (6%)	18,38,41	2.39	4 (22%)
1	PSU	BA	516	1	16,21,22	0.84	1 (6%)	20,30,33	3.62	5 (25%)
1	G7M	BA	527	1	19,26,27	1.19	2 (10%)	19,39,42	2.01	4 (21%)
1	2MG	BA	966	1	19,26,27	1.32	2 (10%)	20,38,41	2.29	8 (40%)
1	5MC	BA	967	1	15,22,23	1.45	1 (6%)	17,32,35	1.03	2 (11%)
12	D2T	BL	89	12	5,9,10	2.36	1 (20%)	3,11,13	1.01	0
22	6MZ	CA	1618	22	18,25,26	1.13	1 (5%)	16,36,39	3.16	4 (25%)
22	2MG	CA	1835	22	19,26,27	1.30	3 (15%)	20,38,41	2.30	8 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PSU	CA	1911	22	16,21,22	1.08	1 (6%)	20,30,33	3.42	5 (25%)
22	3TD	CA	1915	22	16,22,23	1.83	4 (25%)	19,32,35	1.95	5 (26%)
22	PSU	CA	1917	22	16,21,22	1.10	1 (6%)	20,30,33	3.56	5 (25%)
22	5MU	CA	1939	22	14,22,23	0.69	0	16,32,35	2.30	2 (12%)
22	5MC	CA	1962	22	15,22,23	1.46	1 (6%)	17,32,35	1.13	2 (11%)
22	6MZ	CA	2030	22	18,25,26	1.06	1 (5%)	16,36,39	3.40	6 (37%)
22	G7M	CA	2069	22	19,26,27	1.21	1 (5%)	19,39,42	2.06	4 (21%)
22	OMG	CA	2251	22	18,26,27	1.38	2 (11%)	22,38,41	2.16	7 (31%)
22	2MG	CA	2445	22	19,26,27	1.45	3 (15%)	20,38,41	2.40	8 (40%)
22	PSU	CA	2457	22	16,21,22	1.02	1 (6%)	20,30,33	3.51	5 (25%)
22	OMC	CA	2498	56,22	15,22,23	0.71	0	19,31,34	0.83	1 (5%)
22	2MA	CA	2503	22	18,25,26	1.78	3 (16%)	17,37,40	1.61	3 (17%)
22	PSU	CA	2504	22	16,21,22	0.96	1 (6%)	20,30,33	3.77	7 (35%)
22	OMU	CA	2552	22	14,22,23	0.68	0	18,31,34	1.88	1 (5%)
22	PSU	CA	2580	22	16,21,22	1.06	1 (6%)	20,30,33	3.48	6 (30%)
22	PSU	CA	2605	22	16,21,22	0.88	1 (6%)	20,30,33	3.58	6 (30%)
22	1MG	CA	745	22	18,26,27	1.50	2 (11%)	18,39,42	1.85	3 (16%)
22	PSU	CA	746	56,22	16,21,22	0.96	2 (12%)	20,30,33	3.43	6 (30%)
22	5MU	CA	747	22	14,22,23	0.91	1 (7%)	16,32,35	2.08	3 (18%)
22	PSU	CA	955	22	16,21,22	1.09	2 (12%)	20,30,33	3.42	5 (25%)
34	4D4	CN	81	34	10,11,12	1.94	2 (20%)	7,13,15	0.74	0
53	6MZ	DA	1618	53	18,25,26	1.03	1 (5%)	16,36,39	2.89	4 (25%)
53	2MG	DA	1835	53	19,26,27	1.03	2 (10%)	20,38,41	2.58	8 (40%)
53	PSU	DA	1911	53	16,21,22	1.09	1 (6%)	20,30,33	3.29	5 (25%)
53	3TD	DA	1915	53	16,22,23	1.46	3 (18%)	19,32,35	1.67	3 (15%)
53	PSU	DA	1917	53	16,21,22	1.29	2 (12%)	20,30,33	3.63	6 (30%)
53	5MU	DA	1939	53	14,22,23	0.93	1 (7%)	16,32,35	2.52	2 (12%)
53	5MC	DA	1962	53	15,22,23	1.41	2 (13%)	17,32,35	0.96	1 (5%)
53	6MZ	DA	2030	53	18,25,26	0.84	0	16,36,39	3.46	5 (31%)
53	G7M	DA	2069	53	19,26,27	1.10	2 (10%)	19,39,42	2.19	5 (26%)
53	OMG	DA	2251	53	18,26,27	1.21	2 (11%)	22,38,41	1.97	6 (27%)
53	2MG	DA	2445	53	19,26,27	1.52	4 (21%)	20,38,41	2.47	7 (35%)
53	H2U	DA	2449	53	17,21,22	1.35	2 (11%)	21,30,33	2.21	5 (23%)
53	PSU	DA	2457	53	16,21,22	1.35	2 (12%)	20,30,33	3.98	6 (30%)
53	OMC	DA	2498	56,53	15,22,23	0.96	1 (6%)	19,31,34	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	2MA	DA	2503	56,53	18,25,26	1.33	3 (16%)	17,37,40	1.67	3 (17%)
53	PSU	DA	2504	53	16,21,22	1.44	2 (12%)	20,30,33	3.80	5 (25%)
53	OMU	DA	2552	53	14,22,23	0.94	1 (7%)	18,31,34	1.85	1 (5%)
53	PSU	DA	2580	53	16,21,22	1.20	1 (6%)	20,30,33	4.13	7 (35%)
53	PSU	DA	2604	53	16,21,22	1.58	4 (25%)	20,30,33	3.80	6 (30%)
53	PSU	DA	2605	53	16,21,22	1.45	3 (18%)	20,30,33	3.47	6 (30%)
53	1MG	DA	745	53	18,26,27	1.42	2 (11%)	18,39,42	2.03	3 (16%)
53	PSU	DA	746	56,53	16,21,22	1.50	4 (25%)	20,30,33	3.50	7 (35%)
53	5MU	DA	747	53	14,22,23	0.87	1 (7%)	16,32,35	2.11	3 (18%)
53	PSU	DA	955	53	16,21,22	1.40	3 (18%)	20,30,33	3.82	5 (25%)
54	MEQ	DD	150[A]	54	9,9,10	1.17	1 (11%)	7,10,12	1.65	2 (28%)
54	MEQ	DD	150[B]	54	9,9,10	1.23	1 (11%)	7,10,12	1.53	1 (14%)
34	4D4	DN	81[A]	-	10,11,12	1.93	2 (20%)	7,13,15	0.94	0
34	4D4	DN	81[B]	-	10,11,12	1.86	2 (20%)	7,13,15	0.66	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
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	AA	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	AA	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	AA	516	1,56	-	0/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	0/3/25/26	0/3/3/3
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
1	5MC	AA	967	1	-	0/3/25/26	0/2/2/2
12	D2T	AL	89	12	-	0/2/12/14	0/0/0/0
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	BA	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	BA	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	BA	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	BA	1518	1	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	BA	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
1	G7M	BA	527	1	-	0/3/25/26	0/3/3/3
1	2MG	BA	966	1	-	0/5/27/28	0/3/3/3
1	5MC	BA	967	1	-	0/3/25/26	0/2/2/2
12	D2T	BL	89	12	-	0/2/12/14	0/0/0/0
22	6MZ	CA	1618	22	-	0/5/27/28	0/3/3/3
22	2MG	CA	1835	22	-	0/5/27/28	0/3/3/3
22	PSU	CA	1911	22	-	0/7/25/26	0/2/2/2
22	3TD	CA	1915	22	-	0/7/25/26	0/2/2/2
22	PSU	CA	1917	22	-	0/7/25/26	0/2/2/2
22	5MU	CA	1939	22	-	0/3/25/26	0/2/2/2
22	5MC	CA	1962	22	-	0/3/25/26	0/2/2/2
22	6MZ	CA	2030	22	-	0/5/27/28	0/3/3/3
22	G7M	CA	2069	22	-	0/3/25/26	0/3/3/3
22	OMG	CA	2251	22	-	0/5/27/28	0/3/3/3
22	2MG	CA	2445	22	-	0/5/27/28	0/3/3/3
22	PSU	CA	2457	22	-	0/7/25/26	0/2/2/2
22	OMC	CA	2498	56,22	-	0/5/27/28	0/2/2/2
22	2MA	CA	2503	22	-	0/3/25/26	0/3/3/3
22	PSU	CA	2504	22	-	0/7/25/26	0/2/2/2
22	OMU	CA	2552	22	-	0/5/27/28	0/2/2/2
22	PSU	CA	2580	22	-	0/7/25/26	0/2/2/2
22	PSU	CA	2605	22	-	0/7/25/26	0/2/2/2
22	1MG	CA	745	22	-	0/3/25/26	0/3/3/3
22	PSU	CA	746	56,22	-	0/7/25/26	0/2/2/2
22	5MU	CA	747	22	-	0/3/25/26	0/2/2/2
22	PSU	CA	955	22	-	0/7/25/26	0/2/2/2
34	4D4	CN	81	34	-	0/10/12/14	0/0/0/0
53	6MZ	DA	1618	53	-	0/5/27/28	0/3/3/3
53	2MG	DA	1835	53	-	0/5/27/28	0/3/3/3
53	PSU	DA	1911	53	-	0/7/25/26	0/2/2/2
53	3TD	DA	1915	53	-	0/7/25/26	0/2/2/2
53	PSU	DA	1917	53	-	0/7/25/26	0/2/2/2
53	5MU	DA	1939	53	-	0/3/25/26	0/2/2/2
53	5MC	DA	1962	53	-	0/3/25/26	0/2/2/2
53	6MZ	DA	2030	53	-	0/5/27/28	0/3/3/3
53	G7M	DA	2069	53	-	0/3/25/26	0/3/3/3
53	OMG	DA	2251	53	-	0/5/27/28	0/3/3/3
53	2MG	DA	2445	53	-	0/5/27/28	0/3/3/3
53	H2U	DA	2449	53	-	0/7/38/39	0/2/2/2
53	PSU	DA	2457	53	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	OMC	DA	2498	56,53	-	0/5/27/28	0/2/2/2
53	2MA	DA	2503	56,53	-	0/3/25/26	0/3/3/3
53	PSU	DA	2504	53	-	0/7/25/26	0/2/2/2
53	OMU	DA	2552	53	-	0/5/27/28	0/2/2/2
53	PSU	DA	2580	53	-	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
53	1MG	DA	745	53	-	0/3/25/26	0/3/3/3
53	PSU	DA	746	56,53	-	0/7/25/26	0/2/2/2
53	5MU	DA	747	53	-	0/3/25/26	0/2/2/2
53	PSU	DA	955	53	-	0/7/25/26	0/2/2/2
54	MEQ	DD	150[A]	54	-	0/7/9/11	0/0/0/0
54	MEQ	DD	150[B]	54	-	1/7/9/11	0/0/0/0
34	4D4	DN	81[A]	-	-	0/10/12/14	0/0/0/0
34	4D4	DN	81[B]	-	-	0/10/12/14	0/0/0/0

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	CA	1915	3TD	C5-C1'	-5.51	1.47	1.52
53	DA	2604	PSU	C5-C1'	-3.73	1.49	1.52
53	DA	2605	PSU	C5-C1'	-3.66	1.49	1.52
53	DA	1915	3TD	C5-C1'	-3.40	1.49	1.52
53	DA	746	PSU	C5-C1'	-3.24	1.49	1.52
1	AA	527	G7M	O5'-C5'	-2.79	1.40	1.44
53	DA	1917	PSU	C5-C1'	-2.72	1.49	1.52
53	DA	2069	G7M	O5'-C5'	-2.70	1.41	1.44
53	DA	2604	PSU	O5'-C5'	-2.68	1.41	1.44
53	DA	747	5MU	O5'-C5'	-2.63	1.41	1.44
53	DA	746	PSU	C2'-C1'	-2.62	1.50	1.53
53	DA	1915	3TD	C4-N3	-2.47	1.34	1.38
53	DA	2457	PSU	O5'-C5'	-2.45	1.41	1.44
53	DA	2449	H2U	C4-N3	-2.45	1.33	1.37
53	DA	955	PSU	C5-C1'	-2.43	1.50	1.52
22	CA	2445	2MG	O5'-C5'	-2.40	1.41	1.44
53	DA	746	PSU	O4'-C1'	-2.38	1.40	1.44
1	BA	527	G7M	O5'-C5'	-2.30	1.41	1.44
22	CA	747	5MU	O5'-C5'	-2.27	1.41	1.44
53	DA	2498	OMC	C6-N1	-2.25	1.32	1.35
22	CA	1915	3TD	C4-N3	-2.24	1.35	1.38
53	DA	955	PSU	C2'-C1'	-2.22	1.51	1.53
53	DA	1939	5MU	C2-N3	-2.22	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	DA	2552	OMU	C2-N3	-2.21	1.33	1.38
1	BA	1407	5MC	O5'-C5'	-2.13	1.41	1.44
53	DA	2445	2MG	O5'-C5'	-2.12	1.41	1.44
22	CA	746	PSU	O4'-C1'	-2.11	1.41	1.44
53	DA	2504	PSU	C5-C1'	-2.08	1.50	1.52
22	CA	1915	3TD	O4'-C1'	-2.07	1.41	1.44
53	DA	2604	PSU	O4'-C1'	-2.03	1.41	1.44
53	DA	1962	5MC	O5'-C5'	-2.02	1.41	1.44
53	DA	2605	PSU	O5'-C5'	-2.01	1.42	1.44
53	DA	2503	2MA	C5-C4	2.02	1.45	1.40
53	DA	1835	2MG	C5-C4	2.03	1.45	1.40
1	BA	1207	2MG	C2-N2	2.13	1.35	1.34
53	DA	746	PSU	C4-N3	2.16	1.37	1.33
1	BA	516	PSU	C4-N3	2.29	1.37	1.33
22	CA	1835	2MG	C2-N2	2.33	1.36	1.34
1	AA	1207	2MG	C2-N2	2.34	1.36	1.34
22	CA	955	PSU	C5-C1'	2.40	1.54	1.52
34	DN	81[B]	4D4	CZ-NH2	2.42	1.42	1.32
1	BA	1498	UR3	C4-N3	2.42	1.41	1.38
54	DD	150[B]	MEQ	OE1-CD	2.46	1.28	1.23
54	DD	150[A]	MEQ	CA-C	2.47	1.53	1.50
34	DN	81[A]	4D4	CZ-NH2	2.52	1.42	1.32
1	AA	1519	MA6	C5-C4	2.53	1.46	1.40
53	DA	2445	2MG	C2-N2	2.56	1.36	1.34
22	CA	746	PSU	C4-N3	2.66	1.37	1.33
53	DA	1915	3TD	C10-N3	2.67	1.53	1.47
1	BA	1519	MA6	C5-C4	2.71	1.46	1.40
53	DA	745	1MG	C5-C4	2.71	1.46	1.40
1	AA	1516	2MG	C5-C4	2.74	1.46	1.40
53	DA	2251	OMG	C5-C4	2.76	1.46	1.40
53	DA	2605	PSU	C4-N3	2.77	1.38	1.33
53	DA	2604	PSU	C4-N3	2.77	1.38	1.33
22	CA	2605	PSU	C4-N3	2.77	1.38	1.33
34	CN	81	4D4	CZ-NH2	2.79	1.43	1.32
53	DA	2457	PSU	C4-N3	2.85	1.38	1.33
22	CA	2457	PSU	C4-N3	2.89	1.38	1.33
22	CA	1915	3TD	C10-N3	2.91	1.53	1.47
53	DA	1618	6MZ	C5-C4	2.91	1.47	1.40
1	BA	1518	MA6	C5-C4	2.92	1.47	1.40
1	AA	1207	2MG	C5-C4	2.92	1.47	1.40
22	CA	955	PSU	C4-N3	2.93	1.38	1.33
1	AA	1518	MA6	C5-C4	2.94	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	1207	2MG	C5-C4	2.94	1.47	1.40
22	CA	2504	PSU	C4-N3	2.98	1.38	1.33
53	DA	2069	G7M	C6-C5	2.99	1.47	1.41
22	CA	1835	2MG	C5-C4	3.02	1.47	1.40
53	DA	2445	2MG	C5-C4	3.02	1.47	1.40
53	DA	1835	2MG	C6-C5	3.06	1.47	1.41
1	AA	1516	2MG	C6-C5	3.06	1.47	1.41
1	BA	966	2MG	C5-C4	3.13	1.47	1.40
53	DA	2580	PSU	C4-N3	3.14	1.38	1.33
1	AA	516	PSU	C4-N3	3.14	1.38	1.33
1	AA	966	2MG	C5-C4	3.17	1.47	1.40
53	DA	2503	2MA	C6-C5	3.17	1.46	1.41
22	CA	2580	PSU	C4-N3	3.19	1.38	1.33
22	CA	745	1MG	C5-C4	3.21	1.47	1.40
22	CA	2445	2MG	C5-C4	3.23	1.47	1.40
22	CA	1618	6MZ	C5-C4	3.23	1.47	1.40
53	DA	1917	PSU	C4-N3	3.24	1.38	1.33
22	CA	2030	6MZ	C5-C4	3.24	1.47	1.40
1	BA	1516	2MG	C5-C4	3.28	1.47	1.40
1	AA	1207	2MG	C6-C5	3.31	1.47	1.41
22	CA	2251	OMG	C5-C4	3.33	1.48	1.40
53	DA	955	PSU	C4-N3	3.42	1.39	1.33
22	CA	1917	PSU	C4-N3	3.45	1.39	1.33
22	CA	1835	2MG	C6-C5	3.46	1.47	1.41
53	DA	2449	H2U	C2-N1	3.48	1.40	1.35
22	CA	1911	PSU	C4-N3	3.48	1.39	1.33
53	DA	1911	PSU	C4-N3	3.50	1.39	1.33
1	BA	527	G7M	C6-C5	3.56	1.48	1.41
22	CA	2503	2MA	C5-C4	3.60	1.48	1.40
1	AA	966	2MG	C6-C5	3.65	1.48	1.41
53	DA	2251	OMG	C6-C5	3.66	1.48	1.41
53	DA	2503	2MA	C6-N6	3.66	1.35	1.27
53	DA	2504	PSU	C4-N3	3.70	1.39	1.33
53	DA	2445	2MG	C6-C5	3.76	1.48	1.41
1	BA	1516	2MG	C6-C5	3.77	1.48	1.41
22	CA	2251	OMG	C6-C5	3.82	1.48	1.41
22	CA	2503	2MA	C6-N6	3.86	1.36	1.27
22	CA	2069	G7M	C6-C5	3.89	1.48	1.41
1	AA	527	G7M	C6-C5	3.94	1.48	1.41
1	BA	1207	2MG	C6-C5	4.01	1.49	1.41
1	BA	966	2MG	C6-C5	4.03	1.49	1.41
22	CA	2445	2MG	C6-C5	4.14	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	DA	745	1MG	C6-C5	4.18	1.48	1.41
12	AL	89	D2T	CA-C	4.23	1.55	1.50
34	DN	81[B]	4D4	CZ-NE	4.33	1.41	1.33
22	CA	2503	2MA	C6-C5	4.36	1.48	1.41
53	DA	1962	5MC	C5-C4	4.39	1.47	1.41
34	DN	81[A]	4D4	CZ-NE	4.44	1.42	1.33
22	CA	745	1MG	C6-C5	4.47	1.49	1.41
1	AA	967	5MC	C5-C4	4.54	1.48	1.41
34	CN	81	4D4	CZ-NE	4.59	1.42	1.33
22	CA	1962	5MC	C5-C4	5.03	1.48	1.41
1	BA	967	5MC	C5-C4	5.09	1.48	1.41
12	BL	89	D2T	CA-C	5.11	1.57	1.50
1	AA	1407	5MC	C5-C4	5.48	1.49	1.41
1	BA	1407	5MC	C5-C4	5.52	1.49	1.41

All (308) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	2580	PSU	N1-C2-N3	-15.16	117.50	128.40
53	DA	2457	PSU	N1-C2-N3	-14.33	118.09	128.40
53	DA	2604	PSU	N1-C2-N3	-14.03	118.31	128.40
53	DA	955	PSU	N1-C2-N3	-13.16	118.94	128.40
53	DA	2504	PSU	N1-C2-N3	-12.91	119.11	128.40
53	DA	2605	PSU	N1-C2-N3	-12.31	119.54	128.40
22	CA	1917	PSU	N1-C2-N3	-12.21	119.62	128.40
22	CA	955	PSU	N1-C2-N3	-12.06	119.73	128.40
1	BA	516	PSU	N1-C2-N3	-12.05	119.74	128.40
53	DA	1911	PSU	N1-C2-N3	-11.79	119.92	128.40
22	CA	1911	PSU	N1-C2-N3	-11.78	119.93	128.40
1	AA	516	PSU	N1-C2-N3	-11.69	119.99	128.40
53	DA	1917	PSU	N1-C2-N3	-11.67	120.00	128.40
22	CA	2504	PSU	N1-C2-N3	-11.54	120.10	128.40
22	CA	2605	PSU	N1-C2-N3	-11.53	120.11	128.40
22	CA	2580	PSU	N1-C2-N3	-11.52	120.12	128.40
22	CA	2457	PSU	N1-C2-N3	-11.11	120.41	128.40
22	CA	746	PSU	N1-C2-N3	-10.26	121.02	128.40
53	DA	746	PSU	N1-C2-N3	-9.24	121.75	128.40
22	CA	746	PSU	C5-C4-N3	-7.84	119.00	125.43
22	CA	2457	PSU	C5-C4-N3	-7.73	119.08	125.43
53	DA	746	PSU	C5-C4-N3	-7.72	119.10	125.43
53	DA	1917	PSU	C5-C4-N3	-7.48	119.30	125.43
53	DA	2030	6MZ	N3-C2-N1	-7.25	122.54	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	516	PSU	C5-C4-N3	-7.22	119.51	125.43
1	BA	1519	MA6	N3-C2-N1	-7.21	122.58	128.86
22	CA	2605	PSU	C5-C4-N3	-7.10	119.60	125.43
22	CA	2580	PSU	C5-C4-N3	-6.85	119.81	125.43
22	CA	2504	PSU	C5-C4-N3	-6.69	119.94	125.43
1	BA	1518	MA6	N3-C2-N1	-6.68	123.04	128.86
1	AA	1519	MA6	N3-C2-N1	-6.62	123.09	128.86
53	DA	1939	5MU	C5-C4-N3	-6.50	118.07	125.24
22	CA	1917	PSU	C5-C4-N3	-6.50	120.10	125.43
53	DA	955	PSU	C5-C4-N3	-6.46	120.13	125.43
22	CA	1618	6MZ	N3-C2-N1	-6.42	123.26	128.86
22	CA	2030	6MZ	N3-C2-N1	-6.33	123.34	128.86
22	CA	2504	PSU	C5-C1'-C2'	-6.29	104.71	115.55
22	CA	1911	PSU	C5-C4-N3	-6.24	120.31	125.43
1	AA	1402	4OC	CM4-N4-C4	-6.22	117.57	122.94
53	DA	2457	PSU	C5-C4-N3	-6.10	120.43	125.43
1	AA	516	PSU	C5-C4-N3	-6.08	120.44	125.43
53	DA	2504	PSU	C5-C4-N3	-6.08	120.44	125.43
53	DA	2449	H2U	C4-N3-C2	-5.77	120.87	125.81
22	CA	1939	5MU	C5-C4-N3	-5.69	118.97	125.24
22	CA	955	PSU	C5-C4-N3	-5.62	120.82	125.43
53	DA	747	5MU	C5-C4-N3	-5.61	119.06	125.24
53	DA	2605	PSU	C5-C4-N3	-5.61	120.83	125.43
53	DA	1618	6MZ	N3-C2-N1	-5.44	124.12	128.86
1	AA	1518	MA6	N3-C2-N1	-5.40	124.15	128.86
53	DA	2580	PSU	C5-C4-N3	-5.37	121.02	125.43
22	CA	747	5MU	C5-C4-N3	-5.29	119.41	125.24
53	DA	2449	H2U	C5-C6-N1	-5.24	105.26	110.70
53	DA	2445	2MG	C5-C6-N1	-5.12	116.19	123.48
53	DA	1911	PSU	C5-C4-N3	-4.97	121.35	125.43
22	CA	2069	G7M	C5-C6-N1	-4.93	116.47	123.48
1	BA	1516	2MG	CM2-N2-C2	-4.89	117.68	123.63
53	DA	2069	G7M	C5-C6-N1	-4.69	116.81	123.48
53	DA	2604	PSU	C5-C4-N3	-4.67	121.60	125.43
1	BA	1207	2MG	C6-C5-C4	-4.63	116.24	120.84
1	BA	527	G7M	C5-C6-N1	-4.61	116.92	123.48
53	DA	2504	PSU	C5-C1'-C2'	-4.49	107.81	115.55
1	AA	527	G7M	C5-C6-N1	-4.43	117.18	123.48
53	DA	1835	2MG	C6-C5-C4	-4.29	116.57	120.84
1	AA	966	2MG	C5-C6-N1	-4.28	117.39	123.48
22	CA	2445	2MG	C5-C6-N1	-4.27	117.41	123.48
22	CA	1915	3TD	C5-C1'-C2'	-4.23	108.25	115.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	CA	1915	3TD	C5-C6-N1	-4.19	118.95	124.39
1	AA	966	2MG	CM2-N2-C2	-4.18	118.54	123.63
1	AA	1207	2MG	CM2-N2-C2	-4.06	118.69	123.63
22	CA	2251	OMG	C6-C5-C4	-4.06	116.81	120.84
53	DA	1835	2MG	CM2-N2-C2	-4.00	118.76	123.63
1	AA	1207	2MG	C5-C6-N1	-3.97	117.82	123.48
53	DA	2445	2MG	C6-C5-C4	-3.95	116.91	120.84
53	DA	746	PSU	C5-C1'-C2'	-3.95	108.73	115.55
53	DA	2251	OMG	C5-C6-N1	-3.90	117.93	123.48
53	DA	745	1MG	C6-C5-C4	-3.88	117.25	119.92
22	CA	1618	6MZ	C9-N6-C6	-3.87	119.54	122.85
53	DA	1915	3TD	C5-C6-N1	-3.87	119.37	124.39
53	DA	2445	2MG	C4-C5-N7	-3.86	105.68	109.41
22	CA	2605	PSU	C5-C6-N1	-3.82	119.44	124.39
22	CA	1835	2MG	C5-C6-N1	-3.82	118.05	123.48
1	AA	1207	2MG	C6-C5-C4	-3.76	117.10	120.84
22	CA	1835	2MG	C6-C5-C4	-3.76	117.11	120.84
53	DA	2251	OMG	C6-C5-C4	-3.73	117.14	120.84
22	CA	2030	6MZ	C9-N6-C6	-3.73	119.66	122.85
1	AA	1516	2MG	C6-C5-C4	-3.72	117.14	120.84
22	CA	2251	OMG	C5-C6-N1	-3.69	118.23	123.48
22	CA	1618	6MZ	C4-C5-N7	-3.68	105.86	109.41
22	CA	2445	2MG	C6-C5-C4	-3.68	117.19	120.84
1	BA	966	2MG	C5-C6-N1	-3.66	118.28	123.48
1	BA	1207	2MG	C5-C6-N1	-3.61	118.34	123.48
1	BA	966	2MG	C6-C5-C4	-3.61	117.25	120.84
1	BA	1516	2MG	C5-C6-N1	-3.58	118.39	123.48
53	DA	1915	3TD	C5-C1'-C2'	-3.57	109.39	115.55
22	CA	2445	2MG	CM2-N2-C2	-3.55	119.31	123.63
22	CA	2030	6MZ	C4-C5-N7	-3.53	106.00	109.41
22	CA	746	PSU	C5-C6-N1	-3.50	119.85	124.39
22	CA	2457	PSU	C5-C6-N1	-3.50	119.85	124.39
53	DA	2069	G7M	N3-C2-N1	-3.50	122.35	127.46
1	AA	1519	MA6	C4-C5-N7	-3.43	106.10	109.41
22	CA	2251	OMG	N3-C2-N1	-3.34	122.58	127.46
22	CA	2445	2MG	C4-C5-N7	-3.34	106.19	109.41
22	CA	2580	PSU	C5-C6-N1	-3.33	120.07	124.39
53	DA	745	1MG	C4-C5-N7	-3.32	106.21	109.41
54	DD	150[B]	MEQ	CB-CA-C	-3.31	106.20	111.65
1	AA	1516	2MG	CM2-N2-C2	-3.30	119.61	123.63
1	AA	966	2MG	C6-C5-C4	-3.29	117.57	120.84
22	CA	747	5MU	C5-C6-N1	-3.28	118.59	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1516	2MG	C5-C6-N1	-3.28	118.81	123.48
53	DA	2604	PSU	C5-C1'-C2'	-3.28	109.89	115.55
53	DA	1618	6MZ	C4-C5-N7	-3.27	106.25	109.41
22	CA	2605	PSU	C5-C1'-C2'	-3.27	109.90	115.55
53	DA	2457	PSU	C5-C6-N1	-3.26	120.17	124.39
1	BA	1207	2MG	C4-C5-N7	-3.23	106.29	109.41
1	BA	516	PSU	C5-C6-N1	-3.22	120.22	124.39
1	BA	966	2MG	C4-C5-N7	-3.21	106.31	109.41
53	DA	1618	6MZ	C9-N6-C6	-3.20	120.11	122.85
22	CA	955	PSU	C5-C6-N1	-3.18	120.27	124.39
53	DA	1917	PSU	C5-C6-N1	-3.15	120.30	124.39
22	CA	746	PSU	C5-C1'-C2'	-3.13	110.15	115.55
54	DD	150[A]	MEQ	CB-CA-C	-3.12	106.51	111.65
53	DA	2069	G7M	C6-C5-C4	-3.11	117.75	120.84
53	DA	1911	PSU	C5-C6-N1	-3.09	120.38	124.39
22	CA	2504	PSU	C5-C6-N1	-3.06	120.42	124.39
1	BA	1516	2MG	C4-C5-N7	-3.05	106.47	109.41
1	BA	1516	2MG	C6-C5-C4	-3.03	117.83	120.84
1	BA	966	2MG	CM2-N2-C2	-3.03	119.95	123.63
1	AA	527	G7M	C1'-N9-C4	-3.02	121.41	126.64
1	AA	527	G7M	N3-C2-N1	-3.00	123.07	127.46
1	BA	1518	MA6	C4-C5-N7	-3.00	106.51	109.41
53	DA	746	PSU	C5-C6-N1	-2.99	120.51	124.39
53	DA	2605	PSU	C5-C6-N1	-2.97	120.54	124.39
53	DA	2030	6MZ	C1'-N9-C4	-2.97	121.51	126.64
22	CA	1911	PSU	C5-C6-N1	-2.95	120.56	124.39
53	DA	1835	2MG	C4-C5-N7	-2.92	106.59	109.41
22	CA	745	1MG	C4-C5-N7	-2.91	106.60	109.41
53	DA	1917	PSU	C5-C1'-C2'	-2.89	110.56	115.55
53	DA	2030	6MZ	C4-C5-N7	-2.87	106.64	109.41
53	DA	2251	OMG	C4-C5-N7	-2.87	106.64	109.41
53	DA	1835	2MG	C5-C6-N1	-2.83	119.45	123.48
1	BA	1402	4OC	CM4-N4-C4	-2.80	120.52	122.94
22	CA	2069	G7M	N3-C2-N1	-2.80	123.37	127.46
1	AA	966	2MG	C4-C5-N7	-2.76	106.74	109.41
1	AA	527	G7M	C6-C5-C4	-2.75	118.11	120.84
1	BA	1519	MA6	C4-C5-N7	-2.74	106.76	109.41
1	BA	1207	2MG	N3-C2-N1	-2.73	122.10	126.23
53	DA	1835	2MG	N3-C2-N1	-2.72	122.11	126.23
22	CA	1835	2MG	N3-C2-N1	-2.69	122.16	126.23
22	CA	2503	2MA	C4-C5-N7	-2.68	106.82	109.41
1	AA	516	PSU	C5-C6-N1	-2.67	120.93	124.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	1207	2MG	CM2-N2-C2	-2.62	120.44	123.63
1	AA	1207	2MG	C4-C5-N7	-2.60	106.90	109.41
22	CA	1915	3TD	O4'-C1'-C5	-2.60	105.91	109.93
53	DA	2449	H2U	O2-C2-N1	-2.60	119.87	123.12
22	CA	2030	6MZ	C1'-N9-C4	-2.58	122.18	126.64
22	CA	1962	5MC	C5-C6-N1	-2.58	119.36	122.15
1	AA	1207	2MG	N3-C2-N1	-2.57	122.34	126.23
53	DA	2503	2MA	C4-C5-N7	-2.55	106.94	109.41
53	DA	2030	6MZ	C9-N6-C6	-2.54	120.68	122.85
22	CA	1917	PSU	C5-C6-N1	-2.53	121.11	124.39
1	BA	1207	2MG	C1'-N9-C4	-2.52	122.28	126.64
1	BA	527	G7M	N3-C2-N1	-2.52	123.78	127.46
22	CA	1835	2MG	CM2-N2-C2	-2.51	120.57	123.63
53	DA	2604	PSU	C5-C6-N1	-2.49	121.17	124.39
1	AA	1518	MA6	C4-C5-N7	-2.48	107.01	109.41
53	DA	2251	OMG	N3-C2-N1	-2.47	123.85	127.46
22	CA	1835	2MG	C4-C5-N7	-2.46	107.03	109.41
22	CA	745	1MG	C6-C5-C4	-2.46	118.23	119.92
1	AA	1516	2MG	C4-C5-N7	-2.44	107.05	109.41
1	AA	1519	MA6	C1'-N9-C4	-2.41	122.47	126.64
53	DA	2503	2MA	C1'-N9-C4	-2.31	122.64	126.64
22	CA	2251	OMG	C4-C5-N7	-2.31	107.18	109.41
1	AA	967	5MC	C5-C6-N1	-2.29	119.67	122.15
22	CA	2445	2MG	N3-C2-N1	-2.26	122.81	126.23
1	BA	966	2MG	N3-C2-N1	-2.25	122.84	126.23
1	BA	1402	4OC	C5-C4-N3	-2.23	119.48	123.21
53	DA	747	5MU	C5-C6-N1	-2.19	119.78	122.15
1	BA	967	5MC	C5-C6-N1	-2.16	119.81	122.15
54	DD	150[A]	MEQ	OE1-CD-CG	-2.15	117.97	122.01
53	DA	2605	PSU	C5-C1'-C2'	-2.14	111.86	115.55
1	AA	966	2MG	N3-C2-N1	-2.13	123.01	126.23
22	CA	2251	OMG	CM2-O2'-C2'	-2.10	108.80	114.54
53	DA	2445	2MG	N3-C2-N1	-2.09	123.06	126.23
1	BA	1407	5MC	C5-C6-N1	-2.09	119.88	122.15
53	DA	2457	PSU	O2'-C2'-C1'	-2.06	107.54	112.21
22	CA	2503	2MA	C1'-N9-C4	-2.05	123.09	126.64
53	DA	955	PSU	O2'-C2'-C1'	-2.04	107.59	112.21
1	AA	1407	5MC	C5-C6-N1	-2.01	119.97	122.15
1	AA	516	PSU	O2'-C2'-C1'	-2.01	107.66	112.21
53	DA	2580	PSU	O4'-C1'-C5	-2.00	106.83	109.93
53	DA	1962	5MC	N4-C4-N3	2.00	119.96	117.00
1	AA	1519	MA6	N1-C6-N6	2.03	119.15	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	966	2MG	N2-C2-N3	2.04	118.94	116.95
1	AA	1518	MA6	N1-C6-N6	2.06	119.19	117.00
22	CA	2498	OMC	N4-C4-N3	2.10	120.17	116.64
22	CA	2030	6MZ	C5-C6-N6	2.18	124.19	120.33
53	DA	2580	PSU	C4-C5-C1'	2.21	125.42	121.15
1	AA	1516	2MG	N2-C2-N1	2.21	119.10	116.95
53	DA	2580	PSU	O4'-C1'-C2'	2.25	108.07	104.45
1	BA	1407	5MC	N4-C4-N3	2.31	120.41	117.00
22	CA	2445	2MG	N2-C2-N1	2.38	119.26	116.95
22	CA	1915	3TD	O4'-C1'-C2'	2.38	108.27	104.45
22	CA	1835	2MG	N2-C2-N3	2.40	119.28	116.95
1	AA	1407	5MC	N4-C4-N3	2.44	120.61	117.00
1	BA	967	5MC	N4-C4-N3	2.49	120.68	117.00
53	DA	746	PSU	C6-N1-C2	2.53	119.41	115.36
22	CA	2580	PSU	O4'-C1'-C2'	2.63	108.68	104.45
1	BA	1207	2MG	N2-C2-N1	2.74	119.62	116.95
1	AA	1207	2MG	N2-C2-N1	2.78	119.65	116.95
53	DA	2498	OMC	N4-C4-N3	2.84	121.42	116.64
22	CA	2504	PSU	C6-N1-C2	2.91	120.02	115.36
22	CA	1962	5MC	N4-C4-N3	2.95	121.35	117.00
22	CA	746	PSU	C6-N1-C2	2.96	120.10	115.36
53	DA	955	PSU	C6-N1-C2	3.03	120.21	115.36
22	CA	2457	PSU	C6-N1-C2	3.05	120.25	115.36
53	DA	1917	PSU	C6-N1-C2	3.11	120.34	115.36
53	DA	1835	2MG	C6-N1-C2	3.16	120.84	115.18
1	BA	516	PSU	C6-N1-C2	3.18	120.45	115.36
22	CA	2580	PSU	C6-N1-C2	3.21	120.50	115.36
53	DA	2449	H2U	C5-C4-N3	3.27	119.97	116.72
22	CA	1911	PSU	C6-N1-C2	3.28	120.61	115.36
1	AA	516	PSU	C6-N1-C2	3.31	120.66	115.36
1	AA	1516	2MG	C6-N1-C2	3.36	121.20	115.18
53	DA	2445	2MG	N2-C2-N1	3.38	120.23	116.95
22	CA	1917	PSU	C6-N1-C2	3.39	120.78	115.36
1	AA	967	5MC	N4-C4-N3	3.39	122.01	117.00
22	CA	2504	PSU	O4'-C1'-C5	3.41	115.21	109.93
22	CA	2605	PSU	C6-N1-C2	3.43	120.85	115.36
53	DA	2604	PSU	C6-N1-C2	3.46	120.90	115.36
53	DA	2504	PSU	C6-N1-C2	3.47	120.91	115.36
53	DA	2449	H2U	N3-C2-N1	3.54	120.25	116.73
1	BA	1516	2MG	C6-N1-C2	3.56	121.55	115.18
53	DA	2605	PSU	C6-N1-C2	3.58	121.09	115.36
1	BA	1519	MA6	N1-C6-N6	3.59	120.81	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	DA	1911	PSU	C6-N1-C2	3.66	121.22	115.36
22	CA	955	PSU	C6-N1-C2	3.73	121.33	115.36
53	DA	2251	OMG	C6-N1-C2	3.86	121.61	116.06
1	AA	1518	MA6	C2-N1-C6	3.90	121.39	111.82
1	BA	966	2MG	C6-N1-C2	3.91	122.17	115.18
53	DA	1915	3TD	C6-N1-C2	3.91	121.62	115.36
1	AA	966	2MG	C6-N1-C2	4.02	122.39	115.18
1	AA	527	G7M	C6-N1-C2	4.03	121.85	116.06
53	DA	2251	OMG	C2-N3-C4	4.08	119.93	115.16
53	DA	2457	PSU	C6-N1-C2	4.09	121.90	115.36
53	DA	2580	PSU	C6-N1-C2	4.10	121.92	115.36
1	AA	1519	MA6	C2-N1-C6	4.11	121.92	111.82
1	BA	527	G7M	C6-N1-C2	4.11	121.98	116.06
53	DA	2069	G7M	C2-N3-C4	4.13	119.98	115.16
1	BA	1518	MA6	C2-N1-C6	4.14	121.97	111.82
1	BA	1207	2MG	C6-N1-C2	4.16	122.64	115.18
1	AA	1207	2MG	C6-N1-C2	4.20	122.69	115.18
22	CA	2445	2MG	C6-N1-C2	4.24	122.77	115.18
22	CA	1835	2MG	C6-N1-C2	4.29	122.86	115.18
53	DA	1911	PSU	C4-N3-C2	4.31	118.93	115.16
1	BA	1519	MA6	C2-N1-C6	4.33	122.44	111.82
22	CA	1915	3TD	C6-N1-C2	4.36	122.34	115.36
22	CA	2069	G7M	C2-N3-C4	4.36	120.25	115.16
53	DA	2445	2MG	C2-N3-C4	4.38	120.11	115.11
1	AA	1516	2MG	C2-N3-C4	4.39	120.12	115.11
22	CA	2069	G7M	C6-N1-C2	4.43	122.44	116.06
1	BA	527	G7M	C2-N3-C4	4.52	120.43	115.16
1	AA	966	2MG	C2-N3-C4	4.56	120.31	115.11
22	CA	2251	OMG	C2-N3-C4	4.56	120.48	115.16
22	CA	2251	OMG	C6-N1-C2	4.58	122.64	116.06
53	DA	1835	2MG	N2-C2-N1	4.64	121.46	116.95
1	AA	516	PSU	C4-N3-C2	4.73	119.30	115.16
1	AA	1207	2MG	C2-N3-C4	4.76	120.54	115.11
53	DA	2445	2MG	C6-N1-C2	4.77	123.72	115.18
22	CA	955	PSU	C4-N3-C2	4.81	119.36	115.16
53	DA	2069	G7M	C6-N1-C2	4.83	123.01	116.06
53	DA	2605	PSU	C4-N3-C2	4.86	119.41	115.16
22	CA	2503	2MA	C2-N3-C4	4.96	119.69	115.41
22	CA	2445	2MG	C2-N3-C4	4.96	120.77	115.11
53	DA	746	PSU	C4-N3-C2	4.96	119.50	115.16
22	CA	2605	PSU	C4-N3-C2	5.00	119.53	115.16
22	CA	2504	PSU	C4-N3-C2	5.11	119.63	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	1516	2MG	C2-N3-C4	5.15	120.98	115.11
22	CA	2580	PSU	C4-N3-C2	5.16	119.67	115.16
22	CA	1911	PSU	C4-N3-C2	5.18	119.69	115.16
53	DA	2503	2MA	C2-N3-C4	5.18	119.89	115.41
22	CA	1835	2MG	C2-N3-C4	5.18	121.03	115.11
22	CA	747	5MU	C4-N3-C2	5.19	119.69	115.16
1	AA	527	G7M	C2-N3-C4	5.19	121.22	115.16
1	BA	1207	2MG	C2-N3-C4	5.25	121.10	115.11
22	CA	746	PSU	C4-N3-C2	5.25	119.75	115.16
22	CA	2457	PSU	C4-N3-C2	5.27	119.77	115.16
53	DA	2604	PSU	C4-N3-C2	5.44	119.92	115.16
1	BA	966	2MG	C2-N3-C4	5.47	121.36	115.11
53	DA	747	5MU	C4-N3-C2	5.54	120.01	115.16
53	DA	1917	PSU	C4-N3-C2	5.76	120.20	115.16
22	CA	1917	PSU	C4-N3-C2	5.82	120.25	115.16
1	BA	516	PSU	C4-N3-C2	5.87	120.29	115.16
53	DA	2457	PSU	C4-N3-C2	6.04	120.44	115.16
53	DA	2504	PSU	C4-N3-C2	6.19	120.58	115.16
53	DA	746	PSU	O4'-C1'-C5	6.25	119.62	109.93
53	DA	1835	2MG	C2-N3-C4	6.32	122.32	115.11
53	DA	745	1MG	C2-N3-C4	6.36	122.58	115.16
22	CA	745	1MG	C2-N3-C4	6.39	122.62	115.16
53	DA	2580	PSU	C4-N3-C2	6.58	120.91	115.16
22	CA	1939	5MU	C4-N3-C2	6.63	120.95	115.16
53	DA	955	PSU	C4-N3-C2	7.13	121.40	115.16
53	DA	1939	5MU	C4-N3-C2	7.20	121.45	115.16
53	DA	2552	OMU	C4-N3-C2	7.27	120.38	114.13
22	CA	2552	OMU	C4-N3-C2	7.52	120.59	114.13
53	DA	1618	6MZ	C2-N1-C6	8.73	122.22	116.53
22	CA	1618	6MZ	C2-N1-C6	8.88	122.31	116.53
22	CA	2030	6MZ	C2-N1-C6	10.23	123.20	116.53
53	DA	2030	6MZ	C2-N1-C6	10.56	123.41	116.53

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	DD	150[B]	MEQ	CG-CD-NE2-CE

There are no ring outliers.

31 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1402	4OC	1	0
1	AA	1518	MA6	2	0
1	AA	1519	MA6	3	0
1	AA	527	G7M	2	0
1	BA	1402	4OC	2	0
1	BA	1407	5MC	2	0
1	BA	1498	UR3	1	0
1	BA	1516	2MG	1	0
1	BA	1518	MA6	2	0
1	BA	1519	MA6	4	0
1	BA	516	PSU	1	0
1	BA	966	2MG	1	0
1	BA	967	5MC	1	0
22	CA	1618	6MZ	1	0
22	CA	1915	3TD	6	0
22	CA	1939	5MU	1	0
22	CA	1962	5MC	1	0
22	CA	2030	6MZ	2	0
22	CA	2069	G7M	1	0
22	CA	2251	OMG	1	0
22	CA	2445	2MG	2	0
22	CA	2498	OMC	2	0
22	CA	2503	2MA	4	0
22	CA	747	5MU	1	0
34	CN	81	4D4	1	0
53	DA	2030	6MZ	2	0
53	DA	2251	OMG	2	0
53	DA	2498	OMC	2	0
54	DD	150[A]	MEQ	1	0
54	DD	150[B]	MEQ	1	0
34	DN	81[A]	4D4	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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
57	PG4	AA	1670	-	12,12,12	0.81	0	11,11,11	0.41	0
58	MPD	AA	1671	-	7,7,7	0.50	0	9,10,10	0.55	0
59	PUT	AA	1672	-	5,5,5	0.22	0	4,4,4	0.59	0
59	PUT	AA	1673	-	5,5,5	0.23	0	4,4,4	0.53	0
59	PUT	AA	1674	-	5,5,5	0.22	0	4,4,4	0.57	0
59	PUT	AA	1675	-	5,5,5	0.29	0	4,4,4	0.38	0
58	MPD	AA	1676	-	7,7,7	0.66	0	9,10,10	0.55	0
61	PEG	AL	201	-	6,6,6	0.98	0	5,5,5	0.45	0
57	PG4	BA	1642	-	12,12,12	0.80	0	11,11,11	0.42	0
66	EDO	D0	101	-	3,3,3	0.37	0	2,2,2	0.45	0
66	EDO	D1	101	-	3,3,3	0.28	0	2,2,2	0.43	0
64	PGE	D1	102	-	9,9,9	1.06	0	8,8,8	0.31	0
64	PGE	D3	101	-	9,9,9	0.92	0	8,8,8	0.37	0
61	PEG	D3	102	-	6,6,6	1.01	0	5,5,5	0.40	0
62	SPD	DA	3183	-	9,9,9	0.42	0	8,8,8	0.80	0
59	PUT	DA	3184	-	5,5,5	0.30	0	4,4,4	0.34	0
63	1PE	DA	3185	-	15,15,15	0.56	0	14,14,14	0.50	0
64	PGE	DA	3186	-	9,9,9	0.93	0	8,8,8	0.30	0
62	SPD	DA	3187	-	9,9,9	0.42	0	8,8,8	0.91	0
59	PUT	DA	3188	-	5,5,5	0.19	0	4,4,4	0.29	0
59	PUT	DA	3189	-	5,5,5	0.32	0	4,4,4	0.44	0
58	MPD	DA	3190	-	7,7,7	0.61	0	9,10,10	0.61	0
65	ACY	DA	3191	-	1,3,3	2.55	1 (100%)	0,3,3	0.00	-
58	MPD	DA	3192	-	7,7,7	0.36	0	9,10,10	1.32	1 (11%)
57	PG4	DA	3193	-	12,12,12	0.80	0	11,11,11	0.59	0
66	EDO	DA	3194	-	3,3,3	0.32	0	2,2,2	0.48	0
59	PUT	DA	3195	-	5,5,5	0.27	0	4,4,4	0.41	0
65	ACY	DA	3196	-	1,3,3	3.55	1 (100%)	0,3,3	0.00	-
66	EDO	DA	3197	-	3,3,3	0.29	0	2,2,2	0.57	0
66	EDO	DA	3198	-	3,3,3	0.36	0	2,2,2	0.39	0
61	PEG	DA	3199	-	6,6,6	0.93	0	5,5,5	0.59	0
61	PEG	DA	3200	-	6,6,6	1.08	0	5,5,5	0.51	0
61	PEG	DA	3201	-	6,6,6	1.05	0	5,5,5	0.49	0
65	ACY	DA	3202	-	1,3,3	2.45	1 (100%)	0,3,3	0.00	-
63	1PE	DA	3203	-	15,15,15	0.66	0	14,14,14	0.33	0
64	PGE	DA	3204	-	9,9,9	0.98	0	8,8,8	0.55	0
58	MPD	DA	3205	-	7,7,7	0.71	0	9,10,10	1.12	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	PUT	DA	3206	-	5,5,5	0.29	0	4,4,4	0.56	0
62	SPD	DA	3207	-	9,9,9	0.50	0	8,8,8	0.67	0
58	MPD	DA	3208	-	7,7,7	0.48	0	9,10,10	0.31	0
66	EDO	DA	3209	-	3,3,3	0.38	0	2,2,2	0.32	0
66	EDO	DA	3210	-	3,3,3	0.33	0	2,2,2	0.50	0
58	MPD	DA	3211	-	7,7,7	0.48	0	9,10,10	0.91	1 (11%)
67	GUN	DA	3212	-	9,12,12	2.14	2 (22%)	8,17,17	3.56	6 (75%)
59	PUT	DA	3213	-	5,5,5	0.27	0	4,4,4	0.24	0
59	PUT	DA	3214	-	5,5,5	0.25	0	4,4,4	0.47	0
64	PGE	DA	3215	-	9,9,9	0.94	0	8,8,8	0.31	0
66	EDO	DA	3216	-	3,3,3	0.40	0	2,2,2	0.37	0
57	PG4	DA	3217	-	12,12,12	0.74	0	11,11,11	0.54	0
64	PGE	DA	3218	-	9,9,9	0.84	0	8,8,8	0.38	0
61	PEG	DA	3219	-	6,6,6	1.04	0	5,5,5	0.45	0
59	PUT	DA	3220	-	5,5,5	0.20	0	4,4,4	0.51	0
68	TRS	DA	3221	-	7,7,7	0.49	0	9,9,9	0.75	0
59	PUT	DA	3222	-	5,5,5	0.23	0	4,4,4	0.46	0
59	PUT	DA	3223	-	5,5,5	0.34	0	4,4,4	0.47	0
59	PUT	DA	3224	-	5,5,5	0.22	0	4,4,4	0.76	0
62	SPD	DA	3225	-	9,9,9	0.56	0	8,8,8	1.06	1 (12%)
64	PGE	DA	3226	-	9,9,9	0.97	0	8,8,8	0.26	0
61	PEG	DA	3227	-	6,6,6	0.98	0	5,5,5	0.42	0
61	PEG	DA	3228	-	6,6,6	1.06	0	5,5,5	0.17	0
66	EDO	DB	210	-	3,3,3	0.30	0	2,2,2	0.77	0
66	EDO	DB	211	-	3,3,3	0.38	0	2,2,2	0.51	0
66	EDO	DB	212	-	3,3,3	0.35	0	2,2,2	0.46	0
58	MPD	DE	301	-	7,7,7	0.58	0	9,10,10	0.67	0
58	MPD	DE	302	-	7,7,7	0.49	0	9,10,10	0.52	0
58	MPD	DK	201	-	7,7,7	0.51	0	9,10,10	0.72	0
61	PEG	DL	201	-	6,6,6	0.88	0	5,5,5	0.57	0
59	PUT	DM	201	-	5,5,5	0.25	0	4,4,4	0.71	0
58	MPD	DN	201	-	7,7,7	0.51	0	9,10,10	0.81	0
61	PEG	DP	201	-	6,6,6	1.00	0	5,5,5	0.42	0
61	PEG	DQ	201	-	6,6,6	1.02	0	5,5,5	0.48	0
57	PG4	DQ	202	-	12,12,12	0.67	0	11,11,11	0.56	0
57	PG4	DR	202	-	12,12,12	0.85	0	11,11,11	0.41	0
66	EDO	DR	203	-	3,3,3	0.31	0	2,2,2	0.40	0
64	PGE	DS	201	-	9,9,9	0.97	0	8,8,8	0.31	0
57	PG4	DS	202	-	12,12,12	0.77	0	11,11,11	0.32	0
58	MPD	DS	203	-	7,7,7	0.93	1 (14%)	9,10,10	0.56	0
58	MPD	DT	201	-	7,7,7	0.79	0	9,10,10	1.06	0
58	MPD	DT	202	-	7,7,7	0.50	0	9,10,10	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
64	PGE	DU	101	-	9,9,9	0.98	0	8,8,8	0.43	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
57	PG4	AA	1670	-	-	0/10/10/10	0/0/0/0
58	MPD	AA	1671	-	-	0/5/5/5	0/0/0/0
59	PUT	AA	1672	-	-	0/3/3/3	0/0/0/0
59	PUT	AA	1673	-	-	0/3/3/3	0/0/0/0
59	PUT	AA	1674	-	-	0/3/3/3	0/0/0/0
59	PUT	AA	1675	-	-	0/3/3/3	0/0/0/0
58	MPD	AA	1676	-	-	0/5/5/5	0/0/0/0
61	PEG	AL	201	-	-	0/4/4/4	0/0/0/0
57	PG4	BA	1642	-	-	0/10/10/10	0/0/0/0
66	EDO	D0	101	-	-	0/1/1/1	0/0/0/0
66	EDO	D1	101	-	-	0/1/1/1	0/0/0/0
64	PGE	D1	102	-	-	0/7/7/7	0/0/0/0
64	PGE	D3	101	-	-	0/7/7/7	0/0/0/0
61	PEG	D3	102	-	-	0/4/4/4	0/0/0/0
62	SPD	DA	3183	-	-	0/7/7/7	0/0/0/0
59	PUT	DA	3184	-	-	0/3/3/3	0/0/0/0
63	1PE	DA	3185	-	-	0/13/13/13	0/0/0/0
64	PGE	DA	3186	-	-	0/7/7/7	0/0/0/0
62	SPD	DA	3187	-	-	0/7/7/7	0/0/0/0
59	PUT	DA	3188	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3189	-	-	0/3/3/3	0/0/0/0
58	MPD	DA	3190	-	-	0/5/5/5	0/0/0/0
65	ACY	DA	3191	-	-	0/0/0/0	0/0/0/0
58	MPD	DA	3192	-	-	0/5/5/5	0/0/0/0
57	PG4	DA	3193	-	-	0/10/10/10	0/0/0/0
66	EDO	DA	3194	-	-	0/1/1/1	0/0/0/0
59	PUT	DA	3195	-	-	0/3/3/3	0/0/0/0
65	ACY	DA	3196	-	-	0/0/0/0	0/0/0/0
66	EDO	DA	3197	-	-	0/1/1/1	0/0/0/0
66	EDO	DA	3198	-	-	0/1/1/1	0/0/0/0
61	PEG	DA	3199	-	-	0/4/4/4	0/0/0/0
61	PEG	DA	3200	-	-	0/4/4/4	0/0/0/0
61	PEG	DA	3201	-	-	0/4/4/4	0/0/0/0
65	ACY	DA	3202	-	-	0/0/0/0	0/0/0/0
63	1PE	DA	3203	-	-	0/13/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	PGE	DA	3204	-	-	0/7/7/7	0/0/0/0
58	MPD	DA	3205	-	-	0/5/5/5	0/0/0/0
59	PUT	DA	3206	-	-	0/3/3/3	0/0/0/0
62	SPD	DA	3207	-	-	0/7/7/7	0/0/0/0
58	MPD	DA	3208	-	-	0/5/5/5	0/0/0/0
66	EDO	DA	3209	-	-	0/1/1/1	0/0/0/0
66	EDO	DA	3210	-	-	0/1/1/1	0/0/0/0
58	MPD	DA	3211	-	-	0/5/5/5	0/0/0/0
67	GUN	DA	3212	-	-	0/0/0/0	0/2/2/2
59	PUT	DA	3213	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3214	-	-	0/3/3/3	0/0/0/0
64	PGE	DA	3215	-	-	0/7/7/7	0/0/0/0
66	EDO	DA	3216	-	-	0/1/1/1	0/0/0/0
57	PG4	DA	3217	-	-	0/10/10/10	0/0/0/0
64	PGE	DA	3218	-	-	0/7/7/7	0/0/0/0
61	PEG	DA	3219	-	-	0/4/4/4	0/0/0/0
59	PUT	DA	3220	-	-	0/3/3/3	0/0/0/0
68	TRS	DA	3221	-	-	0/9/9/9	0/0/0/0
59	PUT	DA	3222	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3223	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3224	-	-	0/3/3/3	0/0/0/0
62	SPD	DA	3225	-	-	0/7/7/7	0/0/0/0
64	PGE	DA	3226	-	-	0/7/7/7	0/0/0/0
61	PEG	DA	3227	-	-	0/4/4/4	0/0/0/0
61	PEG	DA	3228	-	-	0/4/4/4	0/0/0/0
66	EDO	DB	210	-	-	0/1/1/1	0/0/0/0
66	EDO	DB	211	-	-	0/1/1/1	0/0/0/0
66	EDO	DB	212	-	-	0/1/1/1	0/0/0/0
58	MPD	DE	301	-	-	0/5/5/5	0/0/0/0
58	MPD	DE	302	-	-	0/5/5/5	0/0/0/0
58	MPD	DK	201	-	-	0/5/5/5	0/0/0/0
61	PEG	DL	201	-	-	0/4/4/4	0/0/0/0
59	PUT	DM	201	-	-	0/3/3/3	0/0/0/0
58	MPD	DN	201	-	-	0/5/5/5	0/0/0/0
61	PEG	DP	201	-	-	0/4/4/4	0/0/0/0
61	PEG	DQ	201	-	-	0/4/4/4	0/0/0/0
57	PG4	DQ	202	-	-	0/10/10/10	0/0/0/0
57	PG4	DR	202	-	-	0/10/10/10	0/0/0/0
66	EDO	DR	203	-	-	0/1/1/1	0/0/0/0
64	PGE	DS	201	-	-	0/7/7/7	0/0/0/0
57	PG4	DS	202	-	-	0/10/10/10	0/0/0/0
58	MPD	DS	203	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	MPD	DT	201	-	-	0/5/5/5	0/0/0/0
58	MPD	DT	202	-	-	0/5/5/5	0/0/0/0
64	PGE	DU	101	-	-	0/7/7/7	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	DS	203	MPD	O2-C2	-2.04	1.39	1.44
65	DA	3202	ACY	CH3-C	2.45	1.51	1.48
65	DA	3191	ACY	CH3-C	2.55	1.52	1.48
67	DA	3212	GUN	C5-C4	3.48	1.48	1.40
65	DA	3196	ACY	CH3-C	3.55	1.53	1.48
67	DA	3212	GUN	C6-C5	4.97	1.50	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	DA	3212	GUN	C6-C5-C4	-4.11	116.75	120.84
67	DA	3212	GUN	C4-C5-N7	-3.71	105.82	109.41
58	DA	3192	MPD	CM-C2-C1	-3.23	103.22	110.42
67	DA	3212	GUN	N3-C2-N1	-3.21	122.78	127.46
67	DA	3212	GUN	C5-C6-N1	-3.05	119.14	123.48
62	DA	3225	SPD	C7-C8-C9	-2.27	105.22	114.19
58	DA	3211	MPD	CM-C2-C1	-2.20	105.52	110.42
58	DA	3205	MPD	CM-C2-C1	2.71	116.47	110.42
67	DA	3212	GUN	C6-N1-C2	3.74	121.44	116.06
67	DA	3212	GUN	C2-N3-C4	6.00	122.17	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

42 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	1670	PG4	1	0
59	AA	1673	PUT	1	0
57	BA	1642	PG4	2	0
61	D3	102	PEG	5	0
62	DA	3183	SPD	1	0
63	DA	3185	1PE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	DA	3187	SPD	1	0
59	DA	3189	PUT	1	0
58	DA	3190	MPD	1	0
57	DA	3193	PG4	7	0
66	DA	3194	EDO	3	0
59	DA	3195	PUT	3	0
66	DA	3197	EDO	1	0
66	DA	3198	EDO	3	0
61	DA	3200	PEG	1	0
61	DA	3201	PEG	1	0
65	DA	3202	ACY	1	0
63	DA	3203	1PE	3	0
64	DA	3204	PGE	2	0
58	DA	3205	MPD	3	0
66	DA	3209	EDO	1	0
66	DA	3210	EDO	3	0
58	DA	3211	MPD	1	0
67	DA	3212	GUN	1	0
59	DA	3213	PUT	1	0
59	DA	3214	PUT	2	0
57	DA	3217	PG4	1	0
64	DA	3218	PGE	1	0
59	DA	3220	PUT	1	0
59	DA	3222	PUT	2	0
59	DA	3223	PUT	4	0
59	DA	3224	PUT	2	0
62	DA	3225	SPD	5	0
61	DA	3227	PEG	1	0
66	DB	212	EDO	1	0
58	DN	201	MPD	6	0
61	DP	201	PEG	4	0
61	DQ	201	PEG	1	0
57	DQ	202	PG4	3	0
57	DR	202	PG4	10	0
57	DS	202	PG4	2	0
64	DU	101	PGE	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.20	45 (2%) 51 58	50, 82, 132, 172	0
1	BA	1522/1534 (99%)	0.43	168 (11%) 6 8	64, 105, 192, 222	0
2	AB	224/224 (100%)	2.93	135 (60%) 0 0	74, 117, 124, 132	0
2	BB	224/224 (100%)	3.75	158 (70%) 0 0	74, 114, 123, 130	0
3	AC	206/206 (100%)	1.19	43 (20%) 1 1	77, 88, 100, 105	0
3	BC	206/206 (100%)	3.19	137 (66%) 0 0	99, 117, 150, 166	0
4	AD	205/205 (100%)	0.80	20 (9%) 8 11	70, 91, 116, 125	0
4	BD	205/205 (100%)	0.94	14 (6%) 18 23	64, 76, 86, 91	0
5	AE	155/155 (100%)	0.95	22 (14%) 3 4	68, 79, 89, 95	0
5	BE	150/155 (96%)	1.70	47 (31%) 0 0	77, 91, 103, 114	0
6	AF	106/106 (100%)	0.75	13 (12%) 5 6	65, 92, 100, 102	0
6	BF	100/106 (94%)	2.46	50 (50%) 0 0	92, 104, 113, 117	0
7	AG	151/151 (100%)	2.31	62 (41%) 0 0	90, 117, 127, 132	0
7	BG	151/151 (100%)	6.71	138 (91%) 0 0	111, 153, 177, 185	0
8	AH	129/129 (100%)	0.81	13 (10%) 8 10	69, 82, 95, 103	0
8	BH	129/129 (100%)	1.60	38 (29%) 1 1	72, 111, 132, 139	0
9	AI	127/127 (100%)	2.55	63 (49%) 0 0	81, 111, 124, 130	0
9	BI	127/127 (100%)	5.15	104 (81%) 0 0	130, 152, 171, 177	0
10	AJ	99/99 (100%)	1.98	43 (43%) 0 0	60, 70, 76, 77	0
10	BJ	98/99 (98%)	5.37	81 (82%) 0 0	69, 76, 80, 81	0
11	AK	117/117 (100%)	1.57	41 (35%) 0 0	60, 90, 104, 108	0
11	BK	117/117 (100%)	2.09	52 (44%) 0 0	75, 102, 115, 118	0
12	AL	122/123 (99%)	0.47	4 (3%) 47 54	55, 67, 77, 88	0
12	BL	122/123 (99%)	1.30	25 (20%) 1 1	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%)	2.49	54 (47%)	0	0	84, 112, 124, 128	0
13	BM	114/114 (100%)	8.50	110 (96%)	0	0	190, 219, 233, 235	0
14	AN	100/100 (100%)	2.13	34 (34%)	0	0	80, 100, 134, 140	0
14	BN	100/100 (100%)	6.90	92 (92%)	0	0	126, 174, 220, 227	0
15	AO	88/88 (100%)	0.73	10 (11%)	6	7	69, 82, 93, 98	0
15	BO	88/88 (100%)	1.87	34 (38%)	0	0	80, 105, 118, 125	0
16	AP	82/82 (100%)	1.49	16 (19%)	1	1	70, 85, 104, 113	0
16	BP	82/82 (100%)	2.94	50 (60%)	0	0	84, 106, 122, 126	0
17	AQ	80/80 (100%)	1.04	17 (21%)	1	1	69, 83, 96, 101	0
17	BQ	80/80 (100%)	3.23	50 (62%)	0	0	89, 120, 129, 133	0
18	AR	55/55 (100%)	1.43	15 (27%)	1	1	79, 86, 96, 98	0
18	BR	55/55 (100%)	1.25	12 (21%)	1	1	83, 90, 98, 100	0
19	AS	79/79 (100%)	2.52	41 (51%)	0	0	91, 110, 123, 127	0
19	BS	79/79 (100%)	9.12	71 (89%)	0	0	199, 217, 228, 231	0
20	AT	86/86 (100%)	1.16	17 (19%)	1	1	58, 84, 101, 107	0
20	BT	85/86 (98%)	4.19	64 (75%)	0	0	107, 131, 142, 144	0
21	AU	56/56 (100%)	2.54	31 (55%)	0	0	67, 80, 103, 113	0
21	BU	56/56 (100%)	1.88	22 (39%)	0	0	65, 85, 106, 113	0
22	CA	2876/2904 (99%)	0.63	291 (10%)	8	10	77, 118, 180, 217	0
23	CB	118/120 (98%)	0.85	17 (14%)	3	4	108, 157, 167, 168	0
23	DB	120/120 (100%)	-0.30	0	100	100	37, 58, 73, 81	0
24	CC	271/271 (100%)	2.01	120 (44%)	0	0	83, 107, 126, 131	0
24	DC	271/271 (100%)	1.31	56 (20%)	1	1	35, 59, 71, 78	0
25	CD	209/209 (100%)	2.64	115 (55%)	0	0	87, 108, 121, 126	0
26	CE	201/201 (100%)	4.51	153 (76%)	0	0	90, 157, 187, 196	0
26	DE	201/201 (100%)	0.70	19 (9%)	9	12	33, 57, 72, 78	0
27	CF	177/177 (100%)	8.47	170 (96%)	0	0	167, 172, 175, 176	0
27	DF	177/177 (100%)	0.89	18 (10%)	7	9	58, 75, 91, 94	0
28	CG	176/176 (100%)	5.40	154 (87%)	0	0	108, 120, 130, 134	0
28	DG	176/176 (100%)	0.55	14 (7%)	13	17	49, 62, 71, 75	0
29	CH	149/149 (100%)	3.99	115 (77%)	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%)	3.88	102 (68%) 0 0	65, 128, 133, 154	0
30	CJ	134/134 (100%)	12.56	134 (100%) 0 0	202, 219, 225, 228	0
30	DJ	134/134 (100%)	9.89	130 (97%) 0 0	155, 183, 202, 208	0
31	CK	142/142 (100%)	2.36	75 (52%) 0 0	98, 110, 115, 120	0
31	DK	142/142 (100%)	0.97	19 (13%) 4 5	33, 41, 51, 60	0
32	CL	122/123 (99%)	2.17	48 (39%) 0 0	94, 107, 113, 114	0
32	DL	123/123 (100%)	0.67	5 (4%) 38 45	37, 48, 59, 68	0
33	CM	144/144 (100%)	4.08	115 (79%) 0 0	100, 137, 162, 166	0
33	DM	144/144 (100%)	1.04	27 (18%) 1 2	28, 53, 69, 73	0
34	CN	135/136 (99%)	2.16	56 (41%) 0 0	95, 122, 142, 150	0
34	DN	135/136 (99%)	0.54	5 (3%) 42 49	36, 44, 57, 63	0
35	CO	120/125 (96%)	2.96	79 (65%) 0 0	103, 120, 137, 142	0
35	DO	125/125 (100%)	1.21	25 (20%) 1 1	35, 44, 60, 69	0
36	CP	116/117 (99%)	5.77	106 (91%) 0 0	146, 155, 162, 164	0
36	DP	117/117 (100%)	0.34	1 (0%) 84 86	49, 59, 69, 73	0
37	CQ	114/114 (100%)	2.77	70 (61%) 0 0	110, 116, 124, 131	0
37	DQ	114/114 (100%)	0.84	11 (9%) 9 11	40, 52, 63, 73	0
38	CR	117/117 (100%)	2.46	67 (57%) 0 0	100, 115, 126, 128	0
38	DR	117/117 (100%)	1.41	31 (26%) 1 1	30, 40, 49, 64	0
39	CS	103/103 (100%)	3.51	70 (67%) 0 0	103, 125, 133, 137	0
39	DS	103/103 (100%)	0.80	10 (9%) 8 11	29, 48, 59, 73	0
40	CT	110/110 (100%)	3.13	78 (70%) 0 0	91, 121, 146, 150	0
40	DT	110/110 (100%)	1.13	10 (9%) 10 13	33, 39, 52, 68	0
41	CU	93/93 (100%)	5.65	82 (88%) 0 0	117, 149, 169, 176	0
41	DU	93/93 (100%)	0.64	6 (6%) 20 25	41, 57, 76, 83	0
42	CV	102/102 (100%)	7.45	95 (93%) 0 0	151, 176, 205, 210	0
42	DV	102/102 (100%)	0.42	4 (3%) 40 47	48, 60, 69, 80	0
43	CW	94/94 (100%)	3.52	60 (63%) 0 0	129, 148, 161, 165	0
43	DW	94/94 (100%)	0.41	3 (3%) 48 55	40, 54, 65, 71	0
44	CX	75/76 (98%)	3.40	50 (66%) 0 0	109, 118, 122, 126	0
44	DX	76/76 (100%)	1.08	12 (15%) 2 3	36, 46, 59, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	CY	77/77 (100%)	2.50	39 (50%) 0 0	99, 116, 133, 135	0
45	DY	77/77 (100%)	0.67	4 (5%) 28 34	42, 59, 73, 78	0
46	CZ	62/62 (100%)	5.21	54 (87%) 0 0	158, 174, 193, 199	0
46	DZ	62/62 (100%)	0.52	4 (6%) 20 25	56, 66, 81, 82	0
47	C0	58/58 (100%)	2.16	23 (39%) 0 0	119, 130, 142, 143	0
47	D0	58/58 (100%)	1.18	6 (10%) 7 9	35, 42, 53, 56	0
48	C1	56/56 (100%)	3.35	42 (75%) 0 0	92, 123, 140, 144	0
48	D1	56/56 (100%)	1.29	15 (26%) 1 1	27, 44, 58, 64	0
49	C2	50/51 (98%)	3.67	39 (78%) 0 0	113, 122, 128, 132	0
49	D2	51/51 (100%)	0.82	5 (9%) 8 11	50, 59, 66, 67	0
50	C3	46/46 (100%)	3.31	32 (69%) 0 0	95, 108, 115, 117	0
50	D3	46/46 (100%)	1.27	5 (10%) 6 8	35, 44, 53, 62	0
51	C4	64/64 (100%)	3.38	43 (67%) 0 0	109, 119, 126, 127	0
51	D4	64/64 (100%)	1.71	21 (32%) 0 0	39, 45, 51, 57	0
52	C5	38/38 (100%)	3.10	25 (65%) 0 0	106, 114, 120, 125	0
52	D5	38/38 (100%)	0.60	1 (2%) 56 62	42, 48, 58, 63	0
53	DA	2873/2903 (98%)	0.16	111 (3%) 40 47	30, 49, 130, 199	0
54	DD	208/209 (99%)	1.15	47 (22%) 1 1	29, 44, 58, 63	0
55	DI	135/135 (100%)	5.53	118 (87%) 0 0	89, 123, 152, 159	1 (0%)
All	All	20634/20744 (99%)	1.66	5718 (27%) 1 1	27, 96, 176, 235	1 (0%)

All (5718) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	CJ	32	GLY	65.1
30	CJ	8	TYR	48.8
30	CJ	9	VAL	38.7
30	CJ	11	LEU	31.9
30	CJ	13	VAL	31.2
30	CJ	26	PRO	31.2
30	CJ	42	PHE	29.4
14	BN	34	VAL	28.9
42	CV	26	LYS	28.3
30	CJ	31	GLN	28.2
30	CJ	67	PHE	28.0

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Mol	Chain	Res	Type	RSRZ
7	BG	62	PHE	27.8
30	CJ	69	PHE	27.2
14	BN	21	PHE	26.9
27	CF	156	ILE	25.8
30	CJ	63	ALA	25.1
30	DJ	67	PHE	24.6
30	CJ	62	TYR	23.8
30	DJ	99	GLY	23.6
42	CV	12	ILE	23.5
30	DJ	80	LEU	23.4
27	CF	76	GLY	23.4
30	CJ	99	GLY	22.7
19	BS	68	GLY	22.3
30	CJ	80	LEU	22.3
42	CV	25	VAL	22.0
9	BI	38	TYR	21.9
41	CU	1	MET	21.7
19	BS	74	PHE	21.7
42	CV	50	PRO	21.0
13	BM	84	GLY	21.0
13	BM	75	MET	20.8
30	CJ	35	ILE	20.8
30	DJ	53	LEU	20.5
13	BM	85	CYS	20.3
55	DI	123	ILE	20.3
13	BM	40	ALA	20.3
30	CJ	27	ALA	20.0
19	BS	15	LEU	19.9
46	CZ	11	VAL	19.9
43	CW	94	ALA	19.8
30	DJ	49	ILE	19.8
7	BG	66	LEU	19.7
30	CJ	17	MET	19.7
19	BS	12	ASP	19.6
30	DJ	85	GLY	19.3
27	CF	97	TRP	19.1
30	DJ	100	LYS	19.0
30	DJ	106	LEU	19.0
27	CF	152	LEU	18.9
13	BM	30	SER	18.8
30	DJ	98	VAL	18.8
7	BG	87	VAL	18.7

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Mol	Chain	Res	Type	RSRZ
13	BM	80	LEU	18.6
19	BS	66	MET	18.6
30	DJ	40	LYS	18.5
30	CJ	21	SER	18.4
30	DJ	48	SER	18.3
30	DJ	87	LYS	18.2
30	CJ	33	VAL	18.2
7	BG	51	ALA	18.2
30	CJ	44	ALA	18.1
51	C4	21	GLY	18.1
30	CJ	56	PRO	18.1
14	BN	33	ASP	18.0
42	CV	51	ALA	17.9
14	BN	31	ILE	17.9
42	CV	29	LEU	17.8
30	CJ	22	PRO	17.8
30	CJ	59	ILE	17.7
30	DJ	138	LEU	17.6
55	DI	131	THR	17.6
2	BB	135	LEU	17.5
30	CJ	75	PRO	17.5
30	CJ	10	LYS	17.4
19	BS	46	GLY	17.4
30	DJ	96	ASP	17.3
14	BN	74	LEU	17.3
30	CJ	12	GLN	17.3
42	CV	28	VAL	17.2
13	BM	5	ALA	17.2
19	BS	67	VAL	17.2
30	DJ	94	ASN	17.1
42	CV	62	GLU	17.0
14	BN	25	ALA	16.9
9	BI	40	GLY	16.9
42	CV	39	ILE	16.9
9	BI	58	VAL	16.8
27	CF	155	THR	16.7
55	DI	84	TYR	16.6
30	CJ	20	PRO	16.6
27	CF	117	LEU	16.5
14	BN	43	ASN	16.5
30	CJ	58	VAL	16.5
7	BG	59	LEU	16.5

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Mol	Chain	Res	Type	RSRZ
30	CJ	57	VAL	16.5
26	CE	119	ILE	16.5
27	CF	120	LYS	16.4
13	BM	109	ARG	16.4
30	CJ	30	GLN	16.4
14	BN	36	ALA	16.4
30	DJ	88	SER	16.4
30	CJ	73	THR	16.4
14	BN	42	TRP	16.2
14	BN	30	ILE	16.2
30	CJ	29	GLY	16.2
30	DJ	114	ALA	16.1
27	CF	100	PHE	16.1
42	CV	87	PHE	16.0
13	BM	106	ALA	16.0
7	BG	152	ALA	16.0
14	AN	21	PHE	15.9
30	CJ	60	THR	15.9
20	BT	4	ILE	15.9
14	BN	57	PRO	15.9
13	BM	96	PRO	15.8
27	CF	4	LEU	15.8
19	BS	22	ALA	15.7
19	BS	11	ILE	15.7
13	BM	6	GLY	15.7
10	BJ	77	VAL	15.7
30	DJ	110	ALA	15.6
26	CE	158	PHE	15.5
30	CJ	76	ALA	15.5
43	CW	57	TYR	15.4
27	CF	169	LEU	15.3
27	CF	113	ASP	15.3
30	CJ	64	ASP	15.2
30	CJ	139	VAL	15.2
27	CF	159	THR	15.2
28	CG	168	VAL	15.2
27	CF	58	ALA	15.1
27	CF	28	VAL	15.0
30	DJ	89	GLY	15.0
30	CJ	34	ASN	15.0
7	BG	134	ALA	14.9
28	CG	40	ALA	14.9

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Mol	Chain	Res	Type	RSRZ
27	CF	55	ALA	14.9
27	CF	106	ILE	14.9
19	BS	61	PHE	14.9
55	DI	129	LEU	14.9
30	DJ	76	ALA	14.9
30	DJ	38	PHE	14.9
55	DI	106	PHE	14.9
36	CP	58	ILE	14.9
30	DJ	52	GLY	14.9
30	CJ	68	THR	14.8
30	DJ	54	PRO	14.8
13	BM	32	ALA	14.7
30	CJ	61	VAL	14.7
9	BI	128	SER	14.7
30	DJ	42	PHE	14.7
30	CJ	25	GLY	14.6
30	DJ	139	VAL	14.6
14	BN	28	LYS	14.6
28	CG	52	PHE	14.5
9	BI	47	VAL	14.5
42	CV	13	VAL	14.5
14	BN	58	SER	14.4
19	BS	58	VAL	14.4
27	CF	116	GLY	14.3
27	CF	57	LEU	14.3
19	BS	27	ASP	14.3
42	CV	30	SER	14.3
13	BM	39	ILE	14.3
55	DI	121	SER	14.3
42	CV	36	VAL	14.2
42	CV	37	GLU	14.2
7	BG	141	VAL	14.1
42	CV	52	LEU	14.1
27	CF	32	GLU	14.0
2	BB	40	ILE	14.0
27	CF	176	PRO	13.9
13	BM	51	GLY	13.9
7	BG	98	ALA	13.9
19	BS	60	VAL	13.9
19	BS	38	SER	13.9
55	DI	130	PRO	13.8
55	DI	117	LEU	13.8

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Mol	Chain	Res	Type	RSRZ
7	BG	5	ARG	13.8
30	DJ	68	THR	13.8
26	CE	127	GLU	13.8
26	CE	131	THR	13.8
30	CJ	23	PRO	13.8
20	BT	79	LEU	13.8
26	CE	128	ALA	13.7
30	DJ	79	LEU	13.7
27	CF	40	VAL	13.7
30	CJ	140	VAL	13.7
30	CJ	38	PHE	13.7
27	CF	136	ILE	13.7
7	BG	79	ARG	13.7
26	CE	164	LEU	13.7
27	CF	172	ALA	13.7
29	DH	74	ALA	13.7
30	DJ	22	PRO	13.7
19	BS	26	GLY	13.7
39	CS	103	ALA	13.6
30	DJ	33	VAL	13.6
13	BM	28	THR	13.6
19	BS	39	THR	13.6
30	DJ	13	VAL	13.6
13	BM	77	ILE	13.6
30	DJ	36	MET	13.6
26	CE	12	LEU	13.6
27	CF	128	TYR	13.6
41	CU	83	ALA	13.5
30	DJ	103	ARG	13.5
33	CM	92	LEU	13.5
46	CZ	6	LEU	13.5
28	CG	10	VAL	13.5
30	DJ	69	PHE	13.5
19	BS	25	SER	13.5
7	BG	133	THR	13.4
27	CF	54	ALA	13.4
19	BS	69	HIS	13.4
36	CP	59	ALA	13.4
13	BM	83	LEU	13.4
27	CF	87	CYS	13.4
30	DJ	55	ILE	13.3
30	DJ	93	PRO	13.3

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Mol	Chain	Res	Type	RSRZ
9	BI	59	GLU	13.3
7	BG	50	LEU	13.3
30	DJ	140	VAL	13.2
14	BN	18	ASP	13.2
42	CV	31	SER	13.1
42	CV	75	ALA	13.1
9	BI	37	GLN	13.1
7	BG	46	ALA	13.1
27	CF	22	TYR	13.1
13	BM	45	ILE	13.0
9	AI	130	ARG	13.0
30	CJ	36	MET	13.0
30	DJ	133	ALA	13.0
27	CF	65	PRO	13.0
27	CF	79	ILE	13.0
30	DJ	115	ALA	12.9
30	DJ	9	VAL	12.9
42	CV	20	GLY	12.9
30	DJ	116	ASP	12.9
13	BM	2	ALA	12.9
19	BS	42	PRO	12.9
30	CJ	70	VAL	12.8
41	CU	55	VAL	12.8
27	CF	34	ILE	12.8
30	DJ	86	ILE	12.8
39	CS	27	ILE	12.8
29	CH	13	GLY	12.8
30	DJ	135	SER	12.7
28	CG	102	VAL	12.7
7	BG	65	ALA	12.7
27	CF	8	TYR	12.6
27	CF	13	VAL	12.6
30	CJ	14	ALA	12.6
30	CJ	41	ALA	12.6
19	BS	13	LEU	12.6
32	CL	111	LYS	12.6
13	BM	31	LYS	12.5
3	BC	193	TYR	12.5
30	CJ	65	ARG	12.5
27	CF	7	TYR	12.5
55	DI	128	THR	12.4
19	BS	30	PRO	12.4

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Mol	Chain	Res	Type	RSRZ
3	BC	29	PHE	12.3
10	BJ	87	LEU	12.3
30	CJ	51	LYS	12.3
10	BJ	26	VAL	12.3
19	BS	65	GLU	12.3
27	CF	154	ILE	12.3
30	CJ	109	ILE	12.3
41	CU	45	ALA	12.3
27	CF	12	VAL	12.3
30	DJ	28	LEU	12.2
10	BJ	100	ILE	12.2
30	DJ	47	ASP	12.2
30	CJ	120	ALA	12.2
26	CE	13	THR	12.2
19	BS	29	LYS	12.2
30	DJ	51	LYS	12.2
7	BG	52	GLN	12.1
19	BS	59	PRO	12.2
30	DJ	39	CYS	12.1
30	CJ	71	THR	12.1
13	BM	10	PRO	12.1
13	BM	22	ILE	12.1
28	CG	157	TYR	12.1
14	BN	8	ALA	12.1
3	BC	28	GLU	12.1
13	BM	113	ARG	12.1
36	CP	40	ILE	12.1
30	CJ	87	LYS	12.0
26	CE	121	VAL	12.0
46	CZ	33	ALA	12.0
30	CJ	119	GLY	12.0
2	AB	136	MET	12.0
33	CM	89	VAL	11.9
41	CU	53	VAL	11.9
27	CF	59	ALA	11.9
27	CF	93	GLY	11.9
27	CF	114	PHE	11.8
27	CF	75	ALA	11.8
30	CJ	138	LEU	11.8
42	CV	76	ALA	11.7
30	DJ	120	ALA	11.7
29	CH	139	PHE	11.7

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Mol	Chain	Res	Type	RSRZ
30	CJ	110	ALA	11.7
19	BS	28	LYS	11.7
7	AG	52	GLN	11.7
39	CS	50	GLY	11.7
26	CE	33	VAL	11.7
39	CS	51	VAL	11.6
10	BJ	86	ALA	11.6
19	BS	32	ARG	11.6
28	CG	33	LEU	11.6
28	CG	83	PHE	11.6
29	CH	15	LEU	11.6
9	BI	71	GLY	11.6
42	CV	32	GLY	11.6
30	DJ	58	VAL	11.6
2	BB	67	ILE	11.6
7	BG	129	GLU	11.5
30	DJ	137	GLY	11.5
43	CW	23	ALA	11.5
2	BB	215	GLY	11.5
7	BG	27	VAL	11.5
13	BM	108	THR	11.5
13	BM	36	ALA	11.5
26	CE	126	VAL	11.5
27	CF	37	ASN	11.4
29	DH	139	PHE	11.4
9	BI	130	ARG	11.4
19	BS	63	THR	11.4
13	BM	67	GLY	11.4
55	DI	104	ALA	11.4
14	BN	22	ALA	11.4
30	DJ	101	ILE	11.4
7	BG	45	SER	11.3
30	DJ	122	ILE	11.3
13	BM	46	SER	11.3
14	BN	27	LEU	11.3
41	CU	69	ARG	11.2
30	CJ	97	LYS	11.2
30	CJ	101	ILE	11.2
28	CG	11	VAL	11.2
30	DJ	107	GLN	11.2
13	BM	55	THR	11.2
30	DJ	62	TYR	11.2

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Mol	Chain	Res	Type	RSRZ
41	CU	71	GLY	11.2
36	CP	109	ALA	11.2
33	CM	82	LEU	11.2
14	BN	32	SER	11.2
13	AM	33	ILE	11.2
55	DI	127	ALA	11.2
41	CU	8	LEU	11.1
29	CH	104	THR	11.1
36	CP	117	PHE	11.1
7	BG	49	THR	11.1
25	CD	186	LEU	11.1
13	BM	35	ALA	11.1
55	DI	132	TYR	11.1
2	BB	64	LYS	11.1
27	CF	170	LEU	11.1
7	BG	75	VAL	11.1
14	BN	35	ASN	11.0
43	CW	58	SER	11.0
2	BB	32	PHE	11.0
36	CP	97	PHE	11.0
36	CP	101	GLY	11.0
14	BN	60	GLN	11.0
7	BG	61	ALA	11.0
22	CA	138	U	11.0
30	CJ	98	VAL	11.0
27	CF	111	ILE	11.0
41	CU	50	LEU	11.0
27	CF	147	ASP	11.0
9	BI	69	GLY	10.9
36	CP	21	LEU	10.9
27	CF	143	TYR	10.9
7	BG	150	ALA	10.9
27	CF	130	MET	10.9
29	DH	75	LEU	10.9
29	DH	126	GLY	10.9
30	DJ	102	SER	10.8
13	BM	97	VAL	10.8
19	BS	49	ILE	10.8
13	BM	65	VAL	10.8
16	BP	47	GLU	10.8
28	CG	165	ALA	10.8
7	BG	103	TRP	10.8

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Mol	Chain	Res	Type	RSRZ
16	BP	52	LEU	10.8
20	BT	36	TYR	10.8
19	BS	14	HIS	10.8
26	CE	15	SER	10.8
27	CF	83	TYR	10.7
3	BC	78	GLY	10.7
30	CJ	16	GLY	10.7
36	CP	19	GLN	10.7
27	CF	109	PRO	10.7
2	BB	186	ILE	10.7
13	BM	4	ILE	10.7
30	DJ	34	ASN	10.7
7	BG	44	TYR	10.7
27	CF	173	PHE	10.6
36	CP	22	GLY	10.6
33	CM	116	VAL	10.6
30	CJ	43	ASN	10.6
30	DJ	66	SER	10.6
7	BG	10	ARG	10.6
13	BM	26	GLY	10.6
27	CF	133	ARG	10.6
48	C1	34	SER	10.6
19	BS	51	VAL	10.6
27	CF	80	ARG	10.6
55	DI	124	ASP	10.6
16	BP	81	ALA	10.5
20	BT	81	ALA	10.5
33	CM	144	GLU	10.5
7	BG	88	PRO	10.5
30	DJ	45	LYS	10.5
9	BI	67	VAL	10.5
30	DJ	23	PRO	10.5
30	DJ	44	ALA	10.4
30	CJ	106	LEU	10.4
27	CF	38	MET	10.4
19	BS	76	PRO	10.4
28	CG	161	GLY	10.4
55	DI	136	ILE	10.4
30	CJ	114	ALA	10.4
13	AM	19	LEU	10.4
30	DJ	41	ALA	10.3
10	BJ	20	GLN	10.3

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Mol	Chain	Res	Type	RSRZ
33	CM	90	VAL	10.3
19	BS	40	ILE	10.3
28	CG	91	GLY	10.3
19	BS	48	THR	10.3
27	CF	151	GLY	10.2
26	CE	183	PHE	10.2
27	CF	95	ARG	10.2
34	CN	136	MET	10.2
17	BQ	83	VAL	10.2
27	CF	10	ASP	10.2
33	CM	117	THR	10.2
28	CG	169	VAL	10.2
36	CP	4	LYS	10.2
27	CF	115	ARG	10.2
28	CG	150	ALA	10.2
41	CU	74	ILE	10.2
13	BM	23	TYR	10.2
13	BM	89	LEU	10.2
17	BQ	78	VAL	10.1
7	BG	77	SER	10.1
30	DJ	30	GLN	10.1
55	DI	40	GLU	10.1
7	BG	132	GLY	10.1
13	BM	62	LYS	10.1
41	CU	10	VAL	10.1
27	CF	104	ILE	10.1
27	CF	107	ALA	10.1
35	CO	76	VAL	10.0
29	CH	130	VAL	10.0
36	CP	100	HIS	10.0
49	D2	5	ILE	10.0
27	CF	112	ARG	10.0
36	CP	103	VAL	10.0
27	CF	103	LEU	10.0
7	BG	17	LYS	9.9
13	AM	5	ALA	9.9
27	CF	171	ALA	9.9
29	DH	63	ALA	9.9
14	BN	41	ARG	9.9
42	CV	40	ASN	9.9
2	BB	130	THR	9.9
29	DH	80	ILE	9.9

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Mol	Chain	Res	Type	RSRZ
6	BF	80	PHE	9.9
30	CJ	28	LEU	9.9
44	CX	32	LEU	9.9
30	DJ	14	ALA	9.9
25	CD	74	GLU	9.9
13	BM	61	ALA	9.9
7	BG	85	TYR	9.9
55	DI	113	PHE	9.9
7	BG	80	VAL	9.9
36	CP	39	VAL	9.9
51	C4	58	VAL	9.9
29	CH	14	SER	9.9
10	BJ	99	GLN	9.9
14	BN	37	SER	9.8
14	BN	56	SER	9.8
30	CJ	117	MET	9.8
27	CF	68	THR	9.8
13	BM	7	ILE	9.8
26	CE	190	ALA	9.8
50	C3	36	ALA	9.8
7	BG	72	THR	9.8
9	BI	48	VAL	9.8
13	BM	64	VAL	9.8
28	CG	92	VAL	9.8
30	CJ	96	ASP	9.8
7	BG	83	SER	9.8
33	CM	79	LEU	9.8
7	BG	15	ASP	9.8
30	DJ	131	GLY	9.8
42	CV	63	ALA	9.8
28	CG	84	THR	9.8
7	BG	8	GLY	9.7
28	CG	2	SER	9.7
27	CF	105	THR	9.7
30	CJ	15	ALA	9.7
27	CF	35	THR	9.7
49	C2	36	LEU	9.7
13	BM	63	PHE	9.7
42	CV	35	ILE	9.7
7	BG	73	VAL	9.7
27	CF	39	GLY	9.7
26	CE	172	ALA	9.7

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Mol	Chain	Res	Type	RSRZ
14	BN	24	ARG	9.6
30	CJ	118	THR	9.6
5	BE	99	ALA	9.6
29	CH	10	ALA	9.6
12	BL	16	VAL	9.6
7	BG	125	SER	9.6
44	CX	63	ALA	9.6
46	CZ	63	ALA	9.6
27	CF	6	ASP	9.6
30	DJ	95	LYS	9.6
30	CJ	66	SER	9.6
2	AB	117	LEU	9.6
28	CG	80	THR	9.6
45	CY	20	HIS	9.6
12	AL	124	ALA	9.6
10	AJ	6	ILE	9.5
28	CG	45	HIS	9.5
30	DJ	19	ASN	9.5
9	BI	75	GLN	9.5
7	BG	64	VAL	9.5
42	CV	49	VAL	9.5
12	BL	15	LYS	9.5
28	CG	128	GLN	9.5
13	BM	37	ALA	9.5
27	CF	45	ALA	9.5
28	CG	58	TYR	9.5
30	CJ	121	ASP	9.5
52	C5	21	GLY	9.5
30	DJ	141	GLU	9.5
33	CM	114	GLY	9.5
55	DI	105	LYS	9.4
44	CX	22	GLY	9.4
2	BB	16	PHE	9.4
28	CG	103	ILE	9.4
13	BM	71	ARG	9.4
9	BI	68	LYS	9.4
13	BM	58	ASP	9.4
30	CJ	95	LYS	9.4
25	CD	185	ASN	9.4
30	DJ	43	ASN	9.4
19	BS	3	ARG	9.4
55	DI	118	ILE	9.4

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Mol	Chain	Res	Type	RSRZ
19	BS	23	VAL	9.4
13	BM	93	ARG	9.4
30	DJ	37	GLU	9.4
30	DJ	92	LYS	9.4
27	CF	157	THR	9.4
30	CJ	113	LYS	9.4
30	DJ	27	ALA	9.3
13	BM	48	LEU	9.3
2	AB	60	ILE	9.3
41	CU	47	VAL	9.3
7	BG	112	GLY	9.3
41	CU	51	PHE	9.3
29	DH	81	ALA	9.3
2	AB	111	ILE	9.3
13	BM	94	GLY	9.3
14	BN	4	GLN	9.3
9	BI	127	PHE	9.3
3	BC	37	PHE	9.3
19	AS	5	LEU	9.3
13	BM	17	ILE	9.3
39	CS	63	VAL	9.3
41	CU	43	ILE	9.3
55	DI	35	VAL	9.3
30	CJ	84	ALA	9.3
13	BM	29	ARG	9.3
28	CG	156	PRO	9.3
41	CU	73	ARG	9.3
28	CG	82	GLY	9.3
42	CV	73	PHE	9.2
46	CZ	5	GLU	9.2
22	CA	1067	A	9.2
13	BM	68	ASP	9.2
13	BM	74	SER	9.2
30	CJ	50	GLU	9.2
55	DI	126	LEU	9.2
28	CG	78	GLY	9.2
46	CZ	30	MET	9.2
20	BT	80	THR	9.2
27	CF	86	GLY	9.2
13	BM	90	ARG	9.2
30	DJ	12	GLN	9.2
19	BS	18	LYS	9.2

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Mol	Chain	Res	Type	RSRZ
48	C1	54	VAL	9.2
7	AG	5	ARG	9.2
42	CV	21	LYS	9.2
2	BB	226	SER	9.2
16	AP	45	GLU	9.2
17	BQ	82	ALA	9.1
30	CJ	79	LEU	9.1
46	CZ	60	LYS	9.1
26	CE	8	ALA	9.1
28	CG	76	VAL	9.1
30	CJ	24	VAL	9.1
7	BG	145	ALA	9.1
12	BL	124	ALA	9.1
30	CJ	112	THR	9.1
13	BM	9	ILE	9.1
19	BS	24	GLU	9.1
27	CF	43	ALA	9.1
30	CJ	94	ASN	9.1
35	CO	119	SER	9.1
40	CT	37	THR	9.1
27	CF	138	PHE	9.1
13	BM	43	VAL	9.0
27	CF	108	VAL	9.0
2	AB	225	ARG	9.0
10	BJ	38	GLY	9.0
27	CF	135	GLN	9.0
10	BJ	28	THR	9.0
46	CZ	15	ASN	9.0
29	DH	146	VAL	9.0
10	BJ	8	ILE	9.0
27	CF	142	ASP	9.0
19	BS	57	HIS	9.0
2	BB	139	ARG	9.0
30	DJ	21	SER	9.0
36	CP	110	ALA	9.0
42	CV	43	LYS	8.9
55	DI	119	PRO	8.9
19	BS	64	ASP	8.9
46	CZ	22	LEU	8.9
10	BJ	36	VAL	8.9
42	CV	38	GLY	8.9
55	DI	21	GLY	8.9

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Mol	Chain	Res	Type	RSRZ
41	CU	6	ARG	8.9
9	BI	39	PHE	8.9
16	BP	80	LYS	8.9
9	BI	57	MET	8.9
35	CO	63	ARG	8.9
36	CP	61	GLN	8.9
22	CA	1175	A	8.9
55	DI	50	VAL	8.9
19	BS	17	LYS	8.9
7	BG	102	ARG	8.9
22	CA	613	A	8.9
30	DJ	78	VAL	8.9
55	DI	94	ARG	8.9
30	CJ	83	ALA	8.9
6	BF	54	LEU	8.9
7	BG	118	LEU	8.9
29	DH	76	GLU	8.9
3	BC	192	THR	8.8
7	BG	84	THR	8.8
14	BN	29	ALA	8.8
42	CV	80	ALA	8.8
47	C0	2	ALA	8.8
26	CE	118	LEU	8.8
27	CF	77	PHE	8.8
2	BB	219	ALA	8.8
28	CG	77	ILE	8.8
30	CJ	129	ILE	8.8
10	BJ	90	LEU	8.8
19	BS	47	LEU	8.8
27	CF	31	VAL	8.8
13	BM	12	HIS	8.8
9	AI	90	TYR	8.8
28	CG	9	VAL	8.8
36	CP	54	VAL	8.8
28	CG	68	ALA	8.8
28	CG	112	PRO	8.8
29	CH	105	ALA	8.8
30	DJ	65	ARG	8.8
10	BJ	76	ILE	8.7
26	CE	143	LEU	8.7
42	CV	71	ALA	8.7
51	C4	52	LYS	8.7

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Mol	Chain	Res	Type	RSRZ
10	BJ	88	MET	8.7
22	CA	1068	G	8.7
29	DH	65	ALA	8.7
30	CJ	46	THR	8.7
13	BM	82	ASP	8.7
7	BG	131	LYS	8.7
10	BJ	91	ASP	8.7
14	BN	51	LEU	8.7
26	CE	104	ALA	8.7
28	CG	51	THR	8.7
9	BI	42	GLU	8.7
41	CU	89	GLU	8.7
26	CE	19	PHE	8.7
55	DI	101	LYS	8.6
13	BM	69	LEU	8.6
13	BM	79	ARG	8.6
13	BM	86	TYR	8.6
36	CP	60	GLU	8.6
39	CS	49	ILE	8.6
30	DJ	132	THR	8.6
42	CV	77	THR	8.6
30	CJ	85	GLY	8.6
20	BT	9	LYS	8.6
29	DH	105	ALA	8.6
30	CJ	124	ALA	8.6
30	DJ	121	ASP	8.6
26	CE	136	GLN	8.6
30	CJ	115	ALA	8.6
10	BJ	74	VAL	8.6
10	BJ	97	ASP	8.6
27	CF	122	PHE	8.5
41	CU	67	VAL	8.5
13	AM	114	LYS	8.5
7	BG	135	VAL	8.5
36	CP	49	VAL	8.5
31	CK	97	PRO	8.5
10	BJ	17	LEU	8.5
27	CF	50	LEU	8.5
2	BB	30	PHE	8.5
19	BS	45	ILE	8.5
37	CQ	4	ILE	8.5
35	CO	100	CYS	8.5

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Mol	Chain	Res	Type	RSRZ
9	BI	118	LEU	8.5
36	CP	78	VAL	8.5
41	CU	57	VAL	8.5
29	CH	47	PHE	8.5
38	CR	101	PHE	8.5
7	BG	76	LYS	8.5
27	CF	25	VAL	8.5
49	C2	53	LYS	8.5
14	BN	15	ALA	8.4
27	CF	119	ALA	8.4
36	CP	62	LEU	8.4
10	BJ	34	ALA	8.4
13	BM	34	LEU	8.4
2	AB	139	ARG	8.4
14	BN	39	GLU	8.4
2	BB	12	ALA	8.4
30	CJ	86	ILE	8.4
55	DI	100	ALA	8.4
42	CV	41	LEU	8.4
34	CN	21	ALA	8.4
2	BB	31	ILE	8.4
30	DJ	91	GLY	8.4
28	CG	17	VAL	8.4
9	BI	126	GLN	8.4
29	DH	77	THR	8.4
55	DI	47	GLU	8.4
7	BG	86	GLN	8.4
29	DH	44	ILE	8.3
30	DJ	24	VAL	8.3
42	CV	6	ARG	8.3
13	BM	8	ASN	8.3
27	CF	174	ASP	8.3
33	CM	121	THR	8.3
30	DJ	90	SER	8.3
46	CZ	40	SER	8.3
33	CM	81	ASP	8.3
25	CD	8	LYS	8.3
27	CF	96	MET	8.3
29	DH	138	VAL	8.3
20	BT	77	ALA	8.3
30	CJ	18	ALA	8.3
32	CL	88	ASN	8.2

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Mol	Chain	Res	Type	RSRZ
10	BJ	92	LEU	8.2
33	CM	73	ILE	8.2
34	CN	41	LEU	8.2
9	BI	66	THR	8.2
30	CJ	82	LYS	8.2
27	CF	11	GLU	8.2
26	CE	11	ALA	8.2
13	BM	25	VAL	8.2
7	BG	78	ARG	8.2
46	CZ	58	ASN	8.2
30	DJ	46	THR	8.2
19	BS	71	LEU	8.2
46	CZ	56	LEU	8.2
49	C2	47	VAL	8.2
29	DH	137	GLU	8.2
32	CL	89	ASN	8.2
3	BC	122	SER	8.2
17	BQ	74	THR	8.2
28	CG	105	LEU	8.2
41	CU	72	GLN	8.2
55	DI	38	MET	8.2
33	CM	124	GLY	8.2
2	BB	4	VAL	8.2
36	CP	71	ALA	8.1
7	BG	57	SER	8.1
33	CM	85	VAL	8.1
44	CX	33	ALA	8.1
14	BN	53	ARG	8.1
2	BB	57	LEU	8.1
36	CP	47	VAL	8.1
36	CP	82	ALA	8.1
10	BJ	101	SER	8.1
2	BB	117	LEU	8.1
14	AN	51	LEU	8.1
9	BI	44	ALA	8.1
33	CM	108	ALA	8.1
30	CJ	78	VAL	8.1
42	CV	74	ASN	8.1
19	BS	80	TYR	8.1
9	BI	26	GLY	8.1
30	CJ	88	SER	8.0
14	BN	40	ASP	8.0

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Mol	Chain	Res	Type	RSRZ
20	BT	49	LYS	8.0
30	CJ	100	LYS	8.0
25	CD	14	ILE	8.0
25	CD	96	ILE	8.0
27	CF	27	GLN	8.0
10	BJ	40	ILE	8.0
46	DZ	63	ALA	8.0
10	BJ	102	LEU	8.0
19	BS	16	LEU	8.0
26	CE	173	THR	8.0
27	CF	99	PHE	8.0
28	CG	132	VAL	8.0
42	CV	59	VAL	8.0
38	CR	15	LYS	8.0
42	CV	60	GLU	8.0
36	CP	64	TYR	8.0
29	CH	140	ALA	8.0
29	DH	147	VAL	7.9
20	BT	51	PHE	7.9
2	AB	7	ARG	7.9
36	CP	20	GLU	7.9
30	CJ	55	ILE	7.9
51	C4	22	PHE	7.9
30	CJ	89	GLY	7.9
36	CP	12	THR	7.9
28	CG	69	ARG	7.9
55	DI	71	CYS	7.9
27	CF	91	LEU	7.9
29	CH	3	VAL	7.9
30	DJ	15	ALA	7.9
42	CV	98	SER	7.9
26	CE	138	LEU	7.9
30	DJ	134	ARG	7.9
7	BG	104	ILE	7.8
17	BQ	70	THR	7.8
27	CF	137	ILE	7.8
28	CG	121	ILE	7.8
37	CQ	43	PHE	7.8
19	BS	31	LEU	7.8
29	CH	17	ASP	7.8
55	DI	64	VAL	7.8
19	BS	21	LYS	7.8

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Mol	Chain	Res	Type	RSRZ
30	DJ	97	LYS	7.8
36	CP	50	ALA	7.8
46	CZ	37	LEU	7.8
13	AM	3	ARG	7.8
30	DJ	124	ALA	7.8
2	BB	123	ASP	7.8
26	CE	3	LEU	7.8
40	CT	110	ARG	7.8
7	BG	94	VAL	7.8
26	CE	1	MET	7.8
1	BA	1031	C	7.8
3	BC	146	ALA	7.8
10	BJ	21	ALA	7.8
27	CF	85	ILE	7.8
2	AB	57	LEU	7.8
30	CJ	39	CYS	7.8
25	CD	86	GLU	7.8
55	DI	27	VAL	7.8
33	CM	142	ILE	7.8
51	C4	20	GLY	7.7
10	BJ	93	ALA	7.7
20	BT	85	LYS	7.7
27	CF	118	SER	7.7
30	CJ	136	MET	7.7
7	BG	124	LEU	7.7
6	BF	70	VAL	7.7
26	CE	14	VAL	7.7
43	CW	34	LYS	7.7
55	DI	76	PHE	7.7
19	BS	50	ALA	7.7
13	AM	4	ILE	7.7
3	BC	138	VAL	7.7
29	CH	108	VAL	7.7
48	C1	3	VAL	7.7
13	AM	9	ILE	7.7
28	CG	131	ILE	7.7
39	CS	37	GLU	7.7
9	BI	54	LEU	7.7
27	CF	16	LEU	7.7
29	CH	142	VAL	7.6
29	DH	124	THR	7.6
30	CJ	128	SER	7.6

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Mol	Chain	Res	Type	RSRZ
41	CU	46	ALA	7.6
7	BG	25	LYS	7.6
27	CF	66	LEU	7.6
2	BB	210	VAL	7.6
13	BM	60	VAL	7.6
14	AN	30	ILE	7.6
20	BT	46	ALA	7.6
19	BS	41	PHE	7.6
55	DI	66	GLY	7.6
30	CJ	126	THR	7.6
39	CS	43	ASN	7.6
41	CU	70	HIS	7.6
27	CF	92	ARG	7.6
29	CH	107	GLY	7.6
16	BP	45	GLU	7.6
35	CO	28	LEU	7.6
30	CJ	53	LEU	7.6
32	CL	91	SER	7.6
2	BB	217	VAL	7.6
34	CN	131	VAL	7.6
43	CW	92	VAL	7.6
9	BI	129	LYS	7.6
2	AB	135	LEU	7.6
13	AM	48	LEU	7.6
13	BM	19	LEU	7.6
29	DH	107	GLY	7.5
2	BB	80	VAL	7.5
27	CF	51	ASP	7.5
1	BA	1032	G	7.5
9	BI	21	ILE	7.5
29	CH	20	ASN	7.5
30	CJ	92	LYS	7.5
27	CF	56	ASP	7.5
29	CH	144	VAL	7.5
36	CP	80	GLU	7.5
22	CA	1093	G	7.5
2	BB	63	ARG	7.5
55	DI	120	ALA	7.5
27	CF	129	SER	7.5
29	CH	136	SER	7.5
27	CF	102	ARG	7.5
13	BM	11	ASP	7.5

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Mol	Chain	Res	Type	RSRZ
39	CS	32	THR	7.5
40	CT	36	LEU	7.5
33	CM	15	ALA	7.5
7	AG	20	SER	7.5
44	CX	83	GLU	7.5
3	BC	145	GLY	7.5
29	DH	143	ILE	7.5
28	CG	101	ASN	7.5
20	BT	34	LYS	7.5
42	CV	27	ASN	7.5
25	CD	25	THR	7.5
28	CG	171	THR	7.5
27	CF	15	LYS	7.5
28	CG	107	LEU	7.4
7	BG	148	ASN	7.4
2	BB	11	LYS	7.4
22	CA	1535	A	7.4
44	CX	46	HIS	7.4
1	AA	1030	U	7.4
27	CF	33	LYS	7.4
46	CZ	4	LYS	7.4
40	CT	66	ILE	7.4
42	CV	33	LYS	7.4
26	CE	189	THR	7.4
42	CV	17	LYS	7.4
27	CF	2	ALA	7.4
31	CK	55	ILE	7.4
26	CE	134	LEU	7.4
42	CV	48	PRO	7.4
30	CJ	131	GLY	7.4
55	DI	91	ALA	7.4
14	BN	55	SER	7.4
30	DJ	8	TYR	7.4
27	CF	164	GLU	7.4
30	DJ	50	GLU	7.4
41	CU	2	ILE	7.4
10	BJ	27	GLU	7.3
25	CD	95	SER	7.3
27	CF	153	ASP	7.3
41	CU	37	ASP	7.3
30	CJ	45	LYS	7.3
29	CH	74	ALA	7.3

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Mol	Chain	Res	Type	RSRZ
7	BG	81	GLY	7.3
55	DI	82	ILE	7.3
7	AG	49	THR	7.3
29	CH	12	LEU	7.3
21	AU	3	VAL	7.3
26	CE	28	VAL	7.3
55	DI	92	ALA	7.3
36	CP	67	ASN	7.3
30	CJ	54	PRO	7.3
2	AB	49	MET	7.3
14	BN	73	PHE	7.3
21	AU	12	PHE	7.3
30	CJ	133	ALA	7.3
43	CW	67	GLY	7.3
34	CN	22	GLN	7.3
16	AP	47	GLU	7.3
36	CP	41	ALA	7.3
27	CF	132	VAL	7.3
41	CU	16	VAL	7.3
19	BS	37	ARG	7.3
27	CF	14	LYS	7.3
28	CG	25	THR	7.3
26	CE	77	ILE	7.3
26	CE	175	ILE	7.3
55	DI	75	ALA	7.2
44	CX	79	PHE	7.2
10	BJ	98	VAL	7.2
28	CG	79	VAL	7.2
7	AG	48	GLU	7.2
7	BG	109	ARG	7.2
13	BM	101	ARG	7.2
13	BM	24	GLY	7.2
10	BJ	96	VAL	7.2
33	CM	93	ASN	7.2
41	DU	1	MET	7.2
16	AP	81	ALA	7.2
30	CJ	104	ALA	7.2
19	AS	41	PHE	7.2
34	CN	60	GLN	7.2
30	CJ	77	ALA	7.2
26	CE	165	HIS	7.2
55	DI	45	GLY	7.2

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Mol	Chain	Res	Type	RSRZ
14	BN	75	ARG	7.2
29	DH	61	VAL	7.2
28	CG	106	SER	7.2
40	CT	68	ASP	7.2
36	CP	116	GLN	7.1
1	BA	1021	A	7.1
42	CV	85	PHE	7.1
30	CJ	40	LYS	7.1
30	DJ	128	SER	7.1
9	BI	110	GLN	7.1
30	CJ	49	ILE	7.1
14	AN	46	LEU	7.1
30	DJ	126	THR	7.1
53	DA	2110	G	7.1
1	BA	211	G	7.1
36	CP	63	LYS	7.1
2	BB	126	PHE	7.1
30	CJ	137	GLY	7.1
3	BC	53	SER	7.1
7	BG	20	SER	7.1
2	AB	6	MET	7.1
7	BG	107	ALA	7.1
28	CG	59	ALA	7.1
30	DJ	105	GLN	7.1
41	CU	68	LYS	7.1
3	BC	107	ARG	7.1
7	BG	43	VAL	7.0
9	AI	129	LYS	7.0
30	DJ	123	GLU	7.0
29	CH	135	HIS	7.0
26	CE	153	LEU	7.0
25	CD	73	VAL	7.0
32	CL	110	GLU	7.0
7	BG	18	PHE	7.0
29	CH	145	ASN	7.0
7	BG	58	GLU	7.0
26	CE	122	GLU	7.0
7	BG	111	ARG	7.0
30	DJ	113	LYS	7.0
25	CD	92	VAL	7.0
26	CE	199	MET	7.0
34	CN	59	ARG	7.0

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Mol	Chain	Res	Type	RSRZ
27	CF	90	THR	7.0
2	AB	42	ASN	7.0
29	DH	127	GLU	7.0
14	BN	16	LEU	7.0
42	DV	52	LEU	7.0
2	AB	14	VAL	7.0
14	BN	14	VAL	7.0
27	CF	162	SER	7.0
3	AC	82	GLU	7.0
9	BI	119	ARG	7.0
30	DJ	59	ILE	6.9
25	CD	10	GLY	6.9
41	CU	34	VAL	6.9
9	BI	14	SER	6.9
44	CX	50	ASN	6.9
42	CV	101	GLU	6.9
31	CK	128	ASN	6.9
33	CM	61	LEU	6.9
48	C1	44	THR	6.9
55	DI	67	THR	6.9
19	BS	19	VAL	6.9
28	CG	125	CYS	6.9
33	CM	122	VAL	6.9
9	AI	53	GLU	6.9
27	CF	20	PHE	6.9
3	BC	62	LYS	6.9
39	CS	52	PRO	6.9
31	CK	127	GLY	6.9
35	CO	62	ASN	6.9
42	CV	96	PHE	6.9
3	BC	181	ASP	6.9
22	CA	1536	C	6.9
15	BO	89	ARG	6.9
39	CS	38	VAL	6.9
2	AB	12	ALA	6.9
17	BQ	50	ASN	6.9
27	CF	81	GLN	6.9
52	C5	6	SER	6.9
30	DJ	81	LYS	6.9
2	BB	74	ARG	6.8
11	BK	16	VAL	6.8
10	BJ	45	ARG	6.8

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Mol	Chain	Res	Type	RSRZ
31	CK	137	PRO	6.8
28	CG	148	LEU	6.8
39	CS	88	GLY	6.8
44	CX	47	ALA	6.8
33	CM	78	ARG	6.8
9	AI	88	MET	6.8
17	BQ	17	MET	6.8
2	BB	33	GLY	6.8
30	CJ	37	GLU	6.8
14	AN	36	ALA	6.8
21	AU	53	VAL	6.8
32	CL	35	VAL	6.8
10	BJ	75	ASP	6.8
42	CV	19	LYS	6.8
29	DH	125	THR	6.8
26	CE	129	PRO	6.8
36	CP	25	ARG	6.8
42	CV	82	ARG	6.8
55	DI	72	LEU	6.8
10	AJ	26	VAL	6.8
5	BE	23	LYS	6.8
36	CP	51	ALA	6.8
46	CZ	36	GLN	6.8
7	BG	144	MET	6.8
20	BT	3	ASN	6.8
24	CC	64	ILE	6.8
26	CE	149	ILE	6.8
33	CM	100	ILE	6.8
37	CQ	92	VAL	6.8
40	CT	107	VAL	6.8
3	BC	98	PRO	6.8
29	CH	16	GLY	6.8
29	DH	104	THR	6.8
27	CF	48	LYS	6.8
9	BI	6	TYR	6.8
27	CF	177	PHE	6.8
27	DF	83	TYR	6.8
22	CA	1537	G	6.7
33	CM	19	LEU	6.7
22	CA	281	C	6.7
36	CP	76	LYS	6.7
29	DH	142	VAL	6.7

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Mol	Chain	Res	Type	RSRZ
10	BJ	85	ASP	6.7
37	CQ	85	SER	6.7
27	CF	52	ASN	6.7
27	CF	17	MET	6.7
36	CP	106	LEU	6.7
21	AU	2	PRO	6.7
53	DA	2163	A	6.7
52	C5	33	HIS	6.7
30	DJ	108	GLU	6.7
46	CZ	59	GLU	6.7
13	AM	36	ALA	6.7
29	DH	95	GLY	6.7
11	BK	55	SER	6.7
36	CP	56	LYS	6.7
19	AS	11	ILE	6.7
33	CM	83	ALA	6.7
2	BB	69	PHE	6.7
28	CG	86	LYS	6.7
2	AB	58	ASN	6.7
40	CT	39	THR	6.7
53	DA	2121	G	6.7
42	CV	5	ILE	6.7
30	DJ	31	GLN	6.7
36	CP	111	ARG	6.7
39	CS	22	LEU	6.7
41	CU	60	THR	6.7
26	CE	98	LYS	6.7
14	AN	39	GLU	6.7
29	DH	56	ALA	6.7
14	BN	49	GLN	6.6
2	AB	214	LEU	6.6
6	BF	79	ARG	6.6
18	AR	73	ARG	6.6
41	CU	62	VAL	6.6
3	BC	77	ILE	6.6
50	C3	1	MET	6.6
29	DH	135	HIS	6.6
26	CE	140	ASP	6.6
2	AB	90	PHE	6.6
33	CM	3	LEU	6.6
3	BC	56	VAL	6.6
10	BJ	67	ILE	6.6

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Mol	Chain	Res	Type	RSRZ
29	CH	143	ILE	6.6
10	BJ	56	HIS	6.6
14	BN	17	ALA	6.6
19	BS	44	MET	6.6
27	CF	110	ARG	6.6
22	CA	1870	C	6.6
14	AN	49	GLN	6.6
7	BG	105	VAL	6.6
28	CG	46	ALA	6.6
40	CT	92	ARG	6.6
32	CL	112	PHE	6.6
33	CM	107	PHE	6.6
20	BT	86	LEU	6.6
46	CZ	21	LEU	6.6
1	BA	1020	G	6.6
13	BM	99	GLY	6.6
26	CE	150	THR	6.6
33	CM	4	ASN	6.6
27	CF	175	PHE	6.6
9	BI	34	SER	6.6
26	CE	133	LEU	6.6
10	AJ	93	ALA	6.6
9	BI	116	VAL	6.6
35	CO	29	VAL	6.6
38	CR	39	VAL	6.6
10	BJ	95	GLY	6.6
36	CP	75	GLY	6.6
39	CS	59	ILE	6.6
14	AN	37	SER	6.5
3	BC	102	ASN	6.5
55	DI	97	LYS	6.5
36	CP	53	THR	6.5
38	CR	71	GLN	6.5
17	BQ	61	ILE	6.5
55	DI	73	LYS	6.5
46	CZ	32	ALA	6.5
55	DI	96	PHE	6.5
17	AQ	83	VAL	6.5
39	CS	20	VAL	6.5
53	DA	1172	C	6.5
20	BT	24	ARG	6.5
2	BB	65	GLY	6.5

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Mol	Chain	Res	Type	RSRZ
14	BN	19	LYS	6.5
7	BG	6	VAL	6.5
27	CF	158	THR	6.5
28	CG	49	THR	6.5
24	CC	27	GLY	6.5
43	CW	33	GLY	6.5
14	BN	2	ALA	6.5
42	CV	24	LYS	6.5
55	DI	22	ALA	6.5
55	DI	107	GLU	6.5
19	BS	43	ASN	6.5
26	CE	20	GLY	6.5
19	BS	56	GLN	6.5
6	AF	97	THR	6.4
30	CJ	48	SER	6.4
9	AI	54	LEU	6.4
48	C1	39	LEU	6.4
33	CM	120	VAL	6.4
47	C0	55	VAL	6.4
9	BI	7	TYR	6.4
14	BN	20	TYR	6.4
28	CG	170	ARG	6.4
42	CV	58	ILE	6.4
36	CP	29	HIS	6.4
2	BB	206	ALA	6.4
27	CF	49	LEU	6.4
15	BO	15	PHE	6.4
43	CW	60	VAL	6.4
41	CU	88	LYS	6.4
20	BT	50	ALA	6.4
35	CO	77	ALA	6.4
1	BA	1030	U	6.4
10	BJ	52	LEU	6.4
2	BB	198	PHE	6.4
7	BG	54	SER	6.4
14	BN	82	ILE	6.4
30	CJ	135	SER	6.4
40	CT	54	ALA	6.4
36	CP	99	TYR	6.4
10	BJ	80	THR	6.4
33	CM	102	GLY	6.4
37	CQ	25	THR	6.4

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Mol	Chain	Res	Type	RSRZ
3	BC	80	LYS	6.4
41	CU	91	GLN	6.4
2	BB	225	ARG	6.4
3	BC	27	LYS	6.4
10	BJ	6	ILE	6.4
13	BM	44	LYS	6.4
27	CF	18	THR	6.4
29	DH	123	ARG	6.4
46	CZ	29	ARG	6.4
27	CF	149	VAL	6.4
29	CH	115	VAL	6.4
36	CP	3	LYS	6.4
33	CM	137	ALA	6.4
36	CP	57	ALA	6.4
30	DJ	20	PRO	6.4
10	BJ	37	ARG	6.3
52	C5	12	ARG	6.3
27	CF	47	LYS	6.3
2	AB	10	LEU	6.3
10	BJ	33	GLY	6.3
30	DJ	75	PRO	6.3
35	CO	9	GLN	6.3
27	CF	141	ILE	6.3
18	BR	20	GLU	6.3
13	BM	81	MET	6.3
26	CE	147	LEU	6.3
20	BT	41	ALA	6.3
25	CD	71	ALA	6.3
9	AI	58	VAL	6.3
30	CJ	130	GLU	6.3
9	BI	43	THR	6.3
13	BM	33	ILE	6.3
36	CP	69	ASP	6.3
46	CZ	10	SER	6.3
30	CJ	93	PRO	6.3
50	C3	42	LEU	6.3
41	CU	58	VAL	6.3
33	CM	80	SER	6.3
19	AS	13	LEU	6.3
36	CP	70	ALA	6.3
14	BN	38	ASP	6.3
19	BS	62	VAL	6.3

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Mol	Chain	Res	Type	RSRZ
29	CH	9	VAL	6.3
26	CE	2	GLU	6.3
29	CH	141	LYS	6.3
55	DI	20	LYS	6.3
55	DI	134	GLU	6.3
3	BC	162	ILE	6.3
9	BI	27	LYS	6.3
36	CP	105	ALA	6.3
29	DH	134	VAL	6.3
30	DJ	61	VAL	6.3
2	BB	164	ILE	6.2
36	CP	85	LYS	6.2
55	DI	88	HIS	6.2
29	DH	52	ALA	6.2
43	CW	28	ALA	6.2
26	CE	5	LEU	6.2
41	CU	87	LEU	6.2
11	BK	65	VAL	6.2
7	BG	151	PHE	6.2
25	CD	184	ARG	6.2
33	CM	123	ARG	6.2
41	CU	76	ARG	6.2
43	CW	22	ALA	6.2
2	AB	114	LEU	6.2
7	BG	30	LEU	6.2
32	CL	68	GLY	6.2
7	BG	53	ARG	6.2
2	AB	31	ILE	6.2
27	CF	21	ASN	6.2
30	CJ	90	SER	6.2
29	CH	120	GLY	6.2
10	BJ	16	ARG	6.2
44	CX	55	ARG	6.2
29	DH	108	VAL	6.2
37	CQ	17	VAL	6.2
42	CV	83	VAL	6.2
26	CE	124	PHE	6.2
28	CG	20	ASN	6.2
28	CG	30	ASN	6.2
28	CG	13	ALA	6.2
42	CV	65	ILE	6.2
36	CP	83	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
7	AG	80	VAL	6.2
37	CQ	3	ASN	6.2
6	BF	66	ALA	6.2
26	CE	21	ARG	6.2
28	CG	65	ALA	6.2
13	BM	38	GLY	6.2
24	CC	242	LYS	6.2
27	CF	60	ILE	6.2
41	CU	36	LYS	6.2
2	BB	161	LEU	6.2
13	BM	95	LEU	6.2
7	BG	101	MET	6.2
20	BT	65	GLY	6.2
2	BB	82	ASP	6.1
2	AB	35	ARG	6.1
35	CO	38	LEU	6.1
26	CE	37	ALA	6.1
30	DJ	104	ALA	6.1
40	CT	5	ALA	6.1
27	CF	84	PRO	6.1
2	BB	124	GLY	6.1
28	CG	41	VAL	6.1
27	CF	78	LYS	6.1
44	CX	75	LYS	6.1
53	DA	2168	G	6.1
2	BB	138	THR	6.1
29	DH	96	THR	6.1
53	DA	2165	C	6.1
55	DI	12	VAL	6.1
30	CJ	74	PRO	6.1
9	BI	20	PHE	6.1
55	DI	11	ILE	6.1
24	CC	237	GLY	6.1
43	CW	32	GLY	6.1
9	BI	62	ASP	6.1
26	CE	88	ARG	6.1
28	CG	104	ASN	6.1
26	CE	201	ALA	6.1
26	CE	4	VAL	6.1
39	CS	33	VAL	6.1
30	DJ	73	THR	6.1
2	BB	62	SER	6.1

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Mol	Chain	Res	Type	RSRZ
28	CG	116	GLN	6.1
37	CQ	7	GLN	6.1
26	CE	108	ILE	6.1
20	BT	7	ALA	6.1
49	C2	34	LEU	6.1
9	AI	29	VAL	6.1
29	CH	125	THR	6.1
19	BS	4	SER	6.0
19	BS	53	ASN	6.0
2	BB	136	MET	6.0
3	AC	75	ILE	6.0
10	AJ	86	ALA	6.0
10	BJ	39	PRO	6.0
29	CH	49	ALA	6.0
36	CP	65	THR	6.0
2	BB	213	TYR	6.0
9	AI	93	SER	6.0
49	C2	27	LYS	6.0
44	CX	60	PHE	6.0
29	CH	6	LEU	6.0
7	BG	56	LYS	6.0
18	AR	74	HIS	6.0
22	CA	1094	U	6.0
29	DH	83	LYS	6.0
7	BG	122	ASN	6.0
7	BG	23	LEU	6.0
27	CF	26	MET	6.0
6	BF	69	GLU	6.0
33	CM	106	GLU	6.0
39	CS	36	ALA	6.0
10	BJ	25	ILE	6.0
30	CJ	52	GLY	6.0
35	CO	59	SER	6.0
36	CP	114	GLY	6.0
30	CJ	134	ARG	6.0
49	C2	31	PRO	6.0
14	BN	44	ALA	6.0
29	DH	64	ALA	6.0
49	C2	52	ALA	6.0
9	AI	59	GLU	6.0
13	BM	52	GLN	6.0
13	AM	39	ILE	6.0

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Mol	Chain	Res	Type	RSRZ
8	BH	111	MET	6.0
24	CC	245	VAL	6.0
41	CU	85	VAL	6.0
5	BE	146	ASN	6.0
22	CA	1460	U	6.0
7	AG	83	SER	5.9
43	CW	82	TYR	5.9
28	CG	97	ALA	5.9
46	CZ	18	LEU	5.9
3	BC	85	GLU	5.9
3	BC	127	ARG	5.9
19	AS	8	GLY	5.9
2	AB	75	ALA	5.9
2	BB	116	ASP	5.9
55	DI	98	GLU	5.9
2	BB	128	LYS	5.9
3	BC	103	ILE	5.9
51	C4	15	LYS	5.9
3	BC	144	LEU	5.9
7	BG	4	ARG	5.9
42	CV	14	LEU	5.9
2	BB	14	VAL	5.9
37	CQ	73	VAL	5.9
40	CT	65	ASP	5.9
48	C1	35	GLY	5.9
28	CG	174	ALA	5.9
29	CH	63	ALA	5.9
49	C2	5	ILE	5.9
9	BI	63	LEU	5.9
27	CF	144	ASP	5.9
26	CE	196	VAL	5.9
10	BJ	94	ALA	5.9
27	CF	63	GLN	5.9
28	CG	122	THR	5.9
29	CH	77	THR	5.9
49	C2	48	ILE	5.9
14	AN	27	LEU	5.9
2	AB	221	VAL	5.9
25	CD	104	VAL	5.9
50	C3	33	ARG	5.9
26	CE	26	ALA	5.9
35	CO	111	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
28	CG	34	THR	5.9
26	CE	191	ASP	5.9
41	CU	79	ASP	5.9
25	CD	6	GLY	5.9
55	DI	43	LYS	5.9
11	BK	52	PHE	5.9
35	CO	27	SER	5.9
3	BC	196	ILE	5.9
13	BM	3	ARG	5.9
16	BP	54	LEU	5.9
51	C4	62	LEU	5.9
2	AB	47	VAL	5.9
42	CV	78	GLY	5.8
9	BI	45	ARG	5.8
33	CM	126	ARG	5.8
55	DI	133	GLU	5.8
42	CV	9	ASP	5.8
3	BC	39	VAL	5.8
10	BJ	32	THR	5.8
39	CS	96	VAL	5.8
30	CJ	111	GLN	5.8
35	CO	73	ASN	5.8
29	DH	132	PHE	5.8
14	BN	48	LEU	5.8
29	DH	140	ALA	5.8
36	CP	107	ALA	5.8
37	CQ	91	ALA	5.8
17	BQ	56	GLY	5.8
28	CG	57	GLY	5.8
19	BS	52	HIS	5.8
22	CA	885	C	5.8
6	BF	91	ARG	5.8
27	CF	94	GLU	5.8
36	CP	72	ALA	5.8
24	CC	34	LEU	5.8
37	CQ	23	GLY	5.8
51	C4	18	GLY	5.8
55	DI	49	GLY	5.8
53	DA	2166	U	5.8
27	CF	146	VAL	5.8
27	DF	113	ASP	5.8
52	C5	20	ASP	5.8

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Mol	Chain	Res	Type	RSRZ
53	DA	2146	C	5.8
9	BI	64	TYR	5.8
11	BK	73	ALA	5.8
40	CT	63	GLY	5.8
24	CC	33	LEU	5.8
37	CQ	16	ASP	5.8
47	C0	32	ILE	5.8
55	DI	26	VAL	5.8
43	CW	1	MET	5.8
2	BB	37	LYS	5.8
31	CK	131	ASN	5.8
2	BB	84	ALA	5.8
13	BM	18	ALA	5.8
51	C4	37	ALA	5.8
51	C4	60	ALA	5.8
9	BI	61	LEU	5.8
28	CG	85	LYS	5.8
29	CH	147	VAL	5.8
7	BG	123	GLU	5.7
2	AB	134	ALA	5.7
7	AG	46	ALA	5.7
6	BF	92	THR	5.7
40	CT	99	ARG	5.7
29	CH	132	PHE	5.7
42	CV	95	PHE	5.7
10	AJ	77	VAL	5.7
28	CG	113	VAL	5.7
1	BA	1024	G	5.7
5	BE	91	GLY	5.7
30	DJ	29	GLY	5.7
10	BJ	41	PRO	5.7
55	DI	135	ALA	5.7
9	BI	92	GLU	5.7
9	AI	28	ILE	5.7
10	BJ	10	LEU	5.7
13	AM	34	LEU	5.7
13	BM	56	LEU	5.7
29	CH	11	ASN	5.7
36	CP	35	ILE	5.7
10	BJ	89	ARG	5.7
35	CO	46	ARG	5.7
10	BJ	23	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
30	DJ	84	ALA	5.7
2	AB	130	THR	5.7
27	CF	64	LYS	5.7
28	CG	48	ASN	5.7
55	DI	52	MET	5.7
36	CP	38	GLN	5.7
27	CF	82	GLY	5.7
41	CU	11	LEU	5.7
9	BI	53	GLU	5.7
30	CJ	123	GLU	5.7
55	DI	114	GLU	5.7
29	CH	36	ALA	5.7
41	CU	49	LYS	5.7
1	BA	82	G	5.7
7	AG	151	PHE	5.7
7	AG	56	LYS	5.7
33	CM	91	ASP	5.7
36	CP	73	ALA	5.7
2	AB	74	ARG	5.7
28	CG	129	THR	5.7
9	BI	22	LYS	5.7
26	CE	137	LYS	5.7
33	CM	68	SER	5.7
13	AM	53	ILE	5.7
36	CP	108	ASP	5.7
26	CE	120	VAL	5.7
38	CR	10	ALA	5.6
1	BA	1025	U	5.6
13	BM	20	THR	5.6
16	BP	60	TRP	5.6
49	C2	29	THR	5.6
24	CC	120	VAL	5.6
30	DJ	70	VAL	5.6
22	CA	2121	G	5.6
33	CM	130	GLY	5.6
10	BJ	9	ARG	5.6
55	DI	87	GLU	5.6
22	CA	1095	A	5.6
43	CW	84	PRO	5.6
7	AG	13	LEU	5.6
2	BB	91	PHE	5.6
20	BT	32	ILE	5.6

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Mol	Chain	Res	Type	RSRZ
9	BI	16	ALA	5.6
17	BQ	79	VAL	5.6
20	BT	87	ALA	5.6
28	CG	98	VAL	5.6
43	CW	72	VAL	5.6
28	CG	164	TYR	5.6
36	CP	112	GLU	5.6
40	CT	67	ASP	5.6
10	BJ	31	ARG	5.6
29	CH	27	ARG	5.6
50	C3	22	MET	5.6
22	CA	228	C	5.6
24	CC	213	TRP	5.6
36	CP	18	LEU	5.6
9	AI	24	GLY	5.6
3	BC	42	TYR	5.6
26	CE	151	GLY	5.6
41	CU	28	ASN	5.6
43	CW	56	PHE	5.6
51	C4	2	PRO	5.6
14	AN	40	ASP	5.6
21	AU	57	ALA	5.6
2	BB	212	LEU	5.6
26	CE	200	LEU	5.6
27	CF	89	VAL	5.6
43	CW	48	MET	5.6
5	BE	157	ARG	5.5
19	AS	9	PRO	5.5
30	CJ	127	ARG	5.5
2	BB	156	GLY	5.5
22	CA	2184	A	5.5
29	DH	67	ALA	5.5
50	C3	37	LYS	5.5
46	CZ	14	LEU	5.5
38	CR	30	ARG	5.5
11	BK	74	VAL	5.5
30	DJ	35	ILE	5.5
36	CP	74	VAL	5.5
41	CU	4	GLU	5.5
7	BG	149	LYS	5.5
13	BM	57	ARG	5.5
36	CP	113	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
10	BJ	24	GLU	5.5
2	AB	215	GLY	5.5
2	BB	41	ILE	5.5
25	CD	158	GLY	5.5
42	CV	72	ILE	5.5
16	AP	46	LYS	5.5
4	AD	160	GLU	5.5
30	DJ	74	PRO	5.5
41	CU	15	HIS	5.5
50	C3	27	GLY	5.5
21	AU	4	ILE	5.5
10	BJ	35	GLN	5.5
26	CE	154	ASP	5.5
30	CJ	47	ASP	5.5
3	AC	168	TYR	5.5
9	BI	86	ALA	5.5
10	AJ	34	ALA	5.5
29	DH	59	ALA	5.5
7	BG	116	MET	5.5
22	CA	1107	G	5.5
28	CG	73	ASN	5.5
44	CX	52	GLY	5.5
9	AI	97	GLU	5.5
46	CZ	8	GLU	5.5
22	CA	2106	U	5.5
16	BP	78	VAL	5.5
26	CE	10	SER	5.5
39	CS	93	PHE	5.5
2	BB	216	ALA	5.5
10	BJ	29	ALA	5.5
20	AT	47	ALA	5.5
9	BI	65	ILE	5.4
33	CM	77	ILE	5.4
6	BF	20	GLY	5.4
22	CA	1092	C	5.4
30	DJ	136	MET	5.4
13	BM	76	SER	5.4
26	CE	157	LEU	5.4
2	BB	208	ARG	5.4
7	AG	91	VAL	5.4
11	AK	113	VAL	5.4
40	CT	45	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
2	BB	220	THR	5.4
11	BK	44	TRP	5.4
28	CG	167	GLU	5.4
4	BD	47	ARG	5.4
42	CV	22	ARG	5.4
2	BB	109	GLN	5.4
36	CP	115	LEU	5.4
42	CV	61	LYS	5.4
49	C2	30	LYS	5.4
26	CE	187	VAL	5.4
16	AP	82	ALA	5.4
19	BS	33	THR	5.4
29	CH	59	ALA	5.4
14	BN	69	ARG	5.4
9	AI	60	LYS	5.4
29	DH	66	ASN	5.4
17	BQ	75	LEU	5.4
26	CE	16	GLU	5.4
35	CO	85	PRO	5.4
2	BB	134	ALA	5.4
3	BC	104	ALA	5.4
24	CC	77	VAL	5.4
40	CT	3	THR	5.4
45	CY	67	VAL	5.4
48	C1	25	VAL	5.4
13	BM	53	ILE	5.4
29	CH	72	ILE	5.4
31	CK	1	MET	5.4
42	CV	86	ARG	5.4
47	C0	56	LYS	5.4
20	BT	43	ASP	5.4
1	BA	1534	A	5.4
2	BB	39	HIS	5.4
3	AC	78	GLY	5.4
28	CG	14	GLY	5.4
25	CD	187	LEU	5.4
29	DH	117	LEU	5.4
15	AO	17	ARG	5.4
36	CP	14	ALA	5.4
28	CG	166	ASP	5.4
1	AA	86	G	5.4
27	CF	178	ARG	5.4

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Mol	Chain	Res	Type	RSRZ
28	CG	95	ARG	5.4
2	BB	53	ALA	5.4
3	BC	167	TRP	5.4
22	CA	1087	G	5.4
30	DJ	60	THR	5.4
43	CW	6	ALA	5.4
44	CX	84	ALA	5.4
55	DI	48	ALA	5.4
2	AB	226	SER	5.3
9	BI	4	ASN	5.3
2	BB	111	ILE	5.3
17	BQ	55	ILE	5.3
43	CW	89	ILE	5.3
36	CP	88	LYS	5.3
19	BS	81	ARG	5.3
1	BA	1033	G	5.3
55	DI	89	PRO	5.3
27	CF	134	GLU	5.3
2	BB	218	ALA	5.3
11	BK	63	ALA	5.3
17	BQ	7	THR	5.3
29	DH	58	LEU	5.3
47	C0	24	LEU	5.3
20	BT	82	GLN	5.3
36	CP	66	GLY	5.3
42	CV	79	LYS	5.3
29	CH	131	SER	5.3
30	CJ	132	THR	5.3
33	CM	74	THR	5.3
31	CK	125	TYR	5.3
27	CF	74	VAL	5.3
34	CN	80	VAL	5.3
42	CV	70	VAL	5.3
9	BI	56	ASP	5.3
32	CL	115	ILE	5.3
35	CO	56	LYS	5.3
20	BT	84	ASN	5.3
46	CZ	20	ASN	5.3
26	CE	55	SER	5.3
30	DJ	83	ALA	5.3
7	BG	99	LEU	5.3
9	BI	52	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
35	CO	94	TYR	5.3
15	BO	11	ILE	5.3
11	BK	71	ALA	5.3
6	BF	31	GLY	5.3
41	CU	32	LEU	5.3
53	DA	2114	A	5.3
10	AJ	36	VAL	5.3
7	AG	18	PHE	5.3
8	AH	2	SER	5.3
6	BF	94	HIS	5.3
13	BM	54	ASP	5.3
25	CD	31	ALA	5.3
5	BE	10	GLU	5.3
31	CK	129	GLU	5.3
39	CS	46	GLU	5.3
14	BN	46	LEU	5.3
3	AC	39	VAL	5.2
17	BQ	81	LYS	5.2
1	BA	85	U	5.2
53	DA	2175	C	5.2
39	CS	26	ASP	5.2
27	CF	165	GLU	5.2
9	BI	50	GLN	5.2
9	BI	120	LYS	5.2
14	BN	23	LYS	5.2
22	CA	878	A	5.2
9	AI	63	LEU	5.2
28	CG	117	LEU	5.2
2	AB	123	ASP	5.2
17	BQ	20	SER	5.2
48	C1	46	ASP	5.2
1	BA	1361	G	5.2
22	CA	1171	G	5.2
22	CA	2169	A	5.2
11	AK	96	THR	5.2
16	BP	76	LYS	5.2
20	AT	50	ALA	5.2
30	DJ	112	THR	5.2
33	CM	71	ALA	5.2
48	C1	33	THR	5.2
9	BI	94	LEU	5.2
28	CG	74	SER	5.2

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Mol	Chain	Res	Type	RSRZ
28	CG	87	LEU	5.2
28	CG	153	ARG	5.2
41	CU	5	GLU	5.2
2	BB	7	ARG	5.2
7	BG	137	LYS	5.2
28	CG	172	LYS	5.2
2	BB	58	ASN	5.2
27	CF	23	ASN	5.2
26	CE	174	GLY	5.2
17	BQ	59	VAL	5.2
27	CF	42	GLU	5.2
7	BG	108	ALA	5.2
13	BM	102	THR	5.2
50	C3	32	ALA	5.2
2	BB	35	ARG	5.2
11	BK	51	GLY	5.2
3	AC	83	ASP	5.2
17	BQ	48	ASP	5.2
27	CF	46	ASP	5.2
28	CG	4	VAL	5.2
2	BB	49	MET	5.2
19	BS	75	ALA	5.2
22	CA	2178	C	5.2
34	CN	54	THR	5.2
38	CR	35	ALA	5.2
36	CP	81	ARG	5.2
9	AI	65	ILE	5.2
28	CG	12	PRO	5.2
28	CG	22	GLN	5.2
29	DH	72	ILE	5.2
50	C3	7	PRO	5.2
19	AS	65	GLU	5.2
19	AS	10	PHE	5.2
35	CO	102	PHE	5.2
14	BN	72	GLY	5.2
1	BA	1019	A	5.2
3	BC	33	LEU	5.2
55	DI	125	ARG	5.1
2	BB	44	GLU	5.1
9	AI	55	VAL	5.1
10	BJ	81	GLU	5.1
29	DH	49	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
36	CP	32	PRO	5.1
22	CA	1053	C	5.1
29	DH	145	ASN	5.1
52	C5	13	ASN	5.1
11	AK	110	ILE	5.1
7	AG	109	ARG	5.1
1	BA	1243	C	5.1
6	BF	39	LEU	5.1
7	AG	59	LEU	5.1
22	CA	2170	A	5.1
40	CT	97	LEU	5.1
43	CW	42	LEU	5.1
26	CE	179	SER	5.1
27	CF	145	LYS	5.1
27	CF	44	ILE	5.1
34	CN	61	GLY	5.1
3	BC	130	PHE	5.1
28	CG	50	LEU	5.1
30	DJ	10	LYS	5.1
32	CL	90	ASN	5.1
13	AM	37	ALA	5.1
16	BP	44	SER	5.1
29	CH	56	ALA	5.1
22	CA	316	C	5.1
13	BM	47	GLU	5.1
25	CD	155	VAL	5.1
26	CE	178	VAL	5.1
42	CV	84	GLY	5.1
9	AI	32	GLN	5.1
53	DA	1175	A	5.1
7	BG	13	LEU	5.1
19	AS	22	ALA	5.1
20	BT	38	ALA	5.1
39	CS	25	LEU	5.1
44	CX	25	ARG	5.1
3	BC	84	VAL	5.1
32	CL	69	VAL	5.1
33	CM	46	VAL	5.1
38	CR	23	GLY	5.1
44	CX	31	VAL	5.1
22	CA	2120	G	5.1
7	BG	130	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
8	BH	46	ILE	5.1
7	BG	60	GLU	5.1
8	BH	54	ASP	5.1
28	CG	56	ASP	5.1
46	CZ	16	THR	5.1
1	BA	1244	G	5.1
26	CE	135	ALA	5.1
26	CE	103	GLY	5.1
43	CW	68	LYS	5.1
46	CZ	54	LYS	5.1
36	CP	90	VAL	5.1
45	CY	76	GLU	5.1
2	AB	82	ASP	5.1
9	BI	123	ARG	5.1
28	CG	151	TYR	5.1
30	CJ	122	ILE	5.1
48	C1	55	ILE	5.1
10	BJ	79	PRO	5.1
7	AG	11	LYS	5.1
25	CD	151	THR	5.1
26	CE	34	ALA	5.1
35	CO	88	ALA	5.1
49	C2	16	GLY	5.1
28	CG	130	GLU	5.1
35	CO	10	LEU	5.1
20	BT	70	ASN	5.0
30	CJ	103	ARG	5.0
14	AN	47	LYS	5.0
30	CJ	141	GLU	5.0
37	CQ	5	ILE	5.0
49	C2	21	TYR	5.0
33	CM	30	THR	5.0
35	CO	57	THR	5.0
11	BK	47	ALA	5.0
16	AP	72	ALA	5.0
9	BI	31	ASN	5.0
27	CF	150	ARG	5.0
53	DA	2105	U	5.0
19	AS	16	LEU	5.0
2	AB	227	GLN	5.0
2	BB	131	LYS	5.0
28	CG	62	TRP	5.0

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Mol	Chain	Res	Type	RSRZ
29	CH	138	VAL	5.0
10	AJ	18	ILE	5.0
13	AM	7	ILE	5.0
15	BO	82	ILE	5.0
26	CE	188	MET	5.0
31	CK	21	THR	5.0
4	AD	27	ALA	5.0
10	AJ	89	ARG	5.0
37	CQ	63	LYS	5.0
46	CZ	24	GLU	5.0
10	AJ	98	VAL	5.0
46	CZ	41	HIS	5.0
53	DA	654	A	5.0
9	BI	90	TYR	5.0
38	CR	29	SER	5.0
12	BL	44	LYS	5.0
31	CK	17	VAL	5.0
40	CT	105	VAL	5.0
22	CA	1172	C	5.0
25	CD	118	PHE	5.0
28	CG	111	HIS	5.0
44	CX	68	LYS	5.0
26	CE	67	ARG	5.0
7	BG	19	GLY	5.0
7	BG	48	GLU	5.0
7	BG	71	PRO	5.0
18	AR	20	GLU	5.0
28	CG	32	GLU	5.0
13	AM	52	GLN	5.0
34	CN	23	GLY	5.0
55	DI	122	GLN	5.0
36	CP	28	VAL	5.0
17	BQ	41	THR	5.0
46	CZ	55	THR	5.0
49	C2	35	GLU	5.0
2	AB	32	PHE	5.0
9	BI	23	PRO	5.0
51	C4	14	PHE	5.0
5	BE	159	LYS	4.9
13	AM	31	LYS	4.9
8	BH	39	VAL	4.9
25	CD	26	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
10	BJ	12	ALA	4.9
25	CD	199	SER	4.9
26	CE	41	GLN	4.9
46	CZ	31	GLN	4.9
2	AB	13	GLY	4.9
19	AS	30	PRO	4.9
27	CF	9	LYS	4.9
27	CF	161	LYS	4.9
38	CR	84	LYS	4.9
2	BB	157	LEU	4.9
19	BS	5	LEU	4.9
29	CH	75	LEU	4.9
37	CQ	8	LEU	4.9
28	CG	162	VAL	4.9
7	BG	37	SER	4.9
32	CL	75	SER	4.9
47	C0	3	LYS	4.9
27	CF	29	PRO	4.9
2	AB	151	ILE	4.9
40	CT	35	ILE	4.9
41	CU	52	GLU	4.9
3	BC	40	ARG	4.9
21	BU	33	ARG	4.9
22	CA	2119	A	4.9
26	CE	171	ASP	4.9
43	CW	43	ASP	4.9
41	CU	39	THR	4.9
7	BG	97	ASN	4.9
21	BU	15	ALA	4.9
26	CE	142	ALA	4.9
51	C4	23	LYS	4.9
2	AB	186	ILE	4.9
2	BB	132	LYS	4.9
20	BT	8	LYS	4.9
3	BC	44	THR	4.9
22	CA	318	C	4.9
14	AN	26	GLU	4.9
43	CW	38	LEU	4.9
7	AG	45	SER	4.9
37	CQ	57	SER	4.9
55	DI	18	VAL	4.9
1	BA	1013	G	4.9

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Mol	Chain	Res	Type	RSRZ
13	AM	58	ASP	4.9
22	CA	1170	C	4.9
41	CU	40	LYS	4.9
26	CE	24	ASN	4.9
2	BB	6	MET	4.9
2	AB	124	GLY	4.9
28	CG	28	GLY	4.9
29	DH	39	ALA	4.9
29	DH	88	GLY	4.9
40	CT	32	ALA	4.9
1	BA	207	C	4.9
29	DH	144	VAL	4.9
34	CN	135	VAL	4.9
40	CT	49	LYS	4.9
10	AJ	75	ASP	4.9
49	C2	32	GLU	4.9
5	AE	164	ILE	4.9
29	DH	12	LEU	4.8
28	CG	94	TYR	4.8
14	BN	11	VAL	4.8
22	CA	1084	A	4.8
8	BH	55	THR	4.8
26	CE	17	THR	4.8
28	CG	24	ILE	4.8
22	CA	2104	C	4.8
7	BG	121	ALA	4.8
31	CK	126	ALA	4.8
42	CV	2	ALA	4.8
45	CY	21	ALA	4.8
48	C1	24	ALA	4.8
53	DA	2120	G	4.8
7	AG	26	PHE	4.8
7	BG	143	ARG	4.8
9	BI	55	VAL	4.8
13	BM	92	ARG	4.8
16	BP	56	ARG	4.8
42	CV	11	VAL	4.8
40	CT	16	LYS	4.8
30	CJ	125	MET	4.8
31	CK	3	THR	4.8
17	AQ	55	ILE	4.8
44	CX	61	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
7	AG	79	ARG	4.8
7	BG	70	ARG	4.8
13	BM	78	LYS	4.8
14	BN	81	ARG	4.8
17	BQ	51	ASN	4.8
28	CG	6	LYS	4.8
9	BI	32	GLN	4.8
24	CC	204	VAL	4.8
38	CR	104	VAL	4.8
29	CH	92	GLY	4.8
33	CM	129	LYS	4.8
2	AB	53	ALA	4.8
20	BT	57	ILE	4.8
22	CA	2128	G	4.8
7	BG	9	GLN	4.8
2	AB	43	LEU	4.8
2	AB	129	LEU	4.8
9	BI	91	ASP	4.8
3	BC	148	GLY	4.8
26	CE	169	VAL	4.8
35	CO	74	GLU	4.8
37	DQ	115	ASN	4.8
14	BN	95	GLY	4.8
41	CU	90	GLY	4.8
45	CY	46	PHE	4.8
4	BD	44	ARG	4.8
14	BN	61	ARG	4.8
7	BG	91	VAL	4.8
9	BI	111	VAL	4.8
45	CY	4	VAL	4.8
3	AC	41	GLN	4.8
5	BE	103	THR	4.8
8	AH	54	ASP	4.8
15	BO	7	ALA	4.8
29	DH	100	ALA	4.8
13	BM	73	ILE	4.8
37	CQ	84	ILE	4.8
44	CX	70	GLU	4.8
53	DA	2174	C	4.8
55	DI	116	GLU	4.8
19	BS	72	GLY	4.8
36	CP	7	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
50	C3	12	ARG	4.8
46	CZ	42	LEU	4.7
42	CV	67	VAL	4.7
42	CV	18	ASP	4.7
10	BJ	61	ALA	4.7
13	AM	35	ALA	4.7
25	CD	41	ALA	4.7
2	AB	62	SER	4.7
55	DI	115	GLY	4.7
3	BC	41	GLN	4.7
3	BC	55	ILE	4.7
22	CA	2168	G	4.7
11	BK	75	LYS	4.7
29	DH	149	GLU	4.7
41	CU	14	PRO	4.7
26	CE	18	THR	4.7
24	CC	112	ALA	4.7
29	DH	16	GLY	4.7
15	BO	83	GLU	4.7
26	CE	148	ILE	4.7
30	CJ	116	ASP	4.7
22	CA	41	C	4.7
2	BB	184	PHE	4.7
15	BO	79	THR	4.7
19	AS	23	VAL	4.7
26	CE	167	VAL	4.7
49	C2	23	THR	4.7
18	AR	32	TYR	4.7
30	CJ	81	LYS	4.7
45	CY	78	TYR	4.7
41	DU	52	GLU	4.7
26	CE	7	ASP	4.7
30	DJ	64	ASP	4.7
26	CE	73	ILE	4.7
33	CM	132	ARG	4.7
53	DA	2111	U	4.7
20	BT	64	LYS	4.7
28	CG	99	LYS	4.7
33	CM	143	GLU	4.7
1	BA	210	C	4.7
1	BA	1245	C	4.7
14	AN	22	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
28	CG	21	GLY	4.7
33	CM	98	ALA	4.7
1	BA	1138	G	4.7
26	CE	40	ARG	4.7
13	AM	115	PRO	4.7
22	CA	1406	U	4.7
27	CF	67	ILE	4.7
6	BF	76	THR	4.7
48	C1	23	THR	4.7
3	BC	31	ASP	4.7
47	C0	26	GLY	4.7
26	CE	113	VAL	4.7
26	CE	186	VAL	4.7
29	CH	65	ALA	4.7
14	AN	23	LYS	4.7
24	CC	29	PRO	4.7
13	AM	8	ASN	4.7
41	CU	24	MET	4.7
7	AG	82	GLY	4.6
14	BN	50	THR	4.6
33	CM	135	ILE	4.6
25	CD	40	LEU	4.6
45	CY	71	LEU	4.6
46	CZ	47	ARG	4.6
8	AH	24	ALA	4.6
20	AT	46	ALA	4.6
42	CV	3	ALA	4.6
49	D2	53	LYS	4.6
25	CD	180	VAL	4.6
34	CN	37	GLY	4.6
34	CN	55	ARG	4.6
9	AI	89	GLU	4.6
39	CS	34	GLU	4.6
7	BG	39	ALA	4.6
14	BN	79	LEU	4.6
21	BU	57	ALA	4.6
29	DH	84	ALA	4.6
1	BA	948	C	4.6
1	BA	1359	C	4.6
44	CX	38	VAL	4.6
3	BC	203	PHE	4.6
53	DA	2164	C	4.6

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Mol	Chain	Res	Type	RSRZ
55	DI	16	SER	4.6
7	AG	42	ILE	4.6
20	AT	66	LEU	4.6
24	CC	31	ALA	4.6
3	BC	147	LYS	4.6
2	BB	107	VAL	4.6
2	BB	187	VAL	4.6
9	BI	113	ARG	4.6
13	BM	105	ASN	4.6
29	DH	97	ARG	4.6
9	BI	82	GLY	4.6
44	CX	54	GLY	4.6
2	BB	125	THR	4.6
22	CA	2112	G	4.6
29	CH	52	ALA	4.6
34	CN	56	ALA	4.6
7	BG	7	ILE	4.6
36	CP	2	ASP	4.6
36	CP	34	HIS	4.6
51	C4	59	ILE	4.6
52	C5	16	ILE	4.6
1	BA	1022	A	4.6
2	AB	141	LEU	4.6
15	BO	32	LEU	4.6
29	CH	54	LEU	4.6
3	AC	81	GLY	4.6
13	BM	111	GLY	4.6
17	BQ	23	VAL	4.6
28	CG	43	VAL	4.6
30	DJ	25	GLY	4.6
31	CK	139	VAL	4.6
42	CV	42	VAL	4.6
53	DA	2113	U	4.6
2	AB	77	SER	4.6
3	BC	79	LYS	4.6
14	BN	83	LYS	4.6
2	BB	127	ASP	4.6
27	DF	80	ARG	4.6
51	C4	64	TYR	4.6
28	CG	136	ALA	4.6
30	DJ	63	ALA	4.6
36	CP	37	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
22	CA	1076	C	4.6
22	CA	1868	C	4.6
29	CH	38	PRO	4.6
2	AB	187	VAL	4.6
19	BS	20	GLU	4.6
43	CW	8	VAL	4.6
53	DA	138	U	4.6
44	CX	77	ARG	4.6
13	BM	100	GLN	4.6
22	CA	882	G	4.6
3	BC	30	ALA	4.6
6	AF	105	ALA	4.6
11	AK	103	ALA	4.6
7	AG	81	GLY	4.5
36	CP	84	GLU	4.5
2	AB	85	LEU	4.5
44	CX	82	ILE	4.5
52	C5	10	LEU	4.5
13	AM	85	CYS	4.5
9	BI	122	ARG	4.5
10	BJ	15	HIS	4.5
7	BG	63	GLU	4.5
21	AU	5	LYS	4.5
13	AM	32	ALA	4.5
55	DI	83	ALA	4.5
14	BN	70	PRO	4.5
26	CE	35	TYR	4.5
1	BA	1362	A	4.5
14	AN	31	ILE	4.5
5	BE	70	ASN	4.5
7	AG	64	VAL	4.5
9	AI	48	VAL	4.5
22	CA	2180	U	4.5
50	C3	6	GLN	4.5
53	DA	2132	U	4.5
14	BN	47	LYS	4.5
22	CA	2177	C	4.5
2	AB	69	PHE	4.5
3	BC	131	ARG	4.5
3	BC	132	ARG	4.5
8	BH	44	GLY	4.5
12	BL	14	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
20	BT	63	ALA	4.5
29	CH	81	ALA	4.5
36	CP	16	ARG	4.5
43	CW	54	ALA	4.5
3	BC	94	ILE	4.5
9	BI	87	LEU	4.5
15	BO	67	LEU	4.5
1	AA	1026	G	4.5
22	CA	1071	G	4.5
39	CS	54	VAL	4.5
14	BN	67	THR	4.5
27	CF	71	ARG	4.5
7	AG	8	GLY	4.5
28	CG	120	GLY	4.5
33	CM	16	GLY	4.5
20	BT	72	ALA	4.5
22	CA	2125	G	4.5
53	DA	2115	G	4.5
22	CA	275	C	4.5
22	CA	2174	C	4.5
41	CU	7	LEU	4.5
51	C4	29	LEU	4.5
1	BA	1247	U	4.5
27	CF	125	ARG	4.5
13	AM	16	VAL	4.5
49	C2	17	THR	4.5
17	BQ	54	GLY	4.5
6	AF	32	ALA	4.5
25	CD	85	ALA	4.5
29	DH	136	SER	4.5
40	CT	13	SER	4.5
50	C3	5	PHE	4.5
3	BC	164	ARG	4.5
2	AB	132	LYS	4.5
7	AG	21	GLU	4.5
8	AH	65	TYR	4.5
33	CM	115	GLU	4.5
46	CZ	9	LYS	4.5
43	CW	61	LEU	4.5
45	CY	30	LEU	4.5
55	DI	86	THR	4.5
10	AJ	74	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
29	DH	78	VAL	4.5
43	CW	64	VAL	4.5
2	AB	55	ALA	4.5
14	AN	42	TRP	4.5
6	BF	8	PHE	4.5
3	AC	126	ARG	4.5
28	CG	18	LYS	4.5
1	BA	1304	G	4.5
2	BB	151	ILE	4.4
7	AG	7	ILE	4.4
15	BO	33	THR	4.4
26	CE	180	LEU	4.4
40	CT	69	LEU	4.4
41	CU	21	SER	4.4
44	CX	71	VAL	4.4
10	BJ	7	ARG	4.4
14	BN	9	ARG	4.4
28	CG	35	ARG	4.4
45	DY	77	LYS	4.4
46	CZ	17	GLU	4.4
30	CJ	107	GLN	4.4
53	DA	1077	A	4.4
53	DA	2101	A	4.4
1	BA	1325	C	4.4
2	AB	224	GLY	4.4
28	CG	127	THR	4.4
45	CY	8	THR	4.4
2	AB	68	LEU	4.4
2	BB	108	ARG	4.4
9	BI	35	LEU	4.4
41	CU	3	ARG	4.4
17	AQ	5	ILE	4.4
34	CN	106	ASP	4.4
37	CQ	30	VAL	4.4
55	DI	111	ALA	4.4
10	AJ	49	PHE	4.4
9	BI	36	GLU	4.4
29	CH	97	ARG	4.4
50	C3	35	ARG	4.4
41	CU	29	THR	4.4
7	BG	47	LEU	4.4
22	CA	1176	U	4.4

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Mol	Chain	Res	Type	RSRZ
46	CZ	49	ASP	4.4
33	CM	104	GLN	4.4
41	CU	26	LYS	4.4
22	CA	2105	U	4.4
27	CF	62	GLY	4.4
24	CC	67	PHE	4.4
25	CD	101	PHE	4.4
33	CM	1	MET	4.4
39	CS	1	MET	4.4
41	CU	78	SER	4.4
42	CV	55	PRO	4.4
1	AA	82	G	4.4
22	CA	654	A	4.4
2	AB	45	LYS	4.4
6	BF	93	LYS	4.4
7	BG	139	GLU	4.4
7	BG	82	GLY	4.4
9	AI	50	GLN	4.4
53	DA	1065	U	4.4
35	CO	80	PHE	4.4
3	BC	110	GLU	4.4
37	CQ	60	THR	4.4
41	CU	64	LYS	4.4
15	AO	89	ARG	4.4
31	CK	96	ARG	4.4
25	CD	201	LEU	4.4
50	C3	31	LEU	4.4
7	AG	19	GLY	4.4
11	AK	19	GLY	4.4
31	CK	142	ILE	4.4
32	CL	2	ILE	4.4
17	BQ	57	ASP	4.4
3	BC	129	MET	4.4
17	BQ	16	LYS	4.4
25	CD	11	MET	4.4
29	CH	79	THR	4.4
29	DH	47	PHE	4.4
3	BC	32	ASN	4.3
2	AB	34	ALA	4.3
20	BT	22	ALA	4.3
27	CF	53	ALA	4.3
28	CG	64	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
3	BC	207	ILE	4.3
22	CA	2158	A	4.3
3	AC	42	TYR	4.3
55	DI	68	PRO	4.3
9	BI	124	ARG	4.3
2	AB	11	LYS	4.3
30	DJ	111	GLN	4.3
2	AB	84	ALA	4.3
2	BB	55	ALA	4.3
2	BB	75	ALA	4.3
3	BC	155	GLY	4.3
29	CH	67	ALA	4.3
7	AG	23	LEU	4.3
22	CA	1059	G	4.3
55	DI	59	LEU	4.3
2	AB	67	ILE	4.3
2	AB	164	ILE	4.3
9	BI	79	ILE	4.3
10	AJ	5	ARG	4.3
28	CG	26	ILE	4.3
35	CO	2	ARG	4.3
13	BM	14	HIS	4.3
29	CH	78	VAL	4.3
30	DJ	57	VAL	4.3
39	CS	75	VAL	4.3
50	C3	25	LYS	4.3
21	BU	7	ARG	4.3
41	CU	54	GLU	4.3
44	CX	78	LYS	4.3
2	BB	199	VAL	4.3
25	CD	20	VAL	4.3
22	CA	2402	U	4.3
31	CK	79	GLY	4.3
11	BK	70	CYS	4.3
48	C1	21	ALA	4.3
20	BT	56	PRO	4.3
3	BC	8	ASN	4.3
29	DH	73	ASN	4.3
42	CV	45	HIS	4.3
29	CH	19	VAL	4.3
13	BM	98	ARG	4.3
19	AS	21	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
26	CE	80	SER	4.3
40	CT	31	GLN	4.3
2	BB	8	ASP	4.3
21	BU	56	HIS	4.3
50	C3	18	PHE	4.3
16	BP	48	GLU	4.3
19	AS	47	LEU	4.3
28	CG	37	LEU	4.3
40	CT	33	LEU	4.3
28	CG	3	ARG	4.3
1	AA	78	A	4.3
2	AB	131	LYS	4.3
20	BT	42	GLY	4.3
21	BU	27	GLY	4.3
27	CF	41	GLY	4.3
33	CM	84	LYS	4.3
6	BF	96	VAL	4.3
7	AG	69	VAL	4.3
26	DE	4	VAL	4.3
37	CQ	110	ILE	4.3
53	DA	2103	C	4.3
2	BB	166	ALA	4.3
6	BF	28	ALA	4.3
15	BO	76	ALA	4.3
29	DH	17	ASP	4.3
54	DD	132	ALA	4.3
19	AS	14	HIS	4.3
2	BB	142	GLU	4.2
26	CE	23	PHE	4.2
28	CG	124	GLU	4.2
26	CE	102	ARG	4.2
1	BA	1027	C	4.2
9	AI	82	GLY	4.2
15	AO	16	GLY	4.2
41	CU	22	THR	4.2
7	BG	29	ILE	4.2
22	CA	1083	U	4.2
38	CR	8	VAL	4.2
38	CR	113	ALA	4.2
39	CS	87	GLN	4.2
34	CN	111	GLU	4.2
45	CY	49	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
20	BT	78	ASN	4.2
6	AF	104	LYS	4.2
28	CG	110	SER	4.2
8	BH	130	ALA	4.2
29	DH	69	ALA	4.2
31	CK	75	TYR	4.2
29	DH	133	GLN	4.2
27	CF	124	GLY	4.2
55	DI	90	GLY	4.2
37	CQ	9	GLU	4.2
40	CT	59	GLU	4.2
44	CX	85	GLU	4.2
3	BC	204	LYS	4.2
30	CJ	19	ASN	4.2
10	AJ	102	LEU	4.2
40	CT	19	LEU	4.2
41	CU	27	SER	4.2
8	BH	127	CYS	4.2
1	AA	79	G	4.2
3	BC	64	ILE	4.2
5	BE	120	VAL	4.2
11	BK	21	ALA	4.2
13	AM	43	VAL	4.2
16	BP	20	VAL	4.2
20	AT	62	ALA	4.2
26	CE	193	VAL	4.2
29	CH	80	ILE	4.2
31	CK	54	ILE	4.2
49	C2	12	VAL	4.2
50	C3	9	VAL	4.2
12	BL	123	LYS	4.2
14	BN	54	ASP	4.2
45	CY	55	GLY	4.2
48	C1	52	ARG	4.2
3	BC	119	SER	4.2
22	CA	317	G	4.2
36	CP	45	SER	4.2
2	BB	158	PRO	4.2
22	CA	896	A	4.2
15	BO	12	VAL	4.2
17	BQ	29	VAL	4.2
27	CF	3	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
28	CG	29	LYS	4.2
2	BB	60	ILE	4.2
26	CE	42	GLY	4.2
32	CL	32	TYR	4.2
3	AC	80	LYS	4.2
9	BI	114	LYS	4.2
49	C2	50	LYS	4.2
2	BB	182	PRO	4.2
10	BJ	43	PRO	4.2
54	DD	143	PRO	4.2
3	BC	111	LEU	4.2
28	CG	47	ASP	4.2
28	CG	96	ALA	4.2
31	CK	94	ALA	4.2
9	BI	117	GLY	4.2
25	CD	72	GLY	4.2
29	CH	51	ARG	4.2
30	CJ	91	GLY	4.2
6	BF	29	ILE	4.2
28	CG	75	MET	4.2
45	CY	56	MET	4.2
2	AB	44	GLU	4.2
11	AK	80	LYS	4.2
29	CH	41	LYS	4.2
48	C1	18	SER	4.2
33	CM	118	THR	4.1
26	CE	168	ASP	4.1
28	CG	126	PRO	4.1
29	DH	118	PRO	4.1
43	CW	91	PHE	4.1
50	C3	14	ARG	4.1
13	BM	88	GLY	4.1
2	BB	221	VAL	4.1
28	CG	23	VAL	4.1
52	C5	22	VAL	4.1
54	DD	142	VAL	4.1
2	BB	89	GLN	4.1
43	CW	51	GLN	4.1
55	DI	74	ASP	4.1
10	BJ	48	ARG	4.1
33	CM	69	ARG	4.1
18	BR	51	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
31	CK	16	TYR	4.1
13	BM	72	GLU	4.1
43	CW	35	GLU	4.1
25	CD	87	GLY	4.1
29	DH	85	GLY	4.1
29	CH	106	ALA	4.1
48	D1	2	ALA	4.1
49	C2	15	ALA	4.1
2	BB	214	LEU	4.1
30	CJ	105	GLN	4.1
1	AA	1027	C	4.1
11	AK	86	VAL	4.1
29	CH	110	VAL	4.1
39	CS	72	VAL	4.1
45	CY	13	VAL	4.1
11	AK	23	ILE	4.1
24	CC	74	ILE	4.1
21	AU	21	ARG	4.1
41	CU	42	GLU	4.1
22	CA	1169	A	4.1
28	CG	8	PRO	4.1
1	BA	1006	G	4.1
37	CQ	98	TYR	4.1
41	DU	91	GLN	4.1
38	CR	116	ALA	4.1
9	AI	52	LEU	4.1
22	CA	1066	U	4.1
39	CS	45	GLU	4.1
26	CE	83	VAL	4.1
1	BA	204	G	4.1
1	BA	206	C	4.1
53	DA	2178	C	4.1
5	BE	80	THR	4.1
13	BM	115	PRO	4.1
40	CT	100	THR	4.1
5	BE	53	ALA	4.1
16	BP	58	ALA	4.1
25	CD	30	GLU	4.1
27	CF	101	GLU	4.1
29	DH	86	ASP	4.1
32	CL	16	ALA	4.1
33	CM	134	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
32	CL	108	ARG	4.1
38	CR	11	ARG	4.1
24	CC	28	LYS	4.1
30	CJ	102	SER	4.1
54	DD	161	MET	4.1
9	AI	67	VAL	4.1
26	CE	156	ASN	4.1
19	AS	39	THR	4.1
34	CN	96	ILE	4.1
46	CZ	35	GLY	4.1
54	DD	146	ILE	4.1
26	CE	25	GLU	4.1
28	CG	16	ASP	4.1
39	CS	55	ASP	4.1
40	CT	34	ASP	4.1
7	AG	149	LYS	4.1
48	C1	32	LYS	4.1
29	DH	128	HIS	4.1
45	CY	29	PHE	4.1
25	CD	9	VAL	4.1
3	BC	38	LYS	4.1
1	BA	5	U	4.1
53	DA	2147	A	4.1
53	DA	2181	U	4.1
11	BK	15	GLN	4.0
3	BC	140	ASN	4.0
22	CA	549	G	4.0
29	CH	149	GLU	4.0
1	BA	983	A	4.0
30	DJ	119	GLY	4.0
14	AN	33	ASP	4.0
1	BA	1226	C	4.0
34	CN	101	VAL	4.0
40	CT	50	VAL	4.0
22	CA	361	G	4.0
11	AK	41	ALA	4.0
13	AM	40	ALA	4.0
22	CA	1211	C	4.0
12	BL	60	GLY	4.0
25	CD	19	GLY	4.0
26	CE	56	GLY	4.0
28	CG	108	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
24	CC	30	PHE	4.0
43	CW	2	PHE	4.0
13	AM	20	THR	4.0
1	BA	1287	A	4.0
25	CD	60	VAL	4.0
22	CA	1075	C	4.0
16	BP	4	ILE	4.0
16	BP	57	ILE	4.0
21	AU	25	LYS	4.0
22	CA	139	U	4.0
42	CV	103	ILE	4.0
53	DA	139	U	4.0
9	BI	108	ALA	4.0
7	AG	4	ARG	4.0
2	AB	9	MET	4.0
20	BT	40	GLU	4.0
13	AM	80	LEU	4.0
20	BT	16	LYS	4.0
24	CC	111	LYS	4.0
24	CC	265	LYS	4.0
28	CG	133	LEU	4.0
37	CQ	59	PHE	4.0
2	AB	217	VAL	4.0
6	AF	96	VAL	4.0
21	AU	55	ARG	4.0
27	CF	30	ARG	4.0
53	DA	283	G	4.0
22	CA	1100	C	4.0
11	BK	76	GLU	4.0
24	CC	56	GLY	4.0
26	CE	144	GLU	4.0
29	DH	45	GLU	4.0
22	CA	883	G	4.0
49	C2	24	THR	4.0
1	BA	999	C	4.0
9	BI	103	PHE	4.0
17	BQ	65	ARG	4.0
18	BR	67	LEU	4.0
36	CP	36	TYR	4.0
48	C1	22	LEU	4.0
17	BQ	58	VAL	4.0
43	CW	7	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
21	AU	50	ALA	4.0
22	CA	2305	U	4.0
28	CG	63	ALA	4.0
32	CL	60	ALA	4.0
43	CW	74	ALA	4.0
29	CH	133	GLN	4.0
1	AA	87	C	4.0
23	CB	37	C	4.0
3	BC	70	THR	4.0
10	BJ	83	THR	4.0
5	AE	115	LEU	4.0
36	CP	26	LEU	4.0
2	AB	143	LYS	4.0
28	CG	88	GLN	4.0
28	CG	158	LYS	4.0
53	DA	2135	A	4.0
6	BF	34	GLY	4.0
7	BG	127	ALA	4.0
25	CD	115	GLY	4.0
29	CH	126	GLY	4.0
53	DA	1064	C	4.0
39	DS	103	ALA	4.0
1	BA	1286	U	4.0
53	DA	1176	U	4.0
53	DA	2172	U	4.0
14	BN	94	PRO	4.0
22	CA	2101	A	3.9
13	BM	21	SER	3.9
13	BM	114	LYS	3.9
14	BN	7	LYS	3.9
33	CM	67	THR	3.9
37	CQ	111	LYS	3.9
53	DA	2133	G	3.9
5	BE	158	GLY	3.9
28	CG	31	GLY	3.9
55	DI	99	PHE	3.9
28	CG	54	PRO	3.9
29	DH	129	GLU	3.9
33	CM	21	ARG	3.9
38	CR	99	ALA	3.9
55	DI	25	ALA	3.9
3	BC	46	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
36	CP	27	VAL	3.9
45	CY	58	VAL	3.9
1	AA	83	C	3.9
1	AA	1031	C	3.9
1	BA	1265	C	3.9
22	CA	1044	C	3.9
19	AS	17	LYS	3.9
22	CA	879	G	3.9
48	C1	27	SER	3.9
22	CA	344	A	3.9
3	BC	96	GLY	3.9
17	AQ	52	GLU	3.9
29	CH	116	ARG	3.9
2	BB	114	LEU	3.9
19	AS	64	ASP	3.9
26	CE	36	ALA	3.9
37	CQ	108	ALA	3.9
53	DA	277	G	3.9
39	CS	60	LYS	3.9
41	CU	44	LYS	3.9
9	BI	19	VAL	3.9
24	CC	3	VAL	3.9
37	CQ	33	VAL	3.9
31	CK	138	GLN	3.9
2	BB	211	THR	3.9
30	CJ	108	GLU	3.9
36	CP	55	GLU	3.9
31	CK	83	GLY	3.9
7	BG	126	ASP	3.9
40	CT	109	ASP	3.9
7	BG	16	PRO	3.9
11	AK	102	ALA	3.9
28	CG	5	ALA	3.9
40	CT	51	LEU	3.9
47	D0	2[A]	ALA	3.9
54	DD	152	PRO	3.9
25	CD	156	PHE	3.9
2	BB	38	VAL	3.9
11	BK	77	TYR	3.9
2	AB	137	ARG	3.9
3	BC	126	ARG	3.9
28	CG	36	THR	3.9

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Mol	Chain	Res	Type	RSRZ
48	C1	26	THR	3.9
40	CT	62	ASP	3.9
1	AA	1025	U	3.9
22	CA	1174	U	3.9
17	BQ	73	TRP	3.9
2	BB	148	LEU	3.9
2	AB	16	PHE	3.9
9	AI	20	PHE	3.9
15	BO	10	LYS	3.9
21	AU	19	PHE	3.9
21	BU	12	PHE	3.9
45	CY	35	SER	3.9
46	CZ	34	SER	3.9
55	DI	62	ARG	3.9
29	CH	21	VAL	3.9
29	CH	61	VAL	3.9
51	D4	7	VAL	3.9
13	AM	6	GLY	3.9
18	BR	21	ILE	3.9
33	CM	105	ILE	3.9
1	BA	79	G	3.9
22	CA	914	G	3.9
22	CA	1871	A	3.9
17	BQ	4	LYS	3.9
24	CC	61	ALA	3.9
29	CH	64	ALA	3.9
35	CO	71	ARG	3.9
36	CP	11	ALA	3.9
42	CV	97	LYS	3.9
9	AI	128	SER	3.9
29	DH	90	LEU	3.9
55	DI	5	LEU	3.9
8	AH	48	ASP	3.9
25	CD	181	ASP	3.9
41	CU	92	ASN	3.9
2	BB	56	GLU	3.9
29	CH	137	GLU	3.9
9	AI	27	LYS	3.9
39	CS	101	ILE	3.9
22	CA	1078	U	3.8
14	BN	99	ALA	3.8
1	AA	1032	G	3.8

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Mol	Chain	Res	Type	RSRZ
53	DA	1171	G	3.8
53	DA	2176	A	3.8
2	BB	205	ASP	3.8
3	BC	83	ASP	3.8
35	CO	120	GLU	3.8
36	CP	93	ASP	3.8
9	AI	26	GLY	3.8
9	AI	61	LEU	3.8
20	BT	52	ASN	3.8
13	AM	26	GLY	3.8
25	CD	163	GLY	3.8
37	CQ	40	LEU	3.8
39	CS	67	GLY	3.8
3	AC	101	ILE	3.8
20	BT	67	ILE	3.8
29	DH	87	GLU	3.8
11	AK	17	SER	3.8
25	CD	206	ALA	3.8
27	CF	127	ASN	3.8
24	CC	57	GLY	3.8
22	CA	2146	C	3.8
33	CM	57	LEU	3.8
40	CT	46	LEU	3.8
22	CA	881	G	3.8
3	BC	153	VAL	3.8
8	BH	66	PHE	3.8
14	BN	26	GLU	3.8
16	BP	39	PHE	3.8
33	CM	66	PHE	3.8
52	C5	25	VAL	3.8
2	AB	8	ASP	3.8
2	AB	128	LYS	3.8
5	BE	30	ILE	3.8
38	CR	2	ALA	3.8
39	CS	74	ILE	3.8
50	D3	46	LYS	3.8
6	BF	1	MET	3.8
36	CP	44	GLY	3.8
13	AM	83	LEU	3.8
15	BO	87	LEU	3.8
46	CZ	28	LEU	3.8
46	CZ	43	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
19	BS	77	THR	3.8
28	CG	39	ASP	3.8
24	CC	78	VAL	3.8
28	CG	90	VAL	3.8
33	CM	127	VAL	3.8
42	CV	44	LYS	3.8
46	CZ	45	GLN	3.8
22	CA	1179	G	3.8
9	BI	18	ARG	3.8
13	BM	87	ARG	3.8
33	CM	75	ALA	3.8
6	BF	65	GLU	3.8
9	AI	30	ILE	3.8
12	AL	123	LYS	3.8
14	AN	18	ASP	3.8
29	CH	8	LYS	3.8
3	BC	175	LEU	3.8
29	CH	40	THR	3.8
35	CO	36	THR	3.8
54	DD	138	LEU	3.8
9	BI	25	ASN	3.8
37	DQ	66	ASN	3.8
21	AU	14	VAL	3.8
21	BU	53	VAL	3.8
3	BC	105	GLU	3.8
27	DF	77	PHE	3.8
29	CH	70	GLU	3.8
36	CP	46	GLU	3.8
44	CX	26	PHE	3.8
38	CR	26	GLY	3.8
7	AG	144	MET	3.8
15	AO	11	ILE	3.8
20	BT	83	ILE	3.8
22	CA	2179	C	3.8
53	DA	2158	A	3.8
26	CE	97	ASN	3.8
26	CE	198	GLU	3.8
2	AB	152	LYS	3.8
2	BB	17	GLY	3.8
55	DI	15	VAL	3.8
29	DH	46	PHE	3.8
30	CJ	72	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
37	CQ	6	LYS	3.8
9	BI	17	ALA	3.8
24	CC	251	GLN	3.8
49	C2	46	HIS	3.8
42	CV	99	ASN	3.7
16	BP	50	THR	3.7
39	CS	94	THR	3.7
2	BB	174	LYS	3.7
3	AC	38	LYS	3.7
9	BI	93	SER	3.7
32	CL	109	SER	3.7
22	CA	2117	A	3.7
28	CG	71	LEU	3.7
28	CG	66	GLY	3.7
10	AJ	91	ASP	3.7
14	BN	84	VAL	3.7
28	CG	137	ASP	3.7
32	CL	61	VAL	3.7
7	AG	134	ALA	3.7
19	AS	74	PHE	3.7
55	DI	63	ALA	3.7
45	CY	50	ARG	3.7
53	DA	2156	G	3.7
1	BA	1314	C	3.7
22	CA	142	A	3.7
22	CA	279	A	3.7
22	CA	1407	G	3.7
2	AB	63	ARG	3.7
7	BG	138	ARG	3.7
34	CN	105	MET	3.7
2	BB	45	LYS	3.7
13	AM	63	PHE	3.7
41	CU	9	LYS	3.7
53	DA	2167	U	3.7
9	AI	21	ILE	3.7
31	CK	136	GLN	3.7
36	CP	52	SER	3.7
1	BA	1270	G	3.7
1	BA	1302	C	3.7
1	BA	1357	A	3.7
22	CA	2115	G	3.7
39	CS	44	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
14	BN	101	TRP	3.7
9	AI	94	LEU	3.7
13	AM	56	LEU	3.7
37	DQ	114	LEU	3.7
45	CY	77	LYS	3.7
25	CD	32	ASN	3.7
3	BC	180	ALA	3.7
20	BT	17	ALA	3.7
25	CD	1	MET	3.7
27	CF	70	ALA	3.7
52	C5	7	VAL	3.7
4	AD	20	PHE	3.7
7	BG	90	GLU	3.7
22	CA	1523	U	3.7
25	CD	183	GLU	3.7
27	CF	98	GLU	3.7
9	AI	91	ASP	3.7
32	CL	48	PRO	3.7
44	CX	65	GLY	3.7
48	D1	9	THR	3.7
17	AQ	4	LYS	3.7
31	DK	84	ILE	3.7
51	C4	19	LYS	3.7
35	CO	112	TYR	3.7
55	DI	103	ASN	3.7
2	BB	43	LEU	3.7
22	CA	491	G	3.7
53	DA	2116	G	3.7
20	BT	47	ALA	3.7
29	CH	69	ALA	3.7
26	CE	32	VAL	3.7
38	CR	34	VAL	3.7
55	DI	85	VAL	3.7
2	BB	5	SER	3.7
9	BI	51	PRO	3.7
4	BD	45	LYS	3.7
25	CD	198	GLY	3.7
37	CQ	20	PHE	3.7
22	CA	1074	G	3.7
22	CA	1538	G	3.7
28	CG	19	ILE	3.7
34	CN	73	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
50	C3	26	ASN	3.7
2	AB	154	MET	3.7
9	AI	57	MET	3.7
1	AA	1534	A	3.7
3	AC	89	LYS	3.7
18	BR	30	LYS	3.7
40	CT	48	LYS	3.7
41	CU	61	LEU	3.7
7	BG	2	PRO	3.7
7	BG	119	ARG	3.7
13	AM	57	ARG	3.7
6	BF	18	VAL	3.7
22	CA	2107	G	3.7
22	CA	2159	G	3.7
29	DH	13	GLY	3.7
49	C2	42	VAL	3.7
51	C4	61	CYS	3.7
2	AB	138	THR	3.7
2	AB	162	PHE	3.7
54	DD	121	THR	3.7
22	CA	2103	C	3.6
23	CB	118	C	3.6
43	CW	63	ILE	3.6
48	C1	37	LYS	3.6
1	BA	94	G	3.6
2	BB	76	ALA	3.6
9	BI	46	MET	3.6
17	BQ	34	TYR	3.6
21	BU	55	ARG	3.6
36	CP	102	ARG	3.6
55	DI	51	TYR	3.6
4	AD	163	GLU	3.6
27	CF	166	GLY	3.6
28	CG	61	GLY	3.6
10	AJ	84	VAL	3.6
24	CC	239	ASN	3.6
25	CD	197	THR	3.6
28	CG	44	LYS	3.6
44	CX	43	THR	3.6
2	AB	208	ARG	3.6
1	AA	412	A	3.6
7	AG	58	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
9	AI	72	ILE	3.6
25	CD	27	ILE	3.6
34	CN	126	ILE	3.6
9	BI	70	GLY	3.6
31	CK	53	TYR	3.6
17	BQ	8	LEU	3.6
19	AS	15	LEU	3.6
1	BA	191	G	3.6
53	DA	1063	G	3.6
29	CH	91	PHE	3.6
31	CK	119	PHE	3.6
14	BN	64	CYS	3.6
1	BA	1266	G	3.6
1	BA	1312	G	3.6
2	AB	40	ILE	3.6
7	BG	55	GLY	3.6
11	AK	66	ALA	3.6
13	BM	27	LYS	3.6
25	CD	38	LYS	3.6
36	CP	87	ILE	3.6
42	CV	92	LYS	3.6
22	CA	547	A	3.6
38	CR	47	TYR	3.6
3	BC	178	LEU	3.6
24	DC	205	LEU	3.6
25	CD	99	GLU	3.6
24	CC	228	VAL	3.6
54	DD	155	VAL	3.6
1	BA	942	G	3.6
13	BM	110	LYS	3.6
53	DA	2161	C	3.6
53	DA	2126	A	3.6
2	AB	150	GLY	3.6
3	BC	60	PRO	3.6
6	BF	67	PRO	3.6
28	CG	53	GLY	3.6
10	AJ	23	ALA	3.6
16	BP	65	ALA	3.6
11	AK	97	ILE	3.6
15	AO	18	ASP	3.6
20	BT	12	ILE	3.6
29	CH	7	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
27	CF	5	HIS	3.6
33	CM	35	HIS	3.6
22	CA	893	C	3.6
29	CH	117	LEU	3.6
40	CT	38	TYR	3.6
1	BA	1246	A	3.6
53	DA	2125	G	3.6
25	CD	105	LYS	3.6
2	BB	47	VAL	3.6
22	CA	280	U	3.6
37	CQ	80	VAL	3.6
13	BM	50	GLU	3.6
16	BP	10	GLY	3.6
35	CO	72	ASP	3.6
53	DA	141	G	3.6
29	DH	57	LYS	3.6
31	CK	93	ILE	3.6
40	CT	4	ILE	3.6
43	CW	29	ILE	3.6
3	BC	12	LEU	3.6
10	BJ	71	LEU	3.6
28	CG	67	THR	3.6
19	AS	43	ASN	3.6
22	CA	2175	C	3.6
24	CC	144	VAL	3.6
4	AD	176	GLY	3.6
13	AM	51	GLY	3.6
15	AO	2	SER	3.6
17	BQ	11	ARG	3.6
25	CD	179	ARG	3.6
32	CL	122	VAL	3.6
48	D1	3	VAL	3.6
33	CM	53	GLY	3.6
7	BG	142	HIS	3.5
11	BK	103	ALA	3.5
21	BU	52	ALA	3.5
31	CK	117	ALA	3.5
34	CN	116	ALA	3.5
38	CR	115	ALA	3.5
22	CA	2167	U	3.5
53	DA	546	U	3.5
10	AJ	100	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
22	CA	2799	A	3.5
38	DR	40	ILE	3.5
2	BB	222	ARG	3.5
9	BI	9	THR	3.5
22	CA	356	G	3.5
22	CA	1091	G	3.5
5	BE	15	LEU	3.5
18	AR	68	LEU	3.5
38	CR	33	ARG	3.5
11	BK	80	LYS	3.5
48	C1	51	GLY	3.5
1	BA	90	C	3.5
1	BA	1132	C	3.5
33	DM	35	HIS	3.5
48	C1	15	MET	3.5
6	BF	32	ALA	3.5
9	AI	101	ALA	3.5
35	DO	125	ALA	3.5
1	BA	1356	G	3.5
2	AB	30	PHE	3.5
22	CA	405	U	3.5
22	CA	2904	U	3.5
7	AG	70	ARG	3.5
37	CQ	72	ARG	3.5
7	BG	42	ILE	3.5
11	BK	23	ILE	3.5
19	AS	28	LYS	3.5
20	AT	5	LYS	3.5
43	CW	70	ILE	3.5
39	CS	29	THR	3.5
53	DA	1730	C	3.5
53	DA	2179	C	3.5
3	BC	20	SER	3.5
22	CA	2176	A	3.5
9	BI	89	GLU	3.5
53	DA	2109	U	3.5
24	CC	65	VAL	3.5
14	AN	44	ALA	3.5
16	BP	82	ALA	3.5
27	CF	168	ALA	3.5
50	C3	23	ALA	3.5
22	CA	276	U	3.5

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Mol	Chain	Res	Type	RSRZ
29	CH	46	PHE	3.5
2	AB	147	SER	3.5
3	BC	74	GLY	3.5
22	CA	1042	G	3.5
29	DH	79	THR	3.5
40	CT	103	ILE	3.5
47	C0	39	GLU	3.5
39	CS	91	GLN	3.5
3	BC	87	LEU	3.5
11	AK	82	LEU	3.5
24	DC	213	TRP	3.5
38	CR	61	TRP	3.5
14	AN	53	ARG	3.5
17	BQ	46	VAL	3.5
24	CC	94	VAL	3.5
27	CF	69	LYS	3.5
31	CK	68	LYS	3.5
31	CK	95	ARG	3.5
39	CS	47	VAL	3.5
48	C1	53	LYS	3.5
16	BP	73	ALA	3.5
18	AR	27	ALA	3.5
19	AS	20	GLU	3.5
1	BA	843	U	3.5
8	BH	2	SER	3.5
11	BK	61	PHE	3.5
22	CA	1057	A	3.5
27	CF	131	GLY	3.5
34	CN	28	PHE	3.5
46	CZ	26	PHE	3.5
54	DD	144	GLY	3.5
30	DJ	118	THR	3.5
29	DH	51	ARG	3.5
29	DH	141	LYS	3.5
38	CR	13	ARG	3.5
44	CX	62	LYS	3.5
2	BB	68	LEU	3.5
11	AK	100	LEU	3.5
22	CA	2157	G	3.5
36	CP	48	LEU	3.5
3	AC	170	GLU	3.5
7	AG	63	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
29	CH	127	GLU	3.5
40	CT	61	ASN	3.5
4	AD	142	VAL	3.5
22	CA	2602	A	3.5
24	DC	17	VAL	3.5
28	CG	145	ALA	3.5
29	CH	84	ALA	3.5
36	CP	98	GLN	3.5
2	AB	17	GLY	3.5
24	CC	6	CYS	3.5
26	CE	125	SER	3.5
44	CX	34	GLY	3.5
29	DH	112	LYS	3.5
34	CN	84	LYS	3.5
21	AU	34	ARG	3.5
26	CE	114	ARG	3.5
33	CM	128	THR	3.5
22	CA	436	C	3.5
33	CM	8	PRO	3.5
7	AG	129	GLU	3.5
22	CA	342	A	3.5
14	BN	93	ILE	3.5
29	CH	58	LEU	3.5
33	CM	27	LEU	3.5
34	CN	20	LEU	3.5
35	CO	98	LEU	3.5
38	CR	18	LEU	3.5
24	DC	211	ALA	3.5
27	CF	160	ALA	3.5
31	CK	20	ALA	3.5
3	AC	90	VAL	3.5
45	CY	47	VAL	3.5
51	D4	50	VAL	3.5
25	CD	97	SER	3.5
53	DA	2162	G	3.5
45	CY	57	ARG	3.5
1	AA	84	U	3.4
13	BM	42	ASP	3.4
24	CC	246	THR	3.4
55	DI	4	ASN	3.4
2	BB	200	ILE	3.4
20	BT	76	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
6	AF	61	LEU	3.4
11	AK	21	ALA	3.4
24	CC	105	LEU	3.4
25	CD	119	ALA	3.4
51	C4	65	ALA	3.4
10	BJ	72	ARG	3.4
13	AM	47	GLU	3.4
17	AQ	54	GLY	3.4
17	BQ	52	GLU	3.4
28	CG	149	ARG	3.4
29	CH	60	GLU	3.4
6	BF	10	VAL	3.4
29	CH	134	VAL	3.4
42	CV	100	SER	3.4
44	CX	67	VAL	3.4
54	DD	122	VAL	3.4
2	BB	46	THR	3.4
1	BA	1000	A	3.4
2	BB	51	ASN	3.4
29	CH	73	ASN	3.4
33	DM	30	THR	3.4
9	BI	41	ARG	3.4
29	DH	4	ILE	3.4
32	CL	98	ARG	3.4
2	BB	10	LEU	3.4
8	BH	59	LEU	3.4
13	AM	38	GLY	3.4
10	AJ	101	SER	3.4
21	AU	16	LEU	3.4
25	CD	188	LEU	3.4
33	CM	125	LEU	3.4
37	CQ	114	LEU	3.4
38	CR	38	ALA	3.4
54	DD	119	ALA	3.4
55	DI	32	GLY	3.4
2	AB	39	HIS	3.4
1	AA	1020	G	3.4
4	AD	101	VAL	3.4
21	AU	54	LYS	3.4
47	C0	41	THR	3.4
13	AM	50	GLU	3.4
22	CA	2122	U	3.4

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Mol	Chain	Res	Type	RSRZ
29	CH	123	ARG	3.4
22	CA	2173	A	3.4
10	BJ	49	PHE	3.4
32	CL	113	MET	3.4
2	BB	180	GLY	3.4
3	BC	197	GLY	3.4
9	AI	117	GLY	3.4
15	BO	4	SER	3.4
1	AA	842	U	3.4
19	AS	45	ILE	3.4
27	CF	24	SER	3.4
33	CM	141	LYS	3.4
7	AG	68	ASN	3.4
14	BN	96	LEU	3.4
41	CU	59	ASN	3.4
1	BA	1293	C	3.4
3	BC	58	GLU	3.4
3	AC	136	ARG	3.4
3	BC	26	THR	3.4
25	CD	112	THR	3.4
22	CA	1112	G	3.4
28	CG	114	ASP	3.4
26	CE	141	MET	3.4
32	CL	101	GLY	3.4
38	CR	85	LYS	3.4
54	DD	147	GLY	3.4
3	BC	71	ALA	3.4
28	CG	119	ALA	3.4
30	DJ	77	ALA	3.4
55	DI	102	ALA	3.4
2	AB	171	ILE	3.4
3	AC	77	ILE	3.4
10	AJ	76	ILE	3.4
28	CG	141	ILE	3.4
33	CM	103	ILE	3.4
2	BB	129	LEU	3.4
27	CF	36	LEU	3.4
35	CO	96	ARG	3.4
1	BA	1303	C	3.4
3	BC	116	VAL	3.4
51	C4	36	LYS	3.4
3	BC	194	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
38	DR	32	TYR	3.4
2	BB	191	SER	3.4
28	DG	101	ASN	3.4
47	C0	52	SER	3.4
12	BL	2	ALA	3.4
17	BQ	24	ALA	3.4
55	DI	19	ALA	3.4
22	CA	846	U	3.4
1	AA	1	A	3.4
10	AJ	25	ILE	3.4
51	C4	4	ILE	3.4
4	BD	55	LEU	3.4
28	CG	72	LEU	3.4
35	DO	121	LYS	3.4
6	BF	30	THR	3.4
6	BF	60	VAL	3.4
15	BO	75	VAL	3.4
24	CC	184	VAL	3.4
31	CK	62	VAL	3.4
20	AT	65	GLY	3.4
22	CA	1047	G	3.4
25	CD	166	GLY	3.4
7	BG	68	ASN	3.3
21	AU	51	SER	3.3
18	AR	51	TYR	3.3
19	AS	3	ARG	3.3
53	DA	1067	A	3.3
7	BG	147	ALA	3.3
9	AI	121	ALA	3.3
20	BT	19	LYS	3.3
24	CC	122	ALA	3.3
30	DJ	82	LYS	3.3
38	CR	63	ALA	3.3
39	CS	61	ALA	3.3
44	CX	44	LYS	3.3
52	C5	8	LYS	3.3
2	AB	198	PHE	3.3
29	CH	29	PHE	3.3
29	CH	86	ASP	3.3
54	DD	118	PHE	3.3
8	BH	42	GLU	3.3
1	BA	846	G	3.3

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Mol	Chain	Res	Type	RSRZ
1	BA	1355	G	3.3
26	DE	73	ILE	3.3
11	AK	111	THR	3.3
29	DH	15	LEU	3.3
32	CL	107	LEU	3.3
40	CT	23	LEU	3.3
53	DA	2169	A	3.3
9	AI	25	ASN	3.3
10	BJ	84	VAL	3.3
29	DH	14	SER	3.3
45	CY	74	ARG	3.3
14	BN	12	LYS	3.3
27	CF	88	LYS	3.3
7	AG	85	TYR	3.3
9	BI	112	GLU	3.3
16	AP	58	ALA	3.3
19	AS	24	GLU	3.3
49	C2	49	TYR	3.3
53	DA	1870	C	3.3
22	CA	2802	G	3.3
33	CM	113	ALA	3.3
26	CE	59	PRO	3.3
53	DA	896	A	3.3
36	CP	104	GLN	3.3
19	BS	10	PHE	3.3
13	BM	70	ARG	3.3
7	BG	35	LYS	3.3
14	BN	68	GLY	3.3
33	CM	14	LYS	3.3
33	CM	26	GLY	3.3
1	BA	1271	A	3.3
22	CA	1869	G	3.3
37	CQ	46	VAL	3.3
7	BG	140	ASP	3.3
22	CA	884	U	3.3
28	CG	123	ALA	3.3
28	CG	139	GLN	3.3
16	BP	31	ARG	3.3
31	CK	123	LYS	3.3
2	AB	36	ASN	3.3
42	CV	69	ASN	3.3
1	AA	845	A	3.3

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Mol	Chain	Res	Type	RSRZ
2	BB	133	GLU	3.3
16	BP	77	GLU	3.3
20	BT	75	HIS	3.3
21	AU	24	GLU	3.3
54	DD	156	PHE	3.3
39	CS	102	SER	3.3
31	CK	109	LEU	3.3
2	AB	205	ASP	3.3
33	CM	55	MET	3.3
10	AJ	35	GLN	3.3
35	CO	60	VAL	3.3
38	CR	100	VAL	3.3
22	CA	12	U	3.3
22	CA	1090	A	3.3
38	DR	35	ALA	3.3
55	DI	109	LYS	3.3
53	DA	2124	G	3.3
30	DJ	130	GLU	3.3
11	AK	104	GLY	3.3
1	AA	91	U	3.3
21	AU	56	HIS	3.3
2	AB	86	SER	3.3
47	C0	8	THR	3.3
5	BE	152	MET	3.3
22	CA	1099	G	3.3
22	CA	1168	G	3.3
31	CK	2	LYS	3.3
43	CW	50	MET	3.3
48	C1	57	LYS	3.3
14	AN	24	ARG	3.3
36	CP	30	ARG	3.3
2	AB	80	VAL	3.3
8	BH	110	VAL	3.3
12	BL	91	PRO	3.3
22	CA	1082	U	3.3
24	DC	144	VAL	3.3
28	CG	81	GLU	3.3
31	CK	124	VAL	3.3
35	CO	114	GLU	3.3
52	C5	3	VAL	3.3
3	AC	92	ALA	3.3
13	BM	15	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
29	DH	43	ASN	3.3
55	DI	13	ALA	3.3
39	CS	92	TRP	3.3
2	AB	149	GLY	3.3
24	DC	42	GLY	3.3
54	DD	117	GLY	3.3
25	CD	103	ASP	3.3
25	CD	140	HIS	3.3
48	C1	38	HIS	3.3
1	BA	1310	G	3.3
5	AE	61	GLN	3.3
11	BK	38	GLN	3.3
17	AQ	53	CYS	3.3
43	CW	3	THR	3.3
43	CW	10	LYS	3.3
35	CO	22	ARG	3.3
35	CO	43	GLU	3.3
7	AG	12	ILE	3.3
31	CK	81	ILE	3.3
35	CO	34	ILE	3.3
38	CR	40	ILE	3.3
45	CY	22	LEU	3.3
1	AA	1492	A	3.3
1	BA	460	A	3.3
1	BA	1330	U	3.3
22	CA	546	U	3.3
2	BB	224	GLY	3.2
8	AH	44	GLY	3.2
9	BI	24	GLY	3.2
16	BP	63	GLN	3.2
29	CH	2	GLN	3.2
29	DH	42	LYS	3.2
46	CZ	38	GLN	3.2
52	C5	28	SER	3.2
13	BM	59	GLU	3.2
17	BQ	80	GLU	3.2
30	DJ	127	ARG	3.2
1	BA	84	U	3.2
22	CA	282	A	3.2
53	DA	1089	A	3.2
6	BF	59	TYR	3.2
22	CA	1056	G	3.2

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Mol	Chain	Res	Type	RSRZ
37	CQ	74	PHE	3.2
35	CO	83	LEU	3.2
40	CT	74	ILE	3.2
41	DU	2	ILE	3.2
44	CX	64	ASP	3.2
7	BG	128	ALA	3.2
8	BH	120	GLY	3.2
20	BT	37	ALA	3.2
36	CP	96	GLY	3.2
41	CU	23	ALA	3.2
48	C1	45	ALA	3.2
14	BN	71	HIS	3.2
26	CE	155	GLU	3.2
29	DH	109	GLU	3.2
42	CV	88	GLU	3.2
44	DX	85	GLU	3.2
49	C2	13	SER	3.2
22	CA	2803	G	3.2
1	BA	1038	C	3.2
2	BB	9	MET	3.2
6	AF	102	MET	3.2
24	CC	146	MET	3.2
35	DO	1	MET	3.2
40	CT	98	LYS	3.2
48	D1	8	PRO	3.2
25	CD	68	PHE	3.2
21	AU	29	LEU	3.2
26	CE	27	LEU	3.2
37	CQ	105	GLY	3.2
38	DR	18	LEU	3.2
47	C0	25	LEU	3.2
55	DI	81	LEU	3.2
11	BK	45	ALA	3.2
28	CG	152	ARG	3.2
35	CO	17	ARG	3.2
41	CU	12	ARG	3.2
22	CA	137	U	3.2
2	BB	110	SER	3.2
22	CA	2164	C	3.2
24	DC	220	VAL	3.2
53	DA	2127	G	3.2
1	BA	1274	A	3.2

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Mol	Chain	Res	Type	RSRZ
9	AI	120	LYS	3.2
20	BT	69	LYS	3.2
22	CA	44	A	3.2
21	AU	9	ASN	3.2
2	AB	88	ASP	3.2
37	CQ	12	GLN	3.2
33	CM	119	PRO	3.2
2	AB	21	ARG	3.2
2	AB	213	TYR	3.2
22	CA	1731	G	3.2
28	CG	163	ARG	3.2
39	CS	83	TYR	3.2
49	C2	6	ARG	3.2
54	DD	125	TRP	3.2
1	AA	205	A	3.2
38	CR	106	PHE	3.2
15	BO	19	ALA	3.2
29	CH	82	SER	3.2
47	C0	7	ILE	3.2
47	D0	17	LEU	3.2
9	BI	13	LYS	3.2
10	BJ	11	LYS	3.2
10	BJ	30	LYS	3.2
37	CQ	14	LYS	3.2
42	CV	47	LYS	3.2
7	BG	69	VAL	3.2
14	AN	34	VAL	3.2
38	DR	34	VAL	3.2
55	DI	33	VAL	3.2
10	BJ	14	ASP	3.2
11	AK	59	THR	3.2
19	AS	27	ASP	3.2
34	CN	24	THR	3.2
40	CT	94	ASP	3.2
22	CA	2124	G	3.2
3	BC	179	ARG	3.2
22	CA	2126	A	3.2
38	CR	28	ARG	3.2
33	CM	52	GLY	3.2
34	CN	99	GLY	3.2
3	BC	108	LYS	3.2
28	CG	138	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
27	CF	121	SER	3.2
11	BK	102	ALA	3.2
41	CU	18	GLU	3.2
1	BA	1012	A	3.2
1	BA	1142	G	3.2
7	AG	9	GLN	3.2
8	BH	36	ILE	3.2
16	BP	21	VAL	3.2
29	DH	130	VAL	3.2
51	C4	7	VAL	3.2
9	BI	11	ARG	3.2
55	DI	42	ARG	3.2
1	BA	1028	C	3.2
2	BB	112	LYS	3.2
9	BI	88	MET	3.2
14	BN	78	GLY	3.2
31	CK	82	GLY	3.2
22	CA	1539	U	3.2
53	DA	356	G	3.2
53	DA	1069	A	3.2
26	CE	116	ASP	3.2
40	CT	15	GLN	3.2
43	CW	5	ASN	3.2
38	CR	45	TYR	3.2
2	AB	212	LEU	3.2
3	AC	107	ARG	3.2
1	AA	90	C	3.2
7	BG	26	PHE	3.2
11	BK	53	ARG	3.2
34	CN	112	LEU	3.2
39	CS	39	LEU	3.2
45	DY	22	LEU	3.2
33	DM	23	ILE	3.2
35	CO	97	ILE	3.2
2	BB	183	VAL	3.2
11	AK	75	LYS	3.2
28	DG	177	LYS	3.2
10	BJ	47	GLU	3.1
29	CH	109	GLU	3.1
1	BA	1279	G	3.1
16	BP	49	GLY	3.1
30	DJ	56	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
46	CZ	62	GLY	3.1
5	AE	160	SER	3.1
32	CL	13	ASN	3.1
37	DQ	2	SER	3.1
24	DC	122	ALA	3.1
1	BA	1492	A	3.1
41	CU	33	LYS	3.1
43	CW	46	LYS	3.1
1	BA	1292	G	3.1
1	BA	1491	G	3.1
22	CA	1873	G	3.1
53	DA	549	G	3.1
24	CC	49	ILE	3.1
24	DC	51	THR	3.1
25	CD	133	THR	3.1
35	CO	52	ILE	3.1
39	CS	19	THR	3.1
21	AU	11	PRO	3.1
29	DH	120	GLY	3.1
35	CO	20	MET	3.1
49	C2	40	ASP	3.1
7	BG	96	ARG	3.1
14	BN	63	ARG	3.1
26	CE	107	SER	3.1
33	CM	42	SER	3.1
2	BB	140	GLU	3.1
22	CA	277	G	3.1
22	CA	1734	G	3.1
41	CU	25	GLU	3.1
2	AB	83	ALA	3.1
24	DC	210	ALA	3.1
55	DI	110	ALA	3.1
1	BA	1011	C	3.1
1	BA	1267	C	3.1
22	CA	140	C	3.1
1	AA	85	U	3.1
2	BB	72	THR	3.1
2	BB	99	GLY	3.1
7	BG	38	THR	3.1
8	BH	63	LEU	3.1
11	AK	42	LEU	3.1
15	BO	86	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
22	CA	1089	A	3.1
28	CG	100	GLY	3.1
33	DM	37	GLY	3.1
42	CV	66	GLN	3.1
42	DV	50	PRO	3.1
48	C1	19	HIS	3.1
1	BA	1026	G	3.1
12	BL	56	ARG	3.1
16	AP	44	SER	3.1
22	CA	438	G	3.1
24	DC	216	VAL	3.1
27	DF	72	LYS	3.1
29	DH	19	VAL	3.1
42	DV	49	VAL	3.1
43	CW	24	ASN	3.1
7	BG	41	SER	3.1
31	CK	92	MET	3.1
2	BB	34	ALA	3.1
3	BC	95	ALA	3.1
48	C1	2	ALA	3.1
3	AC	79	LYS	3.1
25	CD	134	HIS	3.1
33	CM	31	GLY	3.1
7	AG	38	THR	3.1
13	BM	107	ARG	3.1
16	BP	51	ARG	3.1
24	CC	48	ARG	3.1
31	CK	110	PRO	3.1
29	CH	55	GLU	3.1
50	C3	13	ASN	3.1
2	AB	91	PHE	3.1
16	BP	75	ILE	3.1
27	CF	61	SER	3.1
36	CP	92	PHE	3.1
40	CT	24	ILE	3.1
44	CX	35	SER	3.1
54	DD	127	PHE	3.1
8	AH	110	VAL	3.1
21	AU	32	VAL	3.1
22	CA	1098	A	3.1
54	DD	145	SER	3.1
1	BA	213	G	3.1

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Mol	Chain	Res	Type	RSRZ
1	BA	1001	C	3.1
11	AK	99	ALA	3.1
29	CH	18	GLN	3.1
29	CH	111	ALA	3.1
43	CW	16	ALA	3.1
43	CW	39	ALA	3.1
24	CC	121	ASP	3.1
29	CH	53	GLU	3.1
31	CK	98	GLU	3.1
1	BA	1441	A	3.1
52	C5	38	GLY	3.1
32	CL	120	PRO	3.1
9	BI	15	SER	3.1
21	BU	16	LEU	3.1
34	CN	27	SER	3.1
3	BC	142	MET	3.1
29	CH	1	MET	3.1
14	BN	77	PHE	3.1
31	DK	81	ILE	3.1
33	DM	103	ILE	3.1
37	DQ	98	TYR	3.1
38	CR	17	ILE	3.1
19	BS	6	LYS	3.1
20	BT	44	LYS	3.1
38	CR	4	VAL	3.1
51	C4	5	LYS	3.1
46	CZ	13	GLU	3.1
1	BA	1029	U	3.1
5	BE	112	ARG	3.1
22	CA	1108	U	3.1
32	CL	30	ARG	3.1
35	CO	118	ARG	3.1
11	BK	67	ALA	3.1
25	CD	44	GLY	3.1
25	CD	102	ALA	3.1
1	BA	1136	C	3.1
2	AB	20	THR	3.1
51	D4	6	THR	3.1
51	D4	61	CYS	3.1
2	BB	152	LYS	3.1
30	DJ	72	LYS	3.1
34	CN	100	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
6	BF	21	MET	3.1
38	CR	59	GLN	3.1
42	CV	46	GLN	3.1
6	BF	72	ASP	3.1
31	CK	13	ARG	3.1
33	CM	33	ARG	3.1
34	CN	25	ASP	3.1
38	DR	24	TYR	3.1
39	DS	75	VAL	3.1
40	CT	85	ILE	3.1
42	CV	81	ASP	3.1
1	BA	1452	C	3.1
7	AG	141	VAL	3.1
7	BG	32	VAL	3.1
24	CC	161	TYR	3.1
46	CZ	7	ARG	3.1
2	BB	146	ASN	3.0
2	BB	149	GLY	3.0
24	CC	119	GLY	3.0
29	CH	128	HIS	3.0
37	CQ	42	ALA	3.0
22	CA	172	A	3.0
29	CH	35	LYS	3.0
31	CK	85	LYS	3.0
6	BF	97	THR	3.0
43	CW	62	THR	3.0
8	BH	5	ASP	3.0
31	CK	120	ARG	3.0
40	DT	110	ARG	3.0
42	CV	94	ARG	3.0
49	C2	28	ARG	3.0
1	BA	1306	A	3.0
22	CA	141	G	3.0
22	CA	1111	A	3.0
29	DH	122	LEU	3.0
53	DA	2123	G	3.0
2	AB	4	VAL	3.0
26	CE	85	PHE	3.0
39	DS	83	TYR	3.0
54	DD	140	HIS	3.0
54	DD	153	GLY	3.0
6	BF	83	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
13	AM	78	LYS	3.0
16	AP	80	LYS	3.0
35	CO	61	ALA	3.0
41	CU	41	ALA	3.0
35	DO	14	SER	3.0
22	CA	359	G	3.0
34	DN	59	ARG	3.0
35	CO	37	THR	3.0
37	CQ	39	ARG	3.0
55	DI	29	ASP	3.0
2	BB	154	MET	3.0
16	BP	40	ASN	3.0
31	CK	111	LYS	3.0
45	CY	16	ASN	3.0
10	AJ	33	GLY	3.0
15	BO	6	GLU	3.0
33	CM	86	GLU	3.0
51	D4	62	LEU	3.0
1	BA	80	A	3.0
2	BB	162	PHE	3.0
3	BC	120	ILE	3.0
14	AN	11	VAL	3.0
26	DE	9	GLN	3.0
9	AI	23	PRO	3.0
3	BC	169	ARG	3.0
13	AM	92	ARG	3.0
20	BT	29	ARG	3.0
2	BB	167	ASP	3.0
25	CD	61	THR	3.0
26	CE	43	THR	3.0
34	CN	129	THR	3.0
28	CG	134	LYS	3.0
8	BH	91	GLU	3.0
9	AI	118	LEU	3.0
33	DM	61	LEU	3.0
14	BN	65	ARG	3.0
2	AB	153	ASP	3.0
2	AB	200	ILE	3.0
3	BC	133	ALA	3.0
25	CD	21	SER	3.0
17	BQ	53	CYS	3.0
17	BQ	64	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	AA	1493	A	3.0
33	CM	109	LYS	3.0
34	CN	58	LYS	3.0
33	CM	10	GLU	3.0
38	DR	25	TYR	3.0
41	CU	56	GLU	3.0
2	BB	119	THR	3.0
50	C3	43	THR	3.0
1	BA	1241	G	3.0
22	CA	291	G	3.0
22	CA	406	G	3.0
23	CB	117	G	3.0
24	CC	179	GLY	3.0
24	DC	215	GLY	3.0
35	CO	7	GLY	3.0
13	AM	79	ARG	3.0
1	BA	958	A	3.0
7	BG	110	LYS	3.0
29	CH	39	ALA	3.0
29	DH	60	GLU	3.0
30	DJ	26	PRO	3.0
44	CX	19	LYS	3.0
35	CO	82	GLU	3.0
47	C0	17	LEU	3.0
55	DI	95	LEU	3.0
21	BU	51	SER	3.0
25	CD	162	ALA	3.0
39	CS	3	ALA	3.0
51	C4	10	ALA	3.0
5	BE	137	VAL	3.0
8	BH	51	VAL	3.0
9	AI	116	VAL	3.0
15	BO	20	ASN	3.0
43	CW	49	ASN	3.0
18	AR	28	THR	3.0
20	BT	20	HIS	3.0
22	CA	1876	A	3.0
3	BC	13	GLY	3.0
11	AK	39	GLY	3.0
24	DC	55	GLY	3.0
51	C4	43	HIS	3.0
54	DD	141	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
55	DI	61	ARG	3.0
3	BC	36	ASP	3.0
6	BF	35	LYS	3.0
1	BA	1018	G	3.0
1	BA	1296	C	3.0
2	BB	223	GLU	3.0
20	BT	15	GLU	3.0
39	CS	23	GLU	3.0
53	DA	2180	U	3.0
14	BN	100	SER	3.0
54	DD	137	SER	3.0
20	BT	66	LEU	3.0
24	CC	174	LEU	3.0
28	DG	105	LEU	3.0
29	CH	5	LEU	3.0
30	DJ	11	LEU	3.0
34	CN	95	LEU	3.0
35	DO	10	LEU	3.0
41	CU	93	LEU	3.0
9	AI	5	GLN	3.0
46	CZ	25	GLN	3.0
5	AE	123	VAL	2.9
7	AG	62	PHE	2.9
9	AI	79	ILE	2.9
14	BN	45	VAL	2.9
24	CC	165	VAL	2.9
45	CY	11	ARG	2.9
45	CY	64	ILE	2.9
20	BT	68	HIS	2.9
22	CA	283	G	2.9
22	CA	315	G	2.9
30	DJ	16	GLY	2.9
26	CE	101	TYR	2.9
30	DJ	17	MET	2.9
34	CN	103	TYR	2.9
5	BE	150	PRO	2.9
40	CT	80	PRO	2.9
3	BC	25	ASN	2.9
5	BE	122	ASN	2.9
7	AG	152	ALA	2.9
38	DR	10	ALA	2.9
55	DI	112	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
4	AD	73	ARG	2.9
10	BJ	73	LEU	2.9
29	DH	54	LEU	2.9
53	DA	881	G	2.9
3	BC	112	ASP	2.9
13	AM	60	VAL	2.9
29	DH	103	VAL	2.9
38	CR	82	GLY	2.9
40	CT	7	HIS	2.9
49	C2	22	THR	2.9
38	DR	9	ILE	2.9
33	DM	55	MET	2.9
1	BA	1365	G	2.9
2	BB	29	PRO	2.9
1	BA	190	A	2.9
2	BB	169	GLU	2.9
7	BG	136	LYS	2.9
22	CA	895	U	2.9
28	DG	48	ASN	2.9
10	BJ	78	GLU	2.9
20	BT	10	ARG	2.9
38	CR	41	LYS	2.9
49	C2	10	LYS	2.9
22	CA	1872	A	2.9
23	CB	57	A	2.9
55	DI	17	GLU	2.9
6	AF	95	ALA	2.9
29	CH	102	ALA	2.9
40	CT	56	ALA	2.9
9	AI	56	ASP	2.9
55	DI	36	ASP	2.9
3	BC	6	HIS	2.9
16	BP	64	GLY	2.9
24	DC	154	LEU	2.9
42	CV	57	GLY	2.9
47	C0	29	LEU	2.9
26	DE	53	THR	2.9
8	BH	104	VAL	2.9
11	AK	129	VAL	2.9
22	CA	1534	U	2.9
26	DE	52	VAL	2.9
38	CR	31	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
9	BI	30	ILE	2.9
39	CS	40	MET	2.9
24	CC	240	PHE	2.9
35	CO	21	PHE	2.9
47	C0	53	PHE	2.9
53	DA	2157	G	2.9
39	CS	48	LYS	2.9
5	AE	93	ARG	2.9
7	AG	57	SER	2.9
9	BI	125	PRO	2.9
32	CL	14	SER	2.9
22	CA	1748	C	2.9
22	CA	1874	C	2.9
22	CA	2181	U	2.9
23	CB	19	C	2.9
24	CC	210	ALA	2.9
11	BK	48	GLY	2.9
22	CA	880	G	2.9
33	CM	49	GLY	2.9
39	CS	8	GLY	2.9
44	CX	21	LEU	2.9
7	BG	106	GLU	2.9
42	CV	54	GLN	2.9
46	CZ	39	GLN	2.9
3	BC	106	VAL	2.9
10	BJ	51	VAL	2.9
11	AK	84	VAL	2.9
40	CT	71	VAL	2.9
45	CY	17	ASN	2.9
35	CO	14	SER	2.9
7	AG	14	PRO	2.9
1	BA	1248	A	2.9
22	CA	2100	G	2.9
38	DR	45	TYR	2.9
53	DA	2100	G	2.9
1	BA	1308	U	2.9
24	DC	190	ALA	2.9
4	BD	166	GLU	2.9
16	AP	48	GLU	2.9
16	BP	46	LYS	2.9
2	BB	87	CYS	2.9
33	CM	48	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
38	CR	92	ARG	2.9
42	CV	15	THR	2.9
11	BK	100	LEU	2.9
35	CO	115	LEU	2.9
1	BA	205	A	2.9
22	CA	1054	A	2.9
1	BA	86	G	2.9
2	BB	147	SER	2.9
14	AN	32	SER	2.9
9	BI	29	VAL	2.9
43	CW	66	ASP	2.9
44	CX	23	VAL	2.9
53	DA	2112	G	2.9
15	BO	36	ILE	2.9
17	BQ	25	ILE	2.9
41	CU	30	ILE	2.9
44	CX	69	PHE	2.9
20	BT	5	LYS	2.9
29	DH	70	GLU	2.9
22	CA	2166	U	2.9
24	CC	233	GLY	2.9
24	DC	47	GLY	2.9
25	CD	94	GLN	2.9
31	DK	115	GLY	2.9
2	BB	61	ALA	2.9
3	AC	113	ALA	2.9
15	BO	17	ARG	2.9
26	CE	192	ALA	2.9
5	AE	122	ASN	2.9
22	CA	1723	G	2.9
24	CC	252	THR	2.9
53	DA	2104	C	2.9
2	AB	54	LEU	2.9
24	CC	272	SER	2.9
29	DH	82	SER	2.9
36	CP	5	SER	2.9
42	CV	89	ASP	2.9
48	C1	31	ASP	2.9
2	AB	56	GLU	2.9
3	AC	62	LYS	2.9
3	BC	161	GLU	2.9
22	CA	2797	U	2.9

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Mol	Chain	Res	Type	RSRZ
25	CD	143	PRO	2.9
38	CR	112	LYS	2.9
43	CW	37	PRO	2.9
48	C1	12	LYS	2.9
34	CN	97	GLN	2.8
11	AK	43	GLY	2.8
33	DM	49	GLY	2.8
55	DI	46	ARG	2.8
2	BB	209	ALA	2.8
25	CD	132	ALA	2.8
33	CM	72	ALA	2.8
39	CS	42	ALA	2.8
43	CW	45	ASP	2.8
7	BG	67	GLU	2.8
22	CA	2660	A	2.8
24	CC	82	GLU	2.8
31	CK	12	LYS	2.8
51	C4	25	LYS	2.8
2	AB	201	PRO	2.8
1	AA	1132	C	2.8
14	AN	96	LEU	2.8
29	CH	118	PRO	2.8
55	DI	23	LEU	2.8
17	BQ	77	ARG	2.8
26	CE	79	ARG	2.8
3	BC	81	GLY	2.8
3	BC	97	VAL	2.8
3	BC	205	GLY	2.8
11	BK	43	GLY	2.8
21	BU	6	VAL	2.8
26	CE	52	VAL	2.8
26	CE	54	GLY	2.8
22	CA	1085	A	2.8
35	DO	13	ASN	2.8
2	AB	209	ALA	2.8
10	BJ	46	LYS	2.8
24	CC	2	ALA	2.8
26	CE	87	ALA	2.8
27	DF	78	LYS	2.8
29	CH	100	ALA	2.8
33	CM	133	ALA	2.8
1	BA	1264	U	2.8

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Mol	Chain	Res	Type	RSRZ
24	CC	103	TYR	2.8
38	CR	25	TYR	2.8
41	CU	48	GLN	2.8
7	AG	92	ARG	2.8
44	CX	74	PRO	2.8
3	AC	43	LEU	2.8
15	BO	70	LEU	2.8
22	CA	1729	U	2.8
37	CQ	97	LEU	2.8
49	C2	11	LEU	2.8
3	BC	159	GLY	2.8
28	CG	38	ASN	2.8
2	AB	92	VAL	2.8
19	AS	12	ASP	2.8
41	CU	31	VAL	2.8
1	AA	844	G	2.8
22	CA	273	G	2.8
7	AG	39	ALA	2.8
10	AJ	94	ALA	2.8
11	BK	110	ILE	2.8
24	CC	54	ILE	2.8
44	DX	84	ALA	2.8
52	C5	14	CYS	2.8
6	BF	46	GLN	2.8
26	CE	75	SER	2.8
36	CP	95	SER	2.8
1	BA	984	C	2.8
2	AB	193	PRO	2.8
22	CA	343	C	2.8
23	CB	30	C	2.8
5	AE	10	GLU	2.8
37	CQ	99	TYR	2.8
8	BH	31	LYS	2.8
9	AI	100	LYS	2.8
28	CG	27	LYS	2.8
52	C5	9	LYS	2.8
22	CA	178	G	2.8
33	DM	22	GLY	2.8
4	BD	68	LEU	2.8
32	CL	8	LEU	2.8
1	BA	1254	A	2.8
1	BA	1340	A	2.8

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Mol	Chain	Res	Type	RSRZ
22	CA	2171	A	2.8
3	AC	106	VAL	2.8
24	DC	195	VAL	2.8
43	CW	12	GLN	2.8
2	BB	160	ALA	2.8
3	BC	14	ILE	2.8
5	BE	69	ARG	2.8
11	AK	107	ILE	2.8
17	BQ	6	ARG	2.8
13	AM	30	SER	2.8
14	BN	80	SER	2.8
20	BT	26	SER	2.8
21	BU	4	ILE	2.8
31	CK	84	ILE	2.8
33	CM	2	ARG	2.8
52	C5	26	ILE	2.8
1	BA	1017	U	2.8
4	BD	148	LYS	2.8
33	CM	29	LYS	2.8
33	DM	64	PHE	2.8
11	BK	111	THR	2.8
22	CA	136	G	2.8
25	CD	23	PRO	2.8
26	CE	89	PRO	2.8
53	DA	1068	G	2.8
35	DO	20	MET	2.8
12	AL	73	ASN	2.8
14	BN	62	ASN	2.8
21	AU	13	ASP	2.8
25	CD	53	GLY	2.8
31	CK	60	ASP	2.8
33	CM	20	GLY	2.8
48	D1	6	ASN	2.8
24	DC	161	TYR	2.8
29	CH	25	TYR	2.8
1	BA	1327	C	2.8
22	CA	145	C	2.8
22	CA	1043	C	2.8
2	AB	19	GLN	2.8
22	CA	2585	U	2.8
31	CK	140	LEU	2.8
25	CD	77	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	BA	1133	G	2.8
3	BC	45	LYS	2.8
3	BC	76	VAL	2.8
9	AI	36	GLU	2.8
13	BM	103	LYS	2.8
26	CE	197	GLU	2.8
33	CM	70	LYS	2.8
37	CQ	37	LYS	2.8
22	CA	272	A	2.8
22	CA	892	A	2.8
38	CR	68	ALA	2.8
1	BA	1009	U	2.8
4	AD	30	THR	2.8
9	AI	51	PRO	2.8
29	CH	4	ILE	2.8
31	CK	50	THR	2.8
38	CR	74	ILE	2.8
2	AB	27	MET	2.8
2	BB	42	ASN	2.8
6	AF	80	PHE	2.8
20	AT	43	ASP	2.8
22	CA	268	C	2.8
22	CA	1064	C	2.8
39	DS	82	HIS	2.8
54	DD	136	ASN	2.8
16	BP	62	GLY	2.8
39	CS	6	GLN	2.8
1	AA	1035	A	2.8
22	CA	2309	A	2.8
29	CH	112	LYS	2.8
43	CW	25	LYS	2.8
53	DA	882	G	2.8
4	BD	171	LEU	2.8
22	CA	1728	C	2.8
7	BG	24	ALA	2.7
16	BP	43	ALA	2.7
25	CD	75	ALA	2.7
26	CE	86	ALA	2.7
29	DH	111	ALA	2.7
33	CM	131	ALA	2.7
38	CR	86	ALA	2.7
50	C3	40	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
52	C5	29	ALA	2.7
7	BG	89	VAL	2.7
11	BK	86	VAL	2.7
15	BO	27	VAL	2.7
25	CD	18	ASP	2.7
38	DR	31	VAL	2.7
29	DH	119	ASN	2.7
9	AI	43	THR	2.7
24	CC	9	THR	2.7
24	CC	219	THR	2.7
1	BA	988	G	2.7
1	BA	1309	G	2.7
1	BA	1316	G	2.7
11	BK	54	GLY	2.7
22	CA	88	G	2.7
22	CA	2163	A	2.7
22	CA	2172	U	2.7
31	CK	86	GLN	2.7
47	D0	32	ILE	2.7
26	CE	123	LYS	2.7
40	CT	28	LYS	2.7
40	CT	73	LYS	2.7
43	CW	41	GLU	2.7
23	CB	35	C	2.7
23	CB	58	A	2.7
24	CC	202	LEU	2.7
32	CL	33	ALA	2.7
40	CT	58	ALA	2.7
40	DT	89	ALA	2.7
54	DD	162	ALA	2.7
55	DI	44	ALA	2.7
22	CA	143	C	2.7
25	CD	24	VAL	2.7
26	CE	106	LYS	2.7
29	DH	115	VAL	2.7
35	DO	9	GLN	2.7
37	CQ	22	PRO	2.7
37	CQ	27	GLU	2.7
40	CT	9	HIS	2.7
48	C1	36	GLU	2.7
14	BN	13	ARG	2.7
29	CH	68	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
33	CM	94	THR	2.7
37	CQ	109	ARG	2.7
40	CT	26	GLY	2.7
40	CT	104	THR	2.7
45	CY	25	THR	2.7
51	C4	16	LYS	2.7
17	AQ	61	ILE	2.7
22	CA	1073	A	2.7
22	CA	1583	A	2.7
22	CA	2127	G	2.7
38	DR	61	TRP	2.7
25	CD	137	SER	2.7
33	DM	40	SER	2.7
8	BH	73	GLU	2.7
8	BH	18	GLN	2.7
6	BF	2	ARG	2.7
11	BK	82	LEU	2.7
20	AT	86	LEU	2.7
24	CC	24	LEU	2.7
26	DE	11	ALA	2.7
28	CG	89	LEU	2.7
28	DG	111	HIS	2.7
38	CR	14	HIS	2.7
40	DT	97	LEU	2.7
5	BE	102	GLY	2.7
38	DR	26	GLY	2.7
3	AC	151	VAL	2.7
24	DC	204	VAL	2.7
29	CH	44	ILE	2.7
33	CM	111	ILE	2.7
47	C0	5	ILE	2.7
2	BB	52	GLU	2.7
15	BO	26	GLU	2.7
18	AR	22	ASP	2.7
8	AH	49	PHE	2.7
39	CS	62	GLU	2.7
40	CT	2	GLU	2.7
44	CX	29	GLU	2.7
2	AB	122	GLN	2.7
5	BE	100	SER	2.7
19	AS	29	LYS	2.7
26	CE	185	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
27	CF	72	LYS	2.7
33	CM	17	LYS	2.7
20	BT	48	GLN	2.7
46	CZ	27	ASN	2.7
42	CV	7	ARG	2.7
4	AD	170	TRP	2.7
19	AS	34	TRP	2.7
15	BO	9	ALA	2.7
18	BR	62	ALA	2.7
20	BT	45	ALA	2.7
23	CB	114	C	2.7
24	CC	53	HIS	2.7
31	DK	77	HIS	2.7
51	C4	26	HIS	2.7
2	AB	219	ALA	2.7
3	AC	74	GLY	2.7
26	CE	76	PRO	2.7
33	DM	43	GLY	2.7
47	C0	42	PRO	2.7
55	DI	93	ALA	2.7
35	DO	100	CYS	2.7
5	BE	88	VAL	2.7
11	AK	16	VAL	2.7
12	BL	87	VAL	2.7
26	CE	96	VAL	2.7
28	CG	15	VAL	2.7
29	CH	146	VAL	2.7
40	CT	82	MET	2.7
42	CV	34	VAL	2.7
38	CR	22	LYS	2.7
45	CY	54	LYS	2.7
7	AG	10	ARG	2.7
8	BH	125	ILE	2.7
11	BK	17	SER	2.7
13	AM	45	ILE	2.7
17	AQ	11	ARG	2.7
20	AT	4	ILE	2.7
24	DC	272	SER	2.7
35	CO	30	ARG	2.7
43	CW	93	ARG	2.7
51	C4	32	ILE	2.7
11	AK	105	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
22	CA	1529	G	2.7
39	CS	53	PHE	2.7
39	DS	77	PHE	2.7
26	CE	29	HIS	2.7
25	CD	205	PRO	2.7
33	DM	34	GLY	2.7
7	BG	40	GLU	2.7
11	BK	68	GLU	2.7
27	DF	45	ALA	2.7
27	DF	75	ALA	2.7
35	CO	32	GLU	2.7
52	C5	5	ALA	2.7
3	BC	201	TRP	2.7
17	BQ	19	LYS	2.7
20	AT	49	LYS	2.7
25	CD	204	LYS	2.7
29	CH	71	LYS	2.7
10	AJ	22	THR	2.7
19	AS	31	LEU	2.7
19	BS	79	THR	2.7
24	CC	95	LEU	2.7
44	DX	21	LEU	2.7
38	DR	76	TYR	2.7
24	DC	6	CYS	2.7
24	DC	188	CYS	2.7
25	CD	164	GLN	2.7
25	CD	170	VAL	2.7
36	CP	43	ASN	2.7
40	CT	18	ARG	2.7
41	DU	92	ASN	2.7
54	DD	172	VAL	2.7
22	CA	1065	U	2.7
24	CC	178	SER	2.7
26	CE	70	SER	2.7
10	AJ	8	ILE	2.7
13	BM	91	HIS	2.7
16	BP	9	HIS	2.7
38	DR	17	ILE	2.7
54	DD	134	HIS	2.7
18	AR	35	GLU	2.7
32	DL	110	GLU	2.7
6	BF	56	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
14	BN	3	LYS	2.7
21	BU	19	PHE	2.7
33	CM	96	LYS	2.7
38	CR	93	LYS	2.7
38	DR	23	GLY	2.7
38	DR	36	PHE	2.7
1	BA	632	U	2.7
22	CA	1101	U	2.7
24	CC	155	ALA	2.7
22	CA	1452	G	2.7
9	BI	33	ARG	2.7
13	AM	113	ARG	2.7
24	CC	156	ARG	2.7
39	CS	78	ARG	2.7
7	AG	118	LEU	2.7
35	CO	107	ASN	2.7
55	DI	3	LEU	2.7
5	BE	25	VAL	2.6
24	CC	220	VAL	2.6
24	DC	137	VAL	2.6
25	CD	122	VAL	2.6
51	D4	51	SER	2.6
1	AA	89	U	2.6
1	BA	1341	U	2.6
2	BB	143	LYS	2.6
22	CA	2132	U	2.6
3	BC	57	ILE	2.6
7	BG	14	PRO	2.6
17	BQ	5	ILE	2.6
22	CA	289	G	2.6
36	CP	86	GLY	2.6
51	D4	56	GLY	2.6
24	CC	247	PRO	2.6
1	BA	1252	A	2.6
22	CA	2322	A	2.6
23	CB	119	A	2.6
7	BG	117	ALA	2.6
10	BJ	13	PHE	2.6
19	AS	32	ARG	2.6
36	CP	77	ALA	2.6
37	CQ	93	ARG	2.6
41	CU	35	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
54	DD	192	ALA	2.6
22	CA	1060	U	2.6
53	DA	884	U	2.6
8	BH	106	THR	2.6
32	CL	106	GLU	2.6
33	CM	136	GLU	2.6
39	CS	31	GLU	2.6
3	AC	178	LEU	2.6
7	BG	22	LEU	2.6
8	BH	40	LEU	2.6
14	AN	48	LEU	2.6
26	DE	10	SER	2.6
35	CO	6	SER	2.6
39	CS	24	LYS	2.6
41	CU	19	LYS	2.6
55	DI	30	SER	2.6
22	CA	2110	G	2.6
53	DA	2136	G	2.6
2	BB	70	VAL	2.6
4	BD	61	VAL	2.6
9	AI	19	VAL	2.6
31	CK	74	TYR	2.6
3	BC	3	GLN	2.6
3	BC	93	ASP	2.6
11	AK	92	GLY	2.6
24	CC	55	GLY	2.6
26	CE	81	GLY	2.6
53	DA	893	C	2.6
9	AI	45	ARG	2.6
32	CL	49	ARG	2.6
33	CM	47	ARG	2.6
48	C1	17	ARG	2.6
17	BQ	21	ILE	2.6
27	DF	85	ILE	2.6
32	CL	99	ILE	2.6
29	DH	148	ALA	2.6
51	C4	48	ALA	2.6
1	BA	1242	G	2.6
22	CA	653	U	2.6
33	CM	64	PHE	2.6
39	CS	35	PHE	2.6
22	CA	1861	G	2.6

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Mol	Chain	Res	Type	RSRZ
14	BN	6	MET	2.6
54	DD	151	THR	2.6
4	AD	138	SER	2.6
17	BQ	72	SER	2.6
22	CA	1531	C	2.6
2	AB	127	ASP	2.6
51	D4	57	LEU	2.6
26	CE	30	GLN	2.6
5	BE	108	GLY	2.6
5	BE	129	GLY	2.6
19	AS	26	GLY	2.6
24	DC	206	GLY	2.6
26	CE	49	ARG	2.6
38	CR	53	ARG	2.6
51	C4	8	ARG	2.6
54	DD	115	GLY	2.6
5	BE	50	TYR	2.6
8	BH	65	TYR	2.6
35	CO	116	VAL	2.6
53	DA	846	U	2.6
12	BL	18	LYS	2.6
14	BN	98	LYS	2.6
26	CE	60	TRP	2.6
26	CE	132	LYS	2.6
22	CA	2165	C	2.6
3	BC	160	ALA	2.6
24	DC	166	ALA	2.6
37	CQ	48	ILE	2.6
38	CR	9	ILE	2.6
1	BA	1007	U	2.6
3	BC	21	THR	2.6
14	BN	5	SER	2.6
20	BT	6	SER	2.6
20	BT	31	PHE	2.6
35	DO	119	SER	2.6
44	CX	45	PHE	2.6
54	DD	165	MET	2.6
18	BR	74	HIS	2.6
31	CK	49	ASP	2.6
1	AA	1036	A	2.6
21	BU	21	ARG	2.6
24	CC	101	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
34	CN	40	ARG	2.6
25	CD	17	GLU	2.6
8	AH	50	LYS	2.6
9	AI	68	LYS	2.6
22	CA	2129	C	2.6
24	CC	81	LEU	2.6
39	CS	73	LYS	2.6
46	CZ	2	LYS	2.6
51	C4	41	LYS	2.6
55	DI	41	LEU	2.6
16	BP	15	PRO	2.6
3	BC	90	VAL	2.6
5	AE	70	ASN	2.6
19	AS	58	VAL	2.6
1	BA	1042	A	2.6
6	BF	57	ALA	2.6
7	AG	127	ALA	2.6
21	AU	30	ALA	2.6
16	BP	42	ILE	2.6
18	AR	59	ILE	2.6
24	CC	135	ILE	2.6
22	CA	287	G	2.6
24	CC	173	THR	2.6
24	CC	238	ARG	2.6
24	DC	54	ILE	2.6
35	CO	113	ILE	2.6
38	DR	65	ILE	2.6
48	D1	5	GLN	2.6
3	BC	82	GLU	2.6
50	C3	41	ARG	2.6
54	DD	171	THR	2.6
14	BN	76	LYS	2.6
33	DM	50	PHE	2.6
34	CN	68	PHE	2.6
35	DO	21	PHE	2.6
3	AC	2	GLY	2.6
3	BC	43	LEU	2.6
13	AM	89	LEU	2.6
13	BM	112	PRO	2.6
29	CH	119	ASN	2.6
34	CN	78	LEU	2.6
35	CO	23	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
22	CA	144	A	2.6
53	DA	613	A	2.6
1	BA	473	U	2.6
1	BA	957	U	2.6
22	CA	2793	C	2.6
53	DA	1066	U	2.6
2	AB	113	ARG	2.6
2	AB	145	GLU	2.6
22	CA	93	G	2.6
7	AG	44	TYR	2.6
13	AM	11	ASP	2.6
13	BM	66	GLU	2.6
26	CE	195	GLN	2.6
26	CE	162	ARG	2.6
28	DG	166	ASP	2.6
54	DD	148	GLN	2.6
24	CC	52	ARG	2.6
19	AS	6	LYS	2.6
32	CL	114	LYS	2.6
35	CO	104	ALA	2.6
36	CP	23	ALA	2.6
38	CR	12	ALA	2.6
45	CY	2	SER	2.6
47	C0	12	SER	2.6
24	CC	51	THR	2.6
30	DJ	117	MET	2.6
32	CL	39	ILE	2.6
48	C1	43	ILE	2.6
1	AA	1009	U	2.6
26	CE	78	TRP	2.6
32	CL	15	GLY	2.6
51	C4	9	GLY	2.6
22	CA	1533	C	2.6
19	BS	9	PRO	2.6
6	BF	44	ARG	2.5
15	BO	74	ASP	2.5
26	CE	176	ASP	2.5
38	CR	60	LEU	2.6
51	C4	55	LEU	2.6
1	AA	88	U	2.5
39	CS	85	LYS	2.5
4	BD	25	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
25	CD	142	VAL	2.5
1	BA	1209	C	2.5
11	AK	73	ALA	2.5
13	BM	49	SER	2.5
22	CA	1045	C	2.5
33	CM	9	ALA	2.5
38	DR	21	ALA	2.5
54	DD	139	SER	2.5
2	AB	211	THR	2.5
6	BF	77	THR	2.5
22	CA	329	G	2.5
24	DC	56	GLY	2.5
14	AN	82	ILE	2.5
25	CD	58	ASN	2.5
1	BA	1212	U	2.5
37	CQ	11	GLU	2.5
1	AA	81	A	2.5
2	AB	64	LYS	2.5
2	BB	90	PHE	2.5
3	BC	18	TRP	2.5
2	AB	192	ASP	2.5
7	AG	143	ARG	2.5
36	CP	89	ASP	2.5
38	CR	102	ASP	2.5
40	CT	84	ARG	2.5
45	CY	3	ARG	2.5
48	C1	7	LYS	2.5
49	D2	30	LYS	2.5
5	BE	115	LEU	2.5
1	BA	212	G	2.5
1	BA	1358	U	2.5
22	CA	1459	G	2.5
53	DA	548	G	2.5
3	BC	66	VAL	2.5
5	AE	56	VAL	2.5
8	AH	25	VAL	2.5
28	CG	7	ALA	2.5
34	CN	26	VAL	2.5
34	CN	93	VAL	2.5
37	DQ	46	VAL	2.5
24	CC	42	GLY	2.5
7	AG	84	THR	2.5

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Mol	Chain	Res	Type	RSRZ
21	AU	43	THR	2.5
22	CA	1103	A	2.5
22	CA	2147	A	2.5
42	CV	90	GLY	2.5
24	DC	191	THR	2.5
36	CP	24	THR	2.5
37	CQ	115	ASN	2.5
31	DK	75	TYR	2.5
33	DM	58	TYR	2.5
45	CY	14	THR	2.5
1	BA	214	C	2.5
23	CB	38	C	2.5
40	CT	27	LYS	2.5
51	D4	64	TYR	2.5
21	BU	17	ARG	2.5
25	CD	141	ARG	2.5
10	AJ	39	PRO	2.5
24	CC	164	ILE	2.5
25	CD	2	ILE	2.5
29	DH	94	ILE	2.5
52	C5	23	ILE	2.5
22	CA	259	G	2.5
31	CK	4	PHE	2.5
34	CN	31	PHE	2.5
19	BS	35	SER	2.5
22	CA	897	C	2.5
22	CA	2795	C	2.5
22	CA	2131	U	2.5
24	CC	45	ASN	2.5
26	CE	47	LYS	2.5
38	DR	7	GLY	2.5
40	CT	6	LYS	2.5
46	DZ	4	LYS	2.5
47	C0	15	GLY	2.5
54	DD	158	GLY	2.5
2	AB	210	VAL	2.5
11	AK	56	ARG	2.5
24	CC	4	VAL	2.5
24	DC	156	ARG	2.5
25	CD	178	VAL	2.5
35	CO	18	GLN	2.5
42	CV	93	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
36	CP	31	THR	2.5
44	DX	41[A]	ARG	2.5
1	BA	1222	G	2.5
22	CA	2123	G	2.5
2	BB	48	PRO	2.5
30	DJ	109	ILE	2.5
2	AB	59	LYS	2.5
3	AC	86	LYS	2.5
14	AN	28	LYS	2.5
26	CE	110	SER	2.5
27	DF	114	PHE	2.5
35	CO	87	PHE	2.5
37	CQ	65	SER	2.5
48	D1	11	SER	2.5
49	C2	19	HIS	2.5
55	DI	24	SER	2.5
12	BL	46	ASN	2.5
1	BA	1278	G	2.5
8	BH	99	LEU	2.5
11	BK	19	GLY	2.5
22	CA	1105	U	2.5
22	CA	1743	G	2.5
33	CM	45	GLY	2.5
33	CM	88	GLY	2.5
36	CP	13	ARG	2.5
39	CS	79	ARG	2.5
46	CZ	52	ARG	2.5
46	DZ	62	GLY	2.5
53	DA	1173	U	2.5
53	DA	1731	G	2.5
3	BC	113	ALA	2.5
10	AJ	21	ALA	2.5
32	CL	37	ASP	2.5
40	CT	89	ALA	2.5
23	CB	49	C	2.5
3	AC	128	VAL	2.5
17	AQ	46	VAL	2.5
24	CC	216	VAL	2.5
31	DK	48	VAL	2.5
41	CU	86	THR	2.5
55	DI	80	THR	2.5
25	CD	88	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
32	CL	67	LYS	2.5
35	CO	42	LYS	2.5
44	CX	72	LYS	2.5
1	AA	1000	A	2.5
1	AA	1004	A	2.5
1	AA	1019	A	2.5
1	BA	461	A	2.5
20	BT	39	ILE	2.5
37	DQ	36	SER	2.5
44	DX	37	ILE	2.5
47	C0	34	HIS	2.5
14	BN	85	ARG	2.5
24	CC	177	ARG	2.5
35	CO	4	ARG	2.5
55	DI	6	GLN	2.5
26	CE	71	GLY	2.5
31	CK	89	PHE	2.5
31	DK	79	GLY	2.5
39	CS	77	PHE	2.5
54	DD	166	GLY	2.5
22	CA	1097	U	2.5
22	CA	2796	U	2.5
24	DC	105	LEU	2.5
31	CK	32	LEU	2.5
38	DR	42	ALA	2.5
39	CS	28	ALA	2.5
51	D4	55	LEU	2.5
21	BU	42	THR	2.5
24	DC	201	MET	2.5
25	CD	165	MET	2.5
7	AG	16	PRO	2.5
24	CC	248	TRP	2.5
37	CQ	29	LYS	2.5
54	DD	133	THR	2.5
38	CR	88	VAL	2.5
53	DA	2145	C	2.5
16	BP	18	GLN	2.5
21	BU	23	CYS	2.5
24	CC	188	CYS	2.5
1	BA	1321	U	2.5
2	BB	21	ARG	2.5
7	BG	95	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
17	BQ	47	HIS	2.5
22	CA	2118	U	2.5
11	AK	72	ASP	2.5
38	DR	47	TYR	2.5
2	AB	180	GLY	2.5
3	BC	9	GLY	2.5
3	BC	10	ILE	2.5
7	BG	12	ILE	2.5
9	AI	8	GLY	2.5
9	AI	92	GLU	2.5
12	BL	92	GLY	2.5
24	DC	12	GLY	2.5
25	CD	28	GLU	2.5
30	DJ	32	GLY	2.5
32	DL	77	ILE	2.5
44	DX	22	GLY	2.5
54	DD	163	GLY	2.5
52	C5	32	LYS	2.5
1	BA	1043	G	2.5
45	CY	69	ALA	2.5
46	CZ	51	ALA	2.5
3	BC	109	PRO	2.4
7	AG	133	THR	2.4
33	CM	6	LEU	2.4
33	DM	57	LEU	2.4
40	CT	72	THR	2.4
4	AD	25	VAL	2.4
5	BE	54	ARG	2.4
7	AG	75	VAL	2.4
11	AK	37	ARG	2.4
21	AU	45	ARG	2.4
25	CD	37	VAL	2.4
37	CQ	81	VAL	2.4
38	CR	6	ARG	2.4
6	BF	42	TRP	2.4
8	BH	21	ASN	2.4
24	CC	134	ASN	2.4
35	DO	11	ASN	2.4
37	CQ	31	TRP	2.4
9	AI	62	ASP	2.4
19	AS	25	SER	2.4
40	CT	81	SER	2.4

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Mol	Chain	Res	Type	RSRZ
42	CV	10	GLU	2.4
4	AD	24	GLY	2.4
11	BK	14	LYS	2.4
20	BT	71	LYS	2.4
22	CA	180	G	2.4
22	CA	1063	G	2.4
24	CC	99	GLY	2.4
5	BE	60	ILE	2.4
16	AP	27	ALA	2.4
24	CC	76	ALA	2.4
25	CD	209	ALA	2.4
26	CE	161	ALA	2.4
1	AA	1029	U	2.4
2	AB	125	THR	2.4
24	CC	11	PRO	2.4
25	CD	152	PRO	2.4
27	CF	139	PRO	2.4
32	CL	31	ARG	2.4
36	CP	15	ARG	2.4
49	C2	39	PHE	2.4
53	DA	2171	A	2.4
2	AB	51	ASN	2.4
2	BB	36	ASN	2.4
16	BP	74	LEU	2.4
16	BP	53	ASP	2.4
27	DF	147	ASP	2.4
43	CW	80	HIS	2.4
2	BB	115	LYS	2.4
3	AC	187	SER	2.4
16	BP	12	LYS	2.4
24	DC	228	VAL	2.4
55	DI	54	VAL	2.4
5	BE	44	GLY	2.4
48	D1	14	GLY	2.4
34	CN	92	TRP	2.4
53	DA	2170	A	2.4
2	AB	223	GLU	2.4
7	BG	21	GLU	2.4
9	BI	28	ILE	2.4
11	AK	98	ARG	2.4
11	BK	121	CYS	2.4
36	CP	8	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
48	D1	10	ARG	2.4
2	AB	61	ALA	2.4
22	CA	548	G	2.4
22	CA	1106	G	2.4
23	CB	54	G	2.4
26	CE	39	ALA	2.4
29	DH	23	ALA	2.4
38	DR	38	ALA	2.4
51	C4	27	ALA	2.4
9	BI	60	LYS	2.4
9	BI	115	LYS	2.4
12	BL	58	THR	2.4
24	CC	18	LYS	2.4
24	DC	218	PRO	2.4
25	CD	126	ASN	2.4
26	CE	53	THR	2.4
31	DK	78	THR	2.4
34	DN	82	MET	2.4
40	DT	87	PRO	2.4
44	CX	24	LYS	2.4
47	C0	40	ASP	2.4
51	C4	63	PRO	2.4
4	AD	182	PHE	2.4
11	AK	61	PHE	2.4
26	DE	85	PHE	2.4
39	CS	82	HIS	2.4
50	D3	5	PHE	2.4
55	DI	69	PHE	2.4
8	BH	92	LEU	2.4
12	BL	7	LEU	2.4
35	CO	65	LEU	2.4
35	DO	44	LEU	2.4
22	CA	1730	C	2.4
24	CC	241	GLY	2.4
48	C1	14	GLY	2.4
51	D4	53	GLY	2.4
53	DA	357	C	2.4
31	CK	73	VAL	2.4
40	CT	20	VAL	2.4
40	CT	47	VAL	2.4
2	AB	222	ARG	2.4
5	BE	145	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
16	BP	25	ARG	2.4
22	CA	2102	G	2.4
34	CN	6	ARG	2.4
49	C2	51	GLU	2.4
48	D1	7	LYS	2.4
1	AA	1037	C	2.4
2	AB	76	ALA	2.4
16	AP	79	ASN	2.4
29	DH	20	ASN	2.4
17	BQ	38	ILE	2.4
22	CA	314	C	2.4
22	CA	351	C	2.4
22	CA	898	C	2.4
35	CO	108	ALA	2.4
35	DO	108	ALA	2.4
39	DS	74	ILE	2.4
49	C2	41	PRO	2.4
51	D4	10	ALA	2.4
32	CL	7	MET	2.4
34	CN	82	MET	2.4
53	DA	140	C	2.4
24	CC	230	HIS	2.4
45	CY	5	CYS	2.4
2	BB	50	PHE	2.4
3	BC	154	SER	2.4
9	BI	96	SER	2.4
22	CA	2130	U	2.4
21	AU	37	PHE	2.4
1	BA	973	G	2.4
5	BE	36	LEU	2.4
9	AI	87	LEU	2.4
20	AT	40	GLU	2.4
25	CD	4	LEU	2.4
29	CH	76	GLU	2.4
33	DM	65	GLY	2.4
35	CO	93	GLY	2.4
14	BN	90	ARG	2.4
19	AS	56	GLN	2.4
9	BI	100	LYS	2.4
10	BJ	82	LYS	2.4
16	BP	36	VAL	2.4
34	CN	133	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
40	CT	83	LYS	2.4
40	DT	50	VAL	2.4
54	DD	170	VAL	2.4
14	AN	38	ASP	2.4
2	BB	93	ASN	2.4
54	DD	167	ASN	2.4
2	AB	48	PRO	2.4
5	BE	110	ALA	2.4
38	CR	118	ALA	2.4
5	AE	24	THR	2.4
22	CA	1177	G	2.4
22	CA	1530	G	2.4
14	AN	55	SER	2.4
18	AR	21	ILE	2.4
19	BS	34	TRP	2.4
38	CR	32	TYR	2.4
49	C2	9	ILE	2.4
2	AB	89	GLN	2.4
5	AE	79	GLY	2.4
10	AJ	20	GLN	2.4
11	AK	38	GLN	2.4
27	DF	178	ARG	2.4
33	DM	31	GLY	2.4
51	C4	53	GLY	2.4
53	DA	358	U	2.4
21	BU	54	LYS	2.4
31	CK	23	LYS	2.4
31	CK	61	LYS	2.4
11	BK	18	ASP	2.4
26	DE	7	ASP	2.4
3	AC	66	VAL	2.4
17	AQ	78	VAL	2.4
24	CC	17	VAL	2.4
25	CD	172	VAL	2.4
6	BF	3	HIS	2.4
3	BC	48	ALA	2.4
9	BI	78	ALA	2.4
24	DC	208	ALA	2.4
3	BC	89	LYS	2.4
24	CC	50	THR	2.4
26	DE	84	THR	2.4
31	CK	69	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
31	CK	78	THR	2.4
34	DN	18[A]	ARG	2.4
35	DO	15	SER	2.4
38	CR	51	ARG	2.4
50	C3	19	ARG	2.4
50	C3	38	GLY	2.4
4	BD	132	ILE	2.4
38	DR	62	ILE	2.4
1	BA	1364	U	2.4
22	CA	2423	U	2.4
31	CK	44	TYR	2.4
1	BA	81	A	2.3
1	BA	1275	A	2.3
1	BA	1294	G	2.4
1	BA	1305	G	2.4
10	BJ	63	ASP	2.4
25	CD	39	ASP	2.4
1	BA	1397	C	2.3
22	CA	1532	A	2.3
22	CA	1582	C	2.3
34	CN	124	LEU	2.3
35	CO	13	ASN	2.3
38	CR	57	PHE	2.3
51	D4	14	PHE	2.3
20	AT	53	GLU	2.3
29	CH	87	GLU	2.3
2	BB	163	VAL	2.3
5	BE	123	VAL	2.3
6	BF	64	VAL	2.3
14	AN	12	LYS	2.3
14	AN	84	VAL	2.3
17	AQ	13	VAL	2.3
22	CA	290	U	2.3
22	CA	1412	U	2.3
25	CD	116	LYS	2.3
25	CD	189	VAL	2.3
25	CD	203	VAL	2.3
32	CL	24	VAL	2.3
29	CH	50	ARG	2.3
38	CR	3	ARG	2.3
24	CC	166	ALA	2.3
31	DK	108	MET	2.3

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Mol	Chain	Res	Type	RSRZ
22	CA	1088	A	2.3
34	CN	107	GLY	2.3
45	DY	15	GLY	2.3
50	C3	4	THR	2.3
50	C3	17	GLY	2.3
7	BG	113	ASP	2.3
5	AE	60	ILE	2.3
5	BE	72	ILE	2.3
40	CT	55	ILE	2.3
16	BP	17	TYR	2.3
33	CM	58	TYR	2.3
7	AG	66	LEU	2.3
25	CD	80	TRP	2.3
9	BI	99	ARG	2.3
10	AJ	4	GLN	2.3
16	BP	32	PHE	2.3
24	CC	63	ARG	2.3
22	CA	345	A	2.3
31	CK	113	PRO	2.3
35	CO	3	HIS	2.3
51	D4	2	PRO	2.3
3	AC	91	VAL	2.3
11	BK	129	VAL	2.3
20	BT	35	VAL	2.3
25	CD	107	VAL	2.3
35	DO	47	VAL	2.3
44	DX	23	VAL	2.3
2	AB	121	SER	2.3
15	BO	13	SER	2.3
49	C2	14	SER	2.3
53	DA	1061	U	2.3
5	AE	99	ALA	2.3
6	BF	27	ALA	2.3
10	AJ	88	MET	2.3
24	CC	235	GLY	2.3
24	DC	235	GLY	2.3
26	CE	152	GLU	2.3
26	DE	87	ALA	2.3
27	DF	43	ALA	2.3
34	CN	29	GLY	2.3
35	CO	1	MET	2.3
42	CV	64	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
42	DV	51	ALA	2.3
55	DI	14	GLU	2.3
39	DS	81	LYS	2.3
1	BA	83	C	2.3
22	CA	320	A	2.3
22	CA	1727	C	2.3
11	BK	56	ARG	2.3
22	CA	358	U	2.3
44	CX	11	ARG	2.3
6	BF	58	HIS	2.3
38	CR	24	TYR	2.3
3	AC	47	LEU	2.3
12	BL	90	LEU	2.3
45	CY	33	LEU	2.3
21	BU	24	GLU	2.3
46	DZ	8	GLU	2.3
3	BC	187	SER	2.3
24	CC	88	SER	2.3
6	AF	103	VAL	2.3
25	CD	3	GLY	2.3
28	DG	10	VAL	2.3
29	DH	110	VAL	2.3
35	DO	26	GLY	2.3
3	BC	134	MET	2.3
8	AH	31	LYS	2.3
16	BP	1	MET	2.3
19	AS	75	ALA	2.3
22	CA	101	A	2.3
22	CA	278	A	2.3
39	CS	58	VAL	2.3
53	DA	2182	U	2.3
35	DO	19	ALA	2.3
38	CR	19	LYS	2.3
43	CW	71	LYS	2.3
51	C4	12	LYS	2.3
52	C5	18	LYS	2.3
2	AB	146	ASN	2.3
22	CA	1546	G	2.3
38	DR	37	GLN	2.3
1	BA	479	U	2.3
2	BB	173	ILE	2.3
6	BF	33	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
10	AJ	27	GLU	2.3
22	CA	1742	U	2.3
53	DA	2131	U	2.3
24	CC	58	HIS	2.3
40	CT	60	HIS	2.3
40	DT	103	ILE	2.3
52	D5	26	ILE	2.3
25	CD	43	ASP	2.3
15	AO	69	TYR	2.3
33	CM	34	GLY	2.3
33	CM	139	GLY	2.3
37	CQ	38	LYS	2.3
3	AC	37	PHE	2.3
22	CA	1724	G	2.3
22	CA	1875	G	2.3
2	AB	70	VAL	2.3
3	BC	173	VAL	2.3
3	BC	195	VAL	2.3
9	AI	111	VAL	2.3
22	CA	1486	U	2.3
16	AP	63	GLN	2.3
24	DC	263	THR	2.3
26	DE	43	THR	2.3
45	CY	27	ARG	2.3
48	C1	9	THR	2.3
54	DD	129	THR	2.3
53	DA	2173	A	2.3
31	CK	80	HIS	2.3
4	AD	148	LYS	2.3
22	CA	360	U	2.3
34	CN	62	LYS	2.3
46	CZ	44	LYS	2.3
51	C4	39	LYS	2.3
51	D4	5	LYS	2.3
53	DA	285	G	2.3
53	DA	545	U	2.3
53	DA	1078	U	2.3
54	DD	154	LYS	2.3
3	AC	14	ILE	2.3
2	AB	65	GLY	2.3
3	BC	2	GLY	2.3
11	BK	90	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
54	DD	195	GLY	2.3
11	BK	109	ASN	2.3
1	BA	1004	A	2.3
1	BA	1236	A	2.3
3	BC	59	ARG	2.3
22	CA	1496	A	2.3
29	CH	30	LEU	2.3
16	BP	7	ALA	2.3
18	BR	27	ALA	2.3
24	CC	89	ALA	2.3
28	DG	13	ALA	2.3
38	CR	36	PHE	2.3
51	D4	22	PHE	2.3
2	AB	196	VAL	2.3
5	AE	88	VAL	2.3
15	AO	22	THR	2.3
25	CD	193	VAL	2.3
43	CW	65	VAL	2.3
44	CX	51	VAL	2.3
1	BA	844	G	2.3
10	AJ	82	LYS	2.3
40	CT	70	LYS	2.3
2	AB	194	ASP	2.3
17	AQ	47	HIS	2.3
31	CK	132	HIS	2.3
22	CA	2183	A	2.3
53	DA	1088	A	2.3
5	AE	57	PRO	2.3
22	CA	1061	U	2.3
9	BI	80	ARG	2.3
14	BN	66	GLN	2.3
39	CS	7	SER	2.3
48	C1	16	ARG	2.3
48	C1	47	GLY	2.3
1	AA	1134	G	2.2
22	CA	308	G	2.2
22	CA	2186	G	2.2
18	AR	29	LEU	2.2
29	DH	8	LYS	2.2
32	DL	32	TYR	2.2
33	CM	138	ALA	2.2
34	CN	94	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
50	D3	1	MET	2.2
1	BA	250	A	2.2
11	AK	46	THR	2.2
11	BK	96	THR	2.2
22	CA	1077	A	2.2
26	DE	13	THR	2.2
37	DQ	60	THR	2.2
12	BL	79	VAL	2.2
27	DF	74	VAL	2.2
45	CY	51	VAL	2.2
2	AB	78	GLU	2.2
4	AD	146	ARG	2.2
37	CQ	21	ARG	2.2
8	BH	53	GLY	2.2
8	BH	68	GLY	2.2
28	DG	82	GLY	2.2
48	C1	6	ASN	2.2
1	BA	1134	G	2.2
22	CA	1224	U	2.2
1	AA	207	C	2.2
1	BA	1263	C	2.2
25	CD	7	LYS	2.2
29	CH	83	LYS	2.2
43	CW	53	LYS	2.2
2	AB	207	ILE	2.2
25	CD	22	ILE	2.2
27	DF	2	ALA	2.2
19	AS	63	THR	2.2
44	CX	59	LEU	2.2
48	D1	22	LEU	2.2
1	AA	1010	U	2.2
1	BA	956	U	2.2
2	AB	184	PHE	2.2
23	CB	40	U	2.2
48	C1	48	TYR	2.2
8	BH	34	VAL	2.2
10	BJ	62	ARG	2.2
13	AM	87	ARG	2.2
17	AQ	79	VAL	2.2
24	CC	153	GLN	2.2
24	DC	221	ARG	2.2
1	AA	1441	A	2.2

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Mol	Chain	Res	Type	RSRZ
1	BA	1317	C	2.2
22	CA	163	C	2.2
22	CA	1046	A	2.2
22	CA	1590	A	2.2
22	CA	2300	C	2.2
24	CC	20	VAL	2.2
35	CO	8	ARG	2.2
37	CQ	113	ARG	2.2
2	AB	174	LYS	2.2
4	AD	46	PRO	2.2
10	AJ	43	PRO	2.2
24	CC	12	GLY	2.2
24	DC	111	LYS	2.2
33	DM	44	GLY	2.2
44	DX	42	GLY	2.2
48	D1	57	LYS	2.2
4	AD	29	ASP	2.2
10	BJ	19	ASP	2.2
29	CH	101	ASP	2.2
22	CA	2114	A	2.2
22	CA	2135	A	2.2
22	CA	2143	C	2.2
31	DK	9	GLU	2.2
53	DA	2128	G	2.2
10	AJ	83	THR	2.2
14	BN	59	ARG	2.2
15	BO	72	ARG	2.2
18	BR	48	ARG	2.2
26	CE	170	ARG	2.2
37	CQ	49	ALA	2.2
44	DX	18	ALA	2.2
31	CK	30	THR	2.2
47	D0	10	THR	2.2
3	BC	124	LEU	2.2
4	BD	199	LEU	2.2
18	AR	55	LEU	2.2
37	CQ	94	LYS	2.2
44	DX	59	LEU	2.2
25	CD	136	ASN	2.2
51	C4	3	LYS	2.2
2	BB	92	VAL	2.2
3	BC	23	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
10	AJ	65	TYR	2.2
41	CU	84	TYR	2.2
16	AP	78	VAL	2.2
24	CC	41	GLY	2.2
26	DE	56	GLY	2.2
31	CK	51	GLY	2.2
33	CM	110	VAL	2.2
37	CQ	61	VAL	2.2
44	DX	38	VAL	2.2
45	CY	7	VAL	2.2
13	AM	54	ASP	2.2
13	AM	82	ASP	2.2
22	CA	366	C	2.2
28	DG	47	ASP	2.2
43	DW	66	ASP	2.2
6	AF	98	GLU	2.2
53	DA	2183	A	2.2
2	BB	137	ARG	2.2
2	BB	227	GLN	2.2
3	AC	88	ARG	2.2
18	AR	43	ARG	2.2
20	AT	61	GLN	2.2
4	AD	177	LYS	2.2
5	BE	126	LYS	2.2
12	BL	77	HIS	2.2
35	CO	16	HIS	2.2
42	CV	4	LYS	2.2
54	DD	123	LYS	2.2
5	BE	148	ASN	2.2
13	AM	2	ALA	2.2
37	DQ	49	ALA	2.2
26	CE	65	THR	2.2
49	D2	48	ILE	2.2
1	BA	161	A	2.2
11	BK	78	GLY	2.2
22	CA	63	A	2.2
22	CA	336	C	2.2
1	BA	1002	G	2.2
1	BA	1010	U	2.2
10	AJ	71	LEU	2.2
10	BJ	42	LEU	2.2
22	CA	1551	A	2.2

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Mol	Chain	Res	Type	RSRZ
34	DN	95	LEU	2.2
1	BA	1139	G	2.2
5	BE	32	SER	2.2
35	CO	101	GLY	2.2
22	CA	2304	G	2.2
31	CK	8	PRO	2.2
38	DR	57	PHE	2.2
43	CW	59	GLU	2.2
2	AB	38	VAL	2.2
3	BC	200	VAL	2.2
13	AM	64	VAL	2.2
55	DI	108	VAL	2.2
2	BB	19	GLN	2.2
2	BB	59	LYS	2.2
7	AG	53	ARG	2.2
11	BK	64	GLN	2.2
17	BQ	30	LYS	2.2
27	DF	95	ARG	2.2
28	CG	160	LYS	2.2
33	CM	36	LYS	2.2
33	CM	41	ARG	2.2
37	CQ	87	LYS	2.2
39	DS	79	ARG	2.2
40	CT	11	ARG	2.2
48	D1	13	ARG	2.2
54	DD	124	ARG	2.2
1	BA	975	A	2.2
22	CA	153	U	2.2
53	DA	897	C	2.2
15	BO	51	HIS	2.2
24	CC	15	HIS	2.2
1	BA	1331	G	2.2
16	BP	27	ALA	2.2
22	CA	619	G	2.2
23	CB	51	G	2.2
29	DH	106	ALA	2.2
34	CN	113	ALA	2.2
35	CO	19	ALA	2.2
51	D4	37	ALA	2.2
4	AD	172	GLU	2.2
27	CF	140	GLU	2.2
31	DK	107	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
35	CO	49	GLU	2.2
18	BR	44	ILE	2.2
32	DL	2	ILE	2.2
33	CM	23	ILE	2.2
35	CO	75	ILE	2.2
35	CO	105	GLY	2.2
24	CC	38	SER	2.2
3	BC	115	LEU	2.2
12	BL	28	PRO	2.2
15	BO	85	LEU	2.2
31	DK	109	LEU	2.2
35	DO	38	LEU	2.2
50	D3	42	LEU	2.2
1	BA	87	C	2.2
1	BA	1137	C	2.2
2	BB	120	GLN	2.2
11	BK	98	ARG	2.2
25	CD	124	ARG	2.2
31	CK	35	ARG	2.2
35	CO	99	LYS	2.2
24	CC	137	VAL	2.2
31	CK	105	VAL	2.2
31	DK	119	PHE	2.2
33	CM	50	PHE	2.2
33	DM	46	VAL	2.2
34	DN	93	VAL	2.2
35	CO	67	PHE	2.2
37	CQ	28	VAL	2.2
1	BA	144	G	2.2
1	BA	1015	G	2.2
22	CA	1062	G	2.2
53	DA	2102	G	2.2
3	BC	19	ASN	2.2
6	BF	11	HIS	2.2
8	AH	38	ASN	2.2
5	AE	65	GLU	2.2
40	CT	52	GLU	2.2
48	D1	15	MET	2.2
3	BC	61	ALA	2.2
24	CC	47	GLY	2.2
26	CE	84	THR	2.2
26	DE	86	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
35	CO	91	ALA	2.2
44	DX	10	THR	2.2
49	D2	4	GLY	2.2
51	D4	11	ALA	2.2
2	AB	28	LYS	2.2
15	BO	2	SER	2.2
24	CC	36	LYS	2.2
54	DD	159	LYS	2.2
3	AC	169	ARG	2.2
7	BG	93	PRO	2.2
24	DC	11	PRO	2.2
37	CQ	10	GLN	2.1
37	CQ	103	ARG	2.2
8	BH	75	ILE	2.1
17	AQ	38	ILE	2.1
20	AT	67	ILE	2.1
17	AQ	75	LEU	2.1
29	DH	6	LEU	2.1
31	DK	36	LEU	2.1
5	AE	114	VAL	2.1
14	AN	20	TYR	2.1
22	CA	1052	C	2.1
24	CC	62	TYR	2.1
32	CL	79	PHE	2.1
33	DM	66	PHE	2.1
52	C5	11	CYS	2.1
53	DA	1728	C	2.1
1	AA	121	U	2.1
5	BE	14	LYS	2.1
40	CT	86	MET	2.1
1	BA	1255	G	2.1
2	BB	176	ALA	2.1
3	BC	72	ARG	2.1
4	BD	2	ALA	2.1
9	AI	33	ARG	2.1
21	AU	18	ARG	2.1
24	CC	190	ALA	2.1
31	DK	112	GLY	2.1
32	CL	81	GLY	2.1
33	DM	21	ARG	2.1
38	CR	73	GLY	2.1
39	DS	78	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	BA	1332	A	2.1
5	AE	162	GLU	2.1
15	AO	6	GLU	2.1
53	DA	2177	C	2.1
4	BD	64	ILE	2.1
5	BE	16	ILE	2.1
24	CC	267	ILE	2.1
32	CL	95	ILE	2.1
53	DA	1070	A	2.1
1	BA	989	U	2.1
10	AJ	90	LEU	2.1
11	BK	81	ASN	2.1
32	CL	9	ASN	2.1
35	CO	54	LEU	2.1
55	DI	60	LEU	2.1
35	DO	16	HIS	2.1
5	BE	114	VAL	2.1
6	AF	89	VAL	2.1
19	AS	67	VAL	2.1
23	CB	9	G	2.1
38	DR	8	VAL	2.1
24	CC	43	ARG	2.1
24	CC	133	ARG	2.1
24	DC	240	PHE	2.1
1	BA	271	C	2.1
24	CC	171	TYR	2.1
40	CT	88	ARG	2.1
50	C3	34	ARG	2.1
22	CA	2111	U	2.1
52	C5	1	MET	2.1
3	AC	61	ALA	2.1
8	BH	43	GLU	2.1
14	BN	88	ALA	2.1
20	AT	37	ALA	2.1
26	DE	50	ALA	2.1
35	DO	25	ALA	2.1
37	CQ	95	ALA	2.1
37	CQ	104	THR	2.1
38	DR	63	ALA	2.1
2	AB	115	LYS	2.1
22	CA	1733	G	2.1
24	CC	37	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
39	CS	71	LYS	2.1
49	C2	25	LYS	2.1
1	BA	4	U	2.1
1	BA	1313	U	2.1
3	BC	182	ILE	2.1
9	BI	107	ASP	2.1
24	CC	104	ILE	2.1
31	CK	76	HIS	2.1
1	BA	78	A	2.1
2	AB	161	LEU	2.1
13	AM	93	ARG	2.1
22	CA	1383	A	2.1
38	DR	28	ARG	2.1
41	DU	69	ARG	2.1
6	BF	68	GLN	2.1
15	AO	60	VAL	2.1
17	BQ	76	VAL	2.1
37	CQ	86	VAL	2.1
37	DQ	47	VAL	2.1
39	CS	4	VAL	2.1
44	CX	42	GLY	2.1
46	CZ	53	VAL	2.1
51	C4	51	SER	2.1
1	BA	1307	U	2.1
24	DC	158	ALA	2.1
37	CQ	18	PRO	2.1
22	CA	1420	A	2.1
40	CT	40	ASN	2.1
2	BB	95	ARG	2.1
11	AK	69	ARG	2.1
18	BR	57	ARG	2.1
9	BI	5	GLN	2.1
1	BA	1008	U	2.1
3	AC	207	ILE	2.1
3	BC	75	ILE	2.1
6	AF	36	ILE	2.1
12	BL	82	ILE	2.1
24	DC	91	ILE	2.1
40	DT	96	ILE	2.1
51	D4	32	ILE	2.1
1	BA	1208	C	2.1
12	BL	84	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
24	DC	41	GLY	2.1
26	DE	64	GLY	2.1
31	DK	82	GLY	2.1
31	DK	83	GLY	2.1
33	DM	19	LEU	2.1
22	CA	2801	G	2.1
53	DA	1062	G	2.1
53	DA	2186	G	2.1
1	BA	1324	A	2.1
15	BO	73	LYS	2.1
22	CA	74	A	2.1
37	DQ	26	VAL	2.1
39	CS	81	LYS	2.1
39	DS	76	LYS	2.1
47	D0	3[A]	LYS	2.1
48	C1	11	SER	2.1
50	C3	8	SER	2.1
24	DC	225	MET	2.1
29	DH	121	VAL	2.1
11	BK	105	PHE	2.1
1	BA	89	U	2.1
11	AK	81	ASN	2.1
13	AM	15	ALA	2.1
22	CA	2833	U	2.1
24	DC	106	ALA	2.1
36	DP	57	ALA	2.1
38	DR	12	ALA	2.1
40	DT	80	PRO	2.1
31	CK	5	THR	2.1
54	DD	126	ASN	2.1
7	AG	60	GLU	2.1
24	CC	214	ARG	2.1
24	DC	60	GLN	2.1
22	CA	1048	A	2.1
1	BA	1023	U	2.1
3	BC	150	LYS	2.1
22	CA	545	U	2.1
26	DE	82	GLY	2.1
31	CK	72	LYS	2.1
35	DO	101	GLY	2.1
53	DA	355	U	2.1
7	AG	37	SER	2.1

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Mol	Chain	Res	Type	RSRZ
12	BL	24	LEU	2.1
24	CC	110	LEU	2.1
24	CC	259	SER	2.1
32	CL	47	ILE	2.1
33	CM	25	SER	2.1
8	BH	95	VAL	2.1
9	AI	47	VAL	2.1
10	AJ	78	GLU	2.1
16	BP	79	ASN	2.1
17	BQ	66	PRO	2.1
43	CW	69	GLU	2.1
44	CX	76	ASN	2.1
12	AL	2	ALA	2.1
19	AS	55	ARG	2.1
20	AT	45	ALA	2.1
22	CA	147	C	2.1
46	CZ	12	GLU	2.1
27	DF	155	THR	2.1
35	DO	122	ALA	2.1
48	C1	50	ARG	2.1
53	DA	1075	C	2.1
24	DC	219	THR	2.1
25	CD	91	THR	2.1
55	DI	10	ALA	2.1
1	BA	1003	G	2.1
16	AP	16	PHE	2.1
3	BC	190	HIS	2.1
22	CA	2735	G	2.1
5	AE	128	TYR	2.1
8	BH	50	LYS	2.1
11	BK	126	LYS	2.1
24	DC	248	TRP	2.1
34	CN	64	TRP	2.1
33	CM	22	GLY	2.1
42	CV	23	GLY	2.1
43	DW	67	GLY	2.1
1	AA	210	C	2.1
6	BF	98	GLU	2.0
8	BH	52	GLU	2.0
25	CD	174	SER	2.0
29	CH	114	GLU	2.0
33	DM	42	SER	2.0

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Mol	Chain	Res	Type	RSRZ
53	DA	142	A	2.0
1	AA	204	G	2.0
5	AE	134	ILE	2.0
6	BF	36	ILE	2.0
9	AI	49	ARG	2.0
10	AJ	67	ILE	2.0
11	AK	18	ASP	2.0
11	BK	72	ASP	2.0
24	CC	130	LEU	2.0
24	DC	49	ILE	2.0
25	CD	146	ILE	2.0
27	DF	26	MET	2.0
31	CK	25	LEU	2.0
38	CR	83	LEU	2.0
38	DR	30	ARG	2.0
47	D0	14	ILE	2.0
3	AC	98	PRO	2.0
10	AJ	99	GLN	2.0
37	CQ	41	GLN	2.0
5	BE	35	ALA	2.0
7	BG	100	ALA	2.0
10	BJ	50	THR	2.0
18	BR	40	VAL	2.0
24	CC	263	THR	2.0
24	DC	173	THR	2.0
31	CK	121	LYS	2.0
33	CM	13	LYS	2.0
34	CN	5	LYS	2.0
37	CQ	70	VAL	2.0
44	CX	66	LYS	2.0
50	C3	44	VAL	2.0
22	CA	357	C	2.0
53	DA	885	C	2.0
53	DA	1076	C	2.0
1	BA	1005	A	2.0
24	CC	196	GLY	2.0
33	DM	24	GLY	2.0
37	CQ	45	GLY	2.0
55	DI	65	GLU	2.0
2	BB	153	ASP	2.0
12	BL	54	ARG	2.0
39	CS	21	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
45	DY	18	ARG	2.0
35	DO	109	PRO	2.0
1	BA	1167	A	2.0
6	BF	47	LEU	2.0
15	BO	57	LEU	2.0
17	AQ	8	LEU	2.0
17	BQ	33	ILE	2.0
40	DT	74	ILE	2.0
40	DT	86	MET	2.0
51	D4	44	LEU	2.0
53	DA	2184	A	2.0
24	DC	224	ALA	2.0
25	CD	110	THR	2.0
26	CE	68	ALA	2.0
34	CN	132	THR	2.0
38	CR	21	ALA	2.0
41	CU	38	ALA	2.0
43	DW	94	ALA	2.0
45	CY	24	ALA	2.0
1	BA	202	G	2.0
8	AH	39	VAL	2.0
22	CA	1587	G	2.0
28	DG	17	VAL	2.0
49	C2	7	GLU	2.0
16	BP	38	PHE	2.0
24	DC	233	GLY	2.0
32	CL	18	ARG	2.0
33	DM	32	GLY	2.0
1	BA	841	C	2.0
2	BB	86	SER	2.0
5	BE	92	SER	2.0
12	BL	78	SER	2.0
14	AN	58	SER	2.0
23	CB	3	C	2.0
28	DG	16	ASP	2.0
24	DC	40	SER	2.0
26	CE	130	LYS	2.0
33	DM	29	LYS	2.0
53	DA	547	A	2.0
22	CA	1466	U	2.0
31	DK	110	PRO	2.0
2	BB	94	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
3	BC	176	HIS	2.0
5	AE	163	GLU	2.0
21	AU	44	GLU	2.0
22	CA	2133	G	2.0
32	DL	7	MET	2.0
53	DA	359	G	2.0
2	BB	172	ALA	2.0
9	AI	16	ALA	2.0
16	AP	4	ILE	2.0
24	DC	116	ILE	2.0
24	DC	155	ALA	2.0
31	DK	117	ALA	2.0
33	CM	97	ALA	2.0
40	CT	64	ALA	2.0
50	C3	24	THR	2.0
50	D3	31	LEU	2.0
51	C4	11	ALA	2.0
51	C4	33	LEU	2.0
55	DI	2	ALA	2.0
3	AC	72	ARG	2.0
5	BE	18	VAL	2.0
9	AI	119	ARG	2.0
10	AJ	7	ARG	2.0
21	AU	33	ARG	2.0
21	BU	47	ARG	2.0
5	BE	119	GLY	2.0
13	AM	99	GLY	2.0
22	CA	89	A	2.0
24	CC	168	ASP	2.0
28	DG	113	VAL	2.0
28	DG	170	ARG	2.0
26	DE	71	GLY	2.0
35	DO	5	LYS	2.0
47	C0	57	VAL	2.0
48	D1	16	ARG	2.0
38	CR	16	LYS	2.0
51	D4	58	VAL	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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
22	1MG	CA	745	24/25	0.88	0.18	-	85,88,93,95	0
53	G7M	DA	2069	24/25	0.97	0.24	-	34,38,43,43	0
1	5MC	BA	967	21/22	0.85	0.15	-	127,132,143,145	0
22	PSU	CA	2605	20/21	0.92	0.17	-	71,79,82,83	0
1	4OC	BA	1402	22/23	0.90	0.18	-	82,86,90,90	0
1	MA6	BA	1518	24/25	0.92	0.15	-	68,73,78,85	0
53	H2U	DA	2449	20/21	0.99	0.24	-	26,32,38,42	0
1	G7M	AA	527	24/25	0.94	0.15	-	64,66,70,75	0
1	MA6	BA	1519	24/25	0.89	0.19	-	67,73,79,81	0
1	2MG	AA	966	24/25	0.94	0.14	-	69,75,80,83	0
53	PSU	DA	2580	20/21	0.98	0.24	-	27,32,38,42	0
22	6MZ	CA	1618	23/24	0.83	0.16	-	91,97,99,100	0
1	2MG	BA	1516	24/25	0.85	0.17	-	67,74,79,83	0
1	2MG	AA	1207	24/25	0.90	0.12	-	89,94,98,100	0
1	UR3	BA	1498	21/22	0.90	0.17	-	69,76,83,83	0
22	6MZ	CA	2030	23/24	0.77	0.28	-	93,99,101,102	0
53	PSU	DA	955	20/21	0.98	0.20	-	28,33,40,40	0
1	PSU	AA	516	20/21	0.95	0.11	-	68,75,81,81	0
22	PSU	CA	2580	20/21	0.93	0.15	-	83,88,90,92	0
53	PSU	DA	2504	20/21	0.98	0.21	-	28,36,44,45	0
1	PSU	BA	516	20/21	0.85	0.13	-	73,79,89,91	0
1	2MG	BA	1207	24/25	0.64	0.18	-	122,126,131,131	0
12	D2T	AL	89	10/11	0.95	0.12	-	59,65,70,77	0
1	5MC	AA	1407	21/22	0.96	0.12	-	51,59,62,63	0
1	5MC	BA	1407	21/22	0.86	0.15	-	86,91,95,96	0
53	PSU	DA	2604	20/21	0.97	0.16	-	33,44,54,57	0
1	4OC	AA	1402	22/23	0.96	0.14	-	59,62,68,70	0
22	5MU	CA	747	21/22	0.88	0.19	-	82,91,96,97	0
22	PSU	CA	1911	20/21	0.78	0.21	-	103,108,113,116	0
53	OMC	DA	2498	21/22	0.97	0.25	-	28,33,38,40	0
53	5MU	DA	747	21/22	0.97	0.24	-	27,36,43,46	0
22	PSU	CA	955	20/21	0.85	0.19	-	100,105,109,110	0
54	MEQ	DD	150[B]	10/11	0.91	0.30	-	28,32,38,39	10
53	6MZ	DA	1618	23/24	0.98	0.24	-	29,36,44,47	0
53	PSU	DA	1911	20/21	0.93	0.11	-	69,74,80,80	0
53	5MC	DA	1962	21/22	0.96	0.14	-	38,48,55,59	0
54	MEQ	DD	150[A]	10/11	0.91	0.30	-	23,32,39,40	10
1	UR3	AA	1498	21/22	0.96	0.15	-	50,58,65,69	0
53	2MA	DA	2503	23/24	0.98	0.23	-	21,37,44,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	PSU	DA	2605	20/21	0.97	0.18	-	38,45,49,50	0
22	5MU	CA	1939	21/22	0.93	0.14	-	70,78,83,83	0
22	PSU	CA	1917	20/21	0.86	0.11	-	102,107,110,112	0
53	3TD	DA	1915	21/22	0.90	0.16	-	76,81,87,94	0
22	OMC	CA	2498	21/22	0.91	0.21	-	90,97,99,102	0
34	4D4	DN	81[B]	12/13	0.94	0.23	-	33,36,40,41	9
12	D2T	BL	89	10/11	0.95	0.14	-	64,74,78,93	0
34	4D4	DN	81[A]	12/13	0.94	0.23	-	33,38,42,43	9
22	2MA	CA	2503	23/24	0.79	0.21	-	87,90,92,94	0
1	MA6	AA	1519	24/25	0.97	0.14	-	51,56,63,67	0
53	6MZ	DA	2030	23/24	0.98	0.27	-	22,30,36,42	0
22	PSU	CA	2504	20/21	0.89	0.17	-	83,87,90,91	0
22	5MC	CA	1962	21/22	0.94	0.14	-	73,78,80,83	0
53	2MG	DA	1835	24/25	0.96	0.16	-	45,50,57,57	0
22	2MG	CA	2445	24/25	0.89	0.19	-	88,92,96,99	0
22	OMU	CA	2552	21/22	0.93	0.23	-	80,85,87,87	0
53	1MG	DA	745	24/25	0.98	0.27	-	25,34,41,44	0
1	2MG	AA	1516	24/25	0.96	0.14	-	47,53,60,67	0
53	PSU	DA	2457	20/21	0.98	0.21	-	31,36,43,45	0
22	G7M	CA	2069	24/25	0.86	0.22	-	88,94,96,100	0
53	PSU	DA	1917	20/21	0.91	0.09	-	63,72,79,84	0
53	OMG	DA	2251	24/25	0.97	0.22	-	23,34,41,43	0
1	G7M	BA	527	24/25	0.93	0.15	-	63,71,78,84	0
53	5MU	DA	1939	21/22	0.97	0.17	-	36,42,45,50	0
22	OMG	CA	2251	24/25	0.86	0.19	-	85,92,95,98	0
1	5MC	AA	967	21/22	0.92	0.19	-	70,76,83,84	0
1	2MG	BA	966	24/25	0.83	0.16	-	128,136,145,147	0
53	OMU	DA	2552	21/22	0.98	0.21	-	35,42,46,49	0
22	2MG	CA	1835	24/25	0.94	0.18	-	74,82,84,86	0
22	3TD	CA	1915	21/22	0.82	0.30	-	109,112,115,116	0
22	PSU	CA	2457	20/21	0.89	0.18	-	91,97,101,102	0
22	PSU	CA	746	20/21	0.81	0.20	-	88,91,95,95	0
1	MA6	AA	1518	24/25	0.96	0.15	-	45,54,59,64	0
34	4D4	CN	81	12/13	0.86	0.20	-	94,97,99,100	0
53	2MG	DA	2445	24/25	0.98	0.23	-	23,32,38,40	0
53	PSU	DA	746	20/21	0.97	0.25	-	28,37,43,44	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
56	MG	DA	3177	1/1	0.84	0.46	45.02	75,75,75,75	0
56	MG	DA	3122	1/1	0.70	0.44	43.21	77,77,77,77	0
56	MG	CA	3025	1/1	0.84	0.65	39.26	92,92,92,92	0
58	MPD	DA	3205	8/8	0.81	0.43	22.02	58,63,68,70	0
56	MG	DA	3119	1/1	0.85	0.28	20.62	66,66,66,66	0
56	MG	DA	3125	1/1	0.88	0.40	15.04	69,69,69,69	0
65	ACY	DA	3202	4/4	0.91	0.51	12.72	53,59,61,64	0
56	MG	DA	3027	1/1	0.96	0.34	11.26	42,42,42,42	0
56	MG	AA	1608	1/1	0.84	0.35	10.95	76,76,76,76	0
56	MG	DA	3022	1/1	0.81	0.31	10.20	40,40,40,40	0
56	MG	AA	1603	1/1	0.60	0.30	10.10	82,82,82,82	0
59	PUT	DA	3222	6/6	0.61	0.24	9.53	62,64,65,68	0
59	PUT	AA	1672	6/6	0.81	0.35	9.49	63,63,66,70	0
59	PUT	DA	3184	6/6	0.83	0.41	9.26	45,52,53,56	0
58	MPD	DA	3192	8/8	0.83	0.33	8.61	56,60,64,66	0
56	MG	CA	3036	1/1	-0.33	0.38	8.57	94,94,94,94	0
56	MG	AA	1642	1/1	0.71	0.24	8.17	88,88,88,88	0
59	PUT	DM	201	6/6	0.91	0.36	8.09	46,49,53,54	0
56	MG	AA	1631	1/1	0.77	0.20	7.81	54,54,54,54	0
64	PGE	D1	102	10/10	0.77	0.39	6.53	61,66,71,74	0
58	MPD	AA	1671	8/8	0.87	0.37	6.36	63,65,70,73	0
56	MG	DA	3035	1/1	0.79	0.40	6.33	38,38,38,38	0
61	PEG	D3	102	7/7	0.90	0.29	6.22	50,54,70,71	0
58	MPD	AA	1676	8/8	0.93	0.24	6.15	60,66,72,76	0
56	MG	DA	3069	1/1	0.92	0.23	5.83	53,53,53,53	0
61	PEG	DA	3200	7/7	0.76	0.31	5.64	52,54,67,67	0
58	MPD	DE	301	8/8	0.78	0.46	5.38	57,67,76,80	0
56	MG	AA	1661	1/1	0.71	0.21	5.18	79,79,79,79	0
59	PUT	DA	3223	6/6	0.67	0.32	5.12	46,49,51,53	0
59	PUT	DA	3214	6/6	0.86	0.30	4.88	49,52,56,57	0
56	MG	CB	202	1/1	0.83	0.23	4.53	86,86,86,86	0
56	MG	CA	3132	1/1	0.79	0.31	4.50	80,80,80,80	0
56	MG	DA	3045	1/1	0.94	0.24	3.82	44,44,44,44	0
56	MG	CA	3150	1/1	0.52	0.29	3.66	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MPD	DA	3208	8/8	0.76	0.22	3.59	56,62,70,74	0
61	PEG	DA	3219	7/7	0.80	0.27	3.58	61,66,70,73	0
62	SPD	DA	3225	10/10	0.92	0.28	3.56	34,45,52,63	0
56	MG	DA	3006	1/1	0.93	0.26	3.32	43,43,43,43	0
56	MG	DA	3048	1/1	0.98	0.29	3.26	35,35,35,35	0
56	MG	DA	3057	1/1	0.89	0.26	3.24	40,40,40,40	0
56	MG	DA	3090	1/1	0.93	0.29	3.19	42,42,42,42	0
66	EDO	DA	3198	4/4	0.81	0.32	3.17	49,53,54,55	0
56	MG	DA	3172	1/1	0.90	0.22	3.16	73,73,73,73	0
57	PG4	DR	202	13/13	0.82	0.29	3.14	47,56,62,65	0
56	MG	CA	3005	1/1	0.72	0.37	3.14	96,96,96,96	0
56	MG	DA	3033	1/1	0.94	0.34	3.13	47,47,47,47	0
59	PUT	DA	3189	6/6	0.86	0.23	3.05	44,48,51,54	0
56	MG	DA	3126	1/1	0.48	0.23	3.05	75,75,75,75	0
56	MG	DA	3011	1/1	0.99	0.36	2.94	33,33,33,33	0
64	PGE	DA	3186	10/10	0.94	0.23	2.87	37,42,58,59	0
56	MG	BA	1632	1/1	0.61	0.20	2.85	68,68,68,68	0
56	MG	DA	3064	1/1	0.94	0.30	2.84	41,41,41,41	0
60	ZN	AB	301	1/1	0.90	0.41	2.76	140,140,140,140	0
56	MG	AA	1611	1/1	0.88	0.23	2.61	63,63,63,63	0
56	MG	DA	3091	1/1	0.97	0.30	2.58	36,36,36,36	0
59	PUT	DA	3220	6/6	0.86	0.24	2.47	56,58,62,67	0
56	MG	DA	3015	1/1	0.91	0.21	2.47	54,54,54,54	0
66	EDO	D0	101	4/4	0.85	0.24	2.41	61,63,66,68	0
57	PG4	DA	3193	13/13	0.83	0.25	2.40	52,56,66,66	0
56	MG	DA	3044	1/1	0.88	0.28	2.36	41,41,41,41	0
56	MG	DA	3108	1/1	0.99	0.24	2.28	38,38,38,38	0
62	SPD	DA	3187	10/10	0.96	0.26	2.28	36,43,46,47	0
56	MG	BA	1605	1/1	0.78	0.22	2.28	81,81,81,81	0
56	MG	DA	3088	1/1	0.98	0.29	2.16	32,32,32,32	0
56	MG	AA	1612	1/1	0.92	0.21	2.05	70,70,70,70	0
56	MG	CA	3002	1/1	0.66	0.30	2.02	91,91,91,91	0
56	MG	DA	3007	1/1	0.98	0.23	1.95	40,40,40,40	0
56	MG	DA	3092	1/1	0.84	0.28	1.91	39,39,39,39	0
56	MG	DA	3056	1/1	0.96	0.23	1.82	44,44,44,44	0
56	MG	AA	1649	1/1	0.92	0.21	1.79	64,64,64,64	0
61	PEG	DQ	201	7/7	0.76	0.24	1.69	63,70,74,76	0
56	MG	AA	1663	1/1	0.67	0.18	1.65	79,79,79,79	0
56	MG	CA	3129	1/1	0.90	0.25	1.63	84,84,84,84	0
56	MG	DA	3014	1/1	0.96	0.26	1.61	36,36,36,36	0
56	MG	CA	3135	1/1	0.87	0.23	1.57	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	BA	1626	1/1	0.80	0.26	1.45	80,80,80,80	0
56	MG	DA	3010	1/1	0.93	0.31	1.42	37,37,37,37	0
56	MG	AA	1637	1/1	0.96	0.22	1.41	57,57,57,57	0
56	MG	DA	3107	1/1	0.97	0.28	1.39	33,33,33,33	0
56	MG	DA	3163	1/1	0.73	0.17	1.39	73,73,73,73	0
59	PUT	DA	3206	6/6	0.71	0.18	1.38	58,61,62,63	0
62	SPD	DA	3207	10/10	0.69	0.21	1.22	57,63,68,70	0
61	PEG	DL	201	7/7	0.93	0.15	1.21	55,58,62,66	0
64	PGE	D3	101	10/10	0.83	0.19	0.89	58,65,67,68	0
63	1PE	DA	3203	16/16	0.89	0.24	0.79	50,55,64,65	0
56	MG	DA	3100	1/1	0.92	0.22	0.74	46,46,46,46	0
66	EDO	D1	101	4/4	0.89	0.17	0.72	47,52,57,63	0
66	EDO	DA	3197	4/4	0.96	0.22	0.67	56,58,62,65	0
56	MG	CA	3088	1/1	0.92	0.19	0.58	68,68,68,68	0
56	MG	CA	3137	1/1	0.85	0.22	0.53	78,78,78,78	0
57	PG4	AA	1670	13/13	0.88	0.17	0.52	52,62,68,68	0
56	MG	DA	3095	1/1	0.89	0.17	0.48	49,49,49,49	0
60	ZN	D5	101	1/1	0.99	0.15	0.40	63,63,63,63	0
56	MG	DA	3029	1/1	0.95	0.25	0.38	41,41,41,41	0
64	PGE	DS	201	10/10	0.75	0.18	0.37	50,56,66,68	0
61	PEG	DA	3201	7/7	0.88	0.23	0.32	53,56,63,66	0
56	MG	DA	3097	1/1	0.84	0.21	0.26	37,37,37,37	0
56	MG	CA	3060	1/1	0.80	0.27	0.20	93,93,93,93	0
57	PG4	DQ	202	13/13	0.87	0.15	0.15	50,58,66,66	0
62	SPD	DA	3183	10/10	0.92	0.18	0.14	42,51,57,57	0
56	MG	AA	1648	1/1	0.89	0.15	0.12	56,56,56,56	0
56	MG	DA	3229	1/1	0.94	0.29	0.10	42,42,42,42	0
58	MPD	DS	203	8/8	0.95	0.25	0.07	41,45,50,53	0
56	MG	DA	3021	1/1	0.84	0.22	-0.02	36,36,36,36	0
56	MG	DA	3082	1/1	0.96	0.22	-0.02	49,49,49,49	0
59	PUT	DA	3195	6/6	0.82	0.17	-0.03	39,46,50,57	0
56	MG	CA	3104	1/1	0.70	0.26	-0.07	83,83,83,83	0
56	MG	CA	3101	1/1	0.85	0.22	-0.28	82,82,82,82	0
63	1PE	DA	3185	16/16	0.89	0.18	-0.32	39,51,68,74	0
58	MPD	DE	302	8/8	0.77	0.23	-0.36	60,65,67,67	0
56	MG	DA	3020	1/1	1.00	0.20	-0.37	30,30,30,30	0
57	PG4	BA	1642	13/13	0.86	0.17	-0.39	52,61,66,69	0
61	PEG	AL	201	7/7	0.93	0.12	-0.49	57,64,71,73	0
64	PGE	DU	101	10/10	0.91	0.13	-0.55	44,60,69,71	0
56	MG	CB	201	1/1	0.64	0.28	-0.58	91,91,91,91	0
56	MG	CA	3013	1/1	0.79	0.21	-0.65	89,89,89,89	0
56	MG	BA	1624	1/1	0.70	0.41	-0.69	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3030	1/1	0.61	0.19	-0.81	74,74,74,74	0
64	PGE	DA	3215	10/10	0.91	0.12	-0.88	56,62,66,70	0
56	MG	AA	1668	1/1	0.97	0.15	-0.93	60,60,60,60	0
57	PG4	DS	202	13/13	0.87	0.15	-0.95	42,48,56,56	0
64	PGE	DA	3204	10/10	0.90	0.21	-0.98	53,61,69,70	0
59	PUT	AA	1673	6/6	0.83	0.10	-0.98	63,64,68,69	0
56	MG	DA	3110	1/1	0.98	0.24	-0.98	33,33,33,33	0
56	MG	CA	3018	1/1	0.46	0.17	-1.14	79,79,79,79	0
56	MG	AA	1677	1/1	0.94	0.09	-1.15	79,79,79,79	0
56	MG	DB	201	1/1	0.93	0.12	-1.21	62,62,62,62	0
56	MG	CA	3010	1/1	0.54	0.19	-1.22	77,77,77,77	0
56	MG	DA	3059	1/1	0.94	0.22	-1.27	42,42,42,42	0
58	MPD	DT	202	8/8	0.86	0.19	-1.29	65,66,75,75	0
67	GUN	DA	3212	11/11	0.84	0.13	-1.31	52,58,63,69	0
56	MG	CA	3122	1/1	0.71	0.14	-1.44	85,85,85,85	0
56	MG	CA	3090	1/1	0.54	0.12	-1.44	80,80,80,80	0
56	MG	CA	3007	1/1	0.76	0.17	-1.64	82,82,82,82	0
56	MG	CA	3099	1/1	0.63	0.17	-1.66	69,69,69,69	0
56	MG	CA	3019	1/1	0.57	0.15	-1.67	81,81,81,81	0
56	MG	AA	1629	1/1	0.70	0.17	-1.79	67,67,67,67	0
56	MG	BA	1612	1/1	0.70	0.10	-1.93	77,77,77,77	0
56	MG	AA	1646	1/1	0.87	0.16	-1.94	59,59,59,59	0
56	MG	CA	3136	1/1	0.76	0.18	-1.96	87,87,87,87	0
60	ZN	C5	101	1/1	0.92	0.04	-2.01	117,117,117,117	0
56	MG	CA	3152	1/1	0.78	0.14	-2.11	77,77,77,77	0
56	MG	CA	3087	1/1	0.78	0.12	-2.20	83,83,83,83	0
56	MG	AA	1656	1/1	0.66	0.08	-2.36	67,67,67,67	0
56	MG	DA	3149	1/1	0.90	0.15	-2.37	62,62,62,62	0
56	MG	CA	3017	1/1	0.86	0.09	-2.39	82,82,82,82	0
57	PG4	DA	3217	13/13	0.87	0.13	-2.40	57,66,72,75	0
56	MG	BA	1602	1/1	0.96	0.14	-2.40	76,76,76,76	0
56	MG	BA	1610	1/1	0.76	0.09	-2.54	69,69,69,69	0
56	MG	CA	3062	1/1	0.54	0.11	-2.54	90,90,90,90	0
56	MG	CA	3038	1/1	0.86	0.14	-2.58	78,78,78,78	0
56	MG	CA	3102	1/1	0.84	0.07	-2.82	78,78,78,78	0
56	MG	CA	3085	1/1	0.82	0.13	-2.83	78,78,78,78	0
56	MG	CA	3084	1/1	0.21	0.11	-2.87	80,80,80,80	0
56	MG	AA	1662	1/1	0.74	0.09	-2.98	74,74,74,74	0
56	MG	CA	3021	1/1	0.62	0.14	-3.03	93,93,93,93	0
56	MG	DA	3123	1/1	0.97	0.13	-3.13	43,43,43,43	0
56	MG	CA	3094	1/1	0.90	0.07	-3.27	68,68,68,68	0
56	MG	CA	3043	1/1	0.94	0.12	-3.41	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1639	1/1	0.90	0.09	-3.43	79,79,79,79	0
56	MG	AA	1644	1/1	0.68	0.12	-3.46	76,76,76,76	0
59	PUT	AA	1674	6/6	0.86	0.11	-3.49	61,62,67,69	0
56	MG	CA	3012	1/1	0.53	0.09	-3.86	69,69,69,69	0
56	MG	CA	3100	1/1	0.93	0.11	-3.87	78,78,78,78	0
56	MG	BA	1615	1/1	0.95	0.08	-3.92	62,62,62,62	0
56	MG	BA	1617	1/1	0.54	0.08	-4.00	82,82,82,82	0
56	MG	DA	3099	1/1	0.93	0.15	-4.17	60,60,60,60	0
56	MG	DA	3001	1/1	0.87	0.13	-4.19	62,62,62,62	0
56	MG	CA	3078	1/1	0.64	0.11	-4.38	85,85,85,85	0
56	MG	DA	3146	1/1	0.94	0.05	-4.61	77,77,77,77	0
56	MG	DA	3079	1/1	0.89	0.10	-4.63	55,55,55,55	0
56	MG	CA	3050	1/1	0.96	0.07	-4.63	65,65,65,65	0
56	MG	CA	3039	1/1	0.62	0.08	-4.65	81,81,81,81	0
56	MG	AA	1643	1/1	0.93	0.10	-4.66	66,66,66,66	0
56	MG	BA	1613	1/1	0.81	0.08	-4.68	65,65,65,65	0
56	MG	CA	3032	1/1	0.82	0.07	-4.69	71,71,71,71	0
56	MG	CA	3051	1/1	0.62	0.10	-4.71	71,71,71,71	0
56	MG	BA	1614	1/1	0.81	0.10	-4.78	77,77,77,77	0
56	MG	DA	3024	1/1	0.92	0.18	-4.79	64,64,64,64	0
56	MG	DA	3003	1/1	0.37	0.09	-4.97	75,75,75,75	0
56	MG	CA	3023	1/1	0.91	0.08	-5.14	75,75,75,75	0
56	MG	DA	3134	1/1	0.98	0.05	-5.51	65,65,65,65	0
56	MG	CA	3143	1/1	0.96	0.05	-5.95	74,74,74,74	0
56	MG	CA	3093	1/1	0.87	0.06	-6.35	91,91,91,91	0
56	MG	AA	1659	1/1	0.78	0.06	-6.36	68,68,68,68	0
56	MG	BA	1601	1/1	0.70	0.10	-6.39	78,78,78,78	0
56	MG	CA	3026	1/1	0.76	0.07	-7.06	75,75,75,75	0
56	MG	BA	1622	1/1	0.96	0.11	-7.20	70,70,70,70	0
56	MG	DA	3093	1/1	0.84	0.09	-7.22	57,57,57,57	0
56	MG	DA	3061	1/1	0.67	0.15	-7.67	60,60,60,60	0
56	MG	CA	3008	1/1	0.87	0.09	-7.97	79,79,79,79	0
56	MG	BA	1608	1/1	0.91	0.04	-8.59	78,78,78,78	0
56	MG	DA	3004	1/1	0.79	0.07	-9.39	66,66,66,66	0
56	MG	DA	3025	1/1	0.94	0.17	-9.61	41,41,41,41	0
56	MG	AA	1653	1/1	0.79	0.09	-10.69	63,63,63,63	0
56	MG	DA	3062	1/1	0.86	0.15	-12.18	50,50,50,50	0
66	EDO	DR	203	4/4	0.84	0.20	-	53,54,57,60	0
56	MG	BA	1621	1/1	0.86	0.17	-	54,54,54,54	0
56	MG	DA	3078	1/1	0.95	0.04	-	72,72,72,72	0
56	MG	DA	3180	1/1	0.74	0.18	-	78,78,78,78	0
56	MG	DA	3109	1/1	0.76	0.64	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1609	1/1	0.71	0.40	-	79,79,79,79	0
56	MG	AA	1628	1/1	0.82	0.46	-	80,80,80,80	0
56	MG	CA	3031	1/1	0.55	0.26	-	90,90,90,90	0
59	PUT	DA	3224	6/6	0.95	0.33	-	43,45,54,60	0
56	MG	DA	3140	1/1	0.82	0.45	-	65,65,65,65	0
66	EDO	DA	3194	4/4	0.84	0.27	-	52,52,52,58	0
56	MG	CA	3106	1/1	0.96	0.40	-	67,67,67,67	0
56	MG	DB	208	1/1	0.79	0.43	-	79,79,79,79	0
56	MG	BA	1620	1/1	0.53	0.08	-	78,78,78,78	0
56	MG	DA	3072	1/1	0.87	0.12	-	53,53,53,53	0
56	MG	DA	3058	1/1	0.88	0.26	-	38,38,38,38	0
56	MG	DA	3142	1/1	0.94	0.50	-	64,64,64,64	0
56	MG	CA	3054	1/1	0.82	0.13	-	83,83,83,83	0
56	MG	CA	3074	1/1	0.54	0.33	-	91,91,91,91	0
66	EDO	DB	210	4/4	0.77	0.24	-	65,67,68,69	0
56	MG	DA	3087	1/1	0.92	0.27	-	31,31,31,31	0
56	MG	AA	1664	1/1	0.73	0.10	-	78,78,78,78	0
56	MG	DA	3182	1/1	0.76	0.49	-	86,86,86,86	0
56	MG	AA	1625	1/1	0.87	0.28	-	70,70,70,70	0
56	MG	CA	3035	1/1	0.19	0.12	-	81,81,81,81	0
56	MG	DA	3026	1/1	0.91	0.30	-	50,50,50,50	0
56	MG	DA	3101	1/1	0.77	0.10	-	51,51,51,51	0
56	MG	BA	1603	1/1	0.87	0.27	-	83,83,83,83	0
65	ACY	DA	3191	4/4	0.89	0.15	-	48,50,52,53	0
56	MG	DA	3066	1/1	0.91	0.24	-	44,44,44,44	0
68	TRS	DA	3221	8/8	0.68	0.17	-	65,69,75,77	0
56	MG	CA	3155	1/1	0.04	0.35	-	93,93,93,93	0
56	MG	DA	3002	1/1	0.72	0.18	-	66,66,66,66	0
56	MG	BA	1631	1/1	0.76	0.10	-	76,76,76,76	0
56	MG	DA	3148	1/1	0.97	0.12	-	66,66,66,66	0
56	MG	CA	3020	1/1	0.70	0.25	-	83,83,83,83	0
56	MG	DA	3036	1/1	0.90	0.19	-	43,43,43,43	0
56	MG	CA	3042	1/1	0.59	0.18	-	70,70,70,70	0
56	MG	CA	3105	1/1	0.88	0.50	-	68,68,68,68	0
56	MG	CA	3073	1/1	-0.09	0.41	-	93,93,93,93	0
56	MG	CA	3027	1/1	0.90	0.34	-	97,97,97,97	0
56	MG	CA	3115	1/1	0.91	0.41	-	73,73,73,73	0
56	MG	DA	3133	1/1	0.92	0.20	-	67,67,67,67	0
56	MG	CA	3071	1/1	0.51	0.20	-	95,95,95,95	0
56	MG	CA	3117	1/1	0.94	0.42	-	79,79,79,79	0
56	MG	CA	3108	1/1	0.95	0.34	-	65,65,65,65	0
56	MG	DA	3046	1/1	0.97	0.21	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	MG	AA	1655	1/1	0.73	0.08	-	77,77,77,77	0
56	MG	CA	3024	1/1	0.91	0.08	-	75,75,75,75	0
56	MG	BA	1616	1/1	0.60	0.08	-	86,86,86,86	0
56	MG	DA	3065	1/1	0.52	0.15	-	70,70,70,70	0
56	MG	DA	3174	1/1	0.84	0.34	-	77,77,77,77	0
56	MG	CA	3044	1/1	0.86	0.08	-	73,73,73,73	0
56	MG	CA	3022	1/1	0.93	0.31	-	78,78,78,78	0
56	MG	DA	3153	1/1	0.72	0.54	-	67,67,67,67	0
56	MG	CA	3142	1/1	0.87	0.28	-	69,69,69,69	0
56	MG	DA	3053	1/1	0.90	0.26	-	38,38,38,38	0
56	MG	CA	3127	1/1	0.90	0.19	-	84,84,84,84	0
56	MG	BA	1627	1/1	0.20	0.23	-	83,83,83,83	0
56	MG	CB	203	1/1	0.63	0.08	-	90,90,90,90	0
56	MG	DA	3051	1/1	0.87	0.14	-	53,53,53,53	0
56	MG	DA	3031	1/1	0.98	0.23	-	34,34,34,34	0
56	MG	DA	3113	1/1	0.90	0.25	-	38,38,38,38	0
56	MG	AA	1618	1/1	0.92	0.52	-	78,78,78,78	0
56	MG	DA	3136	1/1	0.85	0.38	-	74,74,74,74	0
56	MG	CA	3009	1/1	0.83	0.19	-	78,78,78,78	0
56	MG	AA	1605	1/1	0.92	0.41	-	76,76,76,76	0
56	MG	DA	3155	1/1	0.93	0.31	-	66,66,66,66	0
56	MG	CA	3092	1/1	0.77	0.13	-	83,83,83,83	0
56	MG	AA	1667	1/1	0.95	0.13	-	57,57,57,57	0
56	MG	BA	1635	1/1	0.78	0.05	-	72,72,72,72	0
56	MG	DA	3071	1/1	0.95	0.35	-	37,37,37,37	0
56	MG	BA	1638	1/1	0.90	0.25	-	75,75,75,75	0
56	MG	DA	3139	1/1	0.87	0.24	-	57,57,57,57	0
56	MG	CA	3055	1/1	0.76	0.35	-	78,78,78,78	0
56	MG	DA	3157	1/1	0.97	0.19	-	65,65,65,65	0
56	MG	CA	3006	1/1	-0.19	0.72	-	100,100,100,100	0
56	MG	DA	3039	1/1	0.99	0.18	-	39,39,39,39	0
56	MG	CA	3148	1/1	0.95	0.35	-	73,73,73,73	0
56	MG	CA	3040	1/1	0.95	0.13	-	59,59,59,59	0
64	PGE	DA	3218	10/10	0.92	0.14	-	50,55,64,68	0
56	MG	DA	3168	1/1	0.74	0.11	-	77,77,77,77	0
56	MG	AA	1654	1/1	0.59	0.52	-	91,91,91,91	0
56	MG	CA	3139	1/1	0.90	0.21	-	71,71,71,71	0
56	MG	DA	3159	1/1	0.89	0.17	-	62,62,62,62	0
56	MG	DA	3137	1/1	0.74	0.67	-	56,56,56,56	1
56	MG	DA	3016	1/1	0.77	0.14	-	63,63,63,63	0
56	MG	CA	3058	1/1	0.68	0.09	-	76,76,76,76	0
58	MPD	DN	201	8/8	0.75	0.29	-	57,63,66,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3118	1/1	0.86	0.23	-	79,79,79,79	0
56	MG	BA	1618	1/1	0.91	0.08	-	74,74,74,74	0
56	MG	AA	1636	1/1	0.82	0.13	-	81,81,81,81	0
56	MG	DA	3150	1/1	0.88	0.23	-	49,49,49,49	0
56	MG	DB	203	1/1	0.88	0.13	-	51,51,51,51	0
56	MG	CA	3110	1/1	0.91	0.41	-	70,70,70,70	0
56	MG	DB	205	1/1	0.91	0.39	-	74,74,74,74	0
56	MG	DA	3145	1/1	0.78	0.12	-	69,69,69,69	0
56	MG	DA	3049	1/1	0.98	0.24	-	45,45,45,45	0
56	MG	DA	3120	1/1	0.87	0.92	-	75,75,75,75	0
56	MG	DA	3089	1/1	0.97	0.26	-	32,32,32,32	0
56	MG	DA	3032	1/1	0.97	0.29	-	31,31,31,31	0
56	MG	CA	3130	1/1	0.89	0.12	-	78,78,78,78	0
56	MG	AA	1623	1/1	0.59	0.41	-	71,71,71,71	0
56	MG	CA	3112	1/1	0.72	0.46	-	81,81,81,81	0
56	MG	AA	1657	1/1	0.84	0.13	-	77,77,77,77	0
56	MG	BA	1634	1/1	0.93	0.06	-	76,76,76,76	0
56	MG	CA	3015	1/1	0.87	0.27	-	76,76,76,76	0
56	MG	DA	3042	1/1	0.62	0.10	-	75,75,75,75	0
56	MG	DA	3018	1/1	0.90	0.24	-	54,54,54,54	0
56	MG	DA	3005	1/1	0.88	0.14	-	72,72,72,72	0
56	MG	CA	3003	1/1	0.50	0.06	-	80,80,80,80	0
56	MG	DA	3161	1/1	0.89	0.27	-	71,71,71,71	0
56	MG	CA	3056	1/1	0.84	0.12	-	75,75,75,75	0
56	MG	CA	3134	1/1	0.93	0.13	-	79,79,79,79	0
56	MG	CA	3064	1/1	0.84	0.16	-	75,75,75,75	0
56	MG	DA	3170	1/1	0.73	0.32	-	66,66,66,66	0
56	MG	DA	3147	1/1	0.77	0.40	-	73,73,73,73	0
56	MG	CA	3086	1/1	0.11	0.17	-	78,78,78,78	0
56	MG	BA	1619	1/1	0.79	0.06	-	66,66,66,66	0
56	MG	CA	3149	1/1	0.92	0.19	-	69,69,69,69	0
56	MG	DA	3040	1/1	0.93	0.17	-	48,48,48,48	0
64	PGE	DA	3226	10/10	0.87	0.18	-	59,63,67,69	0
56	MG	AA	1633	1/1	0.89	0.12	-	72,72,72,72	0
56	MG	AA	1624	1/1	0.92	0.58	-	80,80,80,80	0
56	MG	DA	3103	1/1	0.80	0.30	-	44,44,44,44	0
56	MG	DA	3173	1/1	0.88	0.26	-	77,77,77,77	0
56	MG	BA	1630	1/1	0.23	0.32	-	98,98,98,98	0
56	MG	CA	3091	1/1	0.80	0.21	-	77,77,77,77	0
56	MG	CA	3069	1/1	0.83	0.06	-	80,80,80,80	0
56	MG	DB	209	1/1	0.93	0.18	-	69,69,69,69	0
56	MG	CA	3133	1/1	0.95	0.27	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1614	1/1	0.85	0.14	-	75,75,75,75	0
56	MG	AA	1607	1/1	0.98	0.29	-	76,76,76,76	0
56	MG	CA	3028	1/1	0.90	0.12	-	69,69,69,69	0
56	MG	BA	1628	1/1	0.91	0.06	-	74,74,74,74	0
56	MG	DA	3131	1/1	0.76	0.17	-	70,70,70,70	0
61	PEG	DA	3228	7/7	0.86	0.26	-	55,58,61,64	0
56	MG	AA	1620	1/1	0.90	0.58	-	72,72,72,72	0
56	MG	DA	3179	1/1	0.88	0.14	-	76,76,76,76	0
56	MG	DA	3019	1/1	0.94	0.27	-	34,34,34,34	0
56	MG	CA	3033	1/1	0.79	0.31	-	90,90,90,90	0
56	MG	DA	3012	1/1	0.45	0.23	-	56,56,56,56	0
56	MG	CA	3097	1/1	0.87	0.10	-	83,83,83,83	0
56	MG	DA	3028	1/1	0.84	0.18	-	49,49,49,49	0
56	MG	DA	3156	1/1	0.83	0.42	-	74,74,74,74	0
61	PEG	DP	201	7/7	0.82	0.14	-	61,65,67,67	0
56	MG	DA	3160	1/1	0.88	0.45	-	71,71,71,71	0
65	ACY	DA	3196	4/4	0.72	0.19	-	59,65,67,71	0
56	MG	CA	3037	1/1	0.11	0.44	-	102,102,102,102	0
56	MG	DA	3143	1/1	0.86	0.11	-	77,77,77,77	0
56	MG	CA	3118	1/1	0.82	0.22	-	87,87,87,87	0
56	MG	BA	1639	1/1	0.70	0.21	-	78,78,78,78	0
56	MG	CA	3098	1/1	0.45	0.07	-	89,89,89,89	0
56	MG	DA	3121	1/1	0.86	0.46	-	85,85,85,85	0
56	MG	DA	3055	1/1	0.96	0.19	-	36,36,36,36	0
56	MG	DA	3105	1/1	0.96	0.23	-	41,41,41,41	0
56	MG	DB	206	1/1	0.72	0.17	-	82,82,82,82	0
56	MG	CA	3080	1/1	0.39	0.17	-	88,88,88,88	0
56	MG	CA	3045	1/1	0.60	0.10	-	80,80,80,80	0
56	MG	CA	3114	1/1	0.88	0.30	-	68,68,68,68	0
56	MG	BA	1633	1/1	0.84	0.34	-	85,85,85,85	0
56	MG	AA	1665	1/1	0.74	0.04	-	78,78,78,78	0
56	MG	CA	3131	1/1	0.91	0.17	-	79,79,79,79	0
56	MG	DA	3181	1/1	0.87	0.45	-	79,79,79,79	0
56	MG	DA	3176	1/1	0.92	0.29	-	70,70,70,70	0
56	MG	CA	3029	1/1	0.94	0.12	-	79,79,79,79	0
56	MG	AA	1669	1/1	0.79	0.08	-	76,76,76,76	0
56	MG	DA	3129	1/1	0.46	0.14	-	70,70,70,70	0
56	MG	CA	3145	1/1	0.02	0.15	-	90,90,90,90	0
66	EDO	DA	3210	4/4	0.82	0.20	-	62,65,69,73	0
56	MG	AA	1638	1/1	0.80	0.17	-	86,86,86,86	0
66	EDO	DA	3209	4/4	0.80	0.29	-	55,59,62,67	0
56	MG	BA	1609	1/1	0.01	0.36	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3083	1/1	0.90	0.21	-	50,50,50,50	0
56	MG	BA	1641	1/1	0.21	0.18	-	86,86,86,86	0
56	MG	AA	1610	1/1	0.27	0.48	-	85,85,85,85	0
56	MG	AA	1602	1/1	0.82	0.23	-	79,79,79,79	0
56	MG	CA	3076	1/1	0.67	0.28	-	83,83,83,83	0
56	MG	DA	3075	1/1	0.90	0.22	-	48,48,48,48	0
56	MG	CA	3075	1/1	0.50	0.18	-	92,92,92,92	0
56	MG	CA	3141	1/1	0.88	0.30	-	77,77,77,77	0
59	PUT	DA	3213	6/6	0.88	0.17	-	49,55,55,58	0
56	MG	AA	1604	1/1	0.70	0.34	-	73,73,73,73	0
56	MG	DA	3117	1/1	0.95	0.31	-	54,54,54,54	0
66	EDO	DB	212	4/4	0.73	0.21	-	59,60,64,64	0
56	MG	CA	3011	1/1	0.80	0.06	-	78,78,78,78	0
58	MPD	DK	201	8/8	0.84	0.13	-	60,66,71,73	0
56	MG	DA	3068	1/1	0.98	0.05	-	70,70,70,70	0
56	MG	BA	1623	1/1	0.78	0.55	-	86,86,86,86	0
56	MG	DA	3052	1/1	0.91	0.10	-	41,41,41,41	0
56	MG	DA	3151	1/1	0.80	0.28	-	80,80,80,80	0
56	MG	DA	3178	1/1	0.64	0.09	-	79,79,79,79	0
56	MG	DA	3127	1/1	0.93	0.46	-	65,65,65,65	0
56	MG	BA	1636	1/1	0.84	0.21	-	83,83,83,83	0
56	MG	DA	3167	1/1	0.82	0.28	-	64,64,64,64	0
56	MG	CA	3153	1/1	0.45	0.23	-	86,86,86,86	0
56	MG	CA	3113	1/1	0.80	0.36	-	63,63,63,63	0
56	MG	CA	3083	1/1	0.44	0.26	-	93,93,93,93	0
56	MG	DR	201	1/1	0.92	0.77	-	66,66,66,66	0
56	MG	AA	1621	1/1	0.70	0.45	-	79,79,79,79	0
56	MG	DA	3104	1/1	0.89	0.20	-	44,44,44,44	0
58	MPD	DA	3190	8/8	0.88	0.19	-	55,64,69,72	0
56	MG	DA	3030	1/1	0.97	0.27	-	34,34,34,34	0
56	MG	DA	3132	1/1	0.93	0.21	-	71,71,71,71	0
56	MG	AA	1622	1/1	0.92	0.35	-	74,74,74,74	0
56	MG	DA	3037	1/1	0.96	0.25	-	37,37,37,37	0
56	MG	AA	1616	1/1	0.55	0.75	-	83,83,83,83	0
56	MG	AA	1601	1/1	0.81	0.31	-	66,66,66,66	0
56	MG	BA	1604	1/1	0.70	0.24	-	75,75,75,75	0
56	MG	AA	1635	1/1	0.93	0.11	-	74,74,74,74	0
56	MG	DA	3112	1/1	0.98	0.25	-	44,44,44,44	0
56	MG	CA	3151	1/1	0.90	0.06	-	82,82,82,82	0
56	MG	DA	3106	1/1	0.83	0.26	-	44,44,44,44	0
56	MG	CA	3004	1/1	0.65	0.39	-	95,95,95,95	0
56	MG	AA	1650	1/1	0.90	0.03	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3009	1/1	0.69	0.10	-	59,59,59,59	0
56	MG	DA	3063	1/1	0.90	0.23	-	42,42,42,42	0
56	MG	CA	3052	1/1	0.67	0.11	-	79,79,79,79	0
56	MG	CA	3057	1/1	0.89	0.10	-	82,82,82,82	0
56	MG	CA	3146	1/1	0.84	0.51	-	60,60,60,60	1
56	MG	DA	3111	1/1	0.77	0.20	-	61,61,61,61	0
56	MG	DA	3141	1/1	0.76	0.27	-	73,73,73,73	0
59	PUT	DA	3188	6/6	0.90	0.30	-	32,39,44,48	0
56	MG	CA	3034	1/1	0.75	0.06	-	82,82,82,82	0
56	MG	DA	3034	1/1	0.95	0.30	-	33,33,33,33	0
56	MG	DA	3060	1/1	0.52	0.07	-	77,77,77,77	0
56	MG	DA	3070	1/1	0.44	0.17	-	52,52,52,52	0
56	MG	CA	3124	1/1	0.66	0.15	-	87,87,87,87	0
56	MG	DA	3102	1/1	0.96	0.34	-	35,35,35,35	0
56	MG	DA	3041	1/1	0.43	0.23	-	50,50,50,50	0
56	MG	DA	3038	1/1	0.82	0.16	-	44,44,44,44	0
56	MG	DA	3138	1/1	0.95	0.24	-	60,60,60,60	0
56	MG	CA	3047	1/1	0.59	0.10	-	77,77,77,77	0
56	MG	DA	3084	1/1	0.95	0.23	-	48,48,48,48	0
56	MG	AA	1606	1/1	0.58	0.19	-	83,83,83,83	0
56	MG	CA	3049	1/1	0.80	0.15	-	64,64,64,64	0
56	MG	CA	3126	1/1	0.95	0.25	-	74,74,74,74	0
56	MG	CA	3061	1/1	0.69	0.40	-	86,86,86,86	0
56	MG	DA	3050	1/1	0.80	0.06	-	55,55,55,55	0
56	MG	DA	3154	1/1	0.91	0.37	-	68,68,68,68	0
56	MG	DA	3165	1/1	0.87	0.37	-	70,70,70,70	0
56	MG	CA	3072	1/1	0.66	0.16	-	92,92,92,92	0
56	MG	C3	101	1/1	-0.16	0.22	-	97,97,97,97	0
56	MG	AA	1634	1/1	0.85	0.07	-	78,78,78,78	0
56	MG	BA	1606	1/1	0.81	0.23	-	85,85,85,85	0
56	MG	DA	3085	1/1	0.82	0.29	-	44,44,44,44	0
56	MG	DA	3128	1/1	0.74	0.30	-	74,74,74,74	0
56	MG	CA	3089	1/1	0.26	0.17	-	80,80,80,80	0
56	MG	AA	1619	1/1	0.91	0.29	-	81,81,81,81	0
56	MG	DA	3162	1/1	0.89	0.16	-	69,69,69,69	0
56	MG	DB	202	1/1	0.98	0.21	-	40,40,40,40	0
56	MG	CA	3121	1/1	0.79	0.14	-	86,86,86,86	0
56	MG	CA	3140	1/1	0.57	0.27	-	76,76,76,76	0
56	MG	DA	3098	1/1	0.95	0.19	-	37,37,37,37	0
56	MG	CA	3116	1/1	0.61	0.41	-	75,75,75,75	0
56	MG	DB	204	1/1	0.89	0.21	-	57,57,57,57	0
56	MG	CA	3125	1/1	0.79	0.09	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3096	1/1	0.79	0.10	-	92,92,92,92	0
56	MG	DA	3115	1/1	0.92	0.17	-	56,56,56,56	0
56	MG	DA	3081	1/1	0.95	0.19	-	52,52,52,52	0
56	MG	AA	1641	1/1	0.78	0.08	-	71,71,71,71	0
56	MG	DA	3124	1/1	0.96	0.51	-	72,72,72,72	0
56	MG	CA	3066	1/1	0.44	0.47	-	85,85,85,85	0
56	MG	DA	3169	1/1	0.89	0.67	-	77,77,77,77	0
56	MG	CA	3119	1/1	0.92	0.06	-	83,83,83,83	0
56	MG	AA	1640	1/1	0.82	0.21	-	65,65,65,65	0
56	MG	CA	3107	1/1	0.79	0.28	-	70,70,70,70	0
56	MG	DA	3086	1/1	0.96	0.08	-	40,40,40,40	0
56	MG	CA	3041	1/1	0.86	0.05	-	72,72,72,72	0
56	MG	AA	1660	1/1	0.89	0.34	-	86,86,86,86	0
56	MG	CA	3001	1/1	0.79	0.16	-	80,80,80,80	0
56	MG	CA	3138	1/1	0.67	0.13	-	80,80,80,80	0
56	MG	CA	3068	1/1	0.54	0.12	-	85,85,85,85	0
56	MG	CA	3154	1/1	0.74	0.17	-	90,90,90,90	0
56	MG	CA	3016	1/1	0.86	0.06	-	71,71,71,71	0
56	MG	DA	3073	1/1	0.96	0.27	-	38,38,38,38	0
56	MG	CA	3144	1/1	0.91	0.31	-	73,73,73,73	0
56	MG	CA	3070	1/1	0.26	0.23	-	90,90,90,90	0
56	MG	CA	3111	1/1	0.82	0.49	-	77,77,77,77	0
56	MG	DA	3152	1/1	0.89	0.43	-	65,65,65,65	0
56	MG	CA	3048	1/1	0.89	0.10	-	74,74,74,74	0
56	MG	BA	1637	1/1	0.90	0.24	-	80,80,80,80	0
56	MG	DA	3043	1/1	0.81	0.18	-	49,49,49,49	0
56	MG	AA	1632	1/1	0.74	0.07	-	79,79,79,79	0
61	PEG	DA	3227	7/7	0.68	0.36	-	57,59,71,73	0
58	MPD	DA	3211	8/8	0.87	0.20	-	54,57,64,66	0
56	MG	CA	3065	1/1	0.92	0.05	-	73,73,73,73	0
56	MG	AA	1652	1/1	0.95	0.25	-	49,49,49,49	0
56	MG	AA	1613	1/1	0.78	0.59	-	80,80,80,80	0
56	MG	AA	1666	1/1	0.91	0.10	-	73,73,73,73	0
56	MG	DA	3166	1/1	0.78	0.18	-	73,73,73,73	0
56	MG	DA	3175	1/1	0.89	0.21	-	72,72,72,72	0
59	PUT	AA	1675	6/6	0.58	0.18	-	65,66,71,72	0
56	MG	CA	3128	1/1	0.84	0.44	-	82,82,82,82	0
56	MG	BA	1607	1/1	0.63	0.12	-	84,84,84,84	0
56	MG	DA	3171	1/1	0.61	0.27	-	76,76,76,76	0
56	MG	DA	3135	1/1	0.93	0.11	-	56,56,56,56	0
56	MG	AA	1627	1/1	0.94	0.38	-	80,80,80,80	0
56	MG	AA	1617	1/1	0.59	0.37	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3067	1/1	0.96	0.10	-	50,50,50,50	0
56	MG	DA	3130	1/1	0.78	0.69	-	77,77,77,77	0
58	MPD	DT	201	8/8	0.74	0.35	-	55,63,66,73	0
56	MG	AA	1651	1/1	0.83	0.10	-	69,69,69,69	0
56	MG	DA	3054	1/1	0.96	0.24	-	35,35,35,35	0
56	MG	AA	1647	1/1	0.07	0.13	-	82,82,82,82	0
56	MG	DA	3076	1/1	0.88	0.09	-	67,67,67,67	0
56	MG	CA	3082	1/1	0.62	0.12	-	79,79,79,79	0
56	MG	CA	3067	1/1	0.80	0.22	-	84,84,84,84	0
56	MG	DA	3114	1/1	0.99	0.19	-	35,35,35,35	0
56	MG	DA	3080	1/1	0.93	0.06	-	61,61,61,61	0
56	MG	CA	3077	1/1	0.82	0.05	-	83,83,83,83	0
56	MG	CA	3081	1/1	0.69	0.08	-	83,83,83,83	0
56	MG	CA	3095	1/1	0.86	0.20	-	71,71,71,71	0
56	MG	CA	3079	1/1	0.01	0.18	-	94,94,94,94	0
56	MG	CA	3120	1/1	0.91	0.35	-	74,74,74,74	0
56	MG	DA	3094	1/1	0.85	0.29	-	38,38,38,38	0
56	MG	CA	3103	1/1	0.60	0.06	-	86,86,86,86	0
56	MG	DA	3008	1/1	0.83	0.16	-	55,55,55,55	0
56	MG	DA	3023	1/1	0.98	0.25	-	41,41,41,41	0
61	PEG	DA	3199	7/7	0.84	0.22	-	49,56,67,67	0
56	MG	BA	1625	1/1	0.10	0.10	-	89,89,89,89	0
56	MG	DA	3144	1/1	0.96	0.10	-	69,69,69,69	0
66	EDO	DA	3216	4/4	0.85	0.22	-	60,61,62,67	0
56	MG	AA	1645	1/1	0.94	0.20	-	67,67,67,67	0
56	MG	CA	3063	1/1	0.82	0.46	-	93,93,93,93	0
56	MG	CA	3147	1/1	0.77	0.17	-	55,55,55,55	1
56	MG	AA	1626	1/1	0.69	0.20	-	84,84,84,84	0
56	MG	BA	1640	1/1	0.95	0.30	-	79,79,79,79	0
56	MG	AA	1615	1/1	0.90	0.45	-	74,74,74,74	0
56	MG	BA	1629	1/1	0.80	0.19	-	77,77,77,77	0
56	MG	DA	3096	1/1	0.91	0.22	-	69,69,69,69	0
56	MG	BA	1611	1/1	0.78	0.16	-	64,64,64,64	0
66	EDO	DB	211	4/4	0.64	0.17	-	68,70,71,73	0
56	MG	DA	3077	1/1	0.76	0.05	-	70,70,70,70	0
56	MG	CA	3109	1/1	0.72	0.37	-	72,72,72,72	0
56	MG	CA	3053	1/1	0.84	0.04	-	80,80,80,80	0
56	MG	DA	3074	1/1	0.97	0.28	-	42,42,42,42	0
56	MG	DA	3158	1/1	0.85	0.10	-	63,63,63,63	0
56	MG	AA	1630	1/1	0.28	0.23	-	86,86,86,86	0
56	MG	AA	1658	1/1	0.53	0.09	-	70,70,70,70	0
56	MG	CA	3059	1/1	0.28	0.52	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3123	1/1	0.91	0.15	-	75,75,75,75	0
56	MG	CA	3046	1/1	0.84	0.20	-	85,85,85,85	0
56	MG	DA	3013	1/1	0.81	0.26	-	52,52,52,52	0
56	MG	CA	3014	1/1	0.86	0.13	-	78,78,78,78	0
56	MG	DA	3116	1/1	0.93	0.11	-	57,57,57,57	0
56	MG	DA	3164	1/1	0.89	0.29	-	70,70,70,70	0
56	MG	DB	207	1/1	0.72	0.15	-	75,75,75,75	0
56	MG	DA	3017	1/1	0.99	0.26	-	36,36,36,36	0
56	MG	DA	3047	1/1	0.86	0.24	-	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.