



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2016 – 08:16 PM EDT

PDB ID : 5J91  
Title : Structure of the Wild-type 70S E coli ribosome bound to Tigecycline  
Authors : Cocozaki, A.; Ferguson, A.  
Deposited on : 2016-04-08  
Resolution : 2.96 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20027939

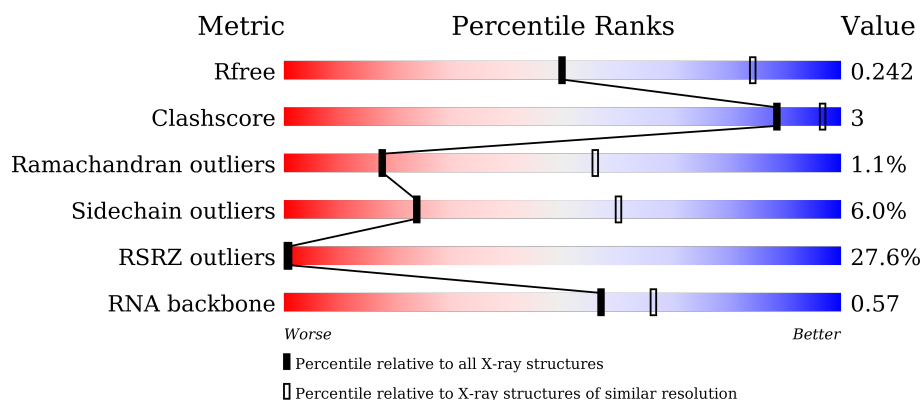
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.96 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)
RNA backbone	2183	1010 (3.36-2.56)

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  $\geq 3$ , 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>7%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
1	BA	1534	<div> <div>26%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>
2	AB	224	<div> <div>32%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
2	BB	224	<div> <div>35%</div> <div>85%</div> <div>13%</div> <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	C1	56	
22	D1	56	
23	C2	51	
23	D2	51	
24	C3	46	
24	D3	46	
25	C4	64	
25	D4	64	
26	C5	38	
26	D5	38	
27	C0	58	
27	D0	58	

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Mol	Chain	Length	Quality of chain
28	CB	120	<div> <div>37%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
28	DB	120	<div> <div>91%</div> <div>8%</div> <div>.</div> </div>
29	CC	272	<div> <div>32%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
29	DC	272	<div> <div>2%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
30	CD	209	<div> <div>63%</div> <div>89%</div> <div>11%</div> <div>.</div> </div>
31	CA	2904	<div> <div>35%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
32	DD	209	<div> <div>89%</div> <div>11%</div> </div>
33	CE	201	<div> <div>70%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
33	DE	201	<div> <div>%</div> <div>91%</div> <div>9%</div> </div>
34	CF	178	<div> <div>85%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
34	DF	178	<div> <div>9%</div> <div>82%</div> <div>17%</div> <div>..</div> </div>
35	CG	176	<div> <div>81%</div> <div>88%</div> <div>12%</div> </div>
35	DG	176	<div> <div>5%</div> <div>88%</div> <div>12%</div> </div>
36	CH	149	<div> <div>53%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
36	DH	149	<div> <div>42%</div> <div>83%</div> <div>17%</div> <div>.</div> </div>
37	CJ	134	<div> <div>95%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
37	DJ	134	<div> <div>82%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
38	CK	142	<div> <div>50%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
38	DK	142	<div> <div>94%</div> <div>6%</div> <div>.</div> </div>
39	CL	123	<div> <div>35%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
39	DL	123	<div> <div>90%</div> <div>8%</div> <div>.</div> </div>
40	CM	144	<div> <div>80%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
40	DM	144	<div> <div>2%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
41	CN	136	<div> <div>26%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
41	DN	136	<div> <div>92%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
42	CO	125	
42	DO	125	
43	CP	117	
43	DP	117	
44	CQ	114	
44	DQ	114	
45	CR	117	
45	DR	117	
46	CS	103	
46	DS	103	
47	CT	110	
47	DT	110	
48	CU	93	
48	DU	93	
49	CV	103	
49	DV	103	
50	CW	94	
50	DW	94	
51	CX	76	
51	DX	76	
52	CY	77	
52	DY	77	
53	CZ	62	
53	DZ	62	
54	DI	135	

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Mol	Chain	Length	Quality of chain
55	DA	2904	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	1607	-	-	-	X
56	MG	AA	1612	-	-	-	X
56	MG	AA	1633	-	-	-	X
56	MG	AA	1642	-	-	-	X
56	MG	AA	1657	-	-	-	X
56	MG	AA	1661	-	-	-	X
56	MG	BA	1612	-	-	-	X
56	MG	BA	1626	-	-	-	X
56	MG	CA	3003	-	-	-	X
56	MG	CA	3022	-	-	-	X
56	MG	CA	3026	-	-	-	X
56	MG	CA	3032	-	-	-	X
56	MG	CA	3037	-	-	-	X
56	MG	CA	3100	-	-	-	X
56	MG	CA	3105	-	-	-	X
56	MG	CA	3110	-	-	-	X
56	MG	CA	3131	-	-	-	X
56	MG	CA	3133	-	-	-	X
56	MG	CA	3137	-	-	-	X
56	MG	CA	3147	-	-	-	X
56	MG	CA	3151	-	-	-	X
56	MG	DA	3038	-	-	-	X
56	MG	DA	3123	-	-	-	X
56	MG	DA	3125	-	-	-	X
56	MG	DA	3127	-	-	-	X
56	MG	DA	3128	-	-	-	X
56	MG	DA	3133	-	-	-	X
56	MG	DA	3148	-	-	-	X
56	MG	DA	3163	-	-	-	X
56	MG	DA	3172	-	-	-	X
56	MG	DA	3182	-	-	-	X
57	PG4	AA	1670	-	-	-	X
57	PG4	BA	1642	-	-	-	X
57	PG4	DA	3193	-	-	-	X
57	PG4	DA	3215	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	PG4	DS	202	-	-	-	X
58	MPD	AA	1671	-	-	-	X
58	MPD	AA	1676	-	-	-	X
58	MPD	DA	3192	-	-	-	X
58	MPD	DA	3203	-	-	-	X
58	MPD	DA	3206	-	-	-	X
58	MPD	DE	301	-	-	-	X
58	MPD	DE	302	-	-	-	X
59	PUT	AA	1672	-	-	-	X
59	PUT	AA	1673	-	-	-	X
59	PUT	AA	1674	-	-	-	X
59	PUT	DA	3189	-	-	-	X
59	PUT	DA	3195	-	-	-	X
59	PUT	DA	3204	-	-	-	X
59	PUT	DA	3211	-	-	-	X
59	PUT	DA	3212	-	-	-	X
59	PUT	DA	3218	-	-	-	X
59	PUT	DA	3220	-	-	-	X
59	PUT	DA	3221	-	-	-	X
62	PEG	AL	201	-	-	-	X
62	PEG	D1	103	-	-	-	X
62	PEG	D3	102	-	-	-	X
62	PEG	DA	3200	-	-	-	X
62	PEG	DA	3217	-	-	-	X
62	PEG	DL	201	-	-	-	X
62	PEG	DQ	201	-	-	-	X
63	EDO	D1	101	-	-	-	X
63	EDO	DA	3001	-	-	-	X
63	EDO	DA	3197	-	-	-	X
63	EDO	DA	3198	-	-	-	X
64	PGE	D1	102	-	-	-	X
64	PGE	D3	101	-	-	-	X
64	PGE	DA	3213	-	-	-	X
64	PGE	DA	3224	-	-	-	X
64	PGE	DD	301	-	-	-	X
64	PGE	DU	101	-	-	-	X
65	SPD	DA	3183	-	-	-	X
65	SPD	DA	3187	-	-	-	X
65	SPD	DA	3205	-	-	-	X
65	SPD	DA	3223	-	-	-	X
66	1PE	DA	3185	-	-	-	X
66	1PE	DA	3202	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
67	ACY	DA	3201	-	-	-	X
68	GUN	DA	3210	-	-	-	X

## 2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 295202 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0	0
			32930	14694	6041	10661	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32908	14684	6036	10655	1533			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	0
			796	498	152	145	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	BJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0	0
			670	414	138	115	3			
20	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

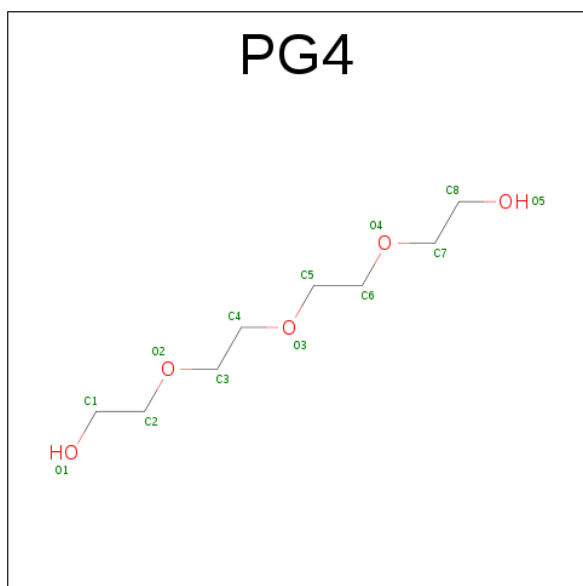
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BA	43	Total	Mg	0	0
			43	43		
56	CA	156	Total	Mg	0	0
			156	156		
56	CB	3	Total	Mg	0	0
			3	3		
56	DM	1	Total	Mg	0	0
			1	1		
56	DR	2	Total	Mg	0	0
			2	2		
56	AA	71	Total	Mg	0	0
			71	71		
56	DA	182	Total	Mg	0	0
			182	182		
56	DB	9	Total	Mg	0	0
			9	9		

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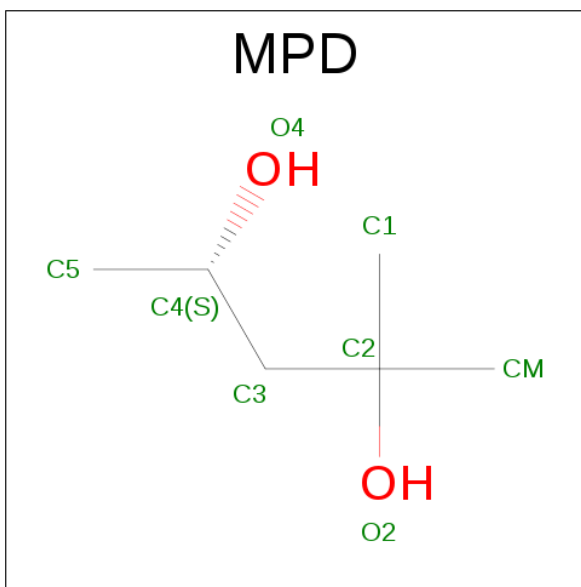
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DD	2	Total	Mg	0	0
			2	2		

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



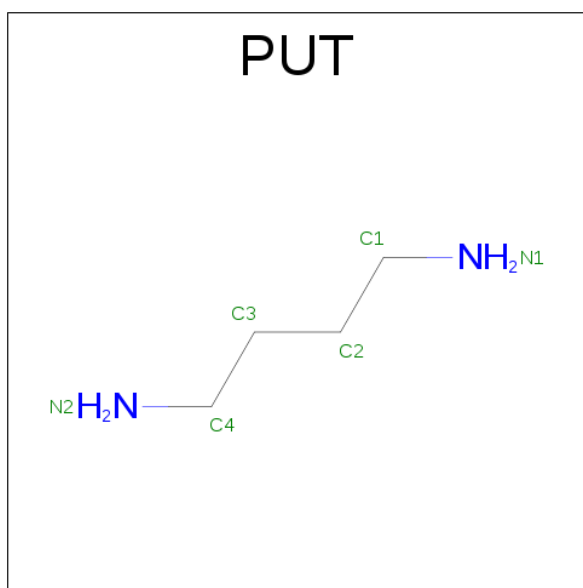
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			13	8	5		
57	BA	1	Total	C	O	0	0
			13	8	5		
57	DQ	1	Total	C	O	0	0
			13	8	5		
57	DR	1	Total	C	O	0	0
			13	8	5		
57	DS	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (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	DE	1	Total	C	O	0	0
			8	6	2		
58	DE	1	Total	C	O	0	0
			8	6	2		
58	DK	1	Total	C	O	0	0
			8	6	2		
58	DN	1	Total	C	O	0	0
			8	6	2		
58	DS	1	Total	C	O	0	0
			8	6	2		
58	DT	1	Total	C	O	0	0
			8	6	2		
58	DT	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		

- Molecule 59 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



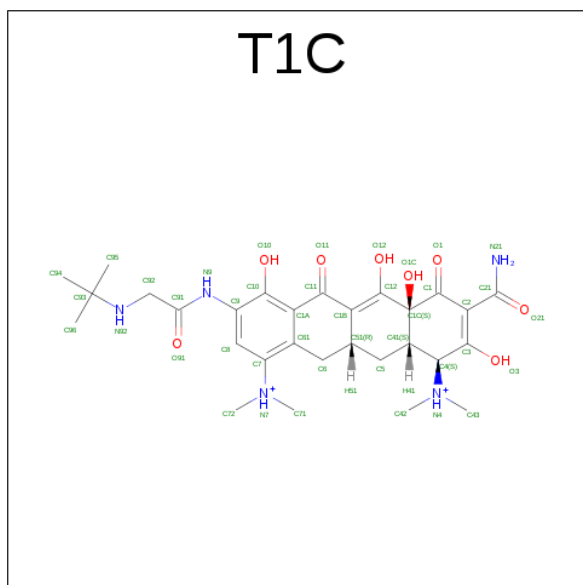
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6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

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

- Molecule 60 is TIGECYCLINE (three-letter code: T1C) (formula: C<sub>29</sub>H<sub>41</sub>N<sub>5</sub>O<sub>8</sub>).



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

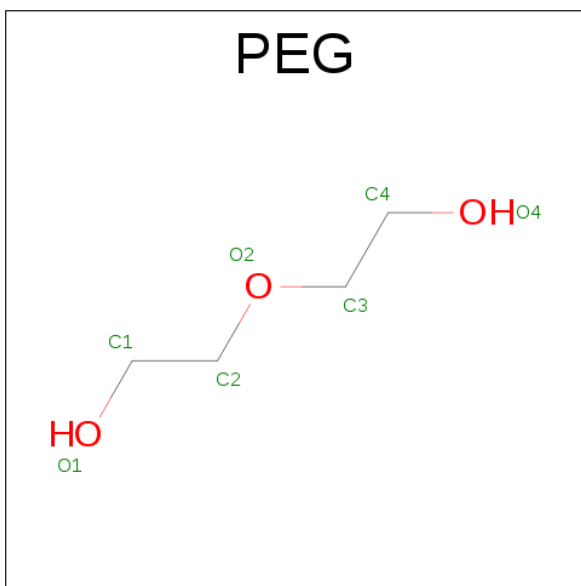
- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 62 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:

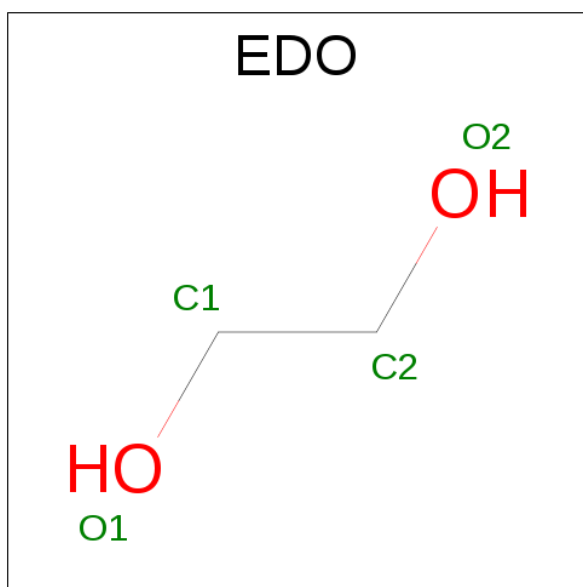


C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



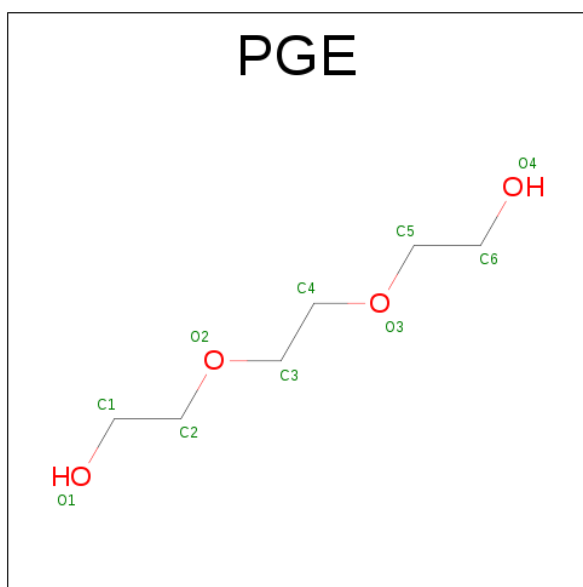
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	AL	1	Total	C	O	0	0
			7	4	3		
62	D1	1	Total	C	O	0	0
			7	4	3		
62	D3	1	Total	C	O	0	0
			7	4	3		
62	DL	1	Total	C	O	0	0
			7	4	3		
62	DP	1	Total	C	O	0	0
			7	4	3		
62	DQ	1	Total	C	O	0	0
			7	4	3		
62	DA	1	Total	C	O	0	0
			7	4	3		
62	DA	1	Total	C	O	0	0
			7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

- Molecule 63 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



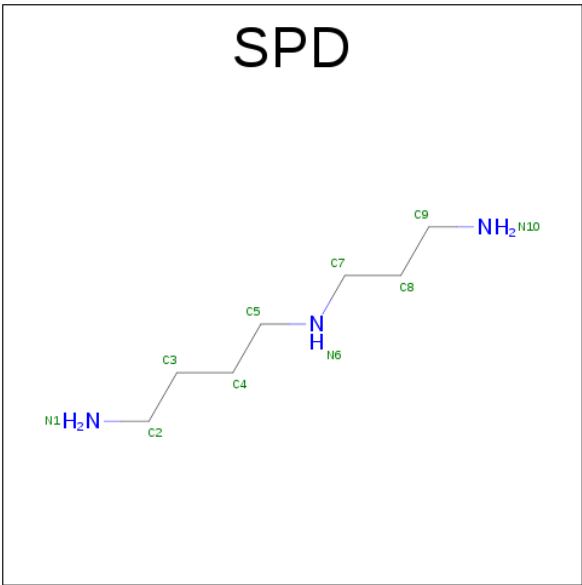
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			4	2	2		
63	DB	1	Total	C	O	0	0
			4	2	2		
63	DB	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4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

- Molecule 64 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



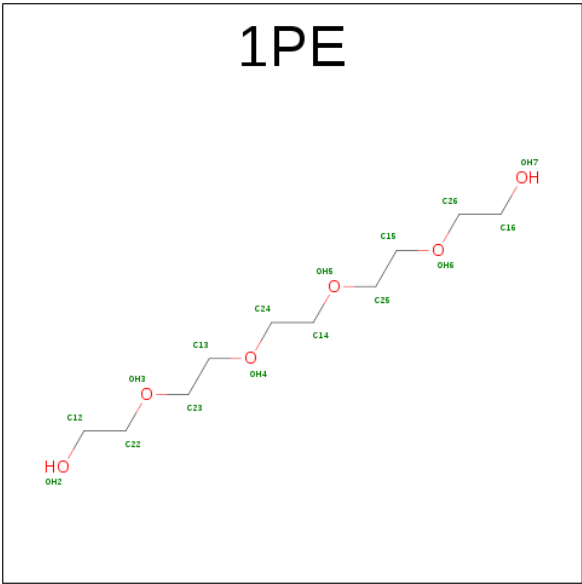
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	D1	1	Total	C	O	0	0
			10	6	4		
64	D3	1	Total	C	O	0	0
			10	6	4		
64	DD	1	Total	C	O	0	0
			10	6	4		
64	DS	1	Total	C	O	0	0
			10	6	4		
64	DU	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0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

- Molecule 65 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



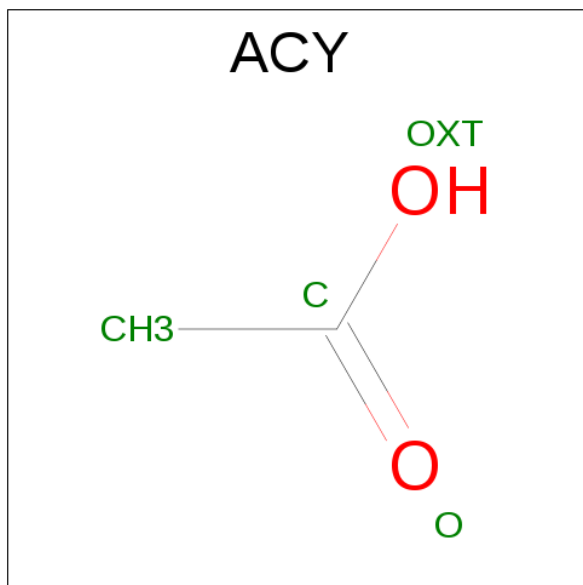
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
65	DA	1	Total	C	N	0	0
			10	7	3		
65	DA	1	Total	C	N	0	0
			10	7	3		
65	DA	1	Total	C	N	0	0
			10	7	3		
65	DA	1	Total	C	N	0	0
			10	7	3		

- Molecule 66 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



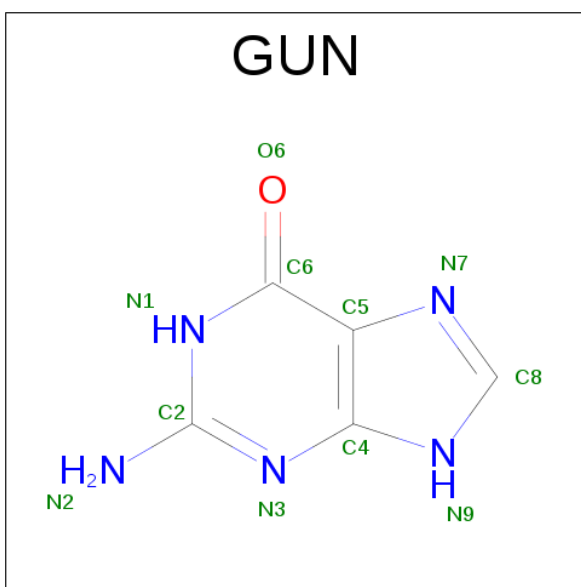
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			16	10	6		
66	DA	1	Total	C	O	0	0
			16	10	6		

- Molecule 67 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



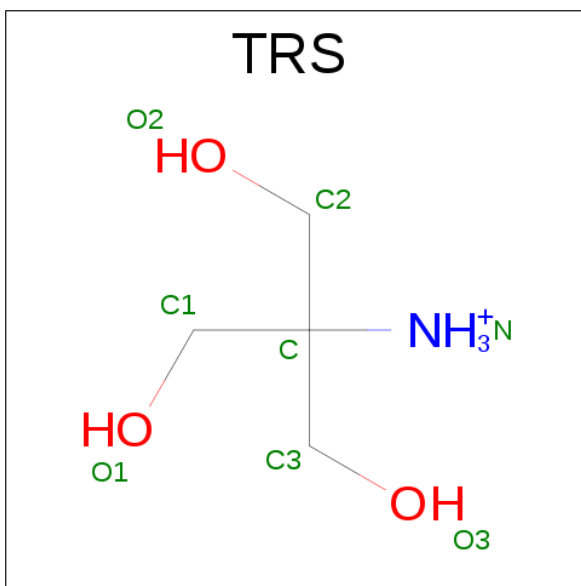
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
67	DA	1	Total	C	O	0	0
			4	2	2		
67	DA	1	Total	C	O	0	0
			4	2	2		
67	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 68 is GUANINE (three-letter code: GUN) (formula: C<sub>5</sub>H<sub>5</sub>N<sub>5</sub>O).



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

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



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

- Molecule 70 is water.

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

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

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

*Continued on next page...*

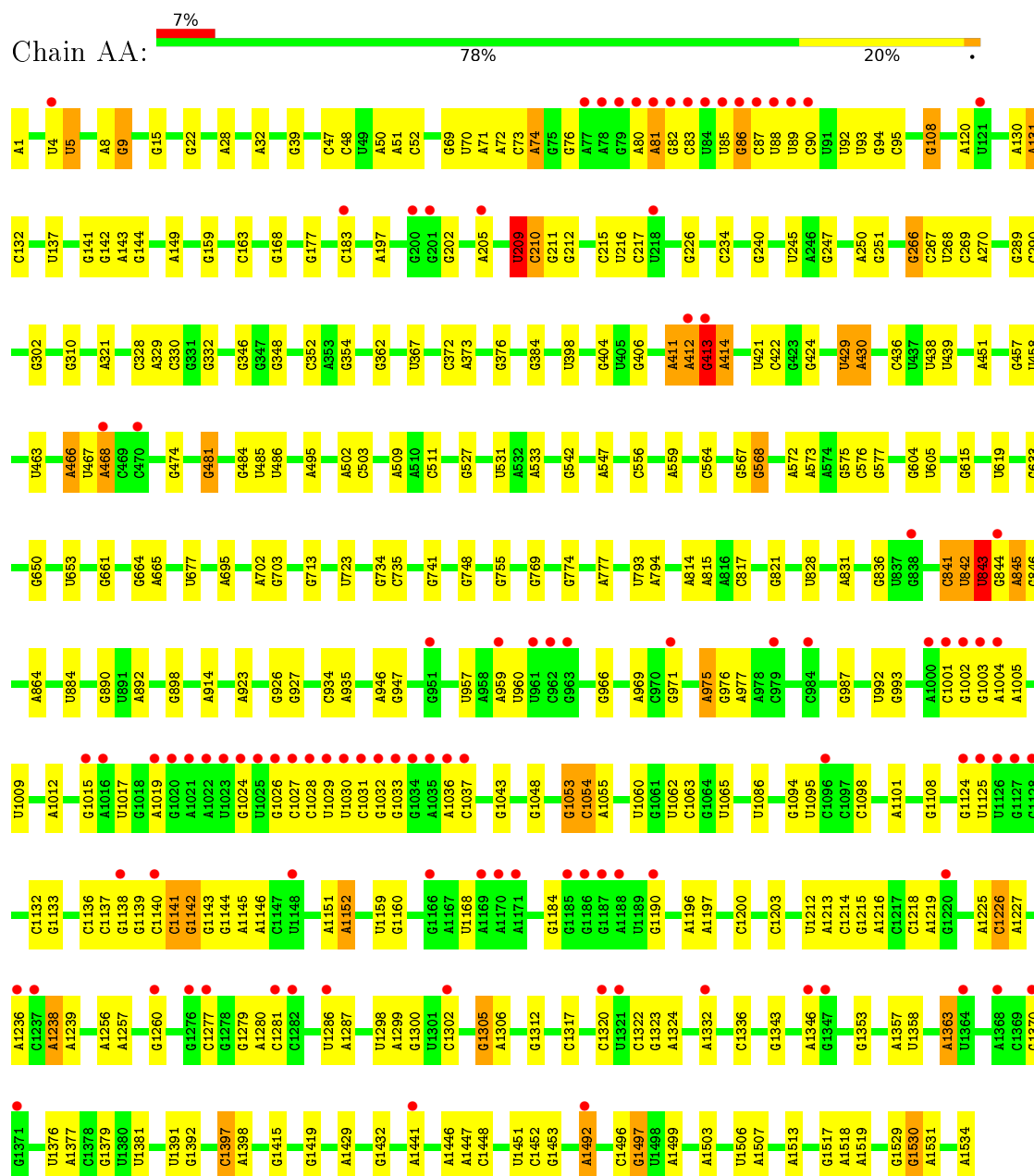
*Continued from previous page...*

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

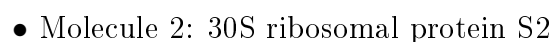
### 3 Residue-property plots

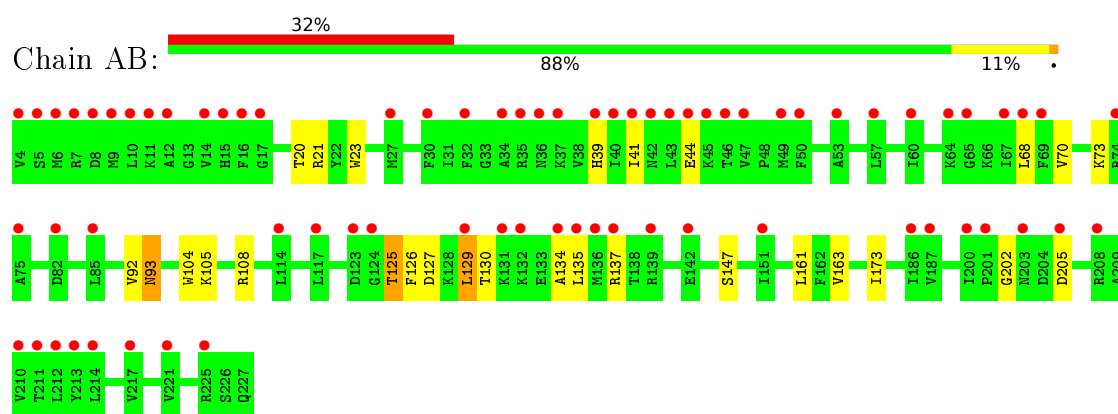
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

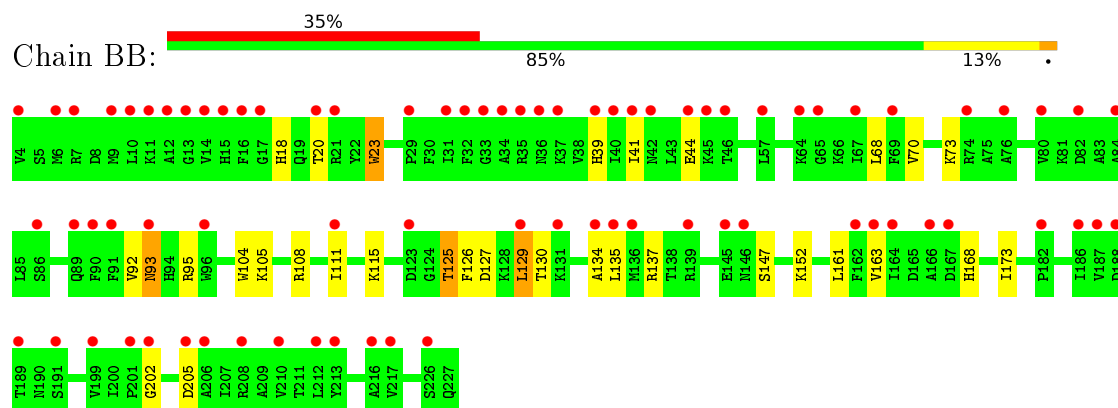


#### • Molecule 1: 16S rRNA

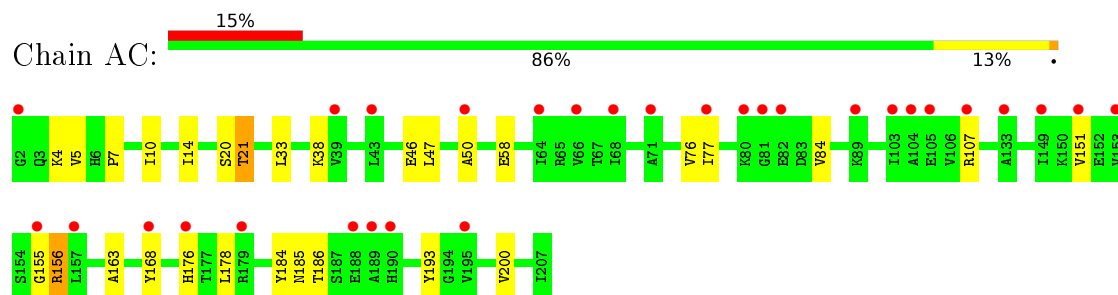




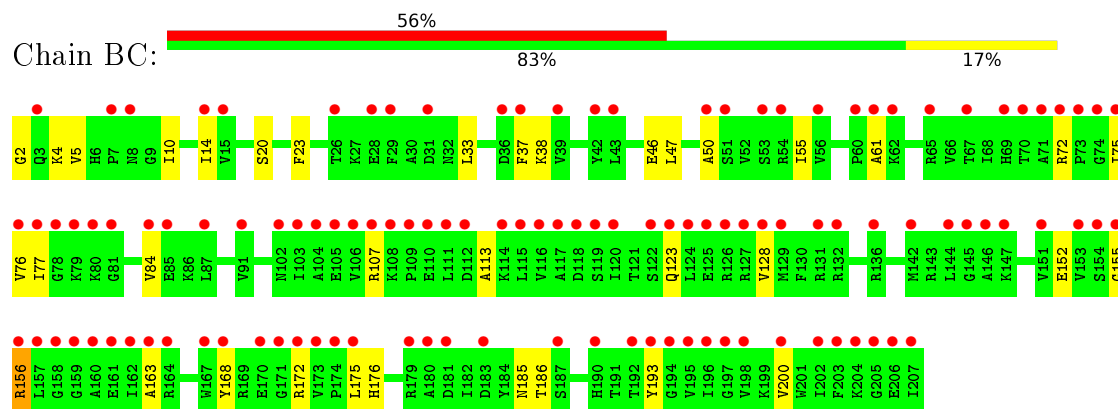
• Molecule 2: 30S ribosomal protein S2



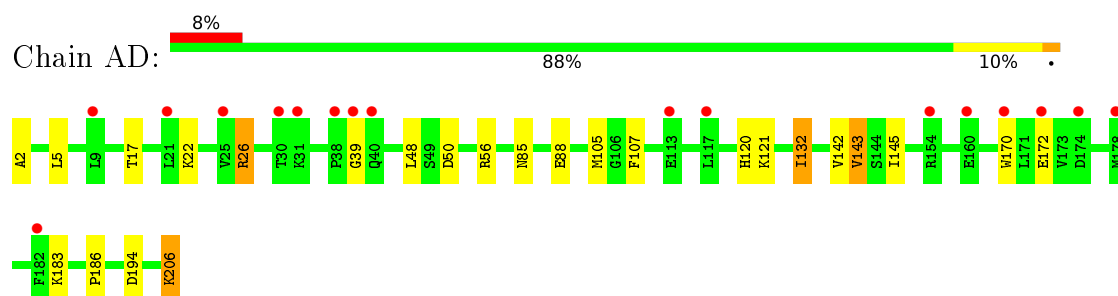
• Molecule 3: 30S ribosomal protein S3



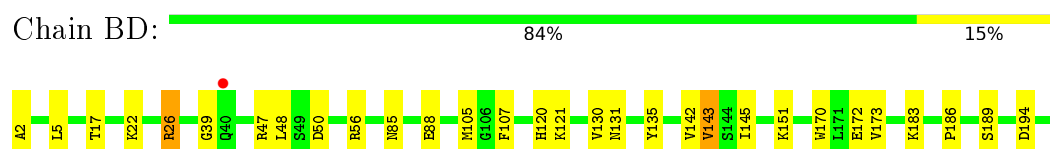
• Molecule 3: 30S ribosomal protein S3



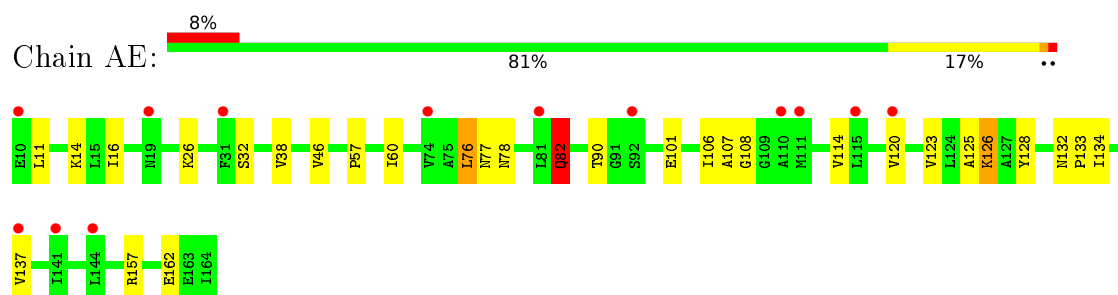
- Molecule 4: 30S ribosomal protein S4



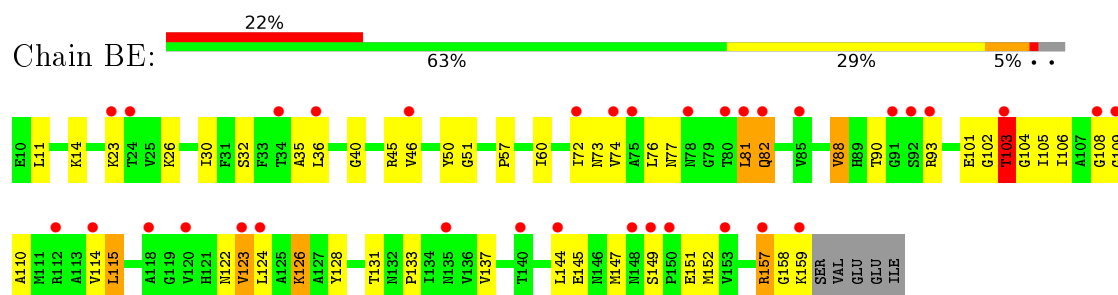
- Molecule 4: 30S ribosomal protein S4



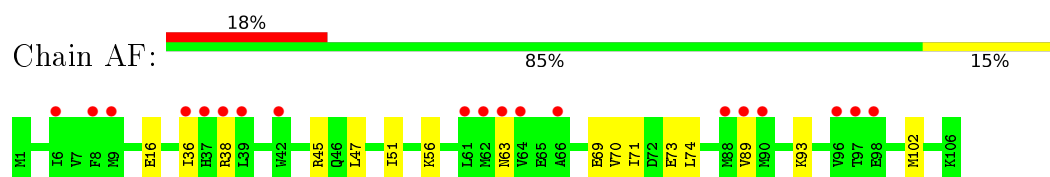
- Molecule 5: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S5

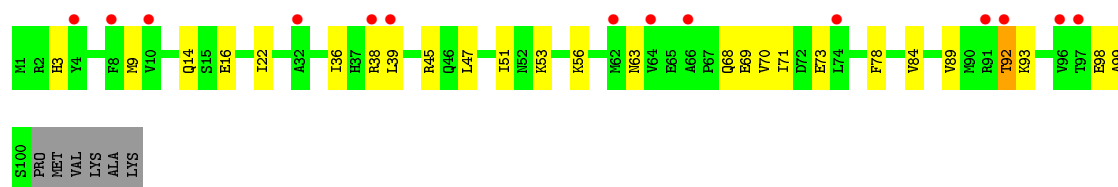


- Molecule 6: 30S ribosomal protein S6

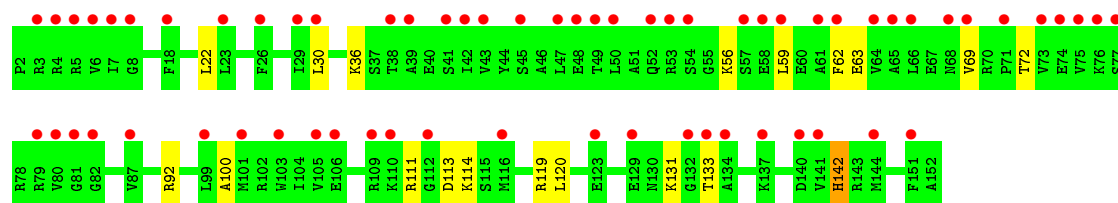
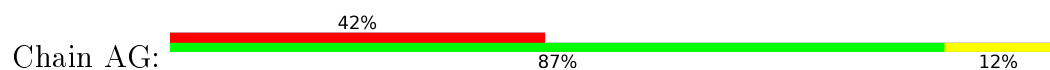


- Molecule 6: 30S ribosomal protein S6

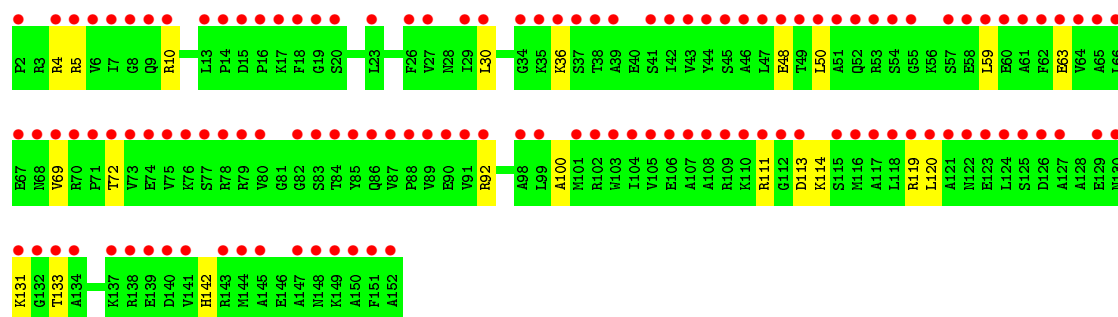
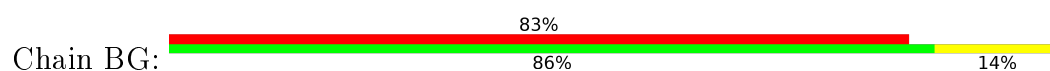




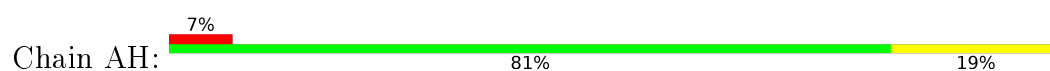
• Molecule 7: 30S ribosomal protein S7



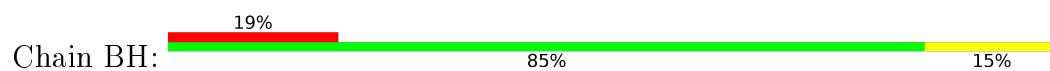
• Molecule 7: 30S ribosomal protein S7



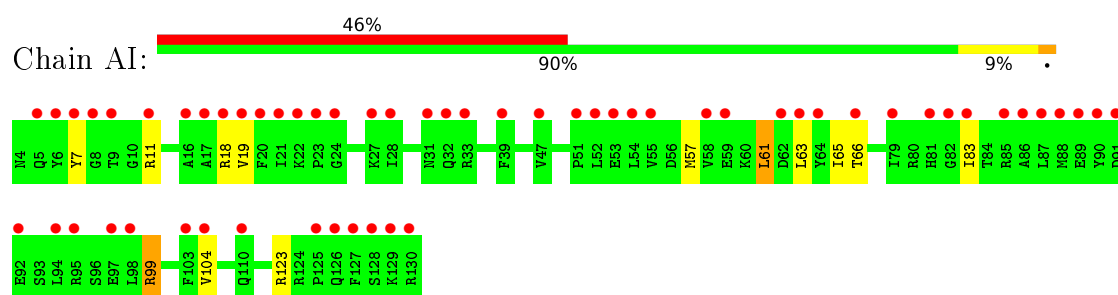
• Molecule 8: 30S ribosomal protein S8



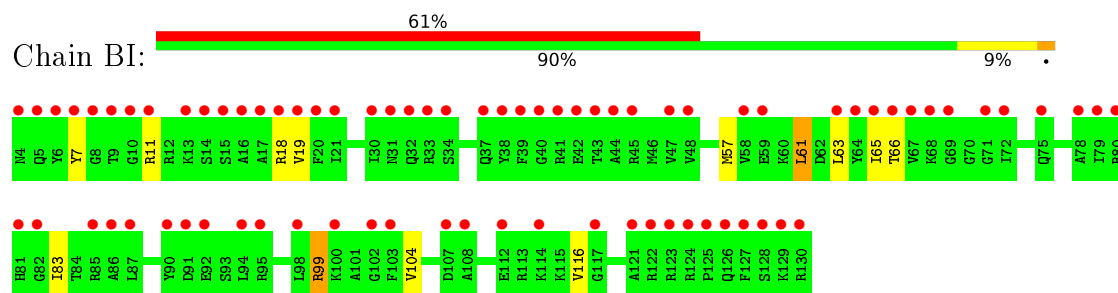
• Molecule 8: 30S ribosomal protein S8



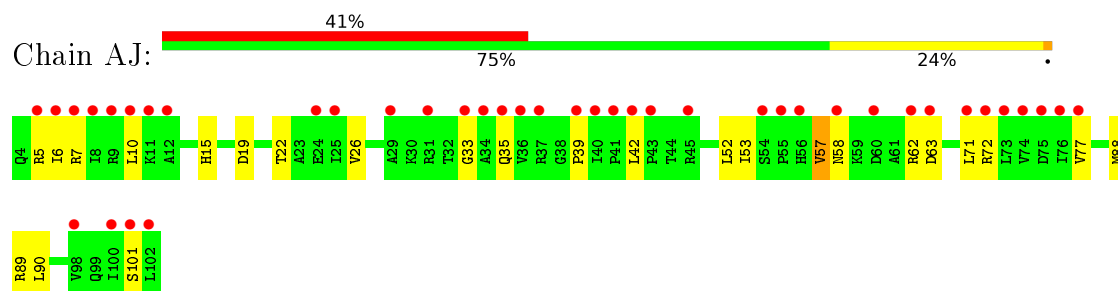
• Molecule 9: 30S ribosomal protein S9



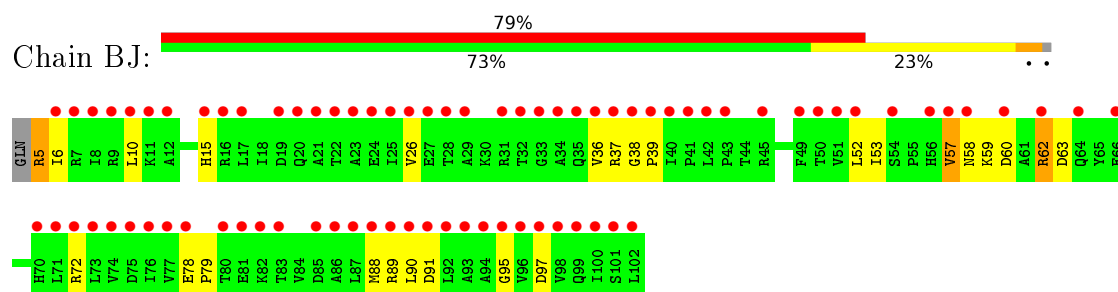
- Molecule 9: 30S ribosomal protein S9



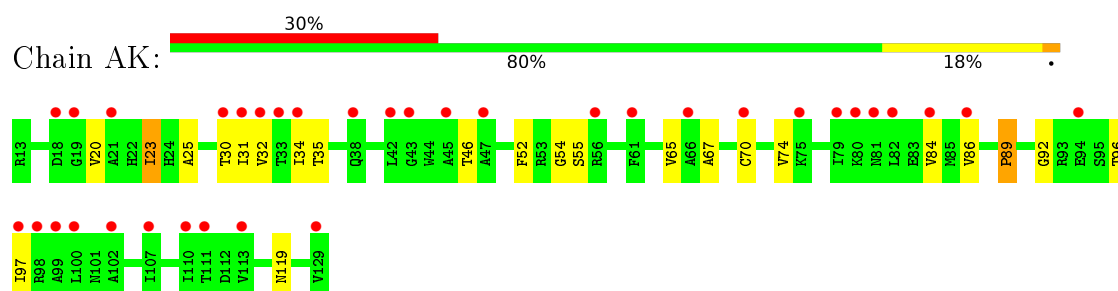
- Molecule 10: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S10

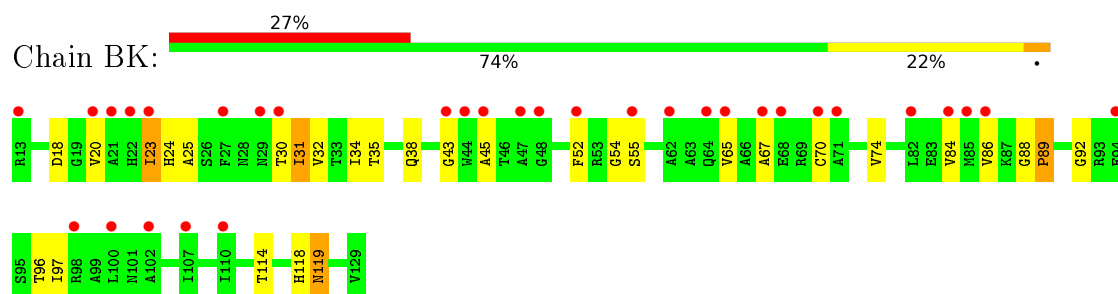


- Molecule 11: 30S ribosomal protein S11

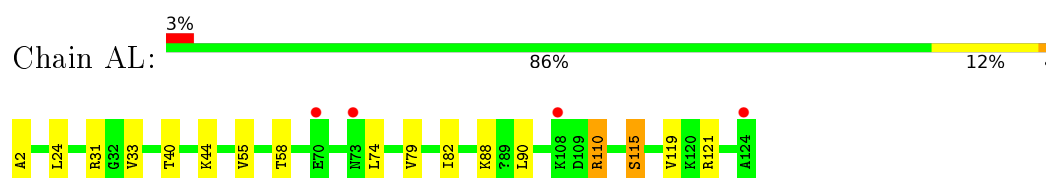




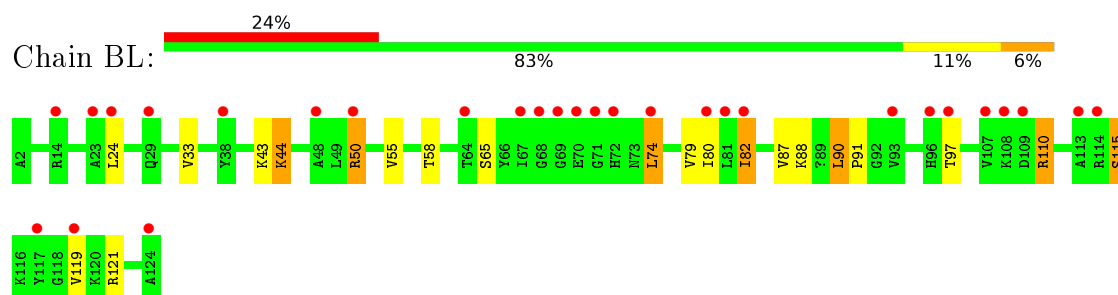
- Molecule 11: 30S ribosomal protein S11



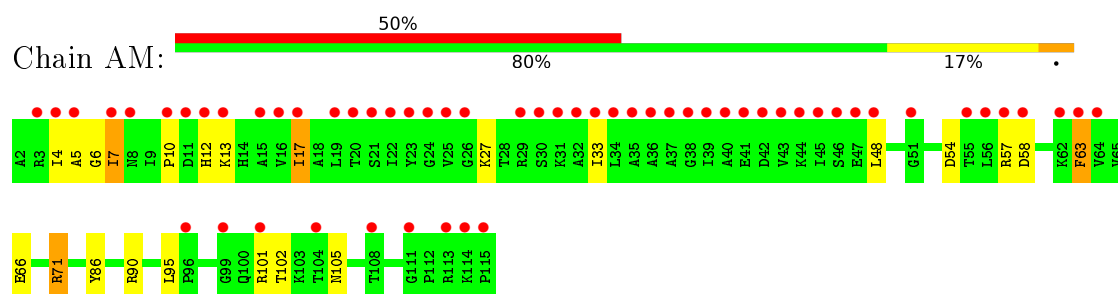
- Molecule 12: 30S ribosomal protein S12



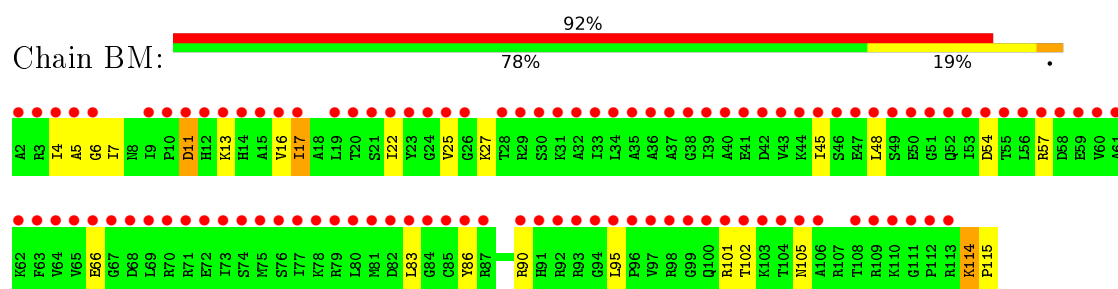
- Molecule 12: 30S ribosomal protein S12



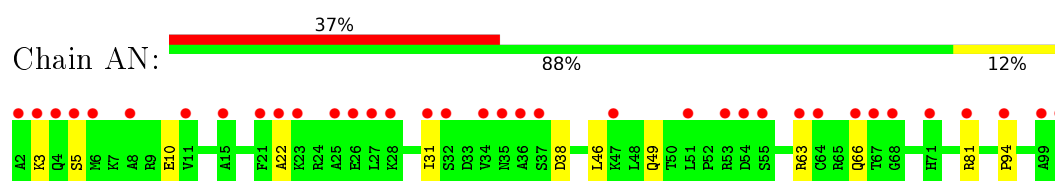
- Molecule 13: 30S ribosomal protein S13



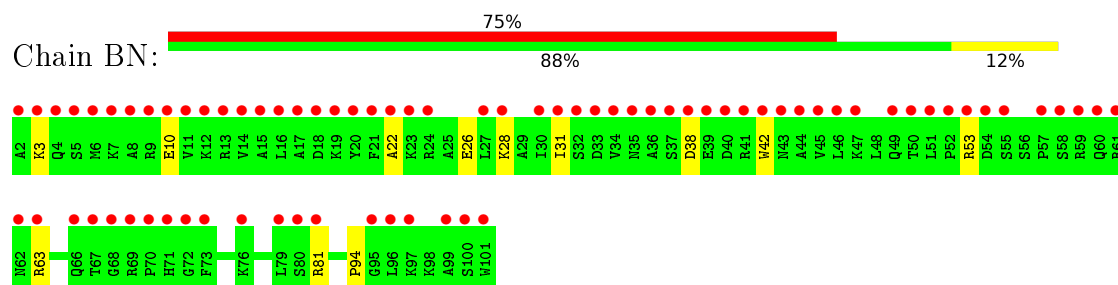
- Molecule 13: 30S ribosomal protein S13



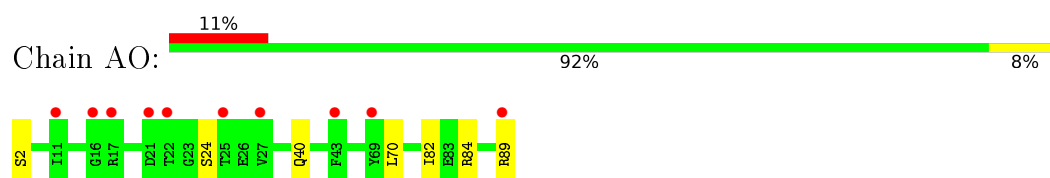
- Molecule 14: 30S ribosomal protein S14



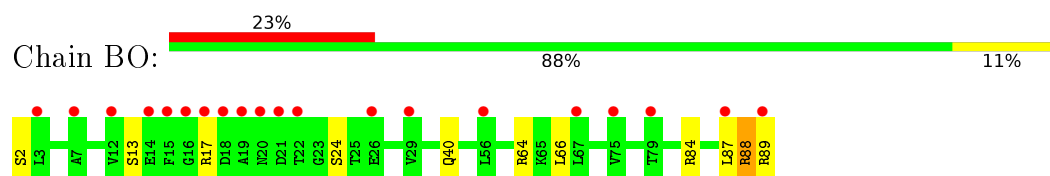
- Molecule 14: 30S ribosomal protein S14



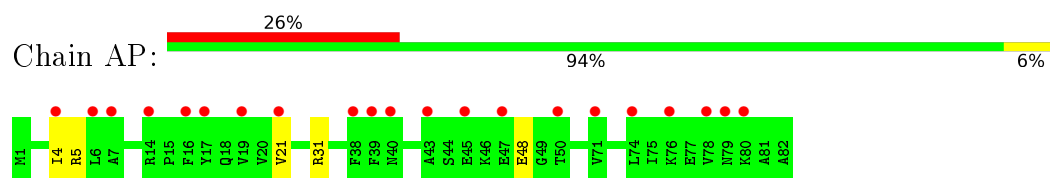
- Molecule 15: 30S ribosomal protein S15



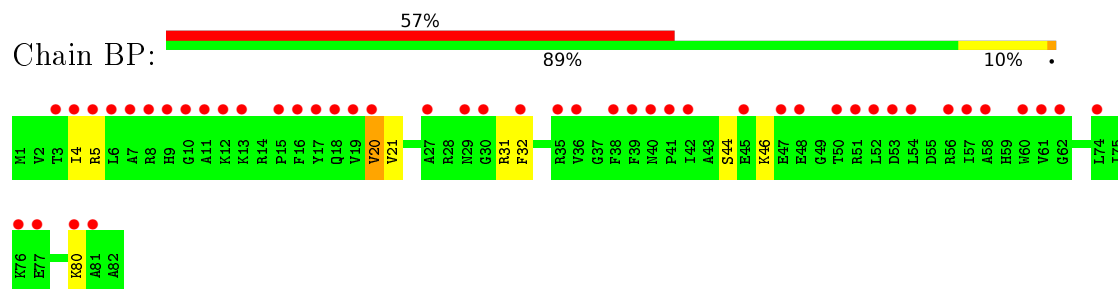
- Molecule 15: 30S ribosomal protein S15



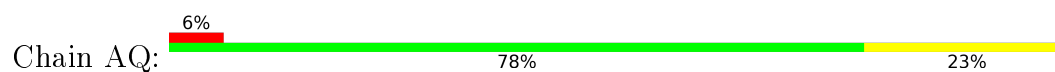
- Molecule 16: 30S ribosomal protein S16



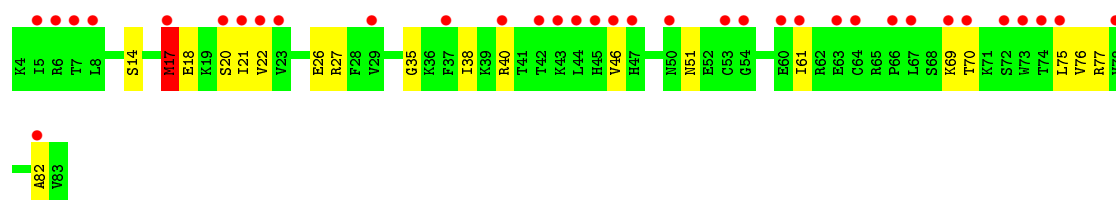
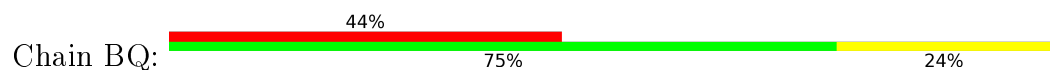
- Molecule 16: 30S ribosomal protein S16



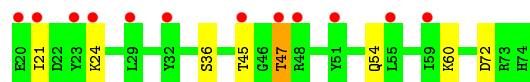
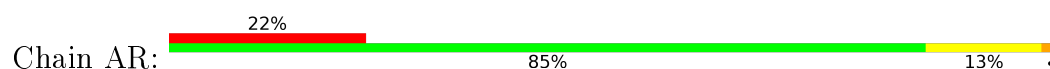
- Molecule 17: 30S ribosomal protein S17



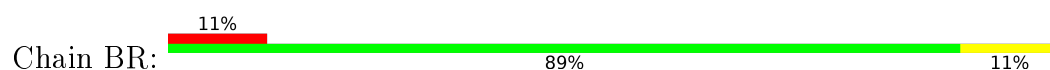
- Molecule 17: 30S ribosomal protein S17



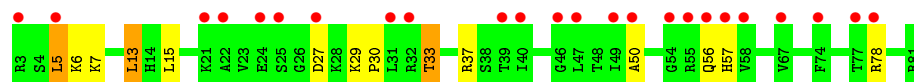
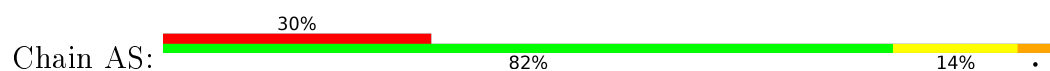
- Molecule 18: 30S ribosomal protein S18



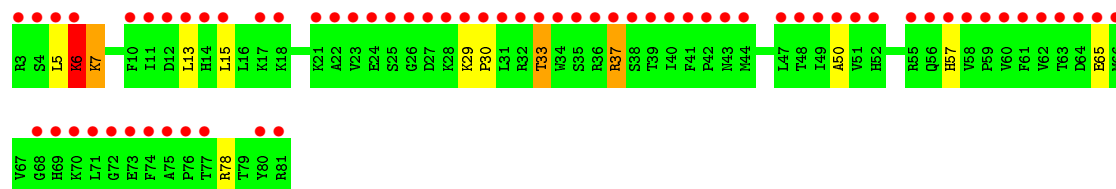
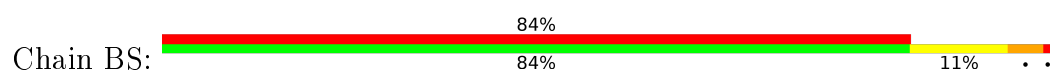
- Molecule 18: 30S ribosomal protein S18



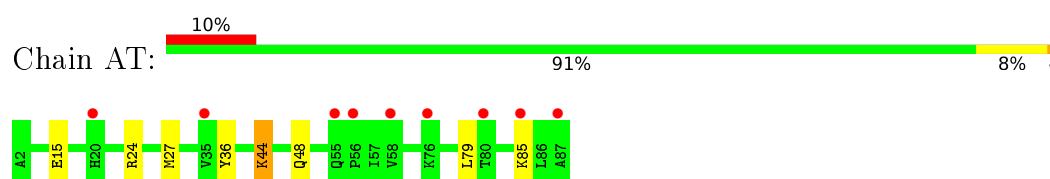
- Molecule 19: 30S ribosomal protein S19



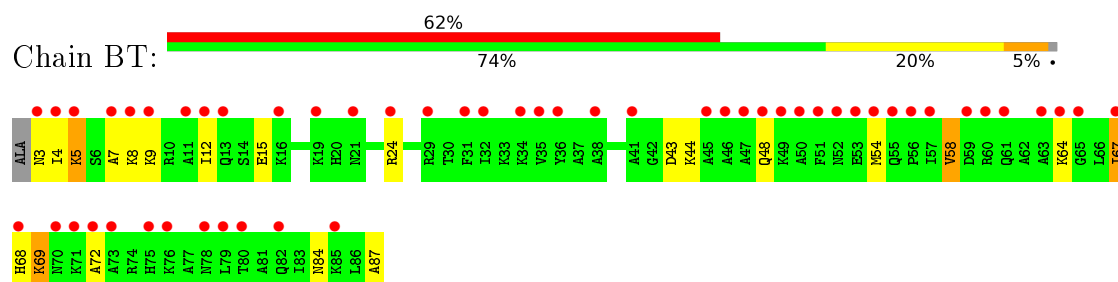
- Molecule 19: 30S ribosomal protein S19



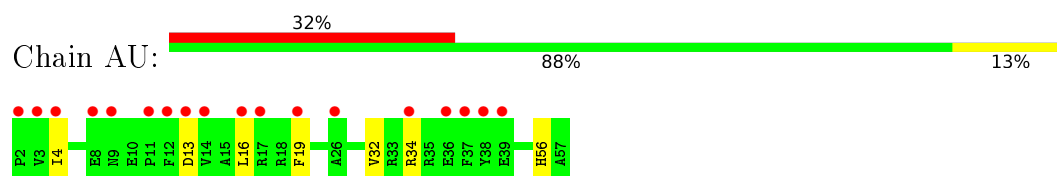
- Molecule 20: 30S ribosomal protein S20



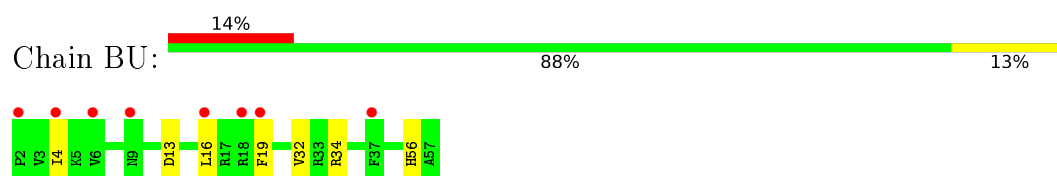
- Molecule 20: 30S ribosomal protein S20



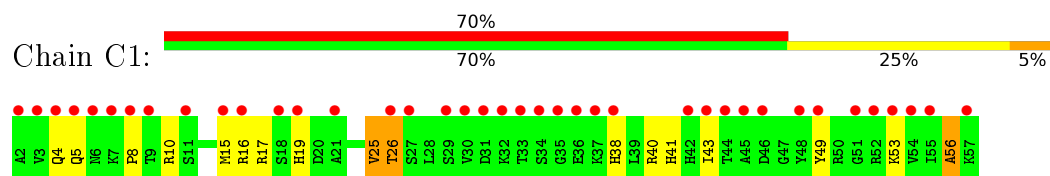
- Molecule 21: 30S ribosomal protein S21



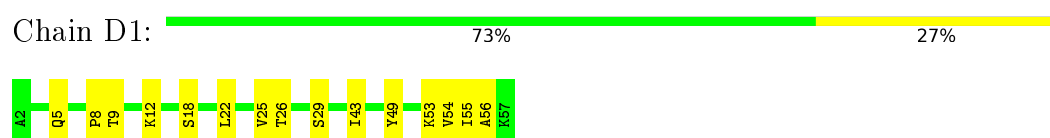
- Molecule 21: 30S ribosomal protein S21



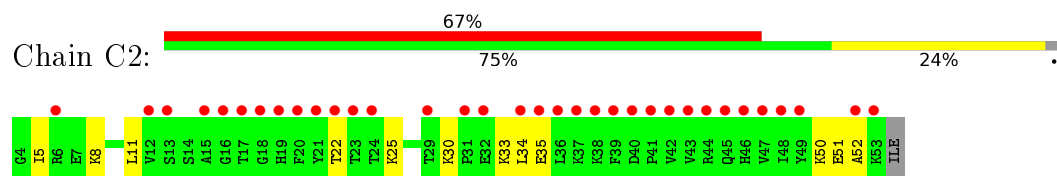
- Molecule 22: 50S ribosomal protein L32



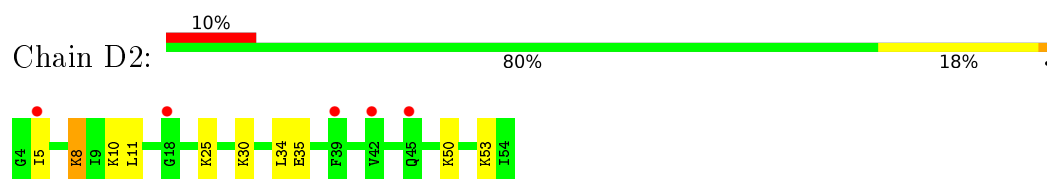
- Molecule 22: 50S ribosomal protein L32



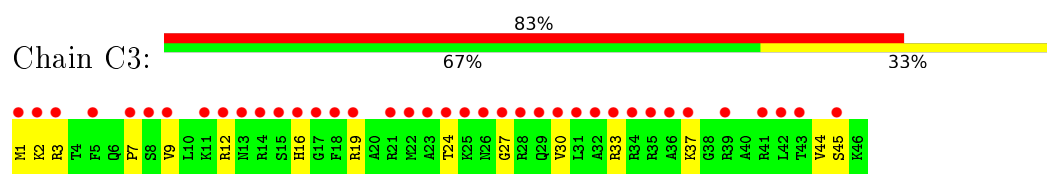
- Molecule 23: 50S ribosomal protein L33



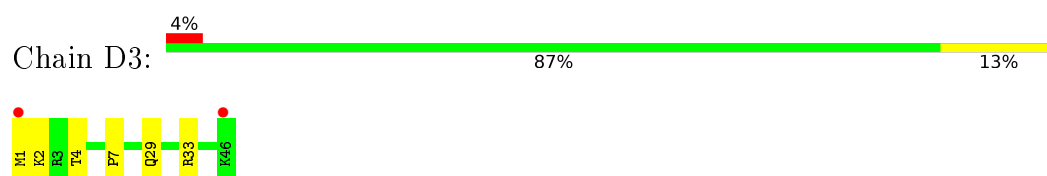
- Molecule 23: 50S ribosomal protein L33



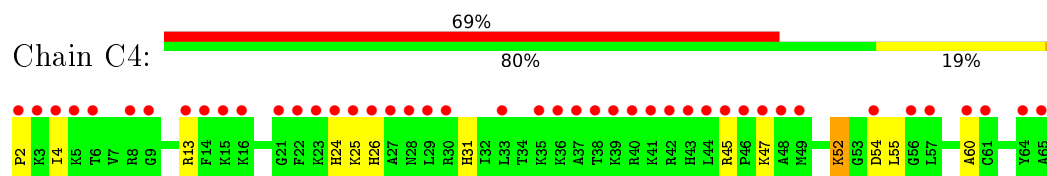
- Molecule 24: 50S ribosomal protein L34



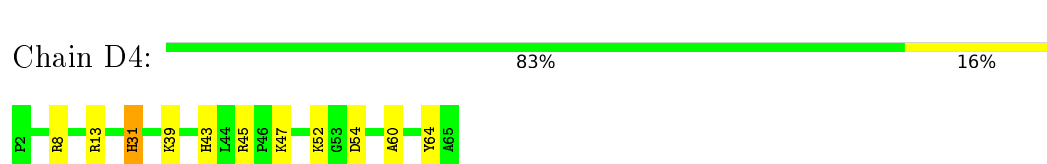
- Molecule 24: 50S ribosomal protein L34



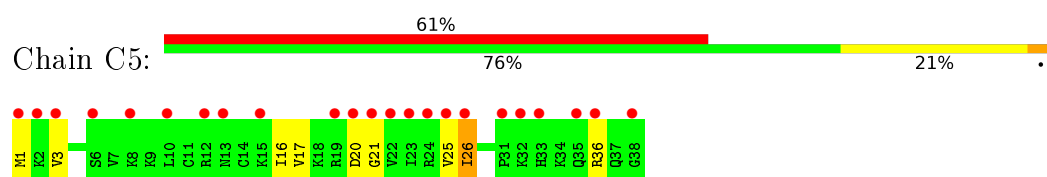
- Molecule 25: 50S ribosomal protein L35



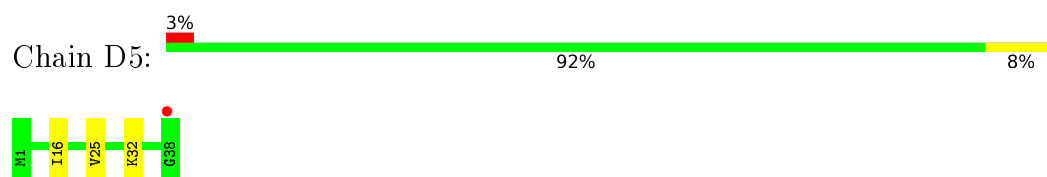
- Molecule 25: 50S ribosomal protein L35



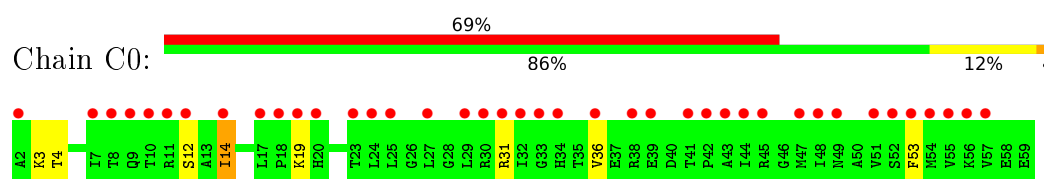
- Molecule 26: 50S ribosomal protein L36



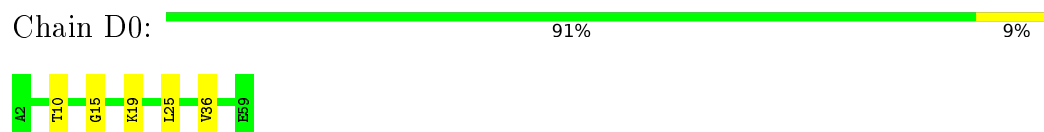
- Molecule 26: 50S ribosomal protein L36



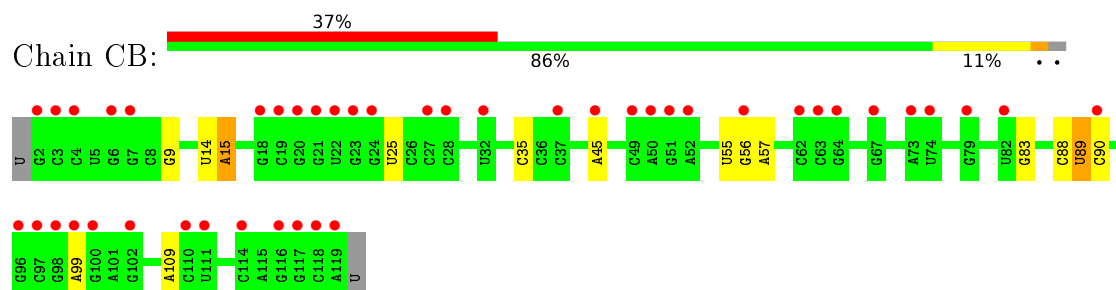
- Molecule 27: 50S ribosomal protein L30



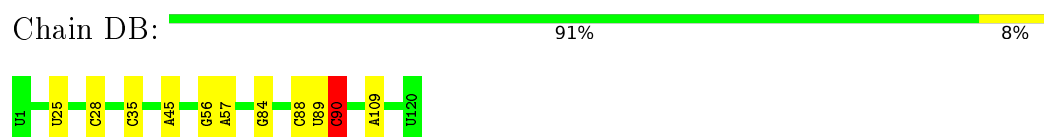
- Molecule 27: 50S ribosomal protein L30



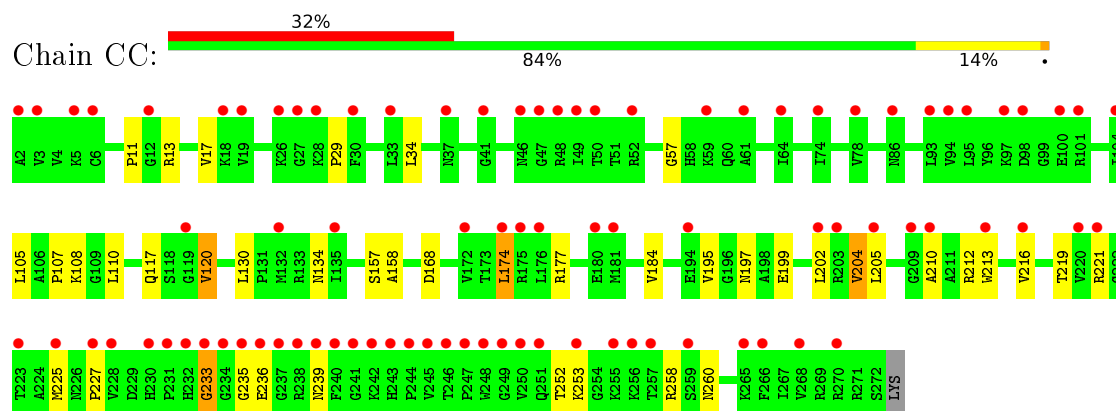
- Molecule 28: 5S rRNA



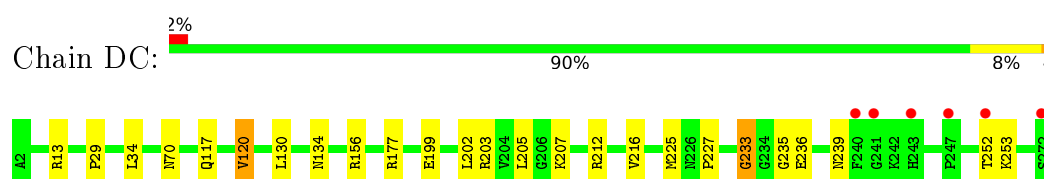
- Molecule 28: 5S rRNA



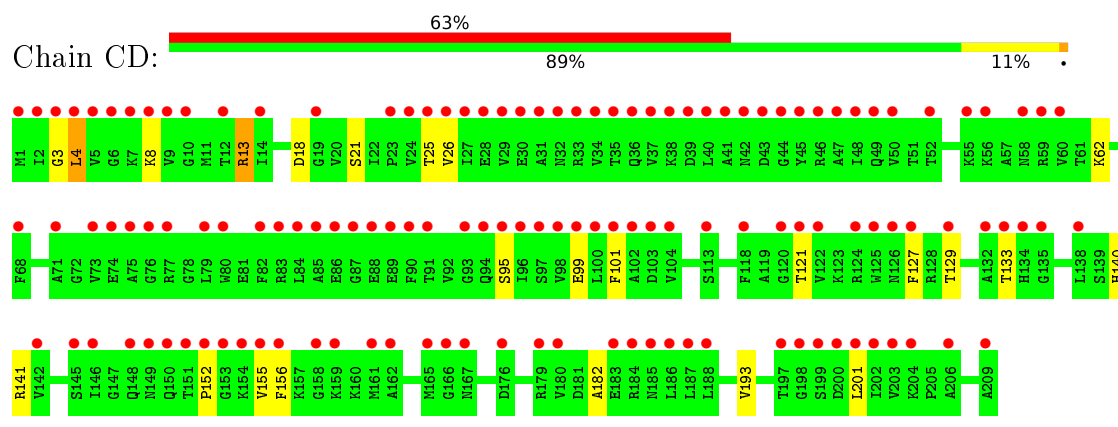
- Molecule 29: 50S ribosomal protein L2



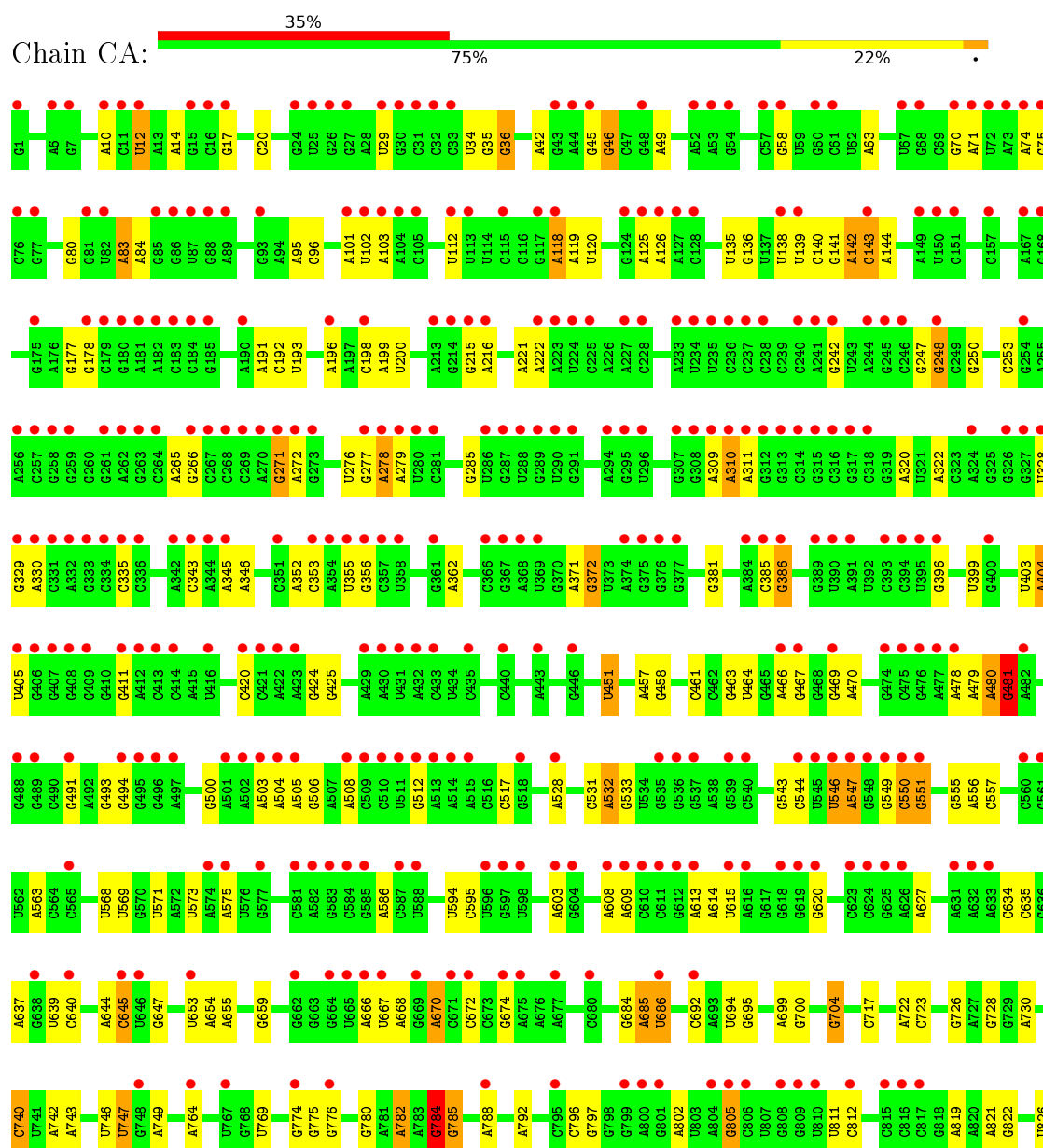
- Molecule 29: 50S ribosomal protein L2



• Molecule 30: 50S ribosomal protein L3

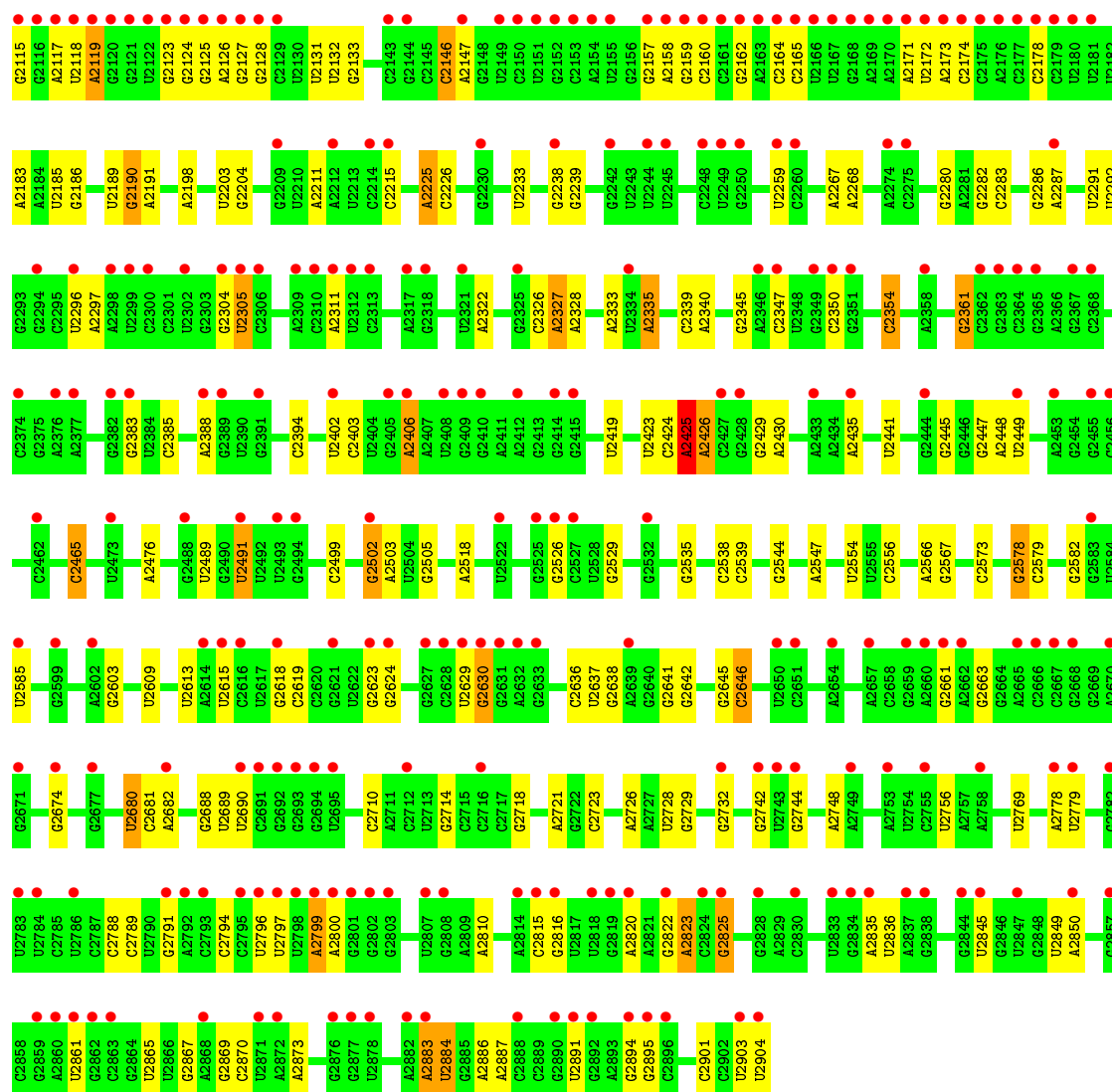


• Molecule 31: 23S rRNA









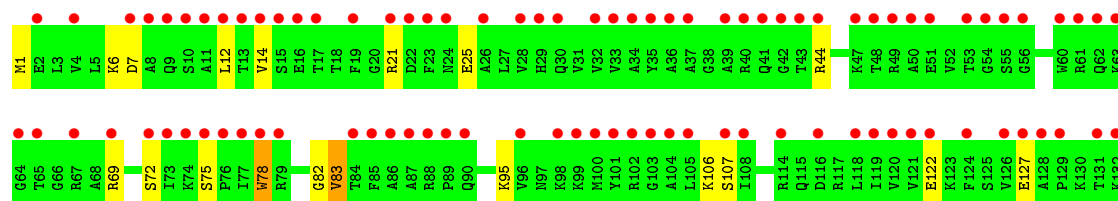
• Molecule 32: 50S ribosomal protein L3

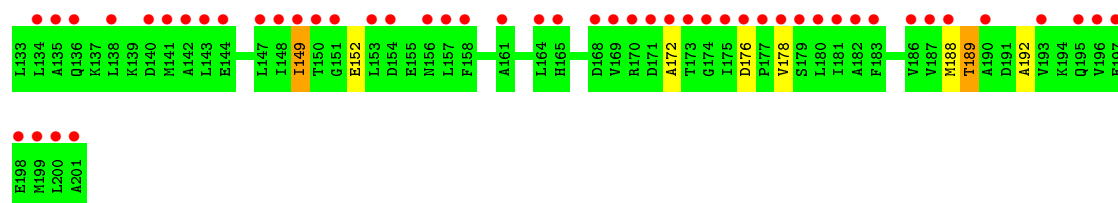
Chain DD: 89% 11%



• Molecule 33: 50S ribosomal protein L4

Chain CE: 70% 87% 11%

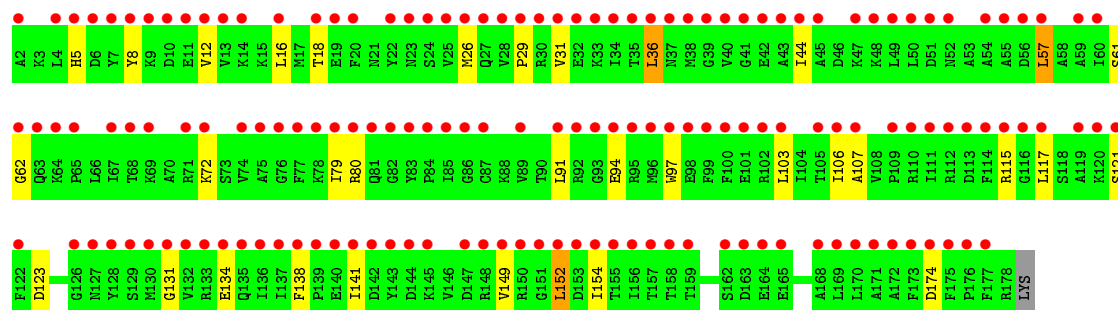
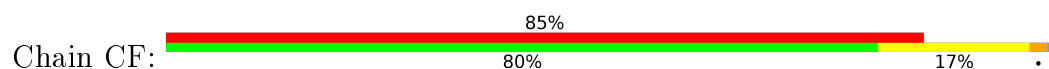




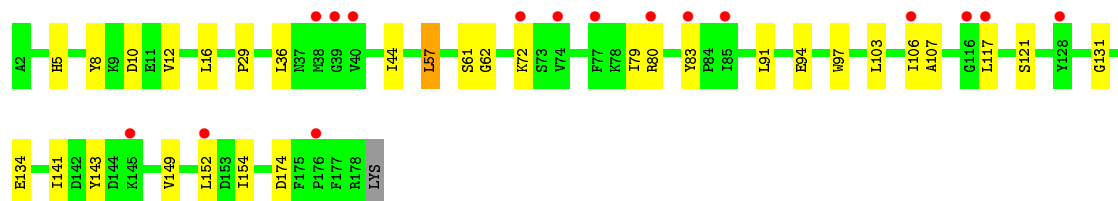
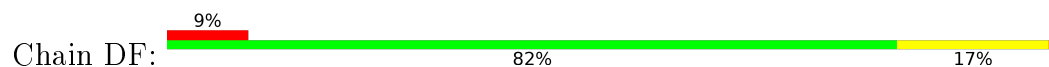
- Molecule 33: 50S ribosomal protein L4



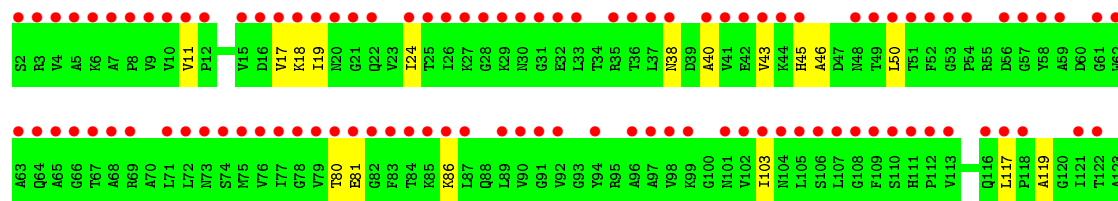
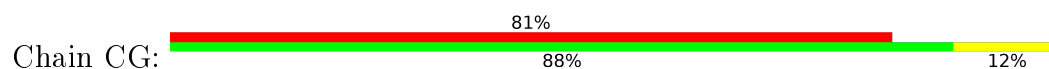
- Molecule 34: 50S ribosomal protein L5

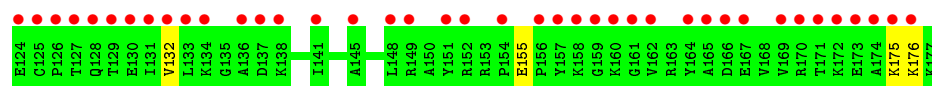


- Molecule 34: 50S ribosomal protein L5

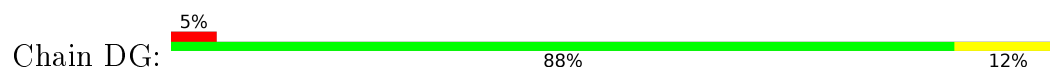


- Molecule 35: 50S ribosomal protein L6

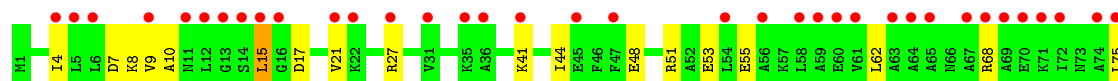
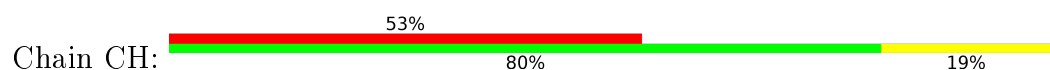




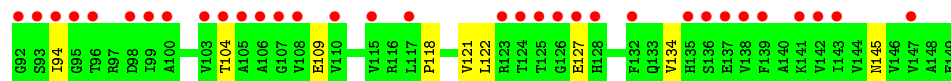
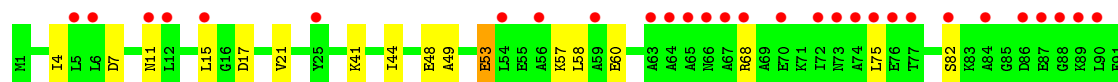
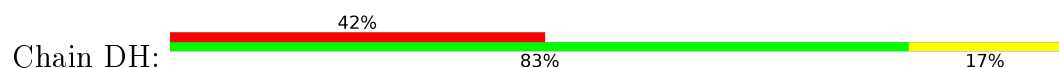
- Molecule 35: 50S ribosomal protein L6



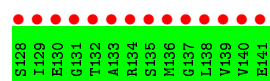
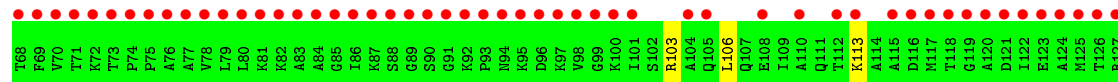
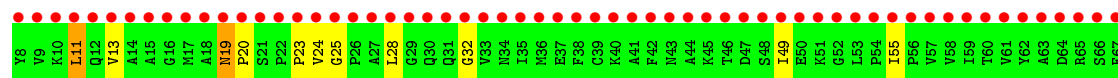
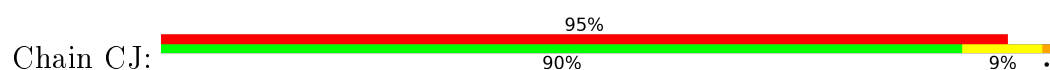
- Molecule 36: 50S ribosomal protein L9



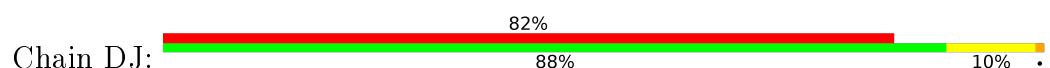
- Molecule 36: 50S ribosomal protein L9

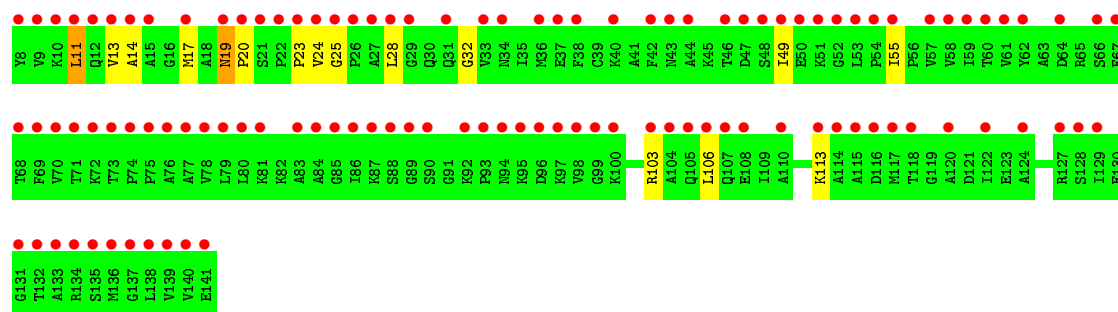


- Molecule 37: 50S ribosomal protein L11

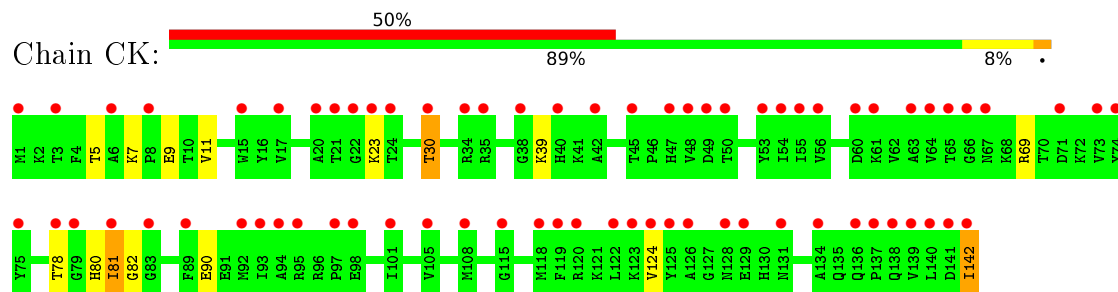


- Molecule 37: 50S ribosomal protein L11

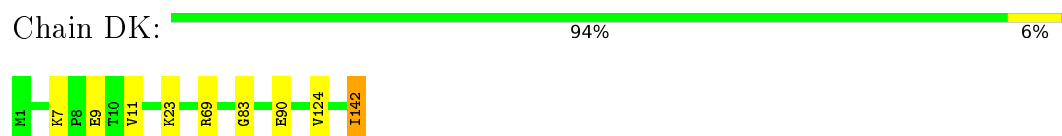




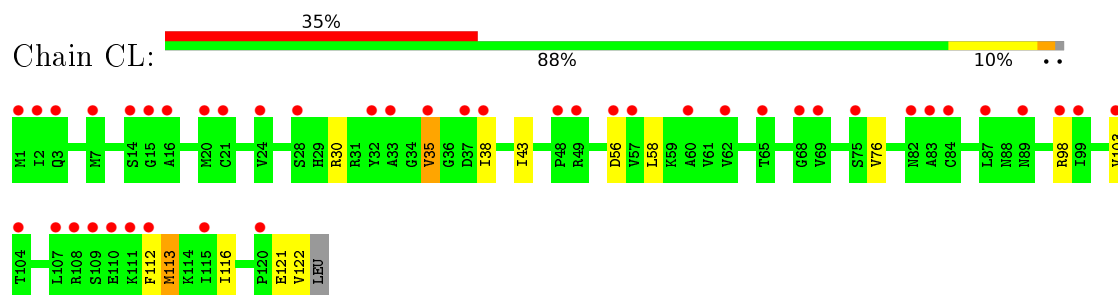
- Molecule 38: 50S ribosomal protein L13



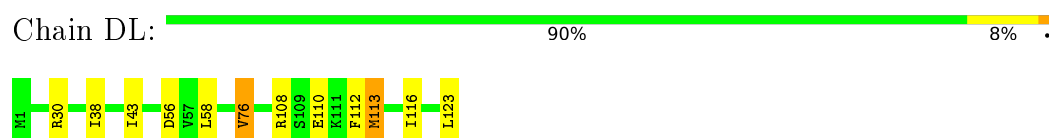
- Molecule 38: 50S ribosomal protein L13



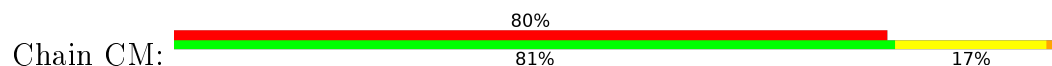
- Molecule 39: 50S ribosomal protein L14

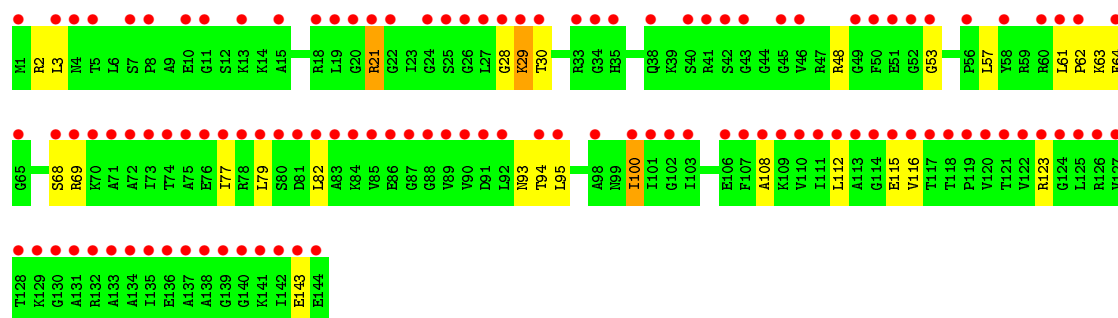


- Molecule 39: 50S ribosomal protein L14

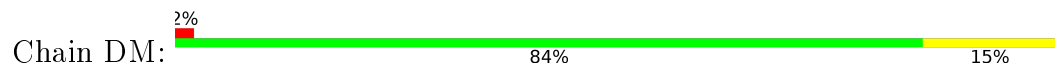


- Molecule 40: 50S ribosomal protein L15

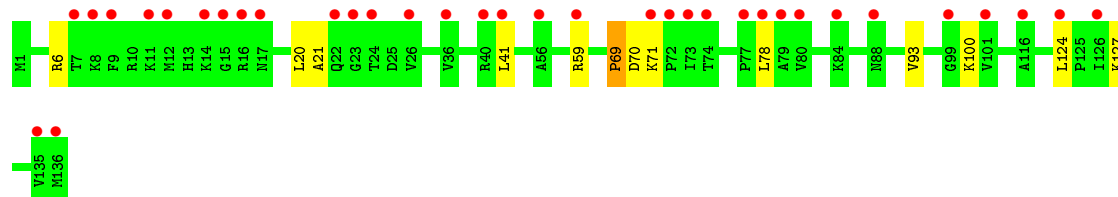




- Molecule 40: 50S ribosomal protein L15



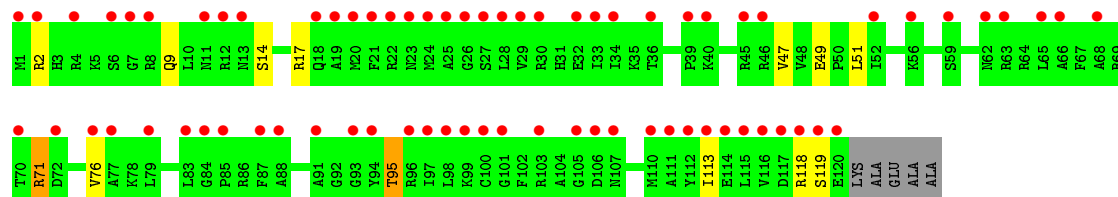
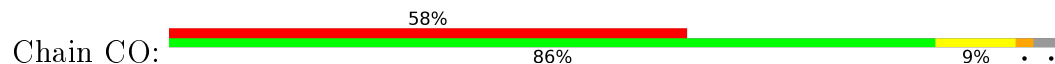
- Molecule 41: 50S ribosomal protein L16



- Molecule 41: 50S ribosomal protein L16



- Molecule 42: 50S ribosomal protein L17

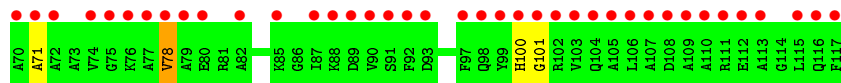
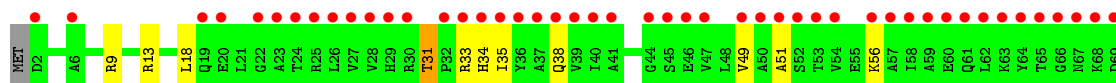
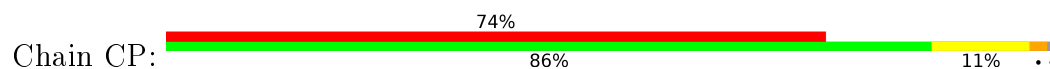


- Molecule 42: 50S ribosomal protein L17

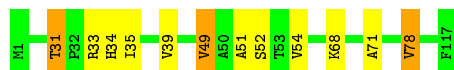




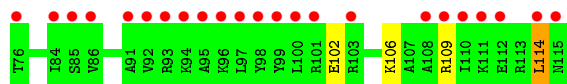
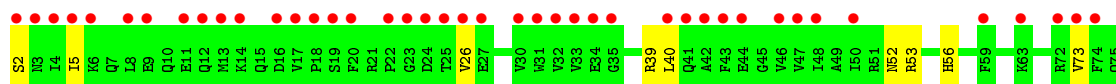
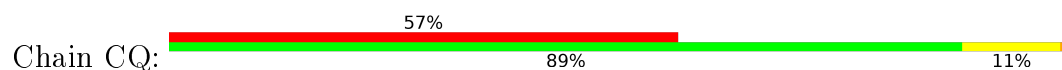
- Molecule 43: 50S ribosomal protein L18



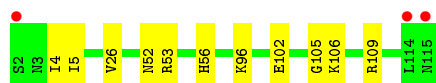
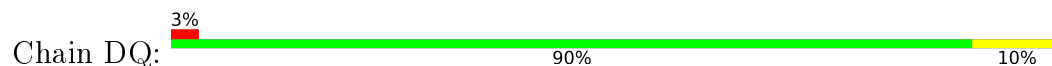
- Molecule 43: 50S ribosomal protein L18



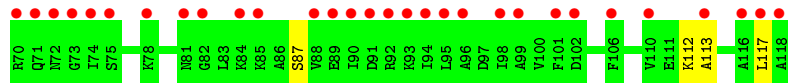
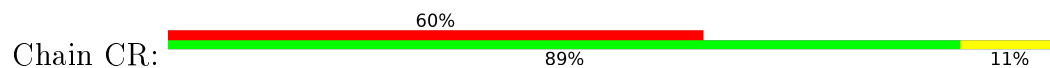
- Molecule 44: 50S ribosomal protein L19



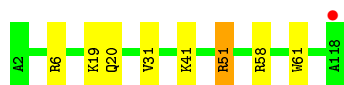
- Molecule 44: 50S ribosomal protein L19



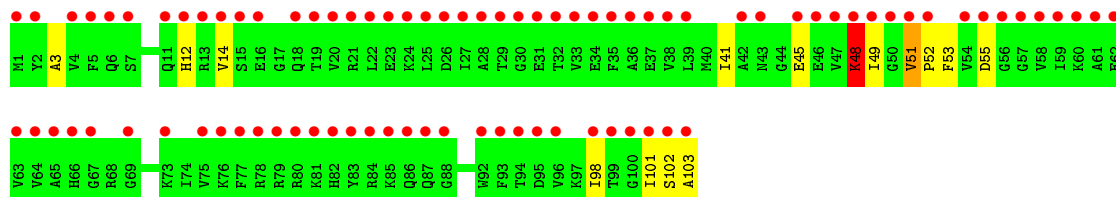
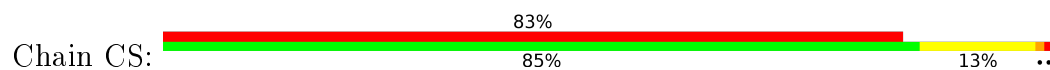
- Molecule 45: 50S ribosomal protein L20



- Molecule 45: 50S ribosomal protein L20



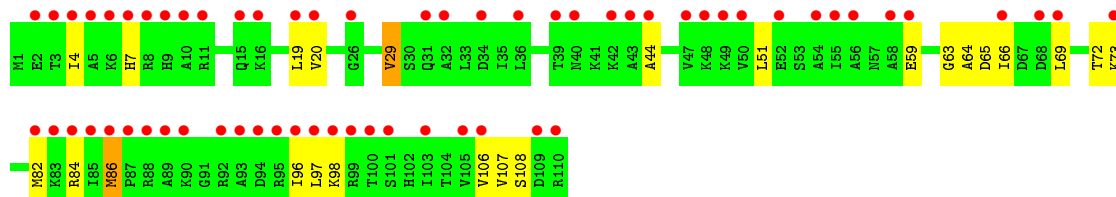
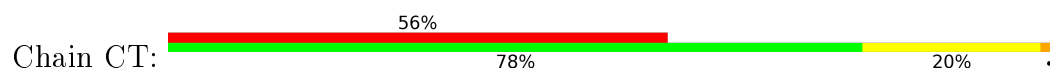
- Molecule 46: 50S ribosomal protein L21



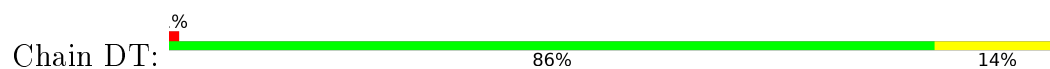
- Molecule 46: 50S ribosomal protein L21



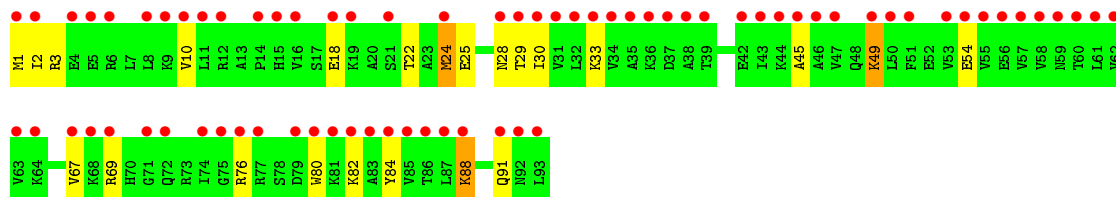
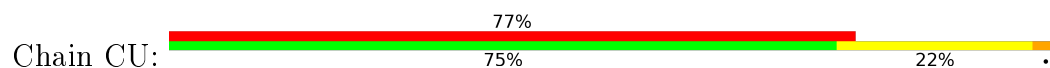
- Molecule 47: 50S ribosomal protein L22



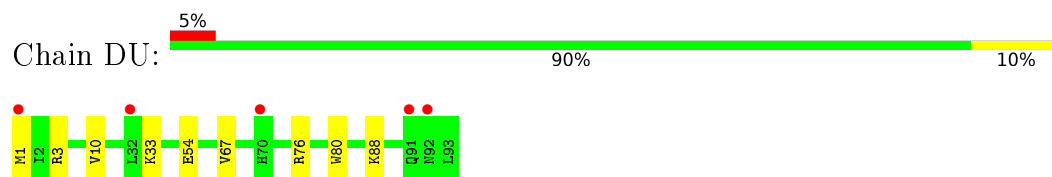
- Molecule 47: 50S ribosomal protein L22



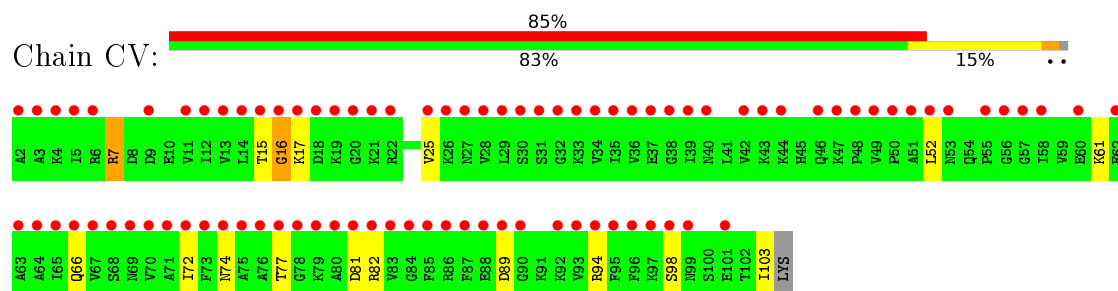
- Molecule 48: 50S ribosomal protein L23



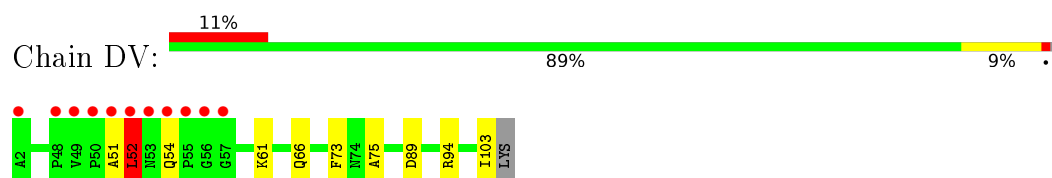
- Molecule 48: 50S ribosomal protein L23



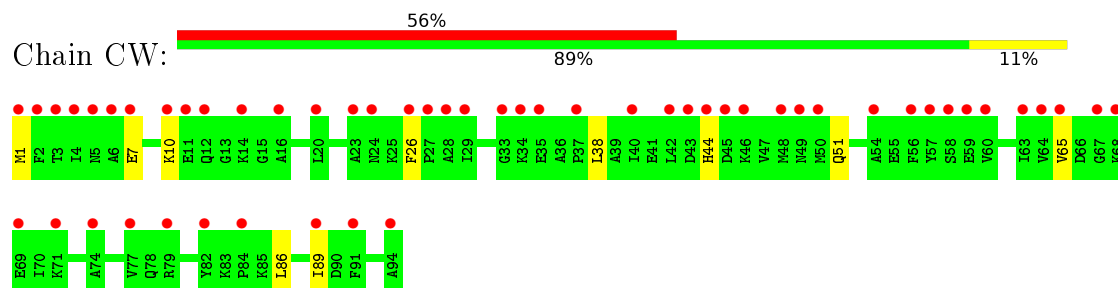
- Molecule 49: 50S ribosomal protein L24



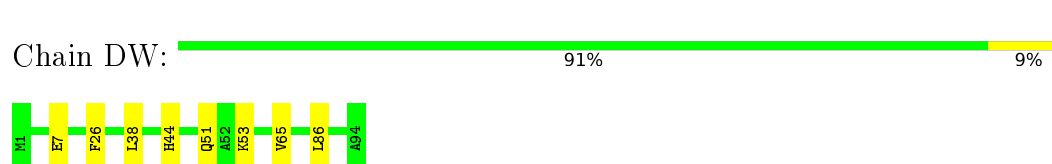
- Molecule 49: 50S ribosomal protein L24



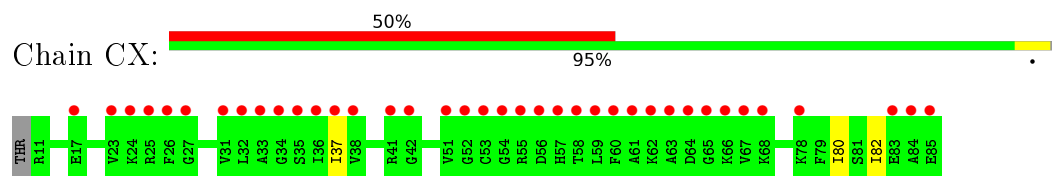
- Molecule 50: 50S ribosomal protein L25



- Molecule 50: 50S ribosomal protein L25

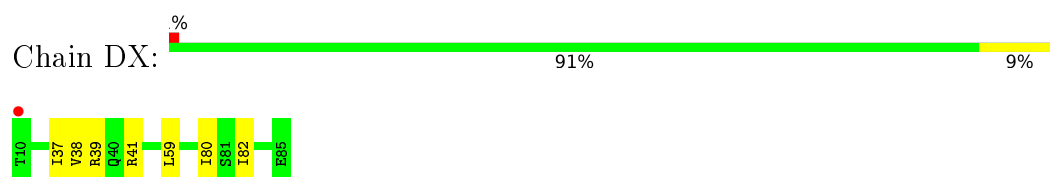


- Molecule 51: 50S ribosomal protein L27

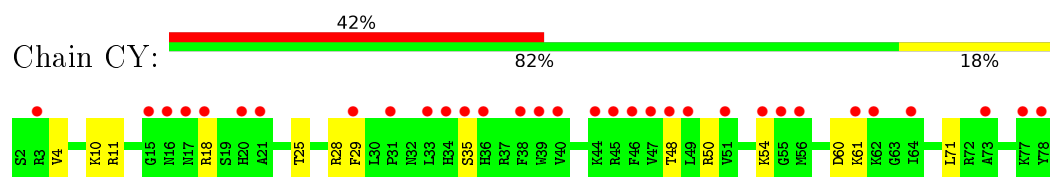


- Molecule 51: 50S ribosomal protein L27

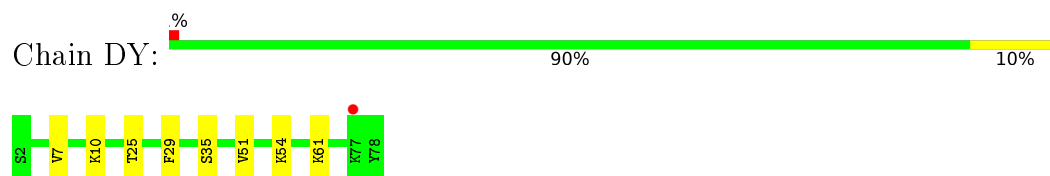




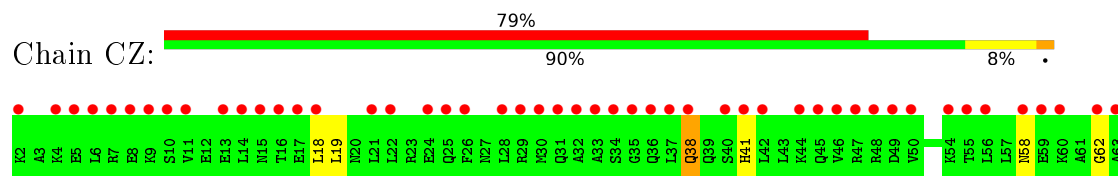
- Molecule 52: 50S ribosomal protein L28



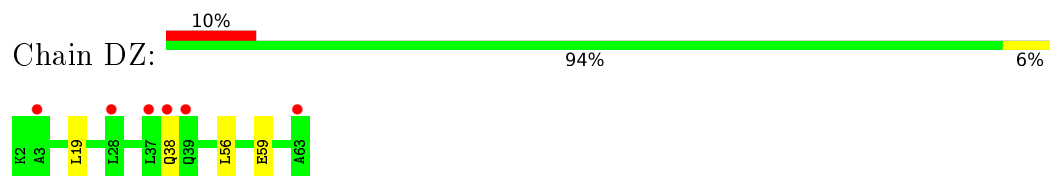
- Molecule 52: 50S ribosomal protein L28



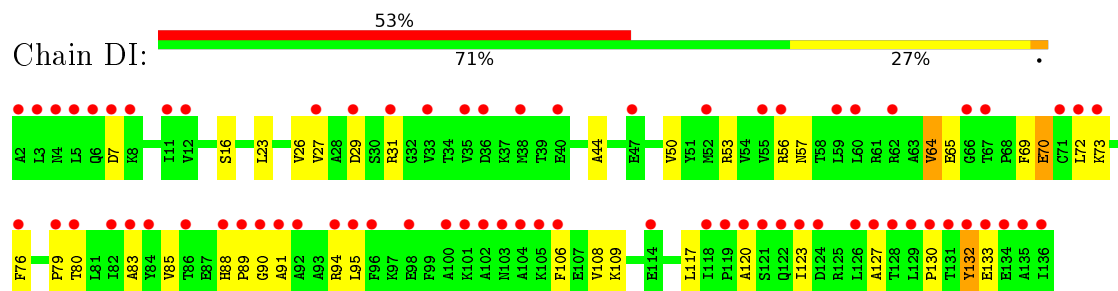
- Molecule 53: 50S ribosomal protein L29



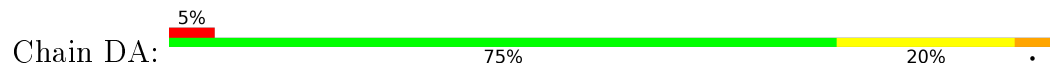
- Molecule 53: 50S ribosomal protein L29



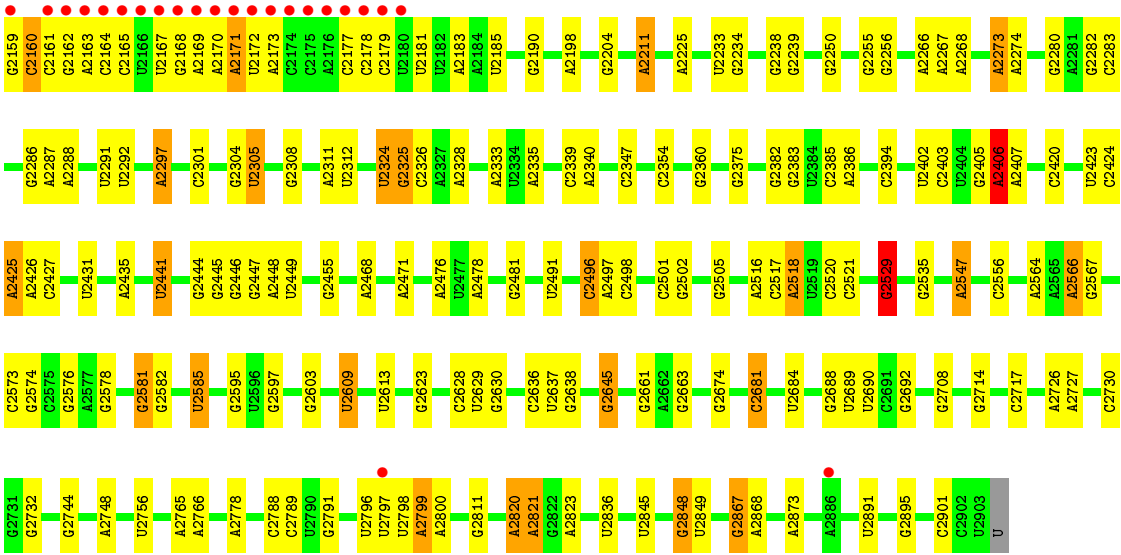
- Molecule 54: 50S ribosomal protein L10



- Molecule 55: 23S rRNA



G2100	U1782	G1975	A1635	A1453	A1284	U1132	A1029	C895	U888	U639	A346	A195	G1
G2102	A1787	U1991	U1636	U1460	A1286	A1134	C1030	C897	A789	C640	A352	A196	A5
G2103	A1787	U1991	A1637	U1460	A1286	A1134	U1033	C898	U790	A644	C353	A199	A6
G2104	A1784	U1993	C1644	G1478	U1294	C1135	A1040	A910	A792	C645	C354	U200	A10
U2105	C1795	U1993	G1645	G1482	G1300	G1137	A1040	A911	A792	U646	U355	C208	U12
U2106	C1997	C1997	U1647	A1482	A1301	U1141	G1047	A911	A800	C647	G356	A207	C11
G2107	A1998	U1648	U1648	A1490	A1301	A1142	G1047	A911	A800	C647	A362	C208	U12
A2108	A1800	C1999	U1649	A1490	A1301	A1142	A1057	C915	G805	U653	A338	G215	G15
U2109	A1802	U2109	G1649	G1492	C1306	C1161	U1058	C915	C806	A654	G370	A216	G15
G2110	A1808	A2014	A1652	C1493	G1309	C1161	U1059	A918	U807	G543	A371	G27	G27
U2111	C1653	U2017	G1653	A1494	G1310	C1164	U1060	A927	U808	C671	G372	A221	G27
U2113	C1816	U2017	A1654	A1494	G1311	A1165	U1061	A927	U809	C672	A371	A222	C31
G2114	U1820	A2020	G1660	U1497	C1320	G1168	G1062	U931	U811	A675	G386	G242	U34
G2115	U1820	C2023	A1508	U1497	C1320	G1168	G1063	U932	C812	A675	U305	G245	G45
G2116	A1829	C2023	A1509	A1508	A1321	G1171	U1065	C946	C816	G684	U306	G245	G46
A2117	A1829	N2030	A1665	G1510	G1324	C1172	U1066	C946	C816	G684	U306	G245	G46
U2118	C1830	U2118	G1666	G1511	G1324	C1172	U1066	C946	C816	G684	U306	G245	G46
A2031	G1831	A2031	G1667	C1512	U1329	U1173	U1067	G956	A819	U686	U399	G248	C57
G2120	G2032	G2032	G1667	C1512	U1329	U1173	U1067	G956	A819	U686	U399	G248	C57
G2121	A1847	A2033	A1672	A1514	C1330	U1175	A1069	A959	A820	G690	U403	G250	G58
U2122	A1848	A2033	G1673	G1515	G1331	U1176	A1070	A959	A821	G690	U403	G250	G58
G2123	A1848	A2033	G1673	G1515	G1331	U1176	A1070	A959	A821	G690	U403	G250	G58
G2124	A1853	C2036	G1674	G1516	G1343	G1177	G1071	A960	G822	G411	G411	G252	U62
G2125	A1853	C2036	C1675	G1516	G1343	G1177	G1071	A960	G822	G411	G411	G252	U62
A2126	U2039	U2039	C1675	G1516	G1343	G1177	G1071	A960	G822	G411	G411	G252	U62
G1869	G1870	G1869	G1681	U1523	C1349	U1181	U1077	G969	U826	C420	G266	G266	A74
G2128	A1871	C2043	G1682	A1532	U1352	U1182	U1078	A972	U827	C420	G266	G266	A74
C2129	A1872	C2044	U1533	A1532	U1352	U1182	U1078	A972	U827	C420	G266	G266	A74
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U2131	G1873	C2044	U1534	A1534	U1352	U1182	U1078	A972	U827	C420	G266	G266	A74
G2048	G1906	G2048	C1704	C1536	U1379	A1189	A1084	A980	U839	U451	U276	U276	A84
U2132	G1906	G2048	C1704	C1536	U1379	A1189	A1084	A980	U839	U451	U276	U276	A84
G1907	G1907	G1907	G1715	G1537	A1383	G1202	G1087	A983	C840	G452	G277	G277	A101
G2133	A1913	A2051	C1727	G1555	A1383	G1202	G1087	A983	C840	G452	G277	G277	A101
A2135	A2052	A2052	C1727	G1555	A1383	G1202	G1087	A983	C840	G452	G277	G277	A101
G2136	C1728	C2053	U1728	A1566	U1391	G1236	A1088	A984	G858	G728	A457	A279	U102
U2137	C1728	C2053	U1728	A1566	U1391	G1236	A1088	A984	G858	G728	A457	A279	U102
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G2138	C2054	C2055	C1730	A1569	U1394	G1238	G1091	A990	U860	C581	G463	C281	U114
G2139	C1731	G2056	G1731	A1569	U1394	G1238	G1091	A990	U860	C581	G463	C281	U114
G2140	C1732	G2056	C1732	U1578	G1416	G1250	G1092	G993	U871	A739	G465	A282	U114
G2141	G1930	A2060	G1733	A1579	C1417	A1253	G1093	G993	U872	A739	G465	A282	U114
A2142	A1931	G2061	A1738	A1583	G1418	A1253	G1094	A996	U872	U744	G465	A282	U114
G2143	A1932	A2062	G1739	U1584	G1424	G1256	A1095	A996	U872	U744	G465	A282	U114
G2144	G1933	G1933	A1739	C1585	G1425	G1256	A1095	A996	U872	U744	G465	A282	U114
G2069	A1936	G2069	A1744	A1586	G1426	U1263	A1098	A996	U872	U744	G465	A282	U114
A2070	A1937	A2070	A1744	A1586	G1426	U1263	A1098	A996	U872	U744	G465	A282	U114
A2071	A1937	A2070	A1744	A1586	G1426	U1263	A1098	A996	U872	U744	G465	A282	U114
U2149	A1938	C2072	G1753	G1588	G1429	G1266	U1097	G997	A878	G748	A479	U135	G136
C2073	A1938	C2072	G1753	G1588	G1429	G1266	U1097	G997	A878	G748	A479	U135	G136
U2150	U1955	U2074	C1761	A1603	G1430	U1267	G1106	U999	C880	A749	A603	G307	U136
C2151	U1955	U2074	C1761	A1603	G1430	U1267	G1106	U999	C880	A749	A603	G307	U136
U2151	U1955	U2074	C1761	A1603	G1430	U1267	G1106	U999	C880	A749	A603	G307	U136
G2152	C1985	A2077	G1764	C1807	A1433	U1268	U1101	A1009	G882	G760	G612	A311	U138
C2153	A1986	C2078	A1773	A1608	A1433	U1268	U1101	A1009	G882	G760	G612	A311	U138
A2154	C1967	A2154	A1773	A1608	A1433	U1268	U1101	A1009	G882	G760	G612	A311	U138
U2086	U2155	U2086	G1776	A1616	G1436	A1272	G1125	A1020	C	G775	G620	A322	C143
G2086	G2086	G2086	G1776	A1616	G1436	A1272	G1125	A1020	C	G775	G620	A322	C143
G2156	U1971	G2086	G1776	A1616	G1436	A1272	G1125	A1020	C	G775	G620	A322	C143
G2157	U1971	G2086	G1776	A1616	G1436	A1272	G1125	A1020	C	G775	G620	A322	C143
G2158	U1971	G2086	G1776	A1616	G1436	A1272	G1125	A1020	C	G775	G620	A322	C143



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.18Å 434.82Å 624.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.51 – 2.96 48.28 – 2.96	Depositor EDS
% Data completeness (in resolution range)	88.6 (48.51-2.96) 88.6 (48.28-2.96)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	21.17 (at 2.96Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, $R_{free}$	0.208 , 0.221 0.226 , 0.242	Depositor DCC
$R_{free}$ test set	4163 reflections (0.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.6	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 89.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	295202	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	123.0	wwPDB-VP

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

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, T1C, 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	1.04	9/36593 (0.0%)	0.86	5/57081 (0.0%)
1	BA	1.05	10/36568 (0.0%)	0.86	5/57042 (0.0%)
2	AB	0.48	0/1784	0.65	0/2403
2	BB	0.48	0/1784	0.65	0/2403
3	AC	0.48	0/1652	0.67	0/2225
3	BC	0.47	0/1652	0.67	0/2225
4	AD	0.44	0/1665	0.69	0/2227
4	BD	0.43	0/1665	0.70	0/2227
5	AE	0.48	0/1157	0.77	0/1557
5	BE	0.51	0/1118	0.81	0/1504
6	AF	0.46	0/881	0.69	0/1189
6	BF	0.47	0/835	0.77	0/1128
7	AG	0.45	0/1196	0.61	0/1602
7	BG	0.46	0/1196	0.62	0/1602
8	AH	0.46	0/989	0.71	0/1326
8	BH	0.46	0/989	0.69	0/1326
9	AI	0.44	0/1034	0.66	0/1375
9	BI	0.44	0/1034	0.65	0/1375
10	AJ	0.44	0/806	0.68	0/1089
10	BJ	0.48	0/797	0.71	0/1077
11	AK	0.46	0/893	0.65	0/1205
11	BK	0.45	0/893	0.68	0/1205
12	AL	0.44	0/960	0.74	0/1286
12	BL	0.47	0/960	0.74	0/1286
13	AM	0.51	0/893	0.72	0/1193
13	BM	0.49	0/893	0.72	0/1193
14	AN	0.46	0/817	0.63	0/1088
14	BN	0.44	0/817	0.63	0/1088
15	AO	0.48	0/722	0.60	0/964
15	BO	0.47	0/722	0.63	0/964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	AP	0.48	0/659	0.70	0/884
16	BP	0.50	0/659	0.76	0/884
17	AQ	0.48	0/658	0.73	0/881
17	BQ	0.51	0/658	0.78	0/881
18	AR	0.53	0/463	0.65	0/621
18	BR	0.50	0/463	0.64	0/621
19	AS	0.46	0/653	0.59	0/877
19	BS	0.45	0/653	0.60	0/877
20	AT	0.48	0/676	0.66	0/895
20	BT	0.52	0/671	0.68	0/888
21	AU	0.45	0/472	0.61	0/627
21	BU	0.43	0/472	0.63	0/627
22	C1	0.49	0/450	0.71	0/599
22	D1	0.61	0/450	0.79	0/599
23	C2	0.46	0/416	0.73	0/554
23	D2	0.51	0/421	0.73	0/561
24	C3	0.46	0/380	0.69	0/498
24	D3	0.55	0/380	0.76	0/498
25	C4	0.46	0/513	0.67	0/676
25	D4	0.56	0/513	0.71	0/676
26	C5	0.43	0/303	0.77	0/397
26	D5	0.53	0/303	0.76	0/397
27	C0	0.52	0/453	0.77	0/605
27	D0	0.62	0/467	0.81	0/623
28	CB	0.98	0/2828	0.88	2/4410 (0.0%)
28	DB	1.13	1/2872 (0.0%)	0.90	0/4478
29	CC	0.45	0/2121	0.76	0/2852
29	DC	0.50	0/2121	0.76	1/2852 (0.0%)
30	CD	0.43	0/1586	0.70	0/2134
31	CA	1.07	44/69165 (0.1%)	0.87	17/107896 (0.0%)
32	DD	0.54	0/1576	0.73	0/2119
33	CE	0.45	0/1571	0.72	0/2113
33	DE	0.52	0/1571	0.72	0/2113
34	CF	0.43	0/1434	0.68	0/1926
34	DF	0.46	0/1434	0.70	0/1926
35	CG	0.42	0/1343	0.66	0/1816
35	DG	0.44	0/1343	0.64	0/1816
36	CH	0.48	0/1121	0.68	0/1515
36	DH	0.48	0/1121	0.68	0/1515
37	CJ	0.48	0/993	0.62	0/1341
37	DJ	0.48	0/993	0.61	0/1341
38	CK	0.43	0/1152	0.70	0/1551
38	DK	0.56	0/1152	0.74	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	CL	0.47	0/947	0.74	0/1268
39	DL	0.54	0/955	0.75	0/1279
40	CM	0.46	0/1062	0.74	1/1413 (0.1%)
40	DM	0.50	0/1062	0.75	1/1413 (0.1%)
41	CN	0.45	0/1081	0.75	1/1443 (0.1%)
41	DN	0.59	0/1092	0.81	0/1457
42	CO	0.46	0/973	0.72	0/1301
42	DO	0.58	0/1006	0.80	0/1345
43	CP	0.43	0/902	0.73	0/1209
43	DP	0.47	0/910	0.73	0/1219
44	CQ	0.41	0/929	0.71	0/1242
44	DQ	0.48	0/929	0.72	0/1242
45	CR	0.48	0/960	0.69	0/1278
45	DR	0.62	0/960	0.76	0/1278
46	CS	0.44	0/829	0.74	0/1107
46	DS	0.55	0/829	0.78	0/1107
47	CT	0.43	0/864	0.74	0/1156
47	DT	0.55	0/864	0.75	0/1156
48	CU	0.44	0/745	0.72	0/994
48	DU	0.48	0/745	0.72	0/994
49	CV	0.44	0/787	0.76	0/1051
49	DV	0.49	0/787	0.77	0/1051
50	CW	0.40	0/766	0.65	0/1025
50	DW	0.50	0/766	0.69	0/1025
51	CX	0.39	0/576	0.65	0/762
51	DX	0.53	0/598	0.73	0/790
52	CY	0.43	0/635	0.73	0/848
52	DY	0.46	0/635	0.72	0/848
53	CZ	0.42	0/502	0.61	0/667
53	DZ	0.43	0/502	0.60	0/667
54	DI	0.51	0/1037	0.74	1/1402 (0.1%)
55	DA	1.27	148/69364 (0.2%)	0.97	26/108207 (0.0%)
All	All	0.98	212/309267 (0.1%)	0.85	60/462210 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	3
1	BA	0	4

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

All (212) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	1020	A	N3-C4	9.93	1.40	1.34
31	CA	1936	A	N9-C4	-9.29	1.32	1.37
31	CA	2095	A	O5'-C5'	-9.00	1.28	1.42
55	DA	539	G	N7-C5	7.77	1.44	1.39
55	DA	12	U	C1'-N1	7.58	1.60	1.48
55	DA	195	A	N9-C4	7.54	1.42	1.37
55	DA	2097	A	O5'-C5'	-7.36	1.31	1.42
55	DA	2050	C	N1-C6	7.35	1.41	1.37
31	CA	769	U	C1'-N1	7.22	1.59	1.48
31	CA	12	U	C1'-N1	7.06	1.59	1.48
55	DA	2585	U	C1'-N1	7.03	1.59	1.48
55	DA	1286	A	N3-C4	7.01	1.39	1.34
31	CA	2425	A	C3'-O3'	6.97	1.51	1.42
55	DA	2060	A	N3-C4	6.87	1.39	1.34
55	DA	2520	C	N1-C6	6.87	1.41	1.37
1	BA	1493	A	C3'-O3'	6.83	1.51	1.42
31	CA	546	U	C1'-N1	6.76	1.58	1.48
55	DA	484	C	C1'-N1	6.76	1.58	1.48
55	DA	1665	A	N7-C5	6.69	1.43	1.39
1	BA	1397	C	N1-C2	6.62	1.46	1.40
55	DA	1787	A	N9-C4	6.58	1.41	1.37
1	BA	5	U	C1'-N1	6.53	1.58	1.48
1	BA	28	A	O5'-C5'	-6.51	1.32	1.42
55	DA	2053	G	C6-N1	6.37	1.44	1.39
55	DA	582	A	N9-C4	6.37	1.41	1.37
55	DA	671	C	C1'-N1	6.33	1.58	1.48
55	DA	1306	C	C1'-N1	6.29	1.58	1.48
31	CA	2225	A	C3'-O3'	6.25	1.50	1.42
55	DA	2547	A	O5'-C5'	-6.23	1.32	1.42
55	DA	998	C	C1'-N1	6.23	1.58	1.48
55	DA	727	A	N3-C4	6.19	1.38	1.34
55	DA	959	A	N3-C4	6.13	1.38	1.34
28	DB	90	C	O5'-C5'	-6.12	1.33	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	28	A	O5'-C5'	-6.11	1.33	1.42
55	DA	2867	G	C3'-O3'	6.10	1.50	1.42
55	DA	372	G	C3'-O3'	6.08	1.50	1.42
55	DA	31	C	N1-C6	6.07	1.40	1.37
55	DA	2547	A	P-O5'	-6.06	1.53	1.59
55	DA	2023	C	N1-C6	6.03	1.40	1.37
55	DA	2521	C	N1-C6	6.01	1.40	1.37
55	DA	1000	A	N3-C4	6.00	1.38	1.34
1	BA	1008	U	O5'-C5'	-6.00	1.33	1.42
55	DA	578	G	N3-C4	5.98	1.39	1.35
55	DA	102	U	N1-C2	5.97	1.44	1.38
55	DA	579	G	C2'-C1'	-5.97	1.46	1.53
55	DA	2717	C	N1-C6	5.96	1.40	1.37
55	DA	1137	G	N3-C4	5.95	1.39	1.35
55	DA	1294	U	O5'-C5'	-5.94	1.33	1.42
55	DA	2297	A	O5'-C5'	-5.93	1.33	1.42
1	AA	1397	C	N1-C6	5.93	1.40	1.37
55	DA	1965	C	C1'-N1	5.92	1.57	1.48
55	DA	972	A	C6-N6	5.90	1.38	1.33
31	CA	253	C	C1'-N1	5.88	1.57	1.48
55	DA	2044	C	N1-C6	5.88	1.40	1.37
55	DA	575	A	N9-C4	5.87	1.41	1.37
1	AA	5	U	C1'-N1	5.86	1.57	1.48
55	DA	969	G	C8-N7	-5.84	1.27	1.30
55	DA	2756	U	C3'-O3'	5.83	1.50	1.42
55	DA	2036	C	N1-C6	5.81	1.40	1.37
55	DA	2518	A	N9-C4	5.80	1.41	1.37
31	CA	1306	C	C1'-N1	5.79	1.57	1.48
55	DA	2447	G	N3-C4	5.79	1.39	1.35
55	DA	2127	G	C3'-O3'	5.79	1.50	1.42
31	CA	2619	C	C1'-N1	5.78	1.57	1.48
55	DA	1635	A	N3-C4	5.77	1.38	1.34
55	DA	1164	C	N1-C6	5.76	1.40	1.37
55	DA	2446	G	N3-C4	5.76	1.39	1.35
31	CA	2579	C	C1'-N1	5.76	1.57	1.48
31	CA	1788	C	C1'-N1	5.74	1.57	1.48
55	DA	984	A	N3-C4	5.70	1.38	1.34
55	DA	2766	A	N9-C4	5.69	1.41	1.37
55	DA	457	A	N3-C4	5.69	1.38	1.34
55	DA	838	C	N1-C6	5.68	1.40	1.37
1	BA	485	U	N1-C2	5.66	1.43	1.38
1	BA	290	C	C1'-N1	5.65	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	821	A	N3-C4	5.65	1.38	1.34
55	DA	1534	U	C1'-N1	5.65	1.57	1.48
55	DA	1311	G	C6-N1	5.63	1.43	1.39
31	CA	1314	C	C1'-N1	5.63	1.57	1.48
55	DA	12	U	N1-C2	5.63	1.43	1.38
55	DA	1267	U	C2-N3	5.63	1.41	1.37
55	DA	744	U	N1-C6	5.60	1.43	1.38
55	DA	2056	G	C6-N1	5.58	1.43	1.39
55	DA	816	C	N1-C6	5.57	1.40	1.37
55	DA	1660	G	O5'-C5'	-5.57	1.33	1.42
55	DA	2426	A	N3-C4	5.57	1.38	1.34
55	DA	823	C	N1-C6	5.56	1.40	1.37
55	DA	990	A	N7-C5	5.55	1.42	1.39
31	CA	1658	C	C1'-N1	5.54	1.57	1.48
55	DA	1920	C	C1'-N1	5.54	1.57	1.48
55	DA	959	A	N9-C4	5.52	1.41	1.37
55	DA	508	A	N3-C4	5.52	1.38	1.34
55	DA	1965	C	C3'-O3'	-5.52	1.34	1.42
55	DA	2425	A	C3'-O3'	5.52	1.49	1.42
55	DA	2576	G	O3'-P	-5.51	1.54	1.61
55	DA	1021	A	N9-C4	5.51	1.41	1.37
55	DA	2821	A	N3-C4	5.51	1.38	1.34
55	DA	2444	G	N7-C5	5.50	1.42	1.39
55	DA	739	A	N3-C4	5.50	1.38	1.34
55	DA	613	A	N9-C4	5.50	1.41	1.37
31	CA	2006	C	C1'-N1	5.49	1.56	1.48
55	DA	196	A	N9-C4	5.48	1.41	1.37
55	DA	809	G	N7-C5	5.48	1.42	1.39
1	BA	575	G	C3'-O3'	5.47	1.49	1.42
55	DA	1265	A	N9-C4	5.46	1.41	1.37
31	CA	2680	U	C3'-O3'	5.46	1.49	1.42
55	DA	2692	G	N3-C4	5.44	1.39	1.35
55	DA	1133	A	O5'-C5'	-5.42	1.34	1.42
31	CA	995	C	O5'-C5'	-5.42	1.34	1.42
31	CA	2146	C	C3'-O3'	5.42	1.49	1.42
55	DA	1189	A	N9-C4	5.42	1.41	1.37
55	DA	12	U	P-O5'	5.41	1.65	1.59
55	DA	561	G	N3-C4	5.41	1.39	1.35
1	AA	1203	C	C1'-N1	5.39	1.56	1.48
31	CA	946	C	C1'-N1	5.39	1.56	1.48
55	DA	810	U	N1-C2	5.39	1.43	1.38
31	CA	2233	U	C1'-N1	5.39	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2823	A	C3'-O3'	5.38	1.49	1.42
31	CA	480	A	N9-C4	5.36	1.41	1.37
55	DA	469	G	N3-C4	5.36	1.39	1.35
31	CA	404	A	C3'-O3'	5.35	1.49	1.42
31	CA	1825	U	C1'-N1	5.34	1.56	1.48
31	CA	451	U	C1'-N1	5.34	1.56	1.48
31	CA	461	C	C1'-N1	5.34	1.56	1.48
55	DA	819	A	N3-C4	5.34	1.38	1.34
55	DA	2036	C	C1'-N1	5.31	1.56	1.48
55	DA	613	A	C3'-O3'	5.31	1.49	1.42
1	BA	842	U	C3'-O3'	5.30	1.49	1.42
55	DA	2077	A	N3-C4	5.30	1.38	1.34
55	DA	653	U	C1'-N1	5.30	1.56	1.48
31	CA	557	C	C1'-N1	5.30	1.56	1.48
55	DA	1030	C	N1-C6	5.29	1.40	1.37
55	DA	962	G	N3-C4	5.29	1.39	1.35
31	CA	1629	U	C1'-N1	5.29	1.56	1.48
55	DA	271	G	C3'-O3'	5.28	1.49	1.42
31	CA	2723	C	C1'-N1	5.28	1.56	1.48
55	DA	1274	A	N7-C5	-5.26	1.36	1.39
31	CA	653	U	C1'-N1	5.26	1.56	1.48
55	DA	2585	U	N1-C2	5.25	1.43	1.38
55	DA	2730	C	N1-C6	5.24	1.40	1.37
31	CA	198	C	C1'-N1	5.24	1.56	1.48
31	CA	1771	C	C1'-N1	5.22	1.56	1.48
31	CA	2646	C	C1'-N1	5.22	1.56	1.48
55	DA	918	A	N3-C4	5.22	1.38	1.34
55	DA	577	G	N3-C4	5.22	1.39	1.35
1	AA	575	G	C3'-O3'	5.22	1.49	1.42
55	DA	1268	A	N3-C4	5.22	1.38	1.34
55	DA	2288	A	N3-C4	5.22	1.38	1.34
55	DA	195	A	N3-C4	5.21	1.38	1.34
55	DA	1584	U	C1'-N1	5.21	1.56	1.48
55	DA	264	C	N1-C2	5.21	1.45	1.40
55	DA	27	G	C6-N1	5.21	1.43	1.39
1	BA	291	U	C1'-N1	5.21	1.56	1.48
55	DA	2521	C	C1'-N1	5.20	1.56	1.48
55	DA	911	A	N3-C4	5.20	1.38	1.34
55	DA	2901	C	C1'-N1	5.20	1.56	1.48
55	DA	1664	A	N9-C4	5.19	1.41	1.37
55	DA	2211	A	C3'-O3'	5.18	1.49	1.42
55	DA	512	G	N9-C4	5.17	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	581	C	C1'-N1	5.17	1.56	1.48
1	AA	15	G	N3-C4	5.17	1.39	1.35
31	CA	1971	U	C1'-N1	5.16	1.56	1.48
55	DA	1675	C	N1-C6	5.16	1.40	1.37
55	DA	1776	G	O5'-C5'	-5.16	1.34	1.42
55	DA	1270	C	N1-C6	5.15	1.40	1.37
55	DA	2354	C	O5'-C5'	-5.15	1.34	1.42
55	DA	2033	A	P-O5'	5.15	1.64	1.59
55	DA	353	C	C1'-N1	5.14	1.56	1.48
55	DA	465	G	N3-C4	5.14	1.39	1.35
55	DA	1607	C	N1-C6	5.13	1.40	1.37
55	DA	2273	A	N3-C4	5.13	1.38	1.34
31	CA	2465	C	C1'-N1	5.13	1.56	1.48
31	CA	2756	U	C3'-O3'	5.13	1.49	1.42
55	DA	672	C	N1-C6	5.12	1.40	1.37
55	DA	2581	G	C3'-O3'	5.12	1.49	1.42
55	DA	562	U	N1-C6	5.12	1.42	1.38
55	DA	792	A	N3-C4	5.12	1.38	1.34
55	DA	1704	C	C1'-N1	5.12	1.56	1.48
55	DA	1965	C	O5'-C5'	-5.12	1.34	1.42
55	DA	1020	A	C6-N1	5.12	1.39	1.35
55	DA	2496	C	O5'-C5'	-5.11	1.34	1.42
1	AA	290	C	C1'-N1	5.11	1.56	1.48
31	CA	672	C	C1'-N1	5.11	1.56	1.48
55	DA	2406	A	P-O5'	5.11	1.64	1.59
55	DA	2427	C	N1-C6	5.11	1.40	1.37
55	DA	2471	A	N3-C4	5.10	1.38	1.34
55	DA	585	G	N9-C4	5.09	1.42	1.38
31	CA	2044	C	C1'-N1	5.08	1.56	1.48
55	DA	1999	C	N1-C6	5.08	1.40	1.37
55	DA	2455	G	C3'-O3'	-5.08	1.35	1.42
31	CA	2354	C	C1'-N1	5.08	1.56	1.48
31	CA	2901	C	C1'-N1	5.07	1.56	1.48
31	CA	1704	C	C1'-N1	5.07	1.56	1.48
55	DA	684	G	N3-C4	5.07	1.39	1.35
55	DA	2708	G	N3-C4	5.06	1.39	1.35
55	DA	2301	C	C1'-N1	5.06	1.56	1.48
55	DA	1437	C	O5'-C5'	-5.05	1.34	1.42
1	AA	209	U	C3'-O3'	5.04	1.49	1.42
55	DA	1253	A	O5'-C5'	-5.04	1.34	1.42
55	DA	114	U	C1'-N1	5.04	1.56	1.48
55	DA	1284	A	N3-C4	5.04	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	692	C	C1'-N1	5.04	1.56	1.48
55	DA	251	A	N3-C4	5.04	1.37	1.34
1	AA	843	U	C1'-N1	5.03	1.56	1.48
55	DA	2585	U	C3'-O3'	5.03	1.49	1.42
55	DA	574	A	O5'-C5'	-5.02	1.34	1.42
55	DA	2061	G	N3-C4	5.02	1.39	1.35
31	CA	20	C	C1'-N1	5.01	1.56	1.48
55	DA	1644	C	C1'-N1	5.01	1.56	1.48
55	DA	1331	G	N3-C4	5.01	1.39	1.35
55	DA	1637	A	N7-C5	5.01	1.42	1.39
31	CA	2215	C	C1'-N1	5.00	1.56	1.48

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	CB	15	A	O4'-C1'-N9	10.06	116.25	108.20
55	DA	512	G	O4'-C1'-N9	8.55	115.04	108.20
1	AA	413	G	C1'-O4'-C4'	-8.26	103.29	109.90
55	DA	784	G	P-O3'-C3'	7.86	129.13	119.70
41	CN	69	PRO	C-N-CA	7.39	140.18	121.70
55	DA	1936	A	O4'-C1'-N9	7.18	113.94	108.20
1	AA	1	A	OP1-P-OP2	-7.13	108.90	119.60
55	DA	2820	A	P-O3'-C3'	7.09	128.21	119.70
55	DA	892	A	OP1-P-OP2	-7.05	109.03	119.60
54	DI	132	TYR	C-N-CA	7.01	139.24	121.70
31	CA	892	A	OP1-P-OP2	-6.96	109.17	119.60
55	DA	1	G	OP1-P-OP2	-6.87	109.29	119.60
1	BA	1362	A	C1'-O4'-C4'	-6.87	104.40	109.90
31	CA	974	G	N9-C1'-C2'	6.74	122.76	114.00
1	BA	2	A	OP1-P-OP2	-6.72	109.52	119.60
31	CA	271	G	P-O3'-C3'	6.49	127.49	119.70
55	DA	271	G	P-O3'-C3'	6.46	127.45	119.70
1	AA	413	G	O4'-C1'-N9	6.44	113.35	108.20
55	DA	2848	G	O4'-C1'-N9	6.20	113.16	108.20
55	DA	1311	G	O4'-C1'-N9	6.05	113.04	108.20
31	CA	2425	A	P-O3'-C3'	5.92	126.80	119.70
31	CA	451	U	C1'-O4'-C4'	-5.89	105.19	109.90
1	BA	842	U	P-O3'-C3'	5.84	126.71	119.70
31	CA	512	G	O4'-C1'-N9	5.82	112.86	108.20
55	DA	1379	U	P-O3'-C3'	5.81	126.67	119.70
31	CA	784	G	P-O3'-C3'	5.76	126.61	119.70
1	BA	485	U	O4'-C1'-N1	5.76	112.81	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	DM	60	ARG	CG-CD-NE	5.73	123.84	111.80
31	CA	1379	U	P-O3'-C3'	5.71	126.55	119.70
55	DA	704	G	O4'-C1'-N9	5.59	112.67	108.20
55	DA	242	G	C3'-C2'-C1'	-5.56	97.05	101.50
55	DA	2406	A	C5'-C4'-O4'	-5.56	102.42	109.10
55	DA	1434	A	O4'-C1'-N9	5.42	112.53	108.20
55	DA	1165	A	O4'-C1'-N9	5.40	112.52	108.20
1	BA	1397	C	C2-N1-C1'	5.39	124.72	118.80
55	DA	27	G	O4'-C1'-N9	5.36	112.49	108.20
29	DC	156	ARG	CB-CG-CD	-5.34	97.71	111.60
31	CA	2225	A	P-O3'-C3'	5.31	126.08	119.70
31	CA	2095	A	C5'-C4'-C3'	-5.28	107.55	116.00
55	DA	2280	G	C4'-C3'-C2'	-5.27	97.33	102.60
31	CA	2035	G	C1'-O4'-C4'	-5.26	105.69	109.90
55	DA	2645	G	O4'-C1'-N9	5.23	112.39	108.20
31	CA	704	G	O4'-C1'-N9	5.20	112.36	108.20
31	CA	2825	G	O4'-C1'-N9	5.19	112.35	108.20
31	CA	242	G	C3'-C2'-C1'	-5.18	97.35	101.50
40	CM	68	SER	C-N-CA	5.18	134.66	121.70
31	CA	2406	A	C5'-C4'-O4'	5.18	115.31	109.10
55	DA	512	G	C1'-O4'-C4'	-5.17	105.76	109.90
55	DA	479	A	C3'-C2'-C1'	-5.17	97.36	101.50
55	DA	807	U	C4'-C3'-C2'	-5.17	97.43	102.60
55	DA	2048	G	C8-N9-C4	-5.15	104.34	106.40
28	CB	89	U	O4'-C1'-N1	5.13	112.31	108.20
55	DA	1238	G	C4'-C3'-C2'	-5.13	97.47	102.60
1	AA	841	C	P-O3'-C3'	5.11	125.83	119.70
1	AA	890	G	C3'-C2'-C1'	-5.08	97.44	101.50
55	DA	1997	C	C4'-C3'-C2'	-5.08	97.52	102.60
31	CA	2447	G	C3'-C2'-C1'	-5.04	97.46	101.50
55	DA	1936	A	C1'-O4'-C4'	-5.03	105.88	109.90
55	DA	2447	G	C3'-C2'-C1'	-5.02	97.48	101.50
31	CA	974	G	C3'-C2'-C1'	-5.01	97.49	101.50

There are no chirality outliers.

All (108) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1432	G	Sidechain
1	AA	362	G	Sidechain
1	AA	898	G	Sidechain
5	AE	82	GLN	Sidechain

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Mol	Chain	Res	Type	Group
1	BA	1432	G	Sidechain
1	BA	362	G	Sidechain
1	BA	575	G	Sidechain
1	BA	898	G	Sidechain
10	BJ	37	ARG	Mainchain
31	CA	1693	U	Sidechain
31	CA	1777	U	Sidechain
31	CA	1936	A	Sidechain
31	CA	1937	A	Sidechain
31	CA	2267	A	Sidechain
31	CA	2638	G	Sidechain
31	CA	2732	G	Sidechain
31	CA	463	G	Sidechain
31	CA	481	G	Sidechain
31	CA	704	G	Sidechain
31	CA	726	G	Sidechain
31	CA	805	G	Sidechain
55	DA	1009	A	Sidechain
55	DA	1142	A	Sidechain
55	DA	1236	G	Sidechain
55	DA	1253	A	Sidechain
55	DA	1283	G	Sidechain
55	DA	1311	G	Sidechain
55	DA	1324	G	Sidechain
55	DA	1343	G	Sidechain
55	DA	1425	G	Sidechain
55	DA	15	G	Sidechain
55	DA	1631	G	Sidechain
55	DA	1645	G	Sidechain
55	DA	1666	G	Sidechain
55	DA	1667	G	Sidechain
55	DA	1672	A	Sidechain
55	DA	1681	G	Sidechain
55	DA	1682	G	Sidechain
55	DA	1693	U	Sidechain
55	DA	1753	G	Sidechain
55	DA	1761	C	Sidechain
55	DA	1779	U	Sidechain
55	DA	1802	A	Sidechain
55	DA	1938	A	Sidechain
55	DA	2037	A	Sidechain
55	DA	2048	G	Sidechain

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Mol	Chain	Res	Type	Group
55	DA	2074	U	Sidechain
55	DA	2078	C	Sidechain
55	DA	221	A	Sidechain
55	DA	2250	G	Sidechain
55	DA	2266	A	Sidechain
55	DA	2267	A	Sidechain
55	DA	2282	G	Sidechain
55	DA	2328	A	Sidechain
55	DA	2375	G	Sidechain
55	DA	2382	G	Sidechain
55	DA	2405	G	Sidechain
55	DA	2468	A	Sidechain
55	DA	2481	G	Sidechain
55	DA	2497	A	Sidechain
55	DA	250	G	Sidechain
55	DA	2516	A	Sidechain
55	DA	2517	C	Sidechain
55	DA	2529	G	Sidechain
55	DA	2564	A	Sidechain
55	DA	2566	A	Sidechain
55	DA	2581	G	Sidechain
55	DA	2582	G	Sidechain
55	DA	2595	G	Sidechain
55	DA	2597	G	Sidechain
55	DA	2638	G	Sidechain
55	DA	2645	G	Sidechain
55	DA	2688	G	Sidechain
55	DA	27	G	Sidechain
55	DA	2727	A	Sidechain
55	DA	2732	G	Sidechain
55	DA	2848	G	Sidechain
55	DA	307	G	Sidechain
55	DA	308	G	Sidechain
55	DA	395	U	Sidechain
55	DA	452	G	Sidechain
55	DA	463	G	Sidechain
55	DA	464	U	Sidechain
55	DA	481	G	Sidechain
55	DA	512	G	Sidechain
55	DA	555	G	Sidechain
55	DA	575	A	Sidechain
55	DA	577	G	Sidechain

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Mol	Chain	Res	Type	Group
55	DA	58	G	Sidechain
55	DA	630	G	Sidechain
55	DA	675	A	Sidechain
55	DA	690	G	Sidechain
55	DA	700	G	Sidechain
55	DA	704	G	Sidechain
55	DA	726	G	Sidechain
55	DA	727	A	Sidechain
55	DA	728	G	Sidechain
55	DA	748	G	Sidechain
55	DA	774	G	Sidechain
55	DA	775	G	Sidechain
55	DA	800	A	Sidechain
55	DA	805	G	Sidechain
55	DA	858	G	Sidechain
55	DA	910	A	Sidechain
55	DA	956	G	Sidechain
55	DA	959	A	Sidechain
55	DA	980	A	Sidechain
55	DA	984	A	Sidechain

## 5.2 Too-close contacts

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	90	0
1	BA	32908	0	16580	97	0
2	AB	1753	0	1780	10	0
2	BB	1753	0	1780	15	0
3	AC	1625	0	1696	14	0
3	BC	1625	0	1696	18	0
4	AD	1643	0	1707	13	0
4	BD	1643	0	1707	17	0
5	AE	1144	0	1185	15	0
5	BE	1105	0	1148	30	0
6	AF	862	0	864	7	0
6	BF	817	0	808	9	0
7	AG	1182	0	1238	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BG	1182	0	1238	4	0
8	AH	979	0	1031	8	0
8	BH	979	0	1031	4	0
9	AI	1022	0	1070	6	0
9	BI	1022	0	1070	6	0
10	AJ	796	0	836	11	0
10	BJ	787	0	828	10	0
11	AK	877	0	887	14	0
11	BK	877	0	887	17	0
12	AL	957	0	1017	7	0
12	BL	957	0	1017	9	0
13	AM	884	0	941	11	0
13	BM	884	0	941	11	0
14	AN	805	0	844	8	0
14	BN	805	0	844	8	0
15	AO	714	0	734	1	0
15	BO	714	0	734	0	0
16	AP	649	0	666	3	0
16	BP	649	0	666	5	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	5	0
18	AR	456	0	478	5	0
18	BR	456	0	478	3	0
19	AS	638	0	665	7	0
19	BS	638	0	665	8	0
20	AT	670	0	719	2	0
20	BT	665	0	714	8	0
21	AU	465	0	491	2	0
21	BU	465	0	491	2	0
22	C1	444	0	458	18	0
22	D1	444	0	458	13	0
23	C2	409	0	440	5	0
23	D2	414	0	442	5	0
24	C3	377	0	418	17	0
24	D3	377	0	418	6	0
25	C4	504	0	572	13	0
25	D4	504	0	572	12	0
26	C5	302	0	340	9	0
26	D5	302	0	340	2	0
27	C0	449	0	488	4	0
27	D0	463	0	504	1	0
28	CB	2529	0	1281	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	DB	2569	0	1301	5	0
29	CC	2082	0	2154	17	0
29	DC	2082	0	2154	11	0
30	CD	1565	0	1616	16	0
31	CA	62229	0	31318	236	0
32	DD	1576	0	1627	16	0
33	CE	1552	0	1619	14	0
33	DE	1552	0	1619	11	0
34	CF	1410	0	1444	16	0
34	DF	1410	0	1444	12	0
35	CG	1323	0	1371	9	0
35	DG	1323	0	1371	9	0
36	CH	1110	0	1148	8	0
36	DH	1110	0	1148	6	0
37	CJ	979	0	1028	4	0
37	DJ	979	0	1028	5	0
38	CK	1129	0	1162	9	0
38	DK	1129	0	1162	5	0
39	CL	938	0	1012	8	0
39	DL	946	0	1023	6	0
40	CM	1053	0	1129	19	0
40	DM	1053	0	1129	15	0
41	CN	1075	0	1154	5	0
41	DN	1092	0	1177	7	0
42	CO	960	0	1000	5	0
42	DO	993	0	1034	5	0
43	CP	892	0	923	7	0
43	DP	900	0	935	9	0
44	CQ	917	0	962	7	0
44	DQ	917	0	962	7	0
45	CR	947	0	1019	13	0
45	DR	947	0	1019	9	0
46	CS	816	0	839	8	0
46	DS	816	0	839	5	0
47	CT	857	0	922	12	0
47	DT	857	0	922	10	0
48	CU	739	0	807	10	0
48	DU	739	0	807	4	0
49	CV	779	0	831	8	0
49	DV	779	0	831	5	0
50	CW	753	0	780	5	0
50	DW	753	0	780	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	CX	569	0	581	1	0
51	DX	591	0	606	5	0
52	CY	625	0	652	8	0
52	DY	625	0	652	4	0
53	CZ	501	0	531	2	0
53	DZ	501	0	531	1	0
54	DI	1023	0	1052	19	0
55	DA	62423	0	31411	173	0
56	AA	71	0	0	0	0
56	BA	43	0	0	0	0
56	CA	156	0	0	0	0
56	CB	3	0	0	0	0
56	DA	182	0	0	0	0
56	DB	9	0	0	0	0
56	DD	2	0	0	0	0
56	DM	1	0	0	0	0
56	DR	2	0	0	0	0
57	AA	13	0	18	1	0
57	BA	13	0	18	0	0
57	DA	26	0	36	2	0
57	DQ	13	0	18	0	0
57	DR	13	0	18	5	0
57	DS	13	0	18	1	0
58	AA	16	0	28	0	0
58	DA	40	0	70	5	0
58	DE	16	0	28	0	0
58	DK	8	0	14	0	0
58	DN	8	0	14	1	0
58	DS	8	0	14	0	0
58	DT	16	0	28	0	0
59	AA	24	0	48	0	0
59	DA	72	0	144	10	0
60	AA	42	0	38	0	0
60	BA	42	0	38	0	0
61	AB	1	0	0	0	0
61	C5	1	0	0	0	0
61	D5	1	0	0	0	0
62	AL	7	0	10	0	0
62	D1	7	0	10	1	0
62	D3	7	0	10	2	0
62	DA	35	0	50	1	0
62	DL	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	DP	7	0	10	1	0
62	DQ	7	0	10	0	0
63	D1	4	0	6	0	0
63	DA	36	0	54	2	0
63	DB	8	0	12	1	0
64	D1	10	0	14	2	0
64	D3	10	0	14	0	0
64	DA	40	0	56	5	0
64	DD	10	0	14	2	0
64	DS	10	0	14	0	0
64	DU	10	0	14	1	0
65	DA	40	0	76	4	0
66	DA	32	0	44	0	0
67	DA	12	0	12	0	0
68	DA	11	0	5	0	0
69	DA	8	0	12	1	0
70	AA	507	0	0	0	0
70	AC	4	0	0	0	0
70	AD	2	0	0	0	0
70	AE	4	0	0	0	0
70	AF	1	0	0	0	0
70	AG	1	0	0	0	0
70	AH	1	0	0	0	0
70	AJ	2	0	0	0	0
70	AK	5	0	0	0	0
70	AL	8	0	0	0	0
70	AM	4	0	0	1	0
70	AN	5	0	0	1	0
70	AO	2	0	0	0	0
70	AP	2	0	0	0	0
70	AR	1	0	0	0	0
70	AS	1	0	0	0	0
70	AT	2	0	0	0	0
70	AU	3	0	0	0	0
70	BA	287	0	0	1	0
70	BD	13	0	0	0	0
70	BE	1	0	0	0	0
70	BF	1	0	0	0	0
70	BK	1	0	0	0	0
70	BL	3	0	0	0	0
70	BN	2	0	0	0	0
70	BO	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	BP	3	0	0	0	0
70	BR	1	0	0	0	0
70	BT	4	0	0	0	0
70	BU	2	0	0	0	0
70	C3	3	0	0	1	0
70	C4	1	0	0	0	0
70	CA	694	0	0	1	0
70	CB	13	0	0	0	0
70	CC	10	0	0	0	0
70	CD	5	0	0	0	0
70	CE	6	0	0	0	0
70	CL	1	0	0	0	0
70	CM	3	0	0	0	0
70	CO	1	0	0	0	0
70	CU	3	0	0	0	0
70	CV	1	0	0	0	0
70	CW	1	0	0	0	0
70	CY	1	0	0	0	0
70	D0	25	0	0	0	0
70	D1	42	0	0	0	0
70	D2	7	0	0	0	0
70	D3	25	0	0	0	0
70	D4	32	0	0	1	0
70	D5	13	0	0	0	0
70	DA	4836	0	0	8	0
70	DB	213	0	0	0	0
70	DC	102	0	0	0	0
70	DD	105	0	0	1	0
70	DE	63	0	0	0	0
70	DF	14	0	0	0	0
70	DG	6	0	0	0	0
70	DH	2	0	0	0	0
70	DK	58	0	0	0	0
70	DL	51	0	0	0	0
70	DM	60	0	0	0	0
70	DN	71	0	0	0	0
70	DO	44	0	0	0	0
70	DP	35	0	0	0	0
70	DQ	27	0	0	1	0
70	DR	64	0	0	0	0
70	DS	51	0	0	0	0
70	DT	70	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	DU	17	0	0	0	0
70	DV	19	0	0	0	0
70	DW	31	0	0	0	0
70	DX	30	0	0	1	0
70	DY	9	0	0	0	0
70	DZ	7	0	0	0	0
All	All	295202	0	194489	1207	0

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

All (1207) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C5:3:VAL:HG11	31:CA:2539:C:H5'	1.32	1.05
46:CS:14:VAL:HG21	46:CS:98:ILE:HG13	1.32	1.05
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.43	0.99
31:CA:1936:A:H2	31:CA:1943:U:H3	1.01	0.98
48:CU:28:ASN:HD21	48:CU:91:GLN:HB3	1.29	0.96
14:AN:66:GLN:HB2	70:AN:205:HOH:O	1.67	0.95
40:CM:82:LEU:HD11	40:CM:116:VAL:HG23	1.52	0.92
24:C3:7:PRO:HB2	31:CA:1309:G:H4'	1.52	0.91
46:CS:14:VAL:CG2	46:CS:98:ILE:HG13	2.00	0.90
5:AE:77:ASN:HB2	5:AE:82:GLN:NE2	1.86	0.90
40:CM:77:ILE:HD11	40:CM:108:ALA:HB1	1.55	0.89
8:BH:87:LYS:HB2	8:BH:125:ILE:HD11	1.55	0.87
22:C1:4:GLN:HA	31:CA:2615:U:C2	2.10	0.86
5:BE:77:ASN:HB2	5:BE:82:GLN:NE2	1.91	0.86
8:AH:87:LYS:HB2	8:AH:125:ILE:HD11	1.58	0.85
31:CA:2796:U:H3	31:CA:2799:A:H61	1.23	0.85
31:CA:1779:U:H5	31:CA:1784:A:N7	1.74	0.85
31:CA:1005:C:O2'	38:CK:30:THR:HG21	1.78	0.84
55:DA:2796:U:H3	55:DA:2799:A:H61	1.21	0.83
1:BA:1305:G:H21	1:BA:1332:A:H2	1.24	0.83
11:BK:88:GLY:H	11:BK:114:THR:HG22	1.43	0.82
2:BB:23:TRP:HB3	2:BB:39:HIS:CE1	2.14	0.82
1:AA:1305:G:H21	1:AA:1332:A:H2	1.23	0.81
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.61	0.81
31:CA:740:C:H5'	31:CA:1784:A:H3'	1.62	0.81
33:CE:149:ILE:HG12	33:CE:188:MET:HG2	1.62	0.81
12:BL:65:SER:HB2	12:BL:82:ILE:HD11	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BM:114:LYS:HB3	13:BM:115:PRO:HD3	1.62	0.80
55:DA:2033:A:H5'	70:DA:4099:HOH:O	1.81	0.80
22:C1:38:HIS:HE1	31:CA:2884:U:O4	1.64	0.80
2:BB:20:THR:HA	2:BB:39:HIS:CE1	2.18	0.79
46:CS:14:VAL:HG21	46:CS:98:ILE:CG1	2.11	0.79
45:DR:20:GLN:CG	57:DR:202:PG4:H42	2.12	0.79
1:BA:9:G:H5'	5:BE:108:GLY:HA3	1.63	0.79
25:C4:60:ALA:O	40:CM:48:ARG:HD2	1.83	0.78
45:DR:20:GLN:HG3	57:DR:202:PG4:H42	1.65	0.78
55:DA:135:U:H3	55:DA:144:A:H61	1.32	0.78
35:CG:24:ILE:HD11	35:CG:43:VAL:HG11	1.66	0.77
35:DG:24:ILE:HD11	35:DG:43:VAL:HG11	1.66	0.77
41:DN:18[A]:ARG:HG2	28:DB:90:C:H5'	1.65	0.77
31:CA:135:U:H3	31:CA:144:A:H61	1.33	0.77
13:BM:22:ILE:HB	13:BM:25:VAL:CG1	2.15	0.77
55:DA:568:U:H1'	55:DA:2030:6MZ:H9C1	1.66	0.77
1:BA:664:G:H22	1:BA:741:G:H1	1.34	0.76
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.67	0.76
39:CL:38:ILE:HD11	39:CL:112:PHE:HZ	1.49	0.76
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.68	0.75
1:AA:664:G:H22	1:AA:741:G:H1	1.34	0.74
10:AJ:7:ARG:HB3	10:AJ:101:SER:HB2	1.69	0.74
4:AD:107:PHE:HB3	4:AD:145:ILE:HD11	1.70	0.74
4:BD:107:PHE:HB3	4:BD:145:ILE:HD11	1.70	0.74
13:BM:83:LEU:HD21	19:BS:65:GLU:HB2	1.70	0.74
31:CA:528:A:C2	31:CA:2043:C:H4'	2.23	0.73
3:BC:123:GLN:HB3	3:BC:128:VAL:HG21	1.69	0.73
1:AA:842:U:H4'	1:AA:843:U:OP1	1.88	0.73
25:D4:54:ASP:HB3	40:DM:57:LEU:HD22	1.70	0.73
1:BA:522:C:H5	12:BL:50:ARG:HH12	1.37	0.73
13:BM:6:GLY:HA3	13:BM:66:GLU:HG3	1.69	0.73
1:BA:1060:U:C5	3:BC:2:GLY:HA3	2.23	0.73
55:DA:2127:G:H4'	55:DA:2128:G:OP1	1.90	0.72
1:AA:1492:A:H5''	12:AL:44:LYS:HG2	1.72	0.71
24:C3:30:VAL:HG13	31:CA:466:A:H5''	1.72	0.71
39:DL:38:ILE:HD11	39:DL:112:PHE:HZ	1.53	0.71
1:AA:73:C:HO2'	1:AA:74:A:H8	1.38	0.70
1:BA:202:G:HO2'	1:BA:468:A:H8	1.39	0.70
47:CT:86:MET:HB2	47:CT:96:ILE:HD11	1.74	0.70
31:CA:1936:A:H2	31:CA:1943:U:N3	1.83	0.70
55:DA:1913:A:H4'	55:DA:1913:A:OP1	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2255:G:H21	69:DA:3219:TRS:H12	1.56	0.70
31:CA:846:U:H1'	31:CA:847:U:H5	1.56	0.70
55:DA:2628:C:H5'	59:DA:3195:PUT:H12	1.73	0.69
31:CA:1478:G:H1	31:CA:1513:U:H3	1.39	0.69
54:DI:64:VAL:HG22	54:DI:69:PHE:HB2	1.75	0.69
39:DL:30:ARG:HD2	55:DA:2674:G:H4'	1.74	0.69
24:C3:19:ARG:HG3	31:CA:126:A:O5'	1.94	0.68
55:DA:1478:G:H1	55:DA:1513:U:H3	1.38	0.68
2:BB:23:TRP:HB3	2:BB:39:HIS:HE1	1.56	0.68
34:CF:36:LEU:HD21	34:CF:91:LEU:HD11	1.76	0.68
59:DA:3195:PUT:H11	70:DA:5703:HOH:O	1.94	0.68
4:BD:201:VAL:HG11	5:BE:103:THR:HB	1.76	0.67
11:BK:88:GLY:N	11:BK:114:THR:HG22	2.09	0.67
22:D1:55:ILE:HD12	42:DO:33:ILE:HD11	1.76	0.67
52:CY:4:VAL:HG22	52:CY:11:ARG:HG3	1.75	0.67
49:DV:52:LEU:HB3	49:DV:54:GLN:HB2	1.76	0.67
31:CA:1250:G:H5''	45:CR:6:ARG:HD3	1.77	0.67
31:CA:45:G:H5''	31:CA:46:G:H5'	1.76	0.67
43:DP:39:VAL:HB	43:DP:49:VAL:HG23	1.76	0.67
1:BA:73:C:HO2'	1:BA:74:A:H8	1.42	0.66
27:C0:12:SER:HB3	31:CA:988:A:P	2.35	0.66
1:BA:502:A:OP1	12:BL:115:SER:HB2	1.95	0.66
1:BA:451:A:H2'	70:BA:1701:HOH:O	1.94	0.66
1:AA:202:G:HO2'	1:AA:468:A:H8	1.44	0.66
40:CM:79:LEU:HD11	40:CM:112:LEU:HD12	1.77	0.66
55:DA:45:G:H5''	55:DA:46:G:H5'	1.77	0.65
43:DP:31:THR:HG21	28:DB:28:C:OP1	1.97	0.65
35:CG:80:THR:HG23	35:CG:81:GLU:H	1.60	0.65
30:CD:133:THR:HG22	31:CA:1993:U:H4'	1.78	0.65
26:C5:3:VAL:HG11	31:CA:2539:C:C5'	2.19	0.64
31:CA:974:G:H8	31:CA:990:A:H62	1.46	0.64
1:AA:502:A:OP1	12:AL:115:SER:HB2	1.97	0.64
12:BL:110:ARG:HB2	12:BL:119:VAL:HG21	1.78	0.64
1:AA:412:A:H3'	1:AA:413:G:H5'	1.79	0.64
1:BA:841:C:H3'	1:BA:842:U:C5'	2.27	0.64
31:CA:372:G:H5''	52:CY:61:LYS:HD3	1.78	0.64
34:DF:61:SER:HB2	34:DF:91:LEU:HD21	1.79	0.64
12:BL:43:LYS:HD2	12:BL:91:PRO:HG3	1.79	0.64
24:C3:12:ARG:HD2	24:C3:44:VAL:HG11	1.80	0.64
31:CA:2394:C:H5''	40:CM:63:LYS:HE2	1.80	0.64
22:C1:43:ILE:HG22	22:C1:49:TYR:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:CF:61:SER:HB2	34:CF:91:LEU:HD21	1.80	0.63
31:CA:17:G:H4'	45:CR:25:TYR:HE2	1.62	0.63
29:CC:29:PRO:HG2	29:CC:34:LEU:HD11	1.80	0.63
31:CA:1105:U:H2'	31:CA:1106:G:C8	2.33	0.63
17:BQ:14:SER:HB3	17:BQ:22:VAL:HG12	1.80	0.63
39:CL:76:VAL:HG12	44:CQ:73:VAL:HB	1.81	0.63
24:D3:7:PRO:HB2	55:DA:1309:G:H4'	1.80	0.63
55:DA:1105:U:H2'	55:DA:1106:G:C8	2.34	0.63
55:DA:31:C:O3'	55:DA:1238:G:H5''	1.98	0.63
40:DM:77:ILE:HD11	40:DM:101:ILE:CG2	2.29	0.63
22:C1:15:MET:HB3	31:CA:2045:C:O3'	1.98	0.63
47:CT:82:MET:HB2	47:CT:98:LYS:HB2	1.79	0.63
55:DA:2256:G:H21	57:DA:3193:PG4:H31	1.63	0.63
20:BT:9:LYS:O	20:BT:12:ILE:HG13	1.98	0.62
24:C3:30:VAL:CG1	31:CA:466:A:H5''	2.29	0.62
45:DR:20:GLN:HG2	57:DR:202:PG4:H51	1.81	0.62
55:DA:1482:G:H1'	55:DA:1509:A:H61	1.65	0.62
26:C5:3:VAL:CG1	31:CA:2539:C:H5'	2.20	0.62
31:CA:2728:U:HO2'	31:CA:2729:G:H8	1.47	0.62
29:DC:29:PRO:HG2	29:DC:34:LEU:HD11	1.82	0.62
17:AQ:17:MET:HG2	17:AQ:20:SER:HB2	1.82	0.62
5:BE:72:ILE:HG12	5:BE:145:GLU:HG3	1.80	0.62
22:C1:8:PRO:HG2	31:CA:1264:A:H5'	1.80	0.62
31:CA:328:U:O3'	49:CV:66:GLN:HG3	2.00	0.62
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	1.80	0.62
1:BA:209:U:H4'	1:BA:210:C:OP2	2.00	0.61
55:DA:788:A:H3'	59:DA:3221:PUT:H41	1.82	0.61
5:AE:77:ASN:HB2	5:AE:82:GLN:HE22	1.62	0.61
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.82	0.61
16:BP:20:VAL:HG13	16:BP:32:PHE:HB2	1.82	0.61
55:DA:1847:A:HO2'	55:DA:1848:A:H8	1.48	0.61
19:BS:6:LYS:HD2	19:BS:7:LYS:H	1.65	0.61
22:D1:43:ILE:HG22	22:D1:49:TYR:HB2	1.83	0.61
64:DD:301:PGE:H12	55:DA:2623:G:OP1	2.01	0.61
2:BB:41:ILE:HD13	2:BB:202:GLY:HA2	1.83	0.61
36:CH:15:LEU:HD22	36:CH:15:LEU:H	1.66	0.61
31:CA:674:G:H1'	33:CE:69:ARG:HD2	1.83	0.61
45:DR:20:GLN:HG2	57:DR:202:PG4:H42	1.81	0.60
12:AL:110:ARG:HB2	12:AL:119:VAL:HG21	1.81	0.60
25:C4:13:ARG:NH1	31:CA:250:G:OP2	2.33	0.60
34:CF:31:VAL:CG1	34:CF:97:TRP:CH2	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DE:48:THR:HG23	33:DE:88:ARG:NH1	2.16	0.60
47:DT:82:MET:HB2	47:DT:98:LYS:HB2	1.82	0.60
29:CC:17:VAL:HB	29:CC:204:VAL:HG13	1.83	0.60
48:DU:80:TRP:HB3	64:DU:101:PGE:H32	1.83	0.60
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.49	0.60
13:AM:33:ILE:HD11	13:AM:63:PHE:HE1	1.66	0.60
1:BA:1323:G:H2'	1:BA:1324:A:C8	2.36	0.60
22:C1:25:VAL:HG13	22:C1:26:THR:H	1.67	0.60
31:CA:1482:G:H1'	31:CA:1509:A:H61	1.66	0.60
47:CT:59:GLU:HA	47:CT:64:ALA:HA	1.82	0.60
1:BA:843:U:H5''	1:BA:843:U:H6	1.67	0.59
31:CA:528:A:H3'	31:CA:528:A:H8	1.67	0.59
6:AF:16:GLU:HB3	4:BD:189:SER:HA	1.83	0.59
1:BA:978:A:HO2'	1:BA:1322:C:H5	1.51	0.59
1:BA:9:G:H4'	5:BE:109:GLY:H	1.66	0.59
31:CA:1779:U:C5	31:CA:1784:A:N7	2.64	0.59
1:AA:1238:A:H5'	1:AA:1336:C:H41	1.68	0.59
2:AB:41:ILE:HD13	2:AB:202:GLY:HA2	1.83	0.59
1:BA:1141:C:HO2'	1:BA:1142:G:H8	1.51	0.59
5:BE:104:GLY:HA3	5:BE:122:ASN:HA	1.83	0.59
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.38	0.59
31:CA:528:A:H3'	31:CA:528:A:C8	2.38	0.59
22:C1:15:MET:SD	31:CA:2045:C:H5''	2.43	0.59
45:DR:19:LYS:HB3	57:DR:202:PG4:H41	1.85	0.59
1:AA:451:A:H61	1:AA:481:G:H5'	1.67	0.59
1:AA:202:G:H21	1:AA:466:A:H61	1.51	0.59
26:C5:16:ILE:HD13	26:C5:25:VAL:HG22	1.85	0.59
33:DE:33:VAL:HG22	58:DA:3192:MPD:H12	1.84	0.59
31:CA:1847:A:HO2'	31:CA:1848:A:H8	1.48	0.58
31:CA:2728:U:O2'	31:CA:2729:G:H5''	2.04	0.58
13:BM:22:ILE:HB	13:BM:25:VAL:HG12	1.86	0.58
11:AK:34:ILE:HG12	11:AK:70:CYS:SG	2.43	0.58
1:BA:841:C:H3'	1:BA:842:U:H5''	1.86	0.58
55:DA:2128:G:H1	55:DA:2160:C:H42	1.52	0.58
1:BA:946:A:H2'	1:BA:947:G:C8	2.38	0.58
5:BE:133:PRO:O	5:BE:137:VAL:HG12	2.02	0.58
42:CO:49:GLU:OE2	42:CO:95:THR:HG22	2.04	0.58
55:DA:12:U:O2	55:DA:12:U:H2'	2.04	0.58
45:DR:31:VAL:HG13	55:DA:580:U:O3'	2.03	0.58
1:AA:946:A:H2'	1:AA:947:G:C8	2.39	0.58
32:DD:114:LYS:HE2	55:DA:2681:C:OP2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:CH:41:LYS:HA	36:CH:44:ILE:HG12	1.86	0.58
55:DA:1105:U:H2'	55:DA:1106:G:H8	1.68	0.58
23:C2:35:GLU:HG2	23:C2:50:LYS:HG2	1.86	0.57
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.86	0.57
29:CC:120:VAL:HG12	29:CC:134:ASN:ND2	2.19	0.57
1:BA:209:U:O2	1:BA:209:U:H2'	2.03	0.57
26:D5:16:ILE:HD13	26:D5:25:VAL:HG22	1.86	0.57
18:AR:36:SER:HA	18:AR:72:ASP:HB3	1.87	0.57
7:BG:113:ASP:HB2	7:BG:119:ARG:HG3	1.86	0.57
24:D3:4:THR:HG22	55:DA:687:C:H1'	1.87	0.57
33:DE:189:THR:HG22	33:DE:192:ALA:H	1.69	0.57
31:CA:1105:U:H2'	31:CA:1106:G:H8	1.68	0.57
31:CA:550:C:H2'	31:CA:551:G:H5''	1.86	0.57
1:AA:1492:A:C5'	12:AL:44:LYS:HG2	2.34	0.57
31:CA:1703:G:H2'	31:CA:1704:C:C6	2.40	0.57
31:CA:310:A:H5''	49:CV:15:THR:HG23	1.86	0.57
36:CH:27:ARG:HH11	52:CY:60:ASP:HA	1.70	0.57
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.87	0.57
1:BA:1238:A:H5'	1:BA:1336:C:H41	1.68	0.57
34:CF:36:LEU:HD21	34:CF:91:LEU:CD1	2.34	0.57
40:CM:82:LEU:HD11	40:CM:116:VAL:CG2	2.32	0.57
48:CU:24:MET:HG2	48:CU:29:THR:O	2.05	0.57
40:CM:28:GLY:O	40:CM:29:LYS:O	2.21	0.57
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.86	0.57
47:CT:66:ILE:HA	47:CT:69:LEU:HD22	1.87	0.57
35:DG:42:GLU:HG2	35:DG:55:ARG:HH21	1.68	0.57
36:DH:41:LYS:HA	36:DH:44:ILE:HG12	1.86	0.57
1:AA:1141:C:HO2'	1:AA:1142:G:H8	1.52	0.57
1:AA:81:A:H61	1:AA:86:G:H1	1.53	0.57
29:DC:120:VAL:HG12	29:DC:134:ASN:ND2	2.20	0.57
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.87	0.56
7:AG:22:LEU:HD12	7:AG:62:PHE:HE2	1.69	0.56
22:C1:5:GLN:HG3	31:CA:2054:A:C2	2.39	0.56
1:BA:451:A:H61	1:BA:481:G:H5'	1.69	0.56
33:CE:189:THR:HG22	33:CE:192:ALA:H	1.70	0.56
5:BE:77:ASN:HB2	5:BE:82:GLN:HE22	1.68	0.56
31:CA:2095:A:H8	31:CA:2095:A:H5''	1.69	0.56
40:DM:77:ILE:HD11	40:DM:101:ILE:HG21	1.87	0.56
55:DA:62:U:O4'	58:DA:3203:MPD:H31	2.05	0.56
1:AA:8:A:C6	4:AD:206:LYS:HB3	2.40	0.56
1:BA:1012:A:H61	1:BA:1017:U:H3	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:DD:146:ILE:HD12	32:DD:155:VAL:HG21	1.88	0.56
44:DQ:96:LYS:HE3	70:DQ:306:HOH:O	2.04	0.56
55:DA:550:C:H2'	55:DA:551:G:H5''	1.87	0.56
1:AA:1277:C:HO2'	1:AA:1279:G:H8	1.53	0.56
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.36	0.56
31:CA:2304:G:H5'	34:CF:121:SER:HB2	1.87	0.56
11:AK:67:ALA:HB2	11:AK:96:THR:HG23	1.88	0.56
23:D2:35:GLU:HG2	23:D2:50:LYS:HG2	1.86	0.56
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.36	0.55
22:C1:17:ARG:NH2	31:CA:1266:G:OP2	2.39	0.55
31:CA:2019:A:H4'	45:CR:34:VAL:HG21	1.87	0.55
41:DN:18[B]:ARG:HG3	28:DB:90:C:H5'	1.89	0.55
1:AA:1012:A:H61	1:AA:1017:U:H3	1.55	0.55
10:AJ:5:ARG:HE	10:AJ:77:VAL:HG22	1.70	0.55
1:BA:1106:G:H5''	3:BC:172:ARG:HG3	1.87	0.55
13:BM:86:TYR:CZ	13:BM:90:ARG:HD2	2.41	0.55
31:CA:457:A:N1	31:CA:470:A:H5''	2.21	0.55
1:BA:619:U:H3	4:BD:131:ASN:HB3	1.71	0.55
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.89	0.55
24:C3:9:VAL:N	31:CA:1309:G:OP1	2.33	0.55
22:D1:8:PRO:HG2	55:DA:1264:A:H5'	1.88	0.55
55:DA:31:C:O2'	55:DA:1238:G:H5'	2.06	0.55
35:DG:175:LYS:HG3	55:DA:2529:G:H4'	1.88	0.55
8:AH:29:SER:HB3	8:AH:57:PRO:HB2	1.88	0.55
5:BE:72:ILE:HG13	5:BE:73:ASN:H	1.72	0.55
1:AA:412:A:H3'	1:AA:413:G:C5'	2.37	0.55
10:AJ:35:GLN:HB2	10:AJ:77:VAL:HB	1.88	0.55
1:BA:1151:A:HO2'	1:BA:1152:A:H8	1.53	0.55
3:BC:77:ILE:HA	3:BC:84:VAL:HG23	1.88	0.55
26:C5:1:MET:HB2	31:CA:2526:G:O2'	2.06	0.55
26:C5:36:ARG:HD3	31:CA:2742:G:OP1	2.07	0.55
4:BD:85:ASN:HB3	4:BD:88:GLU:HB2	1.89	0.55
48:CU:22:THR:HA	48:CU:25:GLU:HG2	1.87	0.55
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	1.89	0.55
31:CA:2822:G:H2'	31:CA:2823:A:H5''	1.88	0.55
55:DA:2297:A:H5''	55:DA:2297:A:C8	2.42	0.55
25:D4:64:TYR:CE2	55:DA:242:G:H5''	2.42	0.55
13:AM:86:TYR:CZ	13:AM:90:ARG:HD2	2.41	0.54
11:BK:67:ALA:HB2	11:BK:96:THR:HG23	1.88	0.54
11:BK:89:PRO:HG3	21:BU:32:VAL:HG11	1.88	0.54
31:CA:2845:U:H5''	44:CQ:52:ASN:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D4:8:ARG:HD3	55:DA:245:G:O6	2.08	0.54
64:D1:102:PGE:H42	47:DT:23:LEU:HD23	1.89	0.54
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.89	0.54
31:CA:2502:G:H5''	31:CA:2503:2MA:H5''	1.90	0.54
1:BA:108:G:N3	1:BA:108:G:H5''	2.23	0.54
65:DA:3223:SPD:H92	65:DA:3223:SPD:H52	1.90	0.54
44:DQ:106:LYS:HA	44:DQ:109:ARG:HD3	1.90	0.54
11:AK:31:ILE:HG12	11:AK:46:THR:HG22	1.88	0.54
16:BP:4:ILE:HG12	16:BP:21:VAL:HG22	1.90	0.54
45:CR:87:SER:HB3	46:CS:52:PRO:HD3	1.90	0.54
5:AE:76:LEU:HD11	5:AE:120:VAL:HG22	1.90	0.54
26:C5:17:VAL:CG1	26:C5:26:ILE:HD12	2.38	0.54
39:DL:76:VAL:CG2	55:DA:2684:U:H4'	2.37	0.54
1:AA:404:G:N7	4:AD:2:ALA:HB3	2.23	0.54
5:BE:72:ILE:HG13	5:BE:73:ASN:N	2.22	0.54
23:D2:8:LYS:HE3	55:DA:2420:C:H5''	1.89	0.54
13:AM:33:ILE:HD11	13:AM:63:PHE:CE1	2.42	0.54
10:BJ:5:ARG:HG2	10:BJ:79:PRO:HG3	1.90	0.54
11:BK:52:PHE:HE2	11:BK:65:VAL:HG21	1.73	0.54
22:C1:4:GLN:HB3	31:CA:2615:U:H1'	1.90	0.54
1:AA:108:G:H5''	1:AA:108:G:N3	2.22	0.54
5:BE:35:ALA:O	5:BE:50:TYR:O	2.26	0.54
31:CA:1394:U:H4'	31:CA:1603:A:H4'	1.90	0.54
48:DU:67:VAL:HG22	48:DU:76:ARG:HG3	1.90	0.54
1:BA:374:A:OP1	1:BA:452:A:N1	2.41	0.53
1:BA:769:G:H4'	1:BA:1513:A:H4'	1.88	0.53
5:BE:126:LYS:HG2	5:BE:128:TYR:CZ	2.44	0.53
33:CE:149:ILE:HD12	33:CE:172:ALA:HA	1.89	0.53
44:CQ:106:LYS:HA	44:CQ:109:ARG:HD3	1.90	0.53
1:AA:1144:G:H21	1:AA:1146:A:H62	1.56	0.53
4:AD:85:ASN:HB3	4:AD:88:GLU:HB2	1.90	0.53
34:CF:31:VAL:HG11	34:CF:97:TRP:CH2	2.43	0.53
1:AA:209:U:H4'	1:AA:210:C:OP2	2.08	0.53
31:CA:1251:C:OP2	45:CR:6:ARG:HD2	2.09	0.53
1:BA:1144:G:H21	1:BA:1146:A:H62	1.56	0.53
6:BF:45:ARG:O	6:BF:56:LYS:HA	2.08	0.53
12:BL:33:VAL:HG22	12:BL:79:VAL:HG22	1.90	0.53
36:CH:4:ILE:HD11	36:CH:44:ILE:HG22	1.90	0.53
3:BC:5:VAL:HG21	3:BC:10:ILE:HD13	1.91	0.53
2:BB:129:LEU:HD13	2:BB:134:ALA:HB2	1.91	0.53
8:BH:29:SER:HB3	8:BH:57:PRO:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:52:PHE:HE2	11:AK:65:VAL:HG21	1.73	0.53
55:DA:2796:U:H3	55:DA:2799:A:N6	1.97	0.53
54:DI:69:PHE:HB3	54:DI:72:LEU:HD12	1.91	0.53
1:AA:735:C:H5'	18:AR:60:LYS:HD3	1.91	0.53
10:AJ:42:LEU:HB2	10:AJ:71:LEU:HB3	1.91	0.53
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.90	0.53
6:BF:38:ARG:HH12	6:BF:99:ALA:HB3	1.74	0.53
44:DQ:52:ASN:O	55:DA:2845:U:H5''	2.09	0.53
2:AB:129:LEU:HD13	2:AB:134:ALA:HB2	1.91	0.53
19:AS:29:LYS:HB3	19:AS:30:PRO:HD2	1.91	0.53
10:BJ:26:VAL:HG21	10:BJ:39:PRO:HD3	1.91	0.53
31:CA:1936:A:C2	31:CA:1943:U:N3	2.59	0.53
25:C4:2:PRO:HD2	31:CA:667:U:O2	2.09	0.52
25:C4:47:LYS:NZ	40:CM:64:PHE:CE1	2.77	0.52
3:AC:5:VAL:HG21	3:AC:10:ILE:HD13	1.92	0.52
31:CA:1847:A:O2'	31:CA:1848:A:H8	1.92	0.52
6:AF:45:ARG:O	6:AF:56:LYS:HA	2.08	0.52
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	1.91	0.52
6:BF:3:HIS:H	6:BF:92:THR:HG23	1.73	0.52
31:CA:2037:A:H2'	31:CA:2038:G:C8	2.44	0.52
22:C1:38:HIS:CE1	31:CA:2884:U:O4	2.54	0.52
31:CA:2796:U:H3	31:CA:2799:A:N6	1.99	0.52
32:DD:128:ARG:HG3	70:DA:7412:HOH:O	2.09	0.52
8:AH:2:SER:HB2	8:AH:4:GLN:HE21	1.75	0.52
13:AM:71:ARG:HH21	34:DF:143:TYR:HB2	1.74	0.52
31:CA:118:A:N3	31:CA:178:G:H1'	2.25	0.52
26:C5:3:VAL:HG12	31:CA:2538:C:O2'	2.10	0.52
43:CP:100:HIS:CD2	43:CP:101:GLY:H	2.28	0.52
35:DG:86:LYS:HG2	35:DG:132:VAL:HG22	1.91	0.52
23:C2:11:LEU:HD21	23:C2:34:LEU:HD23	1.91	0.52
31:CA:2297:A:C8	31:CA:2297:A:H5''	2.45	0.52
24:C3:33:ARG:NE	31:CA:467:G:OP1	2.36	0.52
31:CA:668:A:H2'	31:CA:670:A:H62	1.75	0.52
65:DA:3223:SPD:H92	65:DA:3223:SPD:C5	2.40	0.52
55:DA:74:A:N3	55:DA:74:A:H5''	2.25	0.52
48:DU:54:GLU:HB3	48:DU:88:LYS:HD2	1.92	0.52
1:AA:86:G:H21	1:AA:87:C:H41	1.58	0.52
1:BA:404:G:N7	4:BD:2:ALA:HB3	2.24	0.52
6:BF:38:ARG:NH1	6:BF:99:ALA:HB3	2.24	0.52
22:C1:41:HIS:HE2	31:CA:2884:U:P	2.32	0.52
35:CG:86:LYS:HG2	35:CG:132:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1277:C:O2'	1:AA:1279:G:H8	1.93	0.52
1:AA:845:A:O4'	1:AA:845:A:P	2.68	0.52
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.75	0.52
22:C1:19:HIS:CE1	31:CA:2624:G:H1'	2.45	0.52
33:CE:21:ARG:HD3	33:CE:106:LYS:HB3	1.92	0.52
40:DM:79:LEU:HD11	40:DM:112:LEU:HD12	1.92	0.52
41:DN:81[B]:4D4:H9	55:DA:2496:C:OP2	2.10	0.52
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.45	0.51
10:AJ:26:VAL:HG21	10:AJ:39:PRO:HD3	1.91	0.51
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.76	0.51
11:AK:23:ILE:HD11	11:AK:86:VAL:HG13	1.92	0.51
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.92	0.51
19:BS:29:LYS:HB3	19:BS:30:PRO:HD2	1.93	0.51
31:CA:699:A:H2'	31:CA:700:G:O4'	2.10	0.51
33:DE:21:ARG:HD3	33:DE:106:LYS:HB3	1.91	0.51
29:CC:13:ARG:HD3	31:CA:728:G:H4'	1.92	0.51
43:CP:51:ALA:HB3	43:CP:78:VAL:HG13	1.92	0.51
1:BA:350:G:H5''	20:BT:3:ASN:HD22	1.76	0.51
1:BA:374:A:H5''	1:BA:452:A:N1	2.25	0.51
4:BD:48:LEU:HD21	4:BD:56:ARG:HG3	1.93	0.51
31:CA:17:G:H4'	45:CR:25:TYR:CE2	2.43	0.51
48:CU:54:GLU:HB3	48:CU:88:LYS:HD2	1.92	0.51
32:DD:25:THR:HG21	32:DD:193:VAL:HG22	1.92	0.51
54:DI:44:ALA:HB1	54:DI:95:LEU:HD11	1.91	0.51
11:BK:23:ILE:HD11	11:BK:86:VAL:HG13	1.91	0.51
31:CA:569:U:H5''	31:CA:821:A:C2	2.46	0.51
55:DA:1853:A:N1	55:DA:2087:G:H1'	2.25	0.51
25:D4:8:ARG:CD	55:DA:245:G:O6	2.59	0.51
7:BG:111:ARG:HB3	7:BG:119:ARG:HG2	1.93	0.51
31:CA:1447:C:H2'	31:CA:1448:G:C8	2.46	0.51
31:CA:532:A:N1	31:CA:2020:A:H1'	2.25	0.51
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.92	0.51
1:BA:1218:C:H2'	1:BA:1219:A:C8	2.46	0.51
1:BA:1277:C:O2'	1:BA:1279:G:H8	1.93	0.51
31:CA:12:U:H2'	31:CA:12:U:O2	2.11	0.51
30:CD:25:THR:HG21	30:CD:193:VAL:HG22	1.93	0.51
47:CT:69:LEU:HG	47:CT:107:VAL:HG22	1.92	0.51
22:D1:22:LEU:HD23	62:D1:103:PEG:H31	1.91	0.51
39:DL:38:ILE:HD11	39:DL:112:PHE:CZ	2.42	0.51
11:AK:23:ILE:HG22	11:AK:32:VAL:HG13	1.92	0.51
30:CD:4:LEU:HD22	30:CD:101:PHE:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D4:31:HIS:HB2	70:D4:103:HOH:O	2.10	0.51
43:DP:51:ALA:HB3	43:DP:78:VAL:HG13	1.93	0.51
5:AE:126:LYS:HG2	5:AE:128:TYR:CZ	2.46	0.51
31:CA:998:C:OP2	45:CR:58:ARG:NH2	2.44	0.51
31:CA:2025:C:H2'	31:CA:2026:U:C6	2.46	0.51
31:CA:2189:U:H2'	31:CA:2190:G:H8	1.76	0.51
30:CD:129:THR:HG23	30:CD:140:HIS:O	2.11	0.51
25:D4:60:ALA:O	40:DM:48:ARG:HD2	2.10	0.51
55:DA:1847:A:O2'	55:DA:1848:A:H8	1.93	0.51
47:CT:73:LYS:HB2	47:CT:106:VAL:HB	1.92	0.50
36:DH:4:ILE:HD11	36:DH:44:ILE:HG22	1.93	0.50
12:AL:33:VAL:HG22	12:AL:79:VAL:HG22	1.92	0.50
31:CA:784:G:H5'	31:CA:785:G:OP1	2.10	0.50
38:CK:81:ILE:HG23	38:CK:82:GLY:H	1.76	0.50
1:AA:774:G:H21	57:AA:1670:PG4:H51	1.75	0.50
5:BE:106:ILE:HD11	5:BE:124:LEU:HD23	1.93	0.50
11:BK:23:ILE:HG22	11:BK:32:VAL:HG13	1.93	0.50
20:BT:4:ILE:HA	20:BT:8:LYS:HE2	1.93	0.50
31:CA:335:C:H5''	49:CV:82:ARG:HD3	1.93	0.50
55:DA:1026:G:H2'	55:DA:1027:A:C8	2.45	0.50
34:DF:131:GLY:HA3	55:DA:2305:U:H5''	1.94	0.50
24:C3:19:ARG:NH2	31:CA:125:A:OP2	2.41	0.50
48:CU:18:GLU:H	48:CU:18:GLU:CD	2.15	0.50
35:DG:19:ILE:HG12	35:DG:24:ILE:HG12	1.93	0.50
9:BI:19:VAL:HG22	9:BI:65:ILE:HG22	1.92	0.50
1:AA:1358:U:H3	1:AA:1363:A:H62	1.59	0.50
19:AS:15:LEU:HD13	19:AS:33:THR:HG21	1.93	0.50
54:DI:57:ASN:HB3	54:DI:76:PHE:HB3	1.93	0.50
1:BA:1003:G:H21	1:BA:1005:A:H5'	1.77	0.50
17:BQ:17:MET:HB3	17:BQ:20:SER:HB3	1.93	0.50
23:D2:25:LYS:HE2	23:D2:30:LYS:O	2.12	0.50
43:DP:31:THR:HG21	28:DB:28:C:P	2.51	0.50
3:AC:20:SER:HB3	14:AN:94:PRO:HG3	1.92	0.50
18:AR:45:THR:OG1	18:AR:47:THR:HG22	2.12	0.50
8:BH:2:SER:HB2	8:BH:4:GLN:HE21	1.76	0.50
31:CA:1638:C:H5''	31:CA:2710:C:O2'	2.12	0.50
55:DA:1536:C:H4'	55:DA:1537:G:H5''	1.93	0.50
7:AG:111:ARG:HB3	7:AG:119:ARG:HG2	1.93	0.50
11:BK:43:GLY:HA3	11:BK:74:VAL:HG12	1.93	0.50
31:CA:70:G:H5''	31:CA:112:U:O2	2.12	0.50
55:DA:914:G:H8	55:DA:914:G:H5''	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AI:19:VAL:HG22	9:AI:65:ILE:HG22	1.93	0.49
1:BA:374:A:H5''	1:BA:452:A:C2	2.47	0.49
9:BI:57:MET:HG3	9:BI:61:LEU:HG	1.93	0.49
1:BA:735:C:H5'	18:BR:60:LYS:HD3	1.93	0.49
31:CA:532:A:H2'	31:CA:532:A:N3	2.26	0.49
30:CD:99:GLU:HG2	30:CD:182:ALA:HB2	1.94	0.49
43:DP:68:LYS:HB3	62:DP:201:PEG:H22	1.93	0.49
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.94	0.49
24:C3:24:THR:HG23	24:C3:27:GLY:H	1.77	0.49
34:CF:44:ILE:HG21	34:CF:79:ILE:HG22	1.94	0.49
55:DA:479:A:N3	55:DA:481:G:H5''	2.26	0.49
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	1.94	0.49
7:BG:69:VAL:HG23	7:BG:100:ALA:HB1	1.94	0.49
18:BR:36:SER:HA	18:BR:72:ASP:HB3	1.93	0.49
31:CA:2185:U:H2'	31:CA:2186:G:C8	2.46	0.49
31:CA:2445:2MG:HM21	31:CA:2449:U:O4	2.11	0.49
29:CC:210:ALA:HA	29:CC:213:TRP:CE2	2.47	0.49
22:D1:9:THR:HG21	55:DA:2020:A:H5'	1.94	0.49
41:CN:21:ALA:HB1	41:CN:100:LYS:HG2	1.94	0.49
55:DA:1433:A:O2'	55:DA:1434:A:H5'	2.12	0.49
29:DC:227:PRO:HA	29:DC:233:GLY:HA2	1.95	0.49
54:DI:31:ARG:HB2	54:DI:79:PRO:HG2	1.93	0.49
29:CC:227:PRO:HA	29:CC:233:GLY:HA2	1.95	0.49
35:CG:19:ILE:HG12	35:CG:24:ILE:HG12	1.93	0.49
55:DA:2441:U:O2'	65:DA:3223:SPD:H91	2.13	0.49
1:AA:411:A:P	4:AD:26:ARG:HH12	2.36	0.49
11:AK:84:VAL:HG21	11:AK:97:ILE:HG23	1.95	0.49
1:BA:202:G:H1	1:BA:215:C:H42	1.59	0.49
55:DA:789:A:OP1	59:DA:3221:PUT:H12	2.12	0.49
1:BA:76:G:H1	1:BA:93:U:H3	1.61	0.49
3:BC:113:ALA:O	3:BC:200:VAL:HG11	2.12	0.49
31:CA:1587:G:H2'	31:CA:1588:G:H8	1.78	0.49
28:CB:14:U:H2'	28:CB:15:A:H2	1.76	0.49
1:AA:202:G:O2'	1:AA:468:A:H8	1.95	0.49
1:BA:202:G:O2'	1:BA:468:A:H8	1.95	0.49
1:AA:1003:G:H21	1:AA:1005:A:H5'	1.77	0.49
1:BA:840:C:H2'	1:BA:841:C:O4'	2.13	0.49
47:CT:4:ILE:HG12	47:CT:106:VAL:HG22	1.94	0.49
5:AE:107:ALA:HB2	5:AE:125:ALA:HB3	1.94	0.48
11:AK:34:ILE:HB	11:AK:74:VAL:HG11	1.95	0.48
3:BC:47:LEU:HB3	3:BC:50:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:20:SER:HB3	14:BN:94:PRO:HG3	1.93	0.48
31:CA:1182:G:H2'	31:CA:1183:U:O4'	2.13	0.48
31:CA:479:A:N3	31:CA:481:G:H5''	2.28	0.48
33:CE:75:SER:O	33:CE:78:TRP:HB2	2.13	0.48
39:CL:43:ILE:HD12	39:CL:56:ASP:HB2	1.94	0.48
55:DA:837:C:H5	70:DA:6720:HOH:O	1.95	0.48
28:DB:84:G:H21	63:DB:211:EDO:H11	1.78	0.48
32:DD:99:GLU:HG2	32:DD:182:ALA:HB2	1.94	0.48
15:AO:82:ILE:HG21	15:AO:89:ARG:OXT	2.13	0.48
31:CA:2630:G:O4'	31:CA:2894:G:H1'	2.13	0.48
32:DD:13:ARG:NH1	70:DD:401:HOH:O	2.44	0.48
4:AD:48:LEU:HD21	4:AD:56:ARG:HG3	1.94	0.48
2:BB:73:LYS:HD2	2:BB:168:HIS:HD2	1.77	0.48
3:BC:72:ARG:HB3	3:BC:75:ILE:HG22	1.94	0.48
31:CA:2060:A:N6	33:CE:69:ARG:NH2	2.60	0.48
31:CA:2623:G:H4'	31:CA:2825:G:H8	1.78	0.48
31:CA:914:G:H8	31:CA:914:G:H5''	1.79	0.48
29:CC:177:ARG:HG2	31:CA:1820:U:OP1	2.14	0.48
1:BA:975:A:H8	1:BA:1357:A:HO2'	1.61	0.48
35:CG:80:THR:HG23	35:CG:81:GLU:N	2.24	0.48
9:AI:57:MET:HG3	9:AI:61:LEU:HG	1.94	0.48
1:BA:677:U:H3	1:BA:713:G:H22	1.61	0.48
11:BK:30:THR:HG21	11:BK:92:GLY:HA3	1.96	0.48
31:CA:634:C:H2'	31:CA:635:C:C6	2.49	0.48
28:CB:14:U:H2'	28:CB:15:A:C2	2.49	0.48
25:C4:24:HIS:CG	40:CM:61:LEU:HD13	2.49	0.48
54:DI:50:VAL:HG13	54:DI:85:VAL:HG22	1.95	0.48
43:DP:31:THR:HG22	43:DP:33:ARG:H	1.79	0.48
1:AA:413:G:H5''	1:AA:414:A:H5'	1.96	0.48
24:C3:37:LYS:O	31:CA:458:G:H2'	2.13	0.48
25:D4:64:TYR:CZ	55:DA:242:G:H5''	2.49	0.48
1:AA:975:A:H8	1:AA:1357:A:HO2'	1.59	0.48
2:AB:20:THR:HG22	2:AB:39:HIS:CE1	2.48	0.48
11:AK:30:THR:HG21	11:AK:92:GLY:HA3	1.95	0.48
25:C4:54:ASP:HB3	40:CM:57:LEU:HD22	1.95	0.48
31:CA:247:G:H4'	31:CA:386:G:C5	2.49	0.48
39:CL:38:ILE:HD11	39:CL:112:PHE:CZ	2.38	0.48
47:DT:4:ILE:HG12	47:DT:106:VAL:HG22	1.94	0.48
47:DT:72:THR:HG21	47:DT:108:SER:HB3	1.95	0.48
5:AE:38:VAL:HG11	5:AE:114:VAL:HG22	1.96	0.48
23:D2:11:LEU:HD21	23:D2:34:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:DM:21:ARG:HA	55:DA:811:U:H2'	1.95	0.48
41:DN:41:LEU:HG	41:DN:96:ILE:HG13	1.96	0.48
7:AG:22:LEU:HD12	7:AG:62:PHE:CE2	2.48	0.48
5:BE:36:LEU:HD21	5:BE:137:VAL:HG11	1.95	0.48
22:D1:55:ILE:HD12	42:DO:33:ILE:CD1	2.44	0.48
55:DA:11:C:H2'	55:DA:12:U:H5'	1.95	0.48
32:DD:150[B]:MEQ:HE2	55:DA:2033:A:O5'	2.14	0.48
51:DX:41[A]:ARG:HG3	55:DA:2386:A:N3	2.28	0.48
34:DF:44:ILE:HG21	34:DF:79:ILE:HG22	1.95	0.48
47:DT:73:LYS:HB2	47:DT:106:VAL:HB	1.95	0.48
1:AA:542:G:H5'	4:AD:39:GLY:HA3	1.96	0.47
24:C3:16:HIS:CD2	31:CA:464:U:HO2'	2.32	0.47
34:CF:36:LEU:HB2	34:CF:57:LEU:HD21	1.96	0.47
22:D1:25:VAL:HG11	47:DT:38:TYR:HB2	1.96	0.47
55:DA:1172:C:C5	55:DA:1173:U:H1'	2.49	0.47
45:DR:6:ARG:HD3	55:DA:1250:G:H5''	1.95	0.47
55:DA:1587:G:H2'	55:DA:1588:G:H8	1.79	0.47
5:AE:133:PRO:O	5:AE:137:VAL:HG13	2.14	0.47
1:BA:542:G:H5'	4:BD:39:GLY:HA3	1.96	0.47
17:BQ:76:VAL:HG12	17:BQ:77:ARG:HG3	1.97	0.47
23:C2:25:LYS:HE2	23:C2:30:LYS:O	2.14	0.47
37:CJ:19:ASN:H	37:CJ:20:PRO:HD2	1.80	0.47
31:CA:1364:G:P	52:CY:50:ARG:HH22	2.36	0.47
55:DA:1975:G:H21	64:DA:3224:PGE:C2	2.27	0.47
1:AA:1055:A:H2'	3:AC:156:ARG:HD2	1.96	0.47
6:AF:38:ARG:HE	6:AF:63:ASN:ND2	2.12	0.47
1:BA:1391:U:H2'	1:BA:1392:G:C8	2.49	0.47
32:DD:8:LYS:HB2	32:DD:201:LEU:HD11	1.96	0.47
39:DL:43:ILE:HD12	39:DL:56:ASP:HB2	1.96	0.47
1:BA:1190:G:H5'	3:BC:176:HIS:NE2	2.29	0.47
55:DA:2291:U:H2'	55:DA:2292:U:C6	2.49	0.47
32:DD:105:LYS:NZ	32:DD:106:LYS:HE3	2.30	0.47
37:DJ:103:ARG:HA	37:DJ:106:LEU:HD12	1.96	0.47
11:BK:84:VAL:HG21	11:BK:97:ILE:HG23	1.97	0.47
31:CA:2185:U:H2'	31:CA:2186:G:H8	1.79	0.47
34:CF:8:TYR:HA	34:CF:12:VAL:HB	1.97	0.47
13:AM:4:ILE:HD12	13:AM:10:PRO:HG2	1.95	0.47
31:CA:1141:U:H4'	31:CA:1142:A:O4'	2.15	0.47
25:C4:25:LYS:HD3	40:CM:62:PRO:HG2	1.97	0.47
52:CY:10:LYS:HE3	52:CY:54:LYS:HG2	1.97	0.47
55:DA:789:A:OP1	59:DA:3221:PUT:C1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:269:C:H2'	1:AA:270:A:C8	2.50	0.47
55:DA:1975:G:H21	64:DA:3224:PGE:H2	1.79	0.47
55:DA:644:A:H2'	55:DA:645:C:O4'	2.14	0.47
43:DP:52:SER:OG	43:DP:54:VAL:HG22	2.14	0.47
49:DV:73:PHE:CE2	49:DV:75:ALA:HA	2.49	0.47
31:CA:2030:6MZ:C2	31:CA:2499:C:H5''	2.45	0.47
30:CD:26:VAL:HG21	44:CQ:5:ILE:HG12	1.97	0.47
22:D1:5:GLN:O	55:DA:2017:U:H4'	2.15	0.47
34:DF:8:TYR:HA	34:DF:12:VAL:HB	1.97	0.47
34:DF:36:LEU:HB2	34:DF:57:LEU:HD21	1.96	0.47
36:DH:49:ALA:O	36:DH:53:GLU:HB3	2.15	0.47
37:DJ:19:ASN:H	37:DJ:20:PRO:HD2	1.80	0.47
52:DY:10:LYS:HE3	52:DY:54:LYS:HG2	1.97	0.47
1:BA:269:C:H2'	1:BA:270:A:C8	2.50	0.47
1:BA:846:G:H2'	1:BA:847:G:H8	1.79	0.47
24:C3:3:ARG:HD3	31:CA:1613:G:O2'	2.15	0.47
31:CA:2060:A:N6	33:CE:69:ARG:HH21	2.13	0.47
31:CA:2291:U:H2'	31:CA:2292:U:C6	2.50	0.47
30:CD:155:VAL:HG21	31:CA:2618:G:H21	1.79	0.47
31:CA:608:A:H2'	31:CA:609:A:C8	2.50	0.47
49:CV:74:ASN:HD22	49:CV:77:THR:H	1.63	0.47
32:DD:186:LEU:HD21	44:DQ:4:ILE:HG21	1.95	0.47
1:AA:677:U:H3	1:AA:713:G:H22	1.63	0.47
24:C3:7:PRO:CB	31:CA:1309:G:H4'	2.37	0.47
55:DA:1236:G:N7	59:DA:3189:PUT:H41	2.30	0.47
31:CA:1936:A:H62	31:CA:1963:U:H3	1.60	0.47
31:CA:193:U:H5	70:CA:3372:HOH:O	1.98	0.47
33:CE:1:MET:HG2	33:CE:14:VAL:HG23	1.97	0.47
25:C4:25:LYS:O	40:CM:62:PRO:HD2	2.15	0.47
55:DA:1182:G:H2'	55:DA:1183:U:O4'	2.15	0.47
38:DK:69:ARG:O	38:DK:90:GLU:HB2	2.16	0.47
1:AA:310:G:H5''	16:AP:31:ARG:HB2	1.97	0.46
5:BE:57:PRO:O	5:BE:60:ILE:HG13	2.15	0.46
55:DA:749:A:H4'	55:DA:1271:G:N3	2.29	0.46
33:DE:176:ASP:OD2	33:DE:178:VAL:HG12	2.15	0.46
1:AA:73:C:O2'	1:AA:74:A:H8	1.97	0.46
1:BA:23:C:H5	1:BA:561:U:O4	1.98	0.46
2:BB:73:LYS:HD2	2:BB:168:HIS:CD2	2.51	0.46
1:BA:1055:A:H2'	3:BC:156:ARG:HD2	1.97	0.46
42:CO:47:VAL:O	42:CO:51:LEU:HD23	2.15	0.46
43:CP:31:THR:HG22	43:CP:33:ARG:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DF:121:SER:HB2	55:DA:2304:G:H5'	1.96	0.46
6:AF:47:LEU:HD13	6:AF:51:ILE:HG12	1.97	0.46
31:CA:309:A:H4'	49:CV:16:GLY:HA2	1.97	0.46
31:CA:846:U:H1'	31:CA:847:U:C5	2.44	0.46
34:CF:103:LEU:HA	34:CF:107:ALA:HB3	1.97	0.46
49:CV:7:ARG:O	49:CV:25:VAL:HB	2.15	0.46
55:DA:1180:U:H5''	55:DA:1180:U:H6	1.80	0.46
34:DF:103:LEU:HA	34:DF:107:ALA:HB3	1.97	0.46
21:AU:4:ILE:HG13	21:AU:19:PHE:HA	1.97	0.46
1:BA:202:G:H21	1:BA:466:A:H61	1.62	0.46
19:BS:15:LEU:HD13	19:BS:33:THR:HG21	1.95	0.46
30:CD:152:PRO:HG3	30:CD:156:PHE:CZ	2.51	0.46
51:DX:39:ARG:NH1	70:DX:101:HOH:O	2.48	0.46
1:AA:76:G:H1	1:AA:93:U:H3	1.62	0.46
30:CD:133:THR:CG2	31:CA:1993:U:H4'	2.45	0.46
30:CD:62:LYS:HE2	31:CA:2810:A:H5''	1.98	0.46
31:CA:740:C:H5'	31:CA:1784:A:C3'	2.38	0.46
30:CD:3:GLY:O	30:CD:4:LEU:HD13	2.15	0.46
40:CM:77:ILE:CD1	40:CM:108:ALA:HB1	2.36	0.46
64:D1:102:PGE:H4	70:DT:313:HOH:O	2.15	0.46
55:DA:57:C:H2'	55:DA:58:G:O4'	2.16	0.46
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.50	0.46
1:AA:1190:G:H5'	3:AC:176:HIS:NE2	2.31	0.46
1:BA:1001:C:H2'	1:BA:1002:G:H8	1.81	0.46
21:BU:4:ILE:HG13	21:BU:19:PHE:HA	1.97	0.46
31:CA:1010:A:H5'	45:CR:62:ILE:CG2	2.46	0.46
31:CA:749:A:H4'	31:CA:1271:G:N3	2.29	0.46
29:CC:219:THR:O	31:CA:1789:A:H5''	2.15	0.46
44:CQ:114:LEU:H	44:CQ:114:LEU:HD23	1.81	0.46
31:CA:1250:G:C5'	45:CR:6:ARG:HD3	2.44	0.46
55:DA:102:U:H2'	55:DA:102:U:O2	2.15	0.46
45:CR:58:ARG:HA	45:CR:61:TRP:CE3	2.50	0.46
48:CU:45:ALA:O	48:CU:49:LYS:HG2	2.14	0.46
52:DY:61:LYS:HD3	55:DA:372:G:H5''	1.98	0.46
29:DC:207:LYS:HB2	55:DA:729:G:C6	2.51	0.46
17:AQ:76:VAL:HG12	17:AQ:77:ARG:HG3	1.97	0.46
1:BA:310:G:H5''	16:BP:31:ARG:HB2	1.97	0.46
1:BA:438:U:H5'	4:BD:120:HIS:HB3	1.97	0.46
1:BA:376:G:H5''	16:BP:5:ARG:HB2	1.97	0.46
23:C2:22:THR:HG21	31:CA:2419:U:H5''	1.98	0.46
31:CA:948:C:H1'	31:CA:984:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:235:GLY:HA3	29:CC:239:ASN:HB2	1.97	0.46
35:CG:80:THR:CG2	35:CG:81:GLU:H	2.27	0.46
24:D3:4:THR:HA	55:DA:687:C:O4'	2.14	0.46
40:DM:60:ARG:HD2	55:DA:2360:G:H1'	1.98	0.46
1:AA:216:U:H2'	1:AA:217:C:C6	2.50	0.46
1:BA:1496:C:H2'	1:BA:1497:G:O4'	2.16	0.46
48:CU:67:VAL:HG22	48:CU:76:ARG:HG3	1.98	0.46
23:D2:10:LYS:HE3	23:D2:53:LYS:O	2.16	0.46
1:AA:1054:C:H5''	1:AA:1054:C:H6	1.80	0.46
1:AA:438:U:H5'	4:AD:120:HIS:HB3	1.98	0.46
5:AE:57:PRO:O	5:AE:60:ILE:HG13	2.15	0.46
18:BR:27:ALA:O	18:BR:30:LYS:HG2	2.16	0.46
31:CA:694:U:OP1	31:CA:1569:A:H1'	2.15	0.46
31:CA:833:A:H2'	31:CA:834:G:C8	2.51	0.46
55:DA:2070:A:H2'	55:DA:2071:A:O4'	2.16	0.46
55:DA:2800:A:C2	55:DA:2895:G:H1'	2.51	0.46
55:DA:722:A:H2'	55:DA:723:C:O4'	2.16	0.46
55:DA:871:U:H2'	55:DA:872:U:C6	2.51	0.46
5:AE:16:ILE:HD13	5:AE:137:VAL:HG11	1.97	0.45
1:BA:846:G:H2'	1:BA:847:G:C8	2.51	0.45
9:BI:7:TYR:HE1	9:BI:18:ARG:HB2	1.80	0.45
31:CA:594:U:H2'	31:CA:595:C:C6	2.51	0.45
22:D1:9:THR:CG2	55:DA:2020:A:H5'	2.46	0.45
36:DH:104:THR:HG22	36:DH:109:GLU:HA	1.97	0.45
30:CD:8:LYS:HB2	30:CD:201:LEU:HD11	1.97	0.45
41:CN:69:PRO:O	41:CN:93:VAL:O	2.34	0.45
55:DA:2086:U:H2'	55:DA:2087:G:C8	2.51	0.45
55:DA:2117:A:H61	55:DA:2171:A:H61	1.63	0.45
65:DA:3223:SPD:H82	70:DA:4260:HOH:O	2.16	0.45
29:DC:177:ARG:HG2	55:DA:1820:U:OP1	2.16	0.45
29:DC:235:GLY:HA3	29:DC:239:ASN:HB2	1.98	0.45
10:AJ:52:LEU:HB2	14:AN:81:ARG:HD2	1.99	0.45
1:BA:216:U:H2'	1:BA:217:C:C6	2.51	0.45
1:BA:411:A:P	4:BD:26:ARG:HH12	2.39	0.45
1:BA:1108:G:H5''	3:BC:176:HIS:CE1	2.52	0.45
31:CA:1326:U:H2'	31:CA:1327:A:H8	1.81	0.45
37:CJ:103:ARG:HA	37:CJ:106:LEU:HD12	1.96	0.45
43:CP:31:THR:HG22	43:CP:34:HIS:H	1.81	0.45
55:DA:2628:C:C5'	59:DA:3195:PUT:H12	2.42	0.45
33:DE:1:MET:HG2	33:DE:14:VAL:HG23	1.97	0.45
42:DO:9:GLN:O	42:DO:17:ARG:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:DX:37:ILE:HG21	51:DX:80:ILE:HG21	1.98	0.45
52:DY:7:VAL:HG23	52:DY:51:VAL:HG12	1.98	0.45
1:AA:845:A:H2'	1:AA:846:G:O4'	2.17	0.45
1:AA:923:A:OP1	5:AE:26:LYS:HG2	2.16	0.45
1:BA:1053:G:N7	1:BA:1200:C:H5''	2.32	0.45
2:BB:163:VAL:HG11	2:BB:173:ILE:HD11	1.99	0.45
31:CA:871:U:H2'	31:CA:872:U:C6	2.51	0.45
38:CK:69:ARG:O	38:CK:90:GLU:HB3	2.16	0.45
55:DA:1133:A:N3	59:DA:3212:PUT:H22	2.32	0.45
32:DD:152:PRO:HG3	32:DD:156:PHE:CZ	2.52	0.45
45:DR:58:ARG:HA	45:DR:61:TRP:CE3	2.51	0.45
1:AA:376:G:H5''	16:AP:5:ARG:HB2	1.98	0.45
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	1.97	0.45
31:CA:2296:U:H5	43:CP:9:ARG:NH2	2.14	0.45
27:D0:15:GLY:HA2	55:DA:969:G:O3'	2.16	0.45
55:DA:1509:A:HO2'	55:DA:1510:G:H8	1.64	0.45
33:DE:32:VAL:HG21	40:DM:6:LEU:HD13	1.99	0.45
2:AB:93:ASN:H	2:AB:93:ASN:HD22	1.65	0.45
1:BA:8:A:H1'	5:BE:108:GLY:HA2	1.97	0.45
31:CA:191:A:H2'	31:CA:192:C:C6	2.51	0.45
31:CA:722:A:H2'	31:CA:723:C:O4'	2.16	0.45
47:CT:84:ARG:HB2	47:CT:96:ILE:HB	1.99	0.45
48:CU:28:ASN:ND2	48:CU:91:GLN:HB3	2.14	0.45
35:DG:103:ILE:HD11	35:DG:117:LEU:HD21	1.99	0.45
1:BA:923:A:OP1	5:BE:26:LYS:HG2	2.17	0.45
31:CA:248:G:H5'	31:CA:250:G:N7	2.31	0.45
31:CA:2544:G:H5'	31:CA:2645:G:C2	2.51	0.45
31:CA:381:G:OP1	52:CY:18:ARG:HD3	2.16	0.45
31:CA:674:G:H1'	33:CE:69:ARG:HH11	1.82	0.45
45:CR:112:LYS:HD3	46:CS:48:LYS:HG3	1.99	0.45
55:DA:1168:G:H5''	55:DA:1168:G:H8	1.81	0.45
55:DA:136:G:H1	55:DA:143:C:H42	1.65	0.45
43:DP:35:ILE:HG21	43:DP:71:ALA:HA	1.98	0.45
44:DQ:52:ASN:O	44:DQ:53:ARG:HD3	2.16	0.45
4:AD:172:GLU:HG2	4:AD:183:LYS:HD2	1.99	0.45
8:AH:105:SER:HB2	8:AH:126:ILE:HD11	1.98	0.45
2:BB:93:ASN:H	2:BB:93:ASN:HD22	1.65	0.45
31:CA:1810:A:H2'	31:CA:1811:G:O4'	2.17	0.45
31:CA:1965:C:H5''	31:CA:1966:A:H2'	1.99	0.45
33:CE:176:ASP:OD2	33:CE:178:VAL:HG12	2.16	0.45
46:CS:49:ILE:HB	46:CS:51:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:2609:U:C5	63:DA:3194:EDO:H12	2.52	0.45
1:AA:202:G:H1	1:AA:215:C:H42	1.64	0.45
47:CT:72:THR:HG21	47:CT:108:SER:HB3	1.98	0.45
54:DI:70:GLU:HG2	54:DI:73:LYS:HE3	1.98	0.45
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.82	0.45
31:CA:1775:U:O4	31:CA:1789:A:H2	2.00	0.45
31:CA:278:A:N3	31:CA:278:A:H2'	2.32	0.45
31:CA:826:U:O2'	40:CM:53:GLY:HA3	2.17	0.45
25:C4:47:LYS:NZ	40:CM:64:PHE:CD1	2.75	0.45
24:D3:33:ARG:HG3	62:D3:102:PEG:H31	1.99	0.45
46:DS:8:GLY:HA2	55:DA:1161:C:O2'	2.17	0.45
55:DA:355:U:H2'	55:DA:356:G:H8	1.82	0.45
38:DK:7:LYS:O	38:DK:11:VAL:HG23	2.17	0.45
50:DW:38:LEU:HD21	50:DW:65:VAL:HG11	1.99	0.45
4:BD:172:GLU:HG2	4:BD:183:LYS:HD2	1.99	0.44
31:CA:320:A:H4'	31:CA:322:A:N7	2.32	0.44
31:CA:478:A:H61	31:CA:500:G:H4'	1.81	0.44
55:DA:1283:G:H1'	55:DA:1329:U:O2	2.17	0.44
55:DA:278:A:H2'	55:DA:278:A:N3	2.32	0.44
55:DA:1349:C:O2'	57:DA:3215:PG4:H82	2.16	0.44
55:DA:612:G:H2'	55:DA:614:A:C8	2.52	0.44
29:DC:199:GLU:O	29:DC:202:LEU:HB2	2.17	0.44
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.81	0.44
1:BA:957:U:O2	1:BA:959:A:H8	2.01	0.44
2:BB:68:LEU:HD11	2:BB:92:VAL:HG23	2.00	0.44
22:C1:16:ARG:HA	31:CA:2046:G:C5'	2.47	0.44
1:BA:1493:A:H1'	31:CA:1913:A:H61	1.82	0.44
55:DA:760:G:H4'	55:DA:1776:G:OP1	2.18	0.44
54:DI:132:TYR:H	54:DI:133:GLU:HB2	1.81	0.44
1:AA:957:U:O2	1:AA:959:A:H8	2.01	0.44
1:BA:1054:C:H6	1:BA:1054:C:H5''	1.83	0.44
6:BF:47:LEU:HD13	6:BF:51:ILE:HG12	1.99	0.44
31:CA:1556:C:H2'	31:CA:1557:C:C6	2.52	0.44
31:CA:2641:G:H5''	38:CK:78:THR:HB	1.99	0.44
31:CA:639:U:H2'	31:CA:640:C:C6	2.52	0.44
29:DC:212:ARG:HD2	29:DC:216:VAL:O	2.18	0.44
34:DF:16:LEU:HD13	34:DF:29:PRO:HD2	1.99	0.44
43:DP:31:THR:HG22	43:DP:34:HIS:H	1.80	0.44
1:AA:1053:G:N7	1:AA:1200:C:H5''	2.33	0.44
2:AB:68:LEU:HD11	2:AB:92:VAL:HG23	1.99	0.44
1:BA:1226:C:H2'	13:BM:102:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:73:C:O2'	1:BA:74:A:H8	1.97	0.44
24:C3:2:LYS:NZ	70:C3:101:HOH:O	2.49	0.44
31:CA:811:U:H2'	40:CM:21:ARG:HA	1.99	0.44
51:CX:37:ILE:HG21	51:CX:80:ILE:HG21	1.98	0.44
55:DA:1738:G:HO2'	55:DA:1739:A:H8	1.62	0.44
1:AA:864:A:H4'	5:AE:90:THR:HG23	2.00	0.44
1:AA:9:G:H5'	5:AE:108:GLY:HA3	1.99	0.44
9:AI:99:ARG:HG2	9:AI:104:VAL:HG21	1.99	0.44
13:AM:12:HIS:HB3	70:AM:302:HOH:O	2.17	0.44
11:BK:84:VAL:HG11	11:BK:97:ILE:HG12	2.00	0.44
14:BN:31:ILE:HG23	14:BN:42:TRP:CZ2	2.53	0.44
20:BT:58:VAL:HG13	20:BT:72:ALA:HB1	1.99	0.44
22:C1:53:LYS:HE3	22:C1:56:ALA:HA	1.99	0.44
25:C4:4:ILE:HG23	31:CA:666:A:O2'	2.17	0.44
31:CA:2489:U:HO2'	31:CA:2491:U:H5	1.64	0.44
31:CA:747:5MU:O2	31:CA:2014:A:H1'	2.18	0.44
31:CA:863:A:H2'	31:CA:864:G:C8	2.53	0.44
34:CF:16:LEU:HD13	34:CF:29:PRO:HD2	1.98	0.44
31:CA:2674:G:H4'	39:CL:30:ARG:HD2	2.00	0.44
50:CW:38:LEU:HD21	50:CW:65:VAL:HG11	1.98	0.44
55:DA:1321:A:C2	64:DA:3216:PGE:H12	2.53	0.44
29:DC:203:ARG:HH21	29:DC:205:LEU:HD21	1.82	0.44
33:DE:84:THR:HG21	55:DA:586:A:H5'	1.98	0.44
2:AB:129:LEU:H	2:AB:129:LEU:HG	1.51	0.44
43:CP:35:ILE:HG21	43:CP:71:ALA:HA	1.98	0.44
55:DA:639:U:H2'	55:DA:640:C:C6	2.53	0.44
29:DC:13:ARG:HD3	55:DA:728:G:H4'	2.00	0.44
8:AH:87:LYS:HB2	8:AH:125:ILE:CD1	2.41	0.44
13:AM:17:ILE:H	13:AM:17:ILE:HD12	1.83	0.44
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	2.00	0.44
25:C4:13:ARG:NH1	31:CA:250:G:P	2.91	0.44
31:CA:659:G:H4'	33:CE:95:LYS:HD3	1.99	0.44
36:CH:104:THR:HG22	36:CH:109:GLU:HA	1.98	0.44
55:DA:1831:G:H1'	64:DA:3224:PGE:H22	1.98	0.44
55:DA:493:G:H2'	55:DA:494:G:O4'	2.18	0.44
55:DA:62:U:H5'	58:DA:3203:MPD:H53	2.00	0.44
54:DI:85:VAL:HG21	54:DI:90:GLY:O	2.17	0.44
1:AA:1496:C:H2'	1:AA:1497:G:O4'	2.18	0.44
3:AC:21:THR:HG23	3:AC:58:GLU:HB3	1.99	0.44
11:AK:84:VAL:HG11	11:AK:97:ILE:HG12	1.99	0.44
1:BA:1060:U:H5	3:BC:2:GLY:HA3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C2:33:LYS:HA	23:C2:52:ALA:HB3	2.00	0.44
31:CA:2051:A:H5'	31:CA:2578:G:O4'	2.18	0.44
29:CC:199:GLU:O	29:CC:202:LEU:HB2	2.18	0.44
38:CK:7:LYS:O	38:CK:11:VAL:HG23	2.17	0.44
37:DJ:11:LEU:HD22	37:DJ:24:VAL:HG23	2.00	0.44
20:BT:5:LYS:HB3	20:BT:7:ALA:H	1.82	0.44
31:CA:1469:A:H2'	31:CA:1470:A:C8	2.53	0.44
24:C3:7:PRO:HG3	31:CA:1612:C:H5'	2.00	0.44
31:CA:528:A:C8	31:CA:528:A:C3'	3.00	0.44
31:CA:95:A:H4'	53:CZ:38:GLN:O	2.18	0.44
29:CC:212:ARG:HD2	29:CC:216:VAL:O	2.18	0.44
31:CA:1808:A:N1	52:CY:28:ARG:HD2	2.33	0.44
46:DS:41:ILE:HD13	46:DS:103:ALA:HA	1.99	0.44
49:DV:94:ARG:HB3	49:DV:103:ILE:HD12	1.99	0.44
17:AQ:8:LEU:HD13	17:AQ:25:ILE:HG13	1.99	0.43
4:BD:85:ASN:HA	5:BE:102:GLY:CA	2.31	0.43
14:BN:10:GLU:HG3	14:BN:63:ARG:HD2	2.00	0.43
31:CA:1274:A:N3	31:CA:1297:C:H1'	2.33	0.43
31:CA:1991:U:H2'	31:CA:1992:G:H5''	2.00	0.43
30:CD:13:ARG:HD3	30:CD:21:SER:OG	2.18	0.43
45:CR:113:ALA:O	45:CR:117:LEU:HD12	2.18	0.43
50:CW:51:GLN:HG2	50:CW:86:LEU:HD11	2.00	0.43
41:DN:42:THR:HG22	41:DN:93:VAL:HG12	1.99	0.43
1:AA:1060:U:H4'	10:AJ:53:ILE:HG23	2.00	0.43
14:AN:46:LEU:HA	14:AN:49:GLN:HE21	1.83	0.43
14:AN:10:GLU:HG3	14:AN:63:ARG:HD2	2.00	0.43
16:BP:20:VAL:CG1	16:BP:32:PHE:HB2	2.47	0.43
31:CA:355:U:H2'	31:CA:356:G:H8	1.83	0.43
34:CF:5:HIS:HB2	34:CF:97:TRP:CD1	2.53	0.43
55:DA:1394:U:H4'	55:DA:1603:A:H4'	2.00	0.43
2:AB:163:VAL:HG11	2:AB:173:ILE:HD11	2.00	0.43
2:AB:70:VAL:HB	2:AB:163:VAL:HG22	2.00	0.43
1:BA:1060:U:H4'	10:BJ:53:ILE:HG23	2.00	0.43
1:BA:10:A:OP2	5:BE:131:THR:HG21	2.18	0.43
6:BF:70:VAL:HA	6:BF:73:GLU:HG2	2.00	0.43
10:BJ:52:LEU:HB2	14:BN:81:ARG:HD2	2.00	0.43
31:CA:2623:G:H4'	31:CA:2825:G:C8	2.53	0.43
31:CA:2688:G:H1'	31:CA:2721:A:N6	2.34	0.43
31:CA:532:A:H4'	31:CA:533:G:C8	2.54	0.43
35:CG:17:VAL:HG11	35:CG:50:LEU:HD21	2.00	0.43
1:AA:604:G:H2'	1:AA:605:U:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AL:31:ARG:O	12:AL:58:THR:HG23	2.18	0.43
1:AA:1226:C:H2'	13:AM:102:THR:HB	2.00	0.43
1:BA:1277:C:HO2'	1:BA:1279:G:H8	1.62	0.43
22:D1:53:LYS:HE3	22:D1:56:ALA:HA	2.00	0.43
55:DA:1424:G:H21	64:DA:3213:PGE:H32	1.84	0.43
55:DA:142:A:H2'	55:DA:143:C:C6	2.53	0.43
55:DA:2031:A:C6	55:DA:2498:OMC:H1'	2.53	0.43
34:DF:80:ARG:HB3	34:DF:83:TYR:CE1	2.53	0.43
34:DF:5:HIS:HB2	34:DF:97:TRP:CD1	2.54	0.43
17:AQ:15:ASP:HA	17:AQ:21:ILE:HG22	1.99	0.43
20:AT:44:LYS:H	20:AT:44:LYS:HG3	1.61	0.43
11:BK:24:HIS:HB3	11:BK:31:ILE:HG23	2.00	0.43
13:BM:54:ASP:HA	13:BM:57:ARG:HD2	2.00	0.43
17:BQ:46:VAL:HG11	17:BQ:61:ILE:CG2	2.48	0.43
31:CA:96:C:H4'	53:CZ:41:HIS:CG	2.53	0.43
30:CD:121:THR:HB	30:CD:127:PHE:CD2	2.54	0.43
37:CJ:11:LEU:HD22	37:CJ:24:VAL:HG23	2.00	0.43
39:CL:103:VAL:O	39:CL:122:VAL:HB	2.18	0.43
31:CA:1030:C:OP2	41:CN:127:LYS:HE3	2.19	0.43
42:CO:71:ARG:HG3	42:CO:71:ARG:O	2.19	0.43
49:CV:94:ARG:HB3	49:CV:103:ILE:HD12	1.99	0.43
54:DI:56:ARG:HA	55:DA:1107:G:OP1	2.19	0.43
10:AJ:10:LEU:HB2	10:AJ:72:ARG:HB2	2.00	0.43
3:BC:23:PHE:CD2	10:BJ:97:ASP:HB2	2.54	0.43
8:BH:105:SER:HB2	8:BH:126:ILE:HD11	1.99	0.43
31:CA:142:A:H2'	31:CA:143:C:C6	2.53	0.43
29:CC:225:MET:O	29:CC:233:GLY:O	2.36	0.43
39:CL:113:MET:O	39:CL:116:ILE:HG13	2.18	0.43
31:CA:309:A:O3'	49:CV:16:GLY:HA2	2.18	0.43
55:DA:1028:A:N6	55:DA:1125:G:H2'	2.33	0.43
55:DA:191:A:H2'	55:DA:192:C:C6	2.53	0.43
25:D4:13:ARG:HH11	55:DA:2394:C:H5'	1.82	0.43
55:DA:2849:U:H4'	55:DA:2868:A:C2	2.54	0.43
55:DA:5:A:H2'	55:DA:6:A:C8	2.53	0.43
54:DI:50:VAL:HG22	54:DI:85:VAL:HG13	2.00	0.43
46:DS:44:GLY:O	46:DS:45:GLU:HG2	2.17	0.43
1:BA:502:A:H2'	1:BA:503:C:O4'	2.19	0.43
31:CA:2728:U:O2'	31:CA:2729:G:H8	2.01	0.43
31:CA:493:G:H2'	31:CA:494:G:O4'	2.18	0.43
31:CA:528:A:C2	31:CA:2042:A:H2'	2.54	0.43
55:DA:523:C:H4'	55:DA:540:C:O2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DI:27:VAL:HG13	54:DI:80:THR:HG23	2.00	0.43
45:DR:51:ARG:HH22	55:DA:993:G:P	2.41	0.43
48:DU:33:LYS:HG3	48:DU:80:TRP:CE3	2.53	0.43
3:AC:7:PRO:HD2	3:AC:184:TYR:CD1	2.54	0.43
1:BA:1493:A:H8	1:BA:1493:A:OP2	2.01	0.43
4:BD:105:MET:SD	4:BD:143:VAL:HG22	2.59	0.43
26:C5:17:VAL:HG12	26:C5:26:ILE:HD12	2.01	0.43
31:CA:2636:C:H2'	31:CA:2637:U:C6	2.54	0.43
31:CA:685:A:H5''	31:CA:774:G:O6	2.19	0.43
40:CM:95:LEU:HD22	40:CM:100:ILE:HG12	2.00	0.43
42:CO:9:GLN:O	42:CO:17:ARG:HD3	2.17	0.43
46:CS:3:ALA:HB3	46:CS:101:ILE:HD12	2.01	0.43
55:DA:1654:A:H1'	55:DA:2823:A:H5'	2.00	0.43
34:DF:36:LEU:HD22	34:DF:154:ILE:HG12	2.01	0.43
38:DK:23:LYS:HE2	38:DK:142:ILE:OXT	2.19	0.43
6:AF:70:VAL:HA	6:AF:73:GLU:HG2	2.00	0.43
8:AH:66:PHE:CD2	8:AH:67:GLN:HG2	2.54	0.43
5:BE:40:GLY:HA2	5:BE:45:ARG:O	2.19	0.43
5:BE:88:VAL:HG12	5:BE:93:ARG:HG2	2.00	0.43
1:BA:1152:A:H5'	10:BJ:15:HIS:HB2	2.01	0.43
13:BM:90:ARG:HH21	13:BM:95:LEU:HB3	1.84	0.43
27:C0:53:PHE:CG	28:CB:83:G:H4'	2.54	0.43
31:CA:1168:G:H5''	31:CA:1168:G:H8	1.83	0.43
31:CA:83:A:H2	31:CA:103:A:N7	2.17	0.43
46:DS:83:TYR:CE1	55:DA:1187:G:H5''	2.54	0.43
55:DA:2233:U:H2'	55:DA:2234:G:C8	2.54	0.43
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.54	0.43
1:AA:1376:U:H2'	1:AA:1377:A:C8	2.54	0.43
1:AA:892:A:O2'	1:AA:1415:G:H4'	2.19	0.43
31:CA:1936:A:N6	31:CA:1963:U:H3	2.16	0.43
31:CA:35:G:H2'	31:CA:36:G:O4'	2.19	0.43
30:CD:13:ARG:HH11	44:CQ:56:HIS:HA	1.84	0.43
31:CA:2642:G:H5'	38:CK:80:HIS:CG	2.53	0.43
62:DA:3200:PEG:H32	70:DA:3804:HOH:O	2.18	0.43
32:DD:121:THR:HB	32:DD:127:PHE:CD2	2.54	0.43
35:DG:17:VAL:HG11	35:DG:50:LEU:HD21	2.00	0.43
54:DI:26:VAL:HB	54:DI:83:ALA:HB3	2.01	0.43
41:DN:21:ALA:HB1	41:DN:100:LYS:HG2	2.00	0.43
46:DS:10:LYS:HE3	57:DS:202:PG4:H21	2.00	0.43
50:DW:51:GLN:HG2	50:DW:86:LEU:HD11	2.01	0.43
3:AC:151:VAL:HG12	3:AC:200:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:104:TRP:O	2:BB:108:ARG:HB2	2.19	0.42
9:BI:99:ARG:HG2	9:BI:104:VAL:HG21	2.00	0.42
31:CA:2106:U:H2'	31:CA:2107:G:H8	1.84	0.42
29:CC:105:LEU:H	29:CC:105:LEU:HD12	1.84	0.42
35:CG:103:ILE:HD11	35:CG:117:LEU:HD21	2.01	0.42
24:D3:29:GLN:HG2	62:D3:102:PEG:H21	2.01	0.42
55:DA:1101:U:H2'	55:DA:1102:C:C6	2.54	0.42
55:DA:2326:C:H3'	70:DA:7772:HOH:O	2.18	0.42
1:AA:619:U:C2	4:AD:132:ILE:HD11	2.54	0.42
1:BA:978:A:O2'	1:BA:1322:C:H5	2.00	0.42
5:BE:81:LEU:HB3	5:BE:147:MET:SD	2.58	0.42
12:BL:80:ILE:HD12	12:BL:97:THR:HG22	2.01	0.42
22:C1:4:GLN:CB	31:CA:2615:U:H1'	2.50	0.42
31:CA:136:G:H1	31:CA:143:C:H42	1.65	0.42
31:CA:2815:C:H2'	31:CA:2816:G:O4'	2.19	0.42
38:CK:23:LYS:HE3	38:CK:142:ILE:OXT	2.20	0.42
55:DA:1510:G:H2'	55:DA:1511:G:O4'	2.18	0.42
55:DA:2051:A:H5'	55:DA:2578:G:O4'	2.19	0.42
55:DA:2636:C:H2'	55:DA:2637:U:C6	2.53	0.42
32:DD:13:ARG:HD3	32:DD:21:SER:OG	2.18	0.42
50:DW:26:PHE:CE2	50:DW:44:HIS:HA	2.54	0.42
8:AH:94:LYS:HB3	8:AH:117:ARG:HH22	1.84	0.42
5:BE:74:VAL:HG11	5:BE:144:LEU:HB3	2.01	0.42
34:CF:36:LEU:HD12	34:CF:154:ILE:HG12	2.01	0.42
48:CU:33:LYS:HG3	48:CU:80:TRP:CE3	2.55	0.42
50:CW:26:PHE:CE1	50:CW:44:HIS:HA	2.54	0.42
22:D1:54:VAL:HG23	22:D1:55:ILE:HG12	2.00	0.42
55:DA:1654:A:C1'	55:DA:2823:A:H5'	2.50	0.42
55:DA:1932:A:H2'	55:DA:1933:G:O4'	2.19	0.42
33:DE:48:THR:HG23	33:DE:88:ARG:HH12	1.82	0.42
42:DO:8:ARG:HD3	55:DA:1652:A:OP1	2.18	0.42
1:BA:864:A:H4'	5:BE:90:THR:HG23	2.01	0.42
2:BB:70:VAL:HB	2:BB:163:VAL:HG22	2.00	0.42
3:BC:47:LEU:HD22	3:BC:76:VAL:HG22	2.00	0.42
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	2.01	0.42
31:CA:2869:G:H2'	31:CA:2870:C:O4'	2.19	0.42
31:CA:822:G:O6	31:CA:943:A:H2	2.01	0.42
46:CS:41:ILE:HD13	46:CS:103:ALA:HA	2.00	0.42
55:DA:189:G:N7	63:DA:3197:EDO:H21	2.35	0.42
32:DD:167:ASN:O	64:DD:301:PGE:H52	2.20	0.42
1:BA:49:U:O2	1:BA:362:G:H1'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:604:G:H2'	1:BA:605:U:O4'	2.20	0.42
31:CA:1028:A:N6	31:CA:1125:G:H2'	2.34	0.42
31:CA:1430:G:H2'	31:CA:1431:A:O4'	2.19	0.42
31:CA:2060:A:H62	33:CE:69:ARG:NH2	2.18	0.42
39:CL:121:GLU:HG2	39:CL:122:VAL:HG23	2.02	0.42
1:AA:1305:G:HO2'	1:AA:1306:A:H8	1.65	0.42
3:AC:47:LEU:HD22	3:AC:76:VAL:HG22	2.01	0.42
5:AE:132:ASN:OD1	5:AE:134:ILE:HG22	2.20	0.42
2:BB:129:LEU:H	2:BB:129:LEU:HG	1.53	0.42
10:BJ:10:LEU:HB2	10:BJ:72:ARG:HB2	2.00	0.42
11:BK:25:ALA:HA	11:BK:30:THR:HG22	2.01	0.42
13:BM:17:ILE:HD12	13:BM:17:ILE:H	1.84	0.42
13:BM:11:ASP:HA	13:BM:45:ILE:HD13	2.01	0.42
38:CK:81:ILE:HG23	38:CK:82:GLY:N	2.35	0.42
25:D4:47:LYS:HE3	40:DM:64:PHE:CD1	2.55	0.42
55:DA:2445:2MG:HM21	55:DA:2449:H2U:O4	2.20	0.42
42:DO:67:PHE:O	42:DO:71:ARG:HD2	2.20	0.42
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.55	0.42
22:C1:15:MET:O	31:CA:2045:C:O2'	2.31	0.42
27:C0:31:ARG:HD3	31:CA:1158:C:H5''	2.02	0.42
31:CA:1510:G:H2'	31:CA:1511:G:O4'	2.20	0.42
31:CA:2800:A:C2	31:CA:2895:G:H1'	2.54	0.42
31:CA:686:U:H2'	31:CA:788:A:N1	2.34	0.42
29:CC:57:GLY:HA2	29:CC:213:TRP:HA	2.01	0.42
34:CF:138:PHE:HE1	34:CF:152:LEU:HD21	1.85	0.42
28:CB:55:U:H1'	34:CF:26:MET:HG3	2.01	0.42
55:DA:355:U:H2'	55:DA:356:G:C8	2.55	0.42
29:DC:225:MET:O	29:DC:233:GLY:O	2.38	0.42
49:DV:51:ALA:O	49:DV:52:LEU:HB2	2.19	0.42
1:AA:502:A:H2'	1:AA:503:C:O4'	2.19	0.42
5:AE:77:ASN:HB2	5:AE:82:GLN:HE21	1.74	0.42
20:AT:36:TYR:CE2	20:AT:79:LEU:HD21	2.55	0.42
1:BA:1322:C:O2	1:BA:1322:C:OP1	2.37	0.42
5:BE:157:ARG:HG2	5:BE:158:GLY:N	2.35	0.42
31:CA:2305:U:H5''	34:CF:131:GLY:HA3	2.02	0.42
36:CH:68:ARG:HB3	36:CH:134:VAL:HG21	2.02	0.42
47:CT:20:VAL:HG11	47:CT:44:ALA:HA	2.02	0.42
50:CW:86:LEU:HD13	50:CW:89:ILE:HD11	2.01	0.42
55:DA:825:A:H5''	59:DA:3222:PUT:H12	2.02	0.42
55:DA:984:A:N3	55:DA:984:A:H2'	2.34	0.42
2:AB:104:TRP:O	2:AB:108:ARG:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AD:105:MET:SD	4:AD:143:VAL:HG22	2.60	0.42
1:AA:1322:C:P	19:AS:78:ARG:HH22	2.43	0.42
1:BA:1530:G:H2'	1:BA:1531:A:C8	2.55	0.42
25:C4:26:HIS:HD1	31:CA:2361:G:P	2.43	0.42
31:CA:796:C:H2'	31:CA:797:G:C8	2.54	0.42
36:CH:82:SER:HB2	36:CH:94:ILE:HD11	2.02	0.42
41:CN:41:LEU:HD21	41:CN:124:LEU:HD22	2.02	0.42
24:D3:2:LYS:HE2	55:DA:687:C:H5''	2.02	0.42
55:DA:1555:G:OP1	59:DA:3218:PUT:H41	2.20	0.42
55:DA:1794:A:H2'	55:DA:1795:C:C6	2.54	0.42
55:DA:747:5MU:O2	55:DA:2014:A:H1'	2.20	0.42
47:DT:6:LYS:HB2	55:DA:494:G:H4'	2.01	0.42
40:DM:109:LYS:HG2	40:DM:126:ARG:HB2	2.02	0.42
1:AA:1298:U:H3	7:AG:114:LYS:HA	1.85	0.42
1:AA:1152:A:H5'	10:AJ:15:HIS:HB2	2.02	0.42
11:AK:25:ALA:HA	11:AK:30:THR:HG22	2.02	0.42
5:BE:115:LEU:HG	5:BE:123:VAL:HG21	2.01	0.42
31:CA:1101:U:H2'	31:CA:1102:C:C6	2.54	0.42
33:CE:178:VAL:HG23	40:CM:3:LEU:HD21	2.02	0.42
50:CW:26:PHE:HE1	50:CW:44:HIS:HA	1.85	0.42
55:DA:2406:A:H5'	55:DA:2406:A:C8	2.55	0.42
55:DA:320:A:H4'	55:DA:322:A:N7	2.35	0.42
32:DD:13:ARG:HH11	44:DQ:56:HIS:HA	1.85	0.42
38:DK:7:LYS:HG2	55:DA:538:A:H4'	2.02	0.42
7:AG:72:THR:HG22	7:AG:142:HIS:CE1	2.55	0.41
1:BA:1048:G:H4'	14:BN:3:LYS:HE2	2.02	0.41
31:CA:2074:U:H2'	31:CA:2075:U:C6	2.55	0.41
31:CA:2425:A:H4'	31:CA:2426:A:O5'	2.20	0.41
24:C3:16:HIS:CD2	31:CA:464:U:O2'	2.73	0.41
25:D4:39:LYS:O	25:D4:43:HIS:HD2	2.03	0.41
3:AC:156:ARG:HD3	3:AC:193:TYR:O	2.20	0.41
19:AS:30:PRO:HB2	19:AS:50:ALA:HB2	2.03	0.41
11:BK:45:ALA:HB3	11:BK:70:CYS:HB2	2.02	0.41
44:CQ:52:ASN:O	44:CQ:53:ARG:HD3	2.20	0.41
48:CU:82:LYS:HD3	48:CU:84:TYR:CE1	2.55	0.41
55:DA:136:G:H1	55:DA:143:C:N4	2.18	0.41
25:D4:8:ARG:HG3	55:DA:253:C:N4	2.36	0.41
1:AA:1108:G:H5''	3:AC:176:HIS:ND1	2.36	0.41
1:AA:131:A:H2'	1:AA:132:C:C6	2.56	0.41
1:AA:302:G:O2'	1:AA:556:C:H5''	2.20	0.41
1:AA:1048:G:H4'	14:AN:3:LYS:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BN:31:ILE:HG23	14:BN:42:TRP:HZ2	1.85	0.41
20:BT:67:ILE:O	20:BT:68:HIS:HB2	2.20	0.41
31:CA:136:G:H1	31:CA:143:C:N4	2.19	0.41
31:CA:2339:C:H2'	31:CA:2340:A:C8	2.56	0.41
55:DA:1430:G:H2'	55:DA:1431:A:O4'	2.20	0.41
55:DA:686:U:H2'	55:DA:788:A:N1	2.35	0.41
32:DD:26:VAL:HG21	44:DQ:5:ILE:HG12	2.02	0.41
5:BE:23:LYS:HB3	5:BE:30:ILE:HG23	2.02	0.41
29:CC:221:ARG:NH1	31:CA:1789:A:OP2	2.53	0.41
31:CA:1794:A:H2'	31:CA:1795:C:C6	2.56	0.41
31:CA:2043:C:C6	31:CA:2043:C:H5''	2.55	0.41
31:CA:2106:U:H2'	31:CA:2107:G:C8	2.55	0.41
31:CA:355:U:H2'	31:CA:356:G:C8	2.56	0.41
31:CA:742:A:H2'	31:CA:743:A:C8	2.55	0.41
40:CM:123:ARG:HG3	40:CM:143:GLU:HG3	2.03	0.41
41:CN:71:LYS:HB3	41:CN:93:VAL:O	2.21	0.41
55:DA:1202:G:H1'	58:DA:3192:MPD:HM1	2.02	0.41
55:DA:1418:G:H2'	55:DA:1579:A:N6	2.35	0.41
54:DI:94:ARG:HG2	54:DI:127:ALA:HA	2.02	0.41
1:BA:131:A:H2'	1:BA:132:C:C6	2.56	0.41
1:BA:429:U:H1'	1:BA:430:A:H5''	2.03	0.41
4:BD:130:VAL:HG11	4:BD:135:TYR:CG	2.55	0.41
11:BK:20:VAL:HB	11:BK:35:THR:HG23	2.02	0.41
31:CA:2114:A:N6	31:CA:2119:A:H62	2.18	0.41
27:C0:14:ILE:HG21	31:CA:988:A:C6	2.56	0.41
55:DA:1417:C:H5'	55:DA:1588:G:H1'	2.01	0.41
55:DA:602:A:C6	58:DA:3190:MPD:H31	2.56	0.41
55:DA:792:A:N3	55:DA:2072:C:O2'	2.48	0.41
36:DH:82:SER:HB2	36:DH:94:ILE:HD11	2.02	0.41
47:DT:20:VAL:HG11	47:DT:44:ALA:HA	2.03	0.41
1:AA:1343:G:O2'	9:AI:123:ARG:HD2	2.20	0.41
1:AA:429:U:H1'	1:AA:430:A:H5''	2.02	0.41
13:AM:54:ASP:HA	13:AM:57:ARG:HD2	2.02	0.41
1:BA:1298:U:H3	7:BG:114:LYS:HA	1.86	0.41
14:BN:53:ARG:HH21	19:BS:37:ARG:HH22	1.69	0.41
31:CA:2788:C:H2'	31:CA:2789:C:C6	2.55	0.41
29:CC:174:LEU:CD2	29:CC:184:VAL:HB	2.50	0.41
47:CT:29:VAL:HG22	47:CT:51:LEU:HD11	2.02	0.41
55:DA:2128:G:H1	55:DA:2160:C:N4	2.18	0.41
55:DA:2324:U:H3'	55:DA:2325:G:H5''	2.03	0.41
52:DY:29:PHE:HB3	55:DA:396:G:H1'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:439:U:H5''	4:AD:121:LYS:HD2	2.02	0.41
4:AD:170:TRP:CD2	4:AD:186:PRO:HB3	2.56	0.41
6:AF:102:MET:CE	18:AR:24:LYS:HB3	2.50	0.41
12:BL:87:VAL:HG11	12:BL:90:LEU:HD22	2.02	0.41
20:BT:44:LYS:HB3	20:BT:87:ALA:HB2	2.03	0.41
31:CA:2095:A:H5''	31:CA:2095:A:C8	2.54	0.41
30:CD:141:ARG:HB2	31:CA:1656:C:H5''	2.01	0.41
42:CO:95:THR:HG21	42:CO:113:ILE:HD11	2.02	0.41
47:CT:69:LEU:HG	47:CT:107:VAL:CG2	2.51	0.41
55:DA:138:U:H5'	55:DA:139:U:H5'	2.03	0.41
55:DA:2038:G:H2'	55:DA:2039:U:O4'	2.21	0.41
51:DX:41[B]:ARG:HA	51:DX:41[B]:ARG:HD3	1.94	0.41
9:AI:19:VAL:HG11	9:AI:83:ILE:HA	2.03	0.41
1:BA:1376:U:H2'	1:BA:1377:A:C8	2.55	0.41
4:BD:170:TRP:CD2	4:BD:186:PRO:HB3	2.56	0.41
5:BE:77:ASN:HB2	5:BE:82:GLN:HE21	1.79	0.41
5:BE:82:GLN:HG2	5:BE:149:SER:HA	2.01	0.41
19:BS:30:PRO:HB2	19:BS:50:ALA:HB2	2.02	0.41
31:CA:1722:A:N6	31:CA:1738:G:H1'	2.36	0.41
31:CA:2038:G:H2'	31:CA:2039:U:O4'	2.21	0.41
55:DA:1020:A:C2	55:DA:1141:U:C2	3.08	0.41
55:DA:1515:A:H2'	55:DA:1516:G:O4'	2.20	0.41
55:DA:2097:A:H8	55:DA:2097:A:H5''	1.85	0.41
25:D4:13:ARG:NH1	55:DA:2394:C:H5'	2.36	0.41
33:DE:23:PHE:HE2	33:DE:25:GLU:HG3	1.86	0.41
35:DG:140:VAL:O	35:DG:144:VAL:HG23	2.20	0.41
51:DX:38:VAL:HG12	51:DX:59:LEU:HB2	2.02	0.41
19:AS:5:LEU:HG	19:AS:5:LEU:H	1.75	0.41
1:BA:567:G:H2'	1:BA:568:G:O4'	2.20	0.41
9:BI:19:VAL:HG11	9:BI:83:ILE:HA	2.03	0.41
31:CA:547:A:H2'	31:CA:547:A:N3	2.36	0.41
29:CC:107:PRO:HD2	29:CC:110:LEU:HD22	2.03	0.41
33:DE:178:VAL:HG23	40:DM:3:LEU:HD21	2.01	0.41
36:DH:68:ARG:HB3	36:DH:134:VAL:HG21	2.03	0.41
5:AE:157:ARG:CD	8:AH:43:GLU:O	2.69	0.41
11:AK:20:VAL:HB	11:AK:35:THR:HG23	2.03	0.41
1:BA:216:U:H4'	1:BA:464:U:H4'	2.02	0.41
1:BA:841:C:H3'	1:BA:842:U:C4'	2.51	0.41
31:CA:1636:U:H2'	31:CA:1637:A:C8	2.55	0.41
31:CA:396:G:H1'	52:CY:29:PHE:HB3	2.01	0.41
54:DI:29:ASP:HB3	54:DI:106:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1141:C:O2'	1:AA:1142:G:H8	2.03	0.41
1:AA:831:A:H5''	2:AB:21:ARG:HD3	2.03	0.41
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.85	0.41
1:AA:1216:A:H5''	14:AN:5:SER:HB3	2.02	0.41
1:BA:439:U:H5''	4:BD:121:LYS:HD2	2.02	0.41
11:BK:34:ILE:HG12	11:BK:70:CYS:SG	2.60	0.41
20:BT:69:LYS:H	20:BT:69:LYS:HG3	1.60	0.41
31:CA:2335:A:OP1	43:CP:13:ARG:HD2	2.21	0.41
31:CA:29:U:O5'	31:CA:29:U:H6	2.02	0.41
37:CJ:49:ILE:HG13	37:CJ:55:ILE:HD13	2.03	0.41
55:DA:207:A:H2'	55:DA:208:C:O4'	2.20	0.41
55:DA:2133:G:H21	55:DA:2158:A:N6	2.18	0.41
55:DA:281:C:H2'	55:DA:282:A:C8	2.56	0.41
54:DI:23:LEU:HD13	54:DI:89:PRO:HD3	2.03	0.41
38:DK:9:GLU:HG2	70:DA:3412:HOH:O	2.21	0.41
40:DM:74:THR:HG23	40:DM:107:PHE:HB2	2.02	0.41
40:DM:123:ARG:HG3	40:DM:143:GLU:HG3	2.02	0.41
41:DN:89:VAL:CG1	58:DN:201:MPD:HM3	2.50	0.41
10:AJ:19:ASP:HA	10:AJ:22:THR:HB	2.03	0.40
1:BA:1108:G:H5''	3:BC:176:HIS:ND1	2.36	0.40
6:BF:22:ILE:HG23	6:BF:39:LEU:HD11	2.02	0.40
1:BA:718:A:H5'	11:BK:119:ASN:HB2	2.03	0.40
22:C1:49:TYR:OH	31:CA:2883:A:OP1	2.34	0.40
31:CA:780:G:H2'	31:CA:782:A:N7	2.36	0.40
35:CG:38:ASN:HD22	35:CG:40:ALA:HB3	1.86	0.40
22:D1:8:PRO:HD2	55:DA:1263:U:O2'	2.22	0.40
55:DA:1306:C:H5''	55:DA:1306:C:H6	1.85	0.40
55:DA:2273:A:H2'	55:DA:2274:A:C8	2.55	0.40
55:DA:839:U:H2'	55:DA:840:C:C6	2.56	0.40
35:DG:50:LEU:HD13	35:DG:72:LEU:HD23	2.02	0.40
54:DI:132:TYR:N	54:DI:133:GLU:HB2	2.35	0.40
37:DJ:14:ALA:HB3	37:DJ:17:MET:HB2	2.03	0.40
40:DM:77:ILE:CD1	40:DM:101:ILE:CG2	2.97	0.40
1:AA:568:G:O6	12:AL:2:ALA:HB2	2.21	0.40
1:AA:842:U:H5''	2:BB:115:LYS:HD3	2.03	0.40
10:BJ:59:LYS:HD2	10:BJ:60:ASP:OD1	2.21	0.40
55:DA:1532:A:H5''	55:DA:1532:A:H8	1.85	0.40
54:DI:120:ALA:HA	54:DI:123:ILE:HD11	2.03	0.40
54:DI:65:GLU:HA	54:DI:70:GLU:HG3	2.02	0.40
47:DT:84:ARG:HB2	47:DT:96:ILE:HB	2.02	0.40
1:AA:268:U:H2'	1:AA:269:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:31:ILE:HG12	11:AK:46:THR:CG2	2.51	0.40
14:AN:46:LEU:HD22	19:AS:13:LEU:HG	2.02	0.40
9:BI:116:VAL:HG21	10:BJ:62:ARG:HD3	2.04	0.40
1:BA:1322:C:P	19:BS:78:ARG:HH22	2.43	0.40
25:C4:52:LYS:HA	25:C4:55:LEU:HD12	2.03	0.40
31:CA:1418:G:H2'	31:CA:1579:A:N6	2.36	0.40
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.57	0.40
22:D1:12:LYS:HD2	22:D1:12:LYS:HA	1.86	0.40
39:DL:113:MET:O	39:DL:116:ILE:HG13	2.19	0.40
40:DM:95:LEU:HD11	40:DM:125:LEU:HD21	2.03	0.40
47:DT:72:THR:CG2	47:DT:108:SER:HB3	2.52	0.40
53:DZ:56:LEU:HA	53:DZ:59:GLU:HG2	2.04	0.40
1:AA:234:C:H4'	17:AQ:66:PRO:HG3	2.03	0.40
1:AA:567:G:H2'	1:AA:568:G:O4'	2.21	0.40
1:BA:268:U:H2'	1:BA:269:C:C6	2.56	0.40
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	2.04	0.40
31:CA:1306:C:H5''	31:CA:1306:C:H6	1.86	0.40
36:CH:126:GLY:H	36:CH:146:VAL:HB	1.87	0.40
31:CA:1131:G:OP1	38:CK:82:GLY:HA2	2.21	0.40
45:CR:58:ARG:HH11	45:CR:62:ILE:HD11	1.86	0.40
26:D5:32:LYS:HG2	55:DA:2478:A:H5'	2.03	0.40
55:DA:2788:C:H2'	55:DA:2789:C:C6	2.57	0.40
1:BA:580:C:H2'	1:BA:581:G:O4'	2.21	0.40
6:BF:78:PHE:HA	6:BF:84:VAL:HG11	2.04	0.40
12:BL:74:LEU:HD21	12:BL:80:ILE:HG21	2.03	0.40
31:CA:1101:U:H2'	31:CA:1102:C:H6	1.87	0.40
31:CA:2327:A:H2'	31:CA:2328:A:C8	2.57	0.40
24:C3:37:LYS:NZ	31:CA:469:G:O6	2.53	0.40
31:CA:644:A:H2'	31:CA:645:C:O4'	2.22	0.40
55:DA:2339:C:H2'	55:DA:2340:A:C8	2.57	0.40
37:DJ:49:ILE:HG13	37:DJ:55:ILE:HD13	2.03	0.40
49:DV:66:GLN:HG3	55:DA:328:U:O3'	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	210 (95%)	9 (4%)	3 (1%)	14	49
2	BB	222/224 (99%)	211 (95%)	7 (3%)	4 (2%)	11	42
3	AC	204/206 (99%)	192 (94%)	11 (5%)	1 (0%)	34	74
3	BC	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	19	58
4	AD	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
4	BD	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
5	AE	153/155 (99%)	147 (96%)	5 (3%)	1 (1%)	26	67
5	BE	148/155 (96%)	132 (89%)	12 (8%)	4 (3%)	6	29
6	AF	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
6	BF	98/106 (92%)	91 (93%)	5 (5%)	2 (2%)	9	38
7	AG	149/151 (99%)	137 (92%)	11 (7%)	1 (1%)	26	67
7	BG	149/151 (99%)	140 (94%)	9 (6%)	0	100	100
8	AH	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
8	BH	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
9	AI	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
9	BI	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
10	AJ	97/99 (98%)	88 (91%)	7 (7%)	2 (2%)	9	37
10	BJ	96/99 (97%)	77 (80%)	14 (15%)	5 (5%)	2	12
11	AK	115/117 (98%)	107 (93%)	6 (5%)	2 (2%)	11	43
11	BK	115/117 (98%)	104 (90%)	9 (8%)	2 (2%)	11	43
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
12	BL	120/123 (98%)	114 (95%)	5 (4%)	1 (1%)	24	64
13	AM	112/114 (98%)	103 (92%)	6 (5%)	3 (3%)	6	29
13	BM	112/114 (98%)	102 (91%)	5 (4%)	5 (4%)	3	15
14	AN	98/100 (98%)	88 (90%)	8 (8%)	2 (2%)	9	38
14	BN	98/100 (98%)	90 (92%)	6 (6%)	2 (2%)	9	38
15	AO	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
15	BO	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	16	53
16	AP	80/82 (98%)	74 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	BP	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	7	31
17	AQ	78/80 (98%)	70 (90%)	7 (9%)	1 (1%)	15	51
17	BQ	78/80 (98%)	68 (87%)	5 (6%)	5 (6%)	2	7
18	AR	53/55 (96%)	53 (100%)	0	0	100	100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	15	51
19	BS	77/79 (98%)	68 (88%)	7 (9%)	2 (3%)	7	30
20	AT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
20	BT	83/86 (96%)	79 (95%)	3 (4%)	1 (1%)	16	53
21	AU	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
21	BU	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
22	C1	54/56 (96%)	47 (87%)	4 (7%)	3 (6%)	2	11
22	D1	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	3	17
23	D2	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
24	C3	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	8	34
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	C4	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
25	D4	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
26	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	6	28
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	54 (96%)	0	2 (4%)	4	21
27	D0	57/58 (98%)	56 (98%)	1 (2%)	0	100	100
29	CC	269/272 (99%)	252 (94%)	12 (4%)	5 (2%)	10	40
29	DC	269/272 (99%)	257 (96%)	10 (4%)	2 (1%)	26	67
30	CD	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
32	DD	206/209 (99%)	202 (98%)	4 (2%)	0	100	100
33	CE	199/201 (99%)	191 (96%)	5 (2%)	3 (2%)	13	47
33	DE	199/201 (99%)	194 (98%)	4 (2%)	1 (0%)	34	74
34	CF	175/178 (98%)	168 (96%)	6 (3%)	1 (1%)	30	70
34	DF	175/178 (98%)	169 (97%)	5 (3%)	1 (1%)	30	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	CG	174/176 (99%)	162 (93%)	7 (4%)	5 (3%)	6	27
35	DG	174/176 (99%)	165 (95%)	8 (5%)	1 (1%)	30	70
36	CH	147/149 (99%)	136 (92%)	6 (4%)	5 (3%)	5	22
36	DH	147/149 (99%)	138 (94%)	6 (4%)	3 (2%)	9	38
37	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	5	26
37	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	5	26
38	CK	140/142 (99%)	135 (96%)	4 (3%)	1 (1%)	26	67
38	DK	140/142 (99%)	137 (98%)	2 (1%)	1 (1%)	26	67
39	CL	120/123 (98%)	112 (93%)	7 (6%)	1 (1%)	24	64
39	DL	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	24	64
40	CM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	9	37
40	DM	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
41	CN	133/136 (98%)	125 (94%)	7 (5%)	1 (1%)	24	64
41	DN	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
42	CO	118/125 (94%)	111 (94%)	5 (4%)	2 (2%)	11	43
42	DO	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
43	CP	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
43	DP	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
44	CQ	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
44	DQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	21	61
45	CR	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
45	DR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
46	CS	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	5	26
46	DS	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	19	58
47	CT	108/110 (98%)	101 (94%)	5 (5%)	2 (2%)	10	40
47	DT	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
48	CU	91/93 (98%)	86 (94%)	4 (4%)	1 (1%)	17	56
48	DU	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
49	CV	100/103 (97%)	91 (91%)	4 (4%)	5 (5%)	3	13
49	DV	100/103 (97%)	96 (96%)	2 (2%)	2 (2%)	9	38
50	CW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	DW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
51	CX	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
51	DX	75/76 (99%)	74 (99%)	1 (1%)	0	100	100
52	CY	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
52	DY	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
53	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11	43
53	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
54	DI	133/135 (98%)	114 (86%)	13 (10%)	6 (4%)	3	15
All	All	11407/11635 (98%)	10791 (95%)	485 (4%)	131 (1%)	17	56

All (131) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE
3	AC	156	ARG
13	AM	5	ALA
22	C1	25	VAL
2	BB	126	PHE
3	BC	156	ARG
5	BE	51	GLY
10	BJ	38	GLY
10	BJ	91	ASP
13	BM	7	ILE
16	BP	80	LYS
20	BT	5	LYS
29	CC	158	ALA
29	CC	197	ASN
33	CE	83	VAL
35	CG	119	ALA
35	CG	175	LYS
35	CG	176	LYS
36	CH	10	ALA
37	CJ	19	ASN
38	CK	81	ILE
39	CL	35	VAL
40	CM	29	LYS
41	CN	70	ASP
42	CO	118	ARG
48	CU	88	LYS

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Mol	Chain	Res	Type
49	CV	7	ARG
37	DJ	19	ASN
49	DV	52	LEU
10	AJ	57	VAL
13	AM	105	ASN
14	AN	38	ASP
17	AQ	82	ALA
22	C1	56	ALA
23	C2	5	ILE
23	C2	51	GLU
27	C0	4	THR
27	C0	14	ILE
3	BC	61	ALA
5	BE	110	ALA
6	BF	92	THR
6	BF	98	GLU
10	BJ	57	VAL
12	BL	44	LYS
13	BM	5	ALA
13	BM	105	ASN
13	BM	114	LYS
17	BQ	70	THR
17	BQ	82	ALA
19	BS	6	LYS
29	CC	233	GLY
29	CC	253	LYS
29	DC	233	GLY
29	DC	253	LYS
33	CE	82	GLY
35	CG	46	ALA
37	CJ	25	GLY
40	CM	69	ARG
49	CV	16	GLY
49	CV	17	LYS
35	DG	46	ALA
37	DJ	25	GLY
2	AB	125	THR
2	AB	127	ASP
7	AG	56	LYS
11	AK	54	GLY
11	AK	89	PRO
13	AM	7	ILE

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Mol	Chain	Res	Type
22	C1	26	THR
24	C3	45	SER
2	BB	125	THR
2	BB	127	ASP
5	BE	103	THR
10	BJ	95	GLY
11	BK	54	GLY
11	BK	89	PRO
14	BN	38	ASP
15	BO	88	ARG
17	BQ	17	MET
17	BQ	18	GLU
19	BS	5	LEU
29	CC	108	LYS
33	CE	6	LYS
36	CH	118	PRO
49	CV	89	ASP
33	DE	6	LYS
36	DH	118	PRO
39	DL	108	ARG
46	DS	44	GLY
49	DV	89	ASP
54	DI	70	GLU
54	DI	91	ALA
54	DI	109	LYS
54	DI	130	PRO
5	AE	162	GLU
5	BE	105	ILE
10	BJ	36	VAL
13	BM	4	ILE
36	CH	9	VAL
40	CM	30	THR
42	CO	119	SER
46	CS	55	ASP
47	CT	63	GLY
36	DH	11	ASN
54	DI	88	HIS
19	AS	6	LYS
2	BB	95	ARG
14	BN	22	ALA
36	CH	8	LYS
36	CH	122	LEU

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Mol	Chain	Res	Type
37	CJ	23	PRO
46	CS	48	LYS
46	CS	53	PHE
36	DH	122	LEU
37	DJ	23	PRO
44	DQ	105	GLY
54	DI	108	VAL
14	AN	22	ALA
16	BP	44	SER
35	CG	45	HIS
47	CT	65	ASP
49	CV	52	LEU
53	CZ	62	GLY
38	DK	83	GLY
26	C5	21	GLY
34	CF	62	GLY
37	CJ	32	GLY
34	DF	62	GLY
37	DJ	32	GLY
17	BQ	35	GLY
10	AJ	33	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%)	173 (93%)	13 (7%)	19	53
2	BB	186/186 (100%)	173 (93%)	13 (7%)	19	53
3	AC	170/170 (100%)	159 (94%)	11 (6%)	21	56
3	BC	170/170 (100%)	156 (92%)	14 (8%)	14	44
4	AD	172/172 (100%)	162 (94%)	10 (6%)	25	62
4	BD	172/172 (100%)	160 (93%)	12 (7%)	19	53
5	AE	118/118 (100%)	107 (91%)	11 (9%)	11	37
5	BE	113/118 (96%)	95 (84%)	18 (16%)	3	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AF	92/92 (100%)	86 (94%)	6 (6%)	21	56
6	BF	87/92 (95%)	77 (88%)	10 (12%)	7	26
7	AG	124/124 (100%)	115 (93%)	9 (7%)	17	50
7	BG	124/124 (100%)	109 (88%)	15 (12%)	6	23
8	AH	104/104 (100%)	93 (89%)	11 (11%)	8	29
8	BH	104/104 (100%)	93 (89%)	11 (11%)	8	29
9	AI	105/105 (100%)	100 (95%)	5 (5%)	31	69
9	BI	105/105 (100%)	100 (95%)	5 (5%)	31	69
10	AJ	87/87 (100%)	81 (93%)	6 (7%)	19	54
10	BJ	86/87 (99%)	78 (91%)	8 (9%)	11	37
11	AK	90/90 (100%)	87 (97%)	3 (3%)	45	80
11	BK	90/90 (100%)	83 (92%)	7 (8%)	16	46
12	AL	102/102 (100%)	92 (90%)	10 (10%)	10	34
12	BL	102/102 (100%)	90 (88%)	12 (12%)	6	24
13	AM	92/92 (100%)	83 (90%)	9 (10%)	10	34
13	BM	92/92 (100%)	85 (92%)	7 (8%)	16	48
14	AN	83/83 (100%)	82 (99%)	1 (1%)	78	93
14	BN	83/83 (100%)	82 (99%)	1 (1%)	78	93
15	AO	76/76 (100%)	71 (93%)	5 (7%)	21	55
15	BO	76/76 (100%)	65 (86%)	11 (14%)	4	16
16	AP	65/65 (100%)	64 (98%)	1 (2%)	72	91
16	BP	65/65 (100%)	63 (97%)	2 (3%)	47	81
17	AQ	74/74 (100%)	67 (90%)	7 (10%)	11	36
17	BQ	74/74 (100%)	66 (89%)	8 (11%)	8	28
18	AR	48/48 (100%)	47 (98%)	1 (2%)	61	88
18	BR	48/48 (100%)	47 (98%)	1 (2%)	61	88
19	AS	70/70 (100%)	63 (90%)	7 (10%)	9	32
19	BS	70/70 (100%)	65 (93%)	5 (7%)	18	52
20	AT	65/65 (100%)	59 (91%)	6 (9%)	11	37
20	BT	65/65 (100%)	55 (85%)	10 (15%)	3	14
21	AU	48/48 (100%)	44 (92%)	4 (8%)	14	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	BU	48/48 (100%)	44 (92%)	4 (8%)	14	43
22	C1	47/47 (100%)	45 (96%)	2 (4%)	35	73
22	D1	47/47 (100%)	44 (94%)	3 (6%)	22	57
23	C2	45/46 (98%)	44 (98%)	1 (2%)	60	87
23	D2	45/46 (98%)	43 (96%)	2 (4%)	35	72
24	C3	38/38 (100%)	37 (97%)	1 (3%)	54	84
24	D3	38/38 (100%)	37 (97%)	1 (3%)	54	84
25	C4	51/51 (100%)	48 (94%)	3 (6%)	24	61
25	D4	51/51 (100%)	48 (94%)	3 (6%)	24	61
26	C5	34/34 (100%)	32 (94%)	2 (6%)	24	61
26	D5	34/34 (100%)	34 (100%)	0	100	100
27	C0	48/48 (100%)	45 (94%)	3 (6%)	22	58
27	D0	49/48 (102%)	45 (92%)	4 (8%)	14	44
29	CC	216/217 (100%)	202 (94%)	14 (6%)	21	56
29	DC	216/217 (100%)	210 (97%)	6 (3%)	51	83
30	CD	164/164 (100%)	160 (98%)	4 (2%)	57	86
32	DD	163/163 (100%)	160 (98%)	3 (2%)	66	89
33	CE	165/165 (100%)	152 (92%)	13 (8%)	15	46
33	DE	165/165 (100%)	161 (98%)	4 (2%)	57	86
34	CF	148/149 (99%)	133 (90%)	15 (10%)	9	32
34	DF	148/149 (99%)	137 (93%)	11 (7%)	17	49
35	CG	137/137 (100%)	134 (98%)	3 (2%)	60	87
35	DG	137/137 (100%)	132 (96%)	5 (4%)	42	78
36	CH	114/114 (100%)	101 (89%)	13 (11%)	7	26
36	DH	114/114 (100%)	101 (89%)	13 (11%)	7	26
37	CJ	104/104 (100%)	100 (96%)	4 (4%)	40	76
37	DJ	104/104 (100%)	100 (96%)	4 (4%)	40	76
38	CK	116/116 (100%)	110 (95%)	6 (5%)	29	66
38	DK	116/116 (100%)	114 (98%)	2 (2%)	68	90
39	CL	103/104 (99%)	99 (96%)	4 (4%)	39	75
39	DL	104/104 (100%)	99 (95%)	5 (5%)	31	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	CM	103/103 (100%)	97 (94%)	6 (6%)	25	62
40	DM	103/103 (100%)	99 (96%)	4 (4%)	39	75
41	CN	108/108 (100%)	104 (96%)	4 (4%)	41	77
41	DN	109/108 (101%)	106 (97%)	3 (3%)	51	83
42	CO	100/102 (98%)	95 (95%)	5 (5%)	30	68
42	DO	102/102 (100%)	99 (97%)	3 (3%)	50	82
43	CP	86/87 (99%)	80 (93%)	6 (7%)	19	53
43	DP	87/87 (100%)	84 (97%)	3 (3%)	44	79
44	CQ	99/99 (100%)	93 (94%)	6 (6%)	23	59
44	DQ	99/99 (100%)	97 (98%)	2 (2%)	63	88
45	CR	89/89 (100%)	86 (97%)	3 (3%)	44	79
45	DR	89/89 (100%)	87 (98%)	2 (2%)	60	87
46	CS	84/84 (100%)	79 (94%)	5 (6%)	24	60
46	DS	84/84 (100%)	83 (99%)	1 (1%)	78	93
47	CT	93/93 (100%)	88 (95%)	5 (5%)	27	64
47	DT	93/93 (100%)	92 (99%)	1 (1%)	80	93
48	CU	80/80 (100%)	72 (90%)	8 (10%)	9	32
48	DU	80/80 (100%)	77 (96%)	3 (4%)	40	76
49	CV	83/84 (99%)	79 (95%)	4 (5%)	31	69
49	DV	83/84 (99%)	81 (98%)	2 (2%)	57	86
50	CW	78/78 (100%)	75 (96%)	3 (4%)	40	76
50	DW	78/78 (100%)	76 (97%)	2 (3%)	54	84
51	CX	56/58 (97%)	55 (98%)	1 (2%)	66	89
51	DX	58/58 (100%)	57 (98%)	1 (2%)	68	90
52	CY	67/67 (100%)	63 (94%)	4 (6%)	24	60
52	DY	67/67 (100%)	65 (97%)	2 (3%)	48	82
53	CZ	54/54 (100%)	50 (93%)	4 (7%)	17	49
53	DZ	54/54 (100%)	52 (96%)	2 (4%)	41	77
54	DI	103/103 (100%)	98 (95%)	5 (5%)	31	68
All	All	9461/9484 (100%)	8897 (94%)	564 (6%)	24	60

All (564) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	23	TRP
2	AB	44	GLU
2	AB	73	LYS
2	AB	93	ASN
2	AB	105	LYS
2	AB	125	THR
2	AB	129	LEU
2	AB	130	THR
2	AB	135	LEU
2	AB	137	ARG
2	AB	147	SER
2	AB	161	LEU
2	AB	205	ASP
3	AC	4	LYS
3	AC	14	ILE
3	AC	21	THR
3	AC	33	LEU
3	AC	38	LYS
3	AC	46	GLU
3	AC	107	ARG
3	AC	168	TYR
3	AC	178	LEU
3	AC	185	ASN
3	AC	186	THR
4	AD	5	LEU
4	AD	17	THR
4	AD	22	LYS
4	AD	26	ARG
4	AD	50	ASP
4	AD	132	ILE
4	AD	142	VAL
4	AD	143	VAL
4	AD	194	ASP
4	AD	206	LYS
5	AE	11	LEU
5	AE	14	LYS
5	AE	32	SER
5	AE	46	VAL
5	AE	76	LEU
5	AE	78	ASN
5	AE	82	GLN
5	AE	101	GLU
5	AE	106	ILE

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Mol	Chain	Res	Type
5	AE	123	VAL
5	AE	126	LYS
6	AF	36	ILE
6	AF	69	GLU
6	AF	71	ILE
6	AF	74	LEU
6	AF	89	VAL
6	AF	93	LYS
7	AG	30	LEU
7	AG	36	LYS
7	AG	59	LEU
7	AG	63	GLU
7	AG	92	ARG
7	AG	120	LEU
7	AG	131	LYS
7	AG	133	THR
7	AG	142	HIS
8	AH	3	MET
8	AH	31	LYS
8	AH	47	GLU
8	AH	52	GLU
8	AH	54	ASP
8	AH	60	GLU
8	AH	63	LEU
8	AH	76	GLN
8	AH	90	ASP
8	AH	107	SER
8	AH	108	LYS
9	AI	11	ARG
9	AI	61	LEU
9	AI	63	LEU
9	AI	66	THR
9	AI	99	ARG
10	AJ	6	ILE
10	AJ	62	ARG
10	AJ	63	ASP
10	AJ	88	MET
10	AJ	89	ARG
10	AJ	90	LEU
11	AK	23	ILE
11	AK	55	SER
11	AK	119	ASN

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Mol	Chain	Res	Type
12	AL	24	LEU
12	AL	40	THR
12	AL	55	VAL
12	AL	74	LEU
12	AL	82	ILE
12	AL	88	LYS
12	AL	90	LEU
12	AL	110	ARG
12	AL	115	SER
12	AL	121	ARG
13	AM	7	ILE
13	AM	13	LYS
13	AM	17	ILE
13	AM	27	LYS
13	AM	48	LEU
13	AM	58	ASP
13	AM	63	PHE
13	AM	71	ARG
13	AM	101	ARG
14	AN	31	ILE
15	AO	2	SER
15	AO	24	SER
15	AO	40	GLN
15	AO	70	LEU
15	AO	84	ARG
16	AP	48	GLU
17	AQ	5	ILE
17	AQ	16	LYS
17	AQ	27	ARG
17	AQ	38	ILE
17	AQ	40	ARG
17	AQ	75	LEU
17	AQ	83	VAL
18	AR	47	THR
19	AS	5	LEU
19	AS	7	LYS
19	AS	13	LEU
19	AS	27	ASP
19	AS	33	THR
19	AS	37	ARG
19	AS	56	GLN
20	AT	15	GLU

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Mol	Chain	Res	Type
20	AT	24	ARG
20	AT	27	MET
20	AT	44	LYS
20	AT	48	GLN
20	AT	85	LYS
21	AU	13	ASP
21	AU	16	LEU
21	AU	34	ARG
21	AU	56	HIS
22	C1	10	ARG
22	C1	40	ARG
23	C2	8	LYS
24	C3	1	MET
25	C4	31	HIS
25	C4	45	ARG
25	C4	52	LYS
26	C5	20	ASP
26	C5	26	ILE
27	C0	3	LYS
27	C0	19	LYS
27	C0	36	VAL
2	BB	18	HIS
2	BB	23	TRP
2	BB	44	GLU
2	BB	93	ASN
2	BB	105	LYS
2	BB	125	THR
2	BB	129	LEU
2	BB	130	THR
2	BB	135	LEU
2	BB	137	ARG
2	BB	147	SER
2	BB	161	LEU
2	BB	205	ASP
3	BC	4	LYS
3	BC	14	ILE
3	BC	33	LEU
3	BC	37	PHE
3	BC	38	LYS
3	BC	46	GLU
3	BC	55	ILE
3	BC	107	ARG

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Mol	Chain	Res	Type
3	BC	152	GLU
3	BC	168	TYR
3	BC	175	LEU
3	BC	185	ASN
3	BC	186	THR
3	BC	193	TYR
4	BD	5	LEU
4	BD	17	THR
4	BD	22	LYS
4	BD	26	ARG
4	BD	47	ARG
4	BD	50	ASP
4	BD	142	VAL
4	BD	143	VAL
4	BD	151	LYS
4	BD	173	VAL
4	BD	194	ASP
4	BD	206	LYS
5	BE	11	LEU
5	BE	14	LYS
5	BE	32	SER
5	BE	46	VAL
5	BE	76	LEU
5	BE	81	LEU
5	BE	82	GLN
5	BE	88	VAL
5	BE	101	GLU
5	BE	103	THR
5	BE	114	VAL
5	BE	115	LEU
5	BE	123	VAL
5	BE	126	LYS
5	BE	151	GLU
5	BE	152	MET
5	BE	157	ARG
5	BE	159	LYS
6	BF	9	MET
6	BF	14	GLN
6	BF	16	GLU
6	BF	36	ILE
6	BF	53	LYS
6	BF	68	GLN

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Mol	Chain	Res	Type
6	BF	69	GLU
6	BF	71	ILE
6	BF	89	VAL
6	BF	93	LYS
7	BG	4	ARG
7	BG	5	ARG
7	BG	10	ARG
7	BG	30	LEU
7	BG	36	LYS
7	BG	48	GLU
7	BG	50	LEU
7	BG	59	LEU
7	BG	63	GLU
7	BG	72	THR
7	BG	92	ARG
7	BG	120	LEU
7	BG	131	LYS
7	BG	133	THR
7	BG	142	HIS
8	BH	3	MET
8	BH	47	GLU
8	BH	52	GLU
8	BH	60	GLU
8	BH	76	GLN
8	BH	77	ARG
8	BH	80	ARG
8	BH	83	LEU
8	BH	90	ASP
8	BH	107	SER
8	BH	108	LYS
9	BI	11	ARG
9	BI	61	LEU
9	BI	63	LEU
9	BI	66	THR
9	BI	99	ARG
10	BJ	5	ARG
10	BJ	6	ILE
10	BJ	62	ARG
10	BJ	63	ASP
10	BJ	78	GLU
10	BJ	88	MET
10	BJ	89	ARG

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Mol	Chain	Res	Type
10	BJ	90	LEU
11	BK	18	ASP
11	BK	23	ILE
11	BK	31	ILE
11	BK	38	GLN
11	BK	55	SER
11	BK	118	HIS
11	BK	119	ASN
12	BL	24	LEU
12	BL	44	LYS
12	BL	50	ARG
12	BL	55	VAL
12	BL	58	THR
12	BL	74	LEU
12	BL	82	ILE
12	BL	88	LYS
12	BL	90	LEU
12	BL	110	ARG
12	BL	115	SER
12	BL	121	ARG
13	BM	11	ASP
13	BM	13	LYS
13	BM	16	VAL
13	BM	17	ILE
13	BM	27	LYS
13	BM	48	LEU
13	BM	101	ARG
14	BN	26	GLU
15	BO	2	SER
15	BO	13	SER
15	BO	17	ARG
15	BO	24	SER
15	BO	40	GLN
15	BO	64	ARG
15	BO	66	LEU
15	BO	84	ARG
15	BO	87	LEU
15	BO	88	ARG
15	BO	89	ARG
16	BP	20	VAL
16	BP	46	LYS
17	BQ	17	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	BQ	21	ILE
17	BQ	26	GLU
17	BQ	27	ARG
17	BQ	38	ILE
17	BQ	40	ARG
17	BQ	51	ASN
17	BQ	75	LEU
18	BR	47	THR
19	BS	6	LYS
19	BS	7	LYS
19	BS	13	LEU
19	BS	33	THR
19	BS	37	ARG
20	BT	15	GLU
20	BT	24	ARG
20	BT	43	ASP
20	BT	48	GLN
20	BT	54	MET
20	BT	58	VAL
20	BT	64	LYS
20	BT	67	ILE
20	BT	69	LYS
20	BT	84	ASN
21	BU	13	ASP
21	BU	16	LEU
21	BU	34	ARG
21	BU	56	HIS
22	D1	18	SER
22	D1	26	THR
22	D1	29	SER
23	D2	5	ILE
23	D2	8	LYS
24	D3	1	MET
25	D4	31	HIS
25	D4	45	ARG
25	D4	52	LYS
27	D0	10	THR
27	D0	19	LYS
27	D0	25	LEU
27	D0	36	VAL
29	CC	11	PRO
29	CC	117	GLN

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Mol	Chain	Res	Type
29	CC	120	VAL
29	CC	130	LEU
29	CC	157	SER
29	CC	168	ASP
29	CC	174	LEU
29	CC	195	VAL
29	CC	204	VAL
29	CC	205	LEU
29	CC	236	GLU
29	CC	252	THR
29	CC	258	ARG
29	CC	260	ASN
30	CD	4	LEU
30	CD	13	ARG
30	CD	18	ASP
30	CD	95	SER
29	DC	70	ASN
29	DC	117	GLN
29	DC	120	VAL
29	DC	130	LEU
29	DC	236	GLU
29	DC	252	THR
32	DD	13	ARG
32	DD	18	ASP
32	DD	95	SER
33	CE	7	ASP
33	CE	12	LEU
33	CE	25	GLU
33	CE	44	ARG
33	CE	72	SER
33	CE	78	TRP
33	CE	83	VAL
33	CE	107	SER
33	CE	122	GLU
33	CE	127	GLU
33	CE	149	ILE
33	CE	152	GLU
33	CE	189	THR
34	CF	18	THR
34	CF	36	LEU
34	CF	57	LEU
34	CF	72	LYS

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Mol	Chain	Res	Type
34	CF	80	ARG
34	CF	94	GLU
34	CF	106	ILE
34	CF	115	ARG
34	CF	117	LEU
34	CF	123	ASP
34	CF	134	GLU
34	CF	141	ILE
34	CF	149	VAL
34	CF	152	LEU
34	CF	174	ASP
35	CG	11	VAL
35	CG	18	LYS
35	CG	155	GLU
36	CH	7	ASP
36	CH	15	LEU
36	CH	17	ASP
36	CH	21	VAL
36	CH	48	GLU
36	CH	51	ARG
36	CH	53	GLU
36	CH	55	GLU
36	CH	62	LEU
36	CH	75	LEU
36	CH	121	VAL
36	CH	127	GLU
36	CH	145	ASN
37	CJ	11	LEU
37	CJ	13	VAL
37	CJ	28	LEU
37	CJ	113	LYS
38	CK	5	THR
38	CK	9	GLU
38	CK	30	THR
38	CK	39	LYS
38	CK	124	VAL
38	CK	142	ILE
39	CL	35	VAL
39	CL	58	LEU
39	CL	98	ARG
39	CL	113	MET
40	CM	2	ARG

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Mol	Chain	Res	Type
40	CM	21	ARG
40	CM	93	ASN
40	CM	94	THR
40	CM	100	ILE
40	CM	115	GLU
41	CN	6	ARG
41	CN	20	LEU
41	CN	59	ARG
41	CN	78	LEU
42	CO	2	ARG
42	CO	14	SER
42	CO	71	ARG
42	CO	76	VAL
42	CO	95	THR
43	CP	18	LEU
43	CP	31	THR
43	CP	38	GLN
43	CP	49	VAL
43	CP	56	LYS
43	CP	78	VAL
44	CQ	2	SER
44	CQ	26	VAL
44	CQ	39	ARG
44	CQ	40	LEU
44	CQ	102	GLU
44	CQ	114	LEU
45	CR	16	LYS
45	CR	51	ARG
45	CR	52	GLN
46	CS	12	HIS
46	CS	45	GLU
46	CS	48	LYS
46	CS	51	VAL
46	CS	102	SER
47	CT	7	HIS
47	CT	19	LEU
47	CT	29	VAL
47	CT	86	MET
47	CT	97	LEU
48	CU	1	MET
48	CU	2	ILE
48	CU	3	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
48	CU	10	VAL
48	CU	24	MET
48	CU	30	ILE
48	CU	49	LYS
48	CU	69	ARG
49	CV	61	LYS
49	CV	72	ILE
49	CV	81	ASP
49	CV	98	SER
50	CW	1	MET
50	CW	7	GLU
50	CW	10	LYS
51	CX	82	ILE
52	CY	25	THR
52	CY	35	SER
52	CY	48	THR
52	CY	71	LEU
53	CZ	18	LEU
53	CZ	19	LEU
53	CZ	38	GLN
53	CZ	58	ASN
33	DE	12	LEU
33	DE	107	SER
33	DE	127	GLU
33	DE	189	THR
34	DF	10	ASP
34	DF	57	LEU
34	DF	72	LYS
34	DF	94	GLU
34	DF	106	ILE
34	DF	117	LEU
34	DF	134	GLU
34	DF	141	ILE
34	DF	149	VAL
34	DF	152	LEU
34	DF	174	ASP
35	DG	3	ARG
35	DG	11	VAL
35	DG	18	LYS
35	DG	56	ASP
35	DG	155	GLU
36	DH	7	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	DH	15	LEU
36	DH	17	ASP
36	DH	21	VAL
36	DH	48	GLU
36	DH	53	GLU
36	DH	57	LYS
36	DH	58	LEU
36	DH	60	GLU
36	DH	75	LEU
36	DH	121	VAL
36	DH	127	GLU
36	DH	145	ASN
37	DJ	11	LEU
37	DJ	13	VAL
37	DJ	28	LEU
37	DJ	113	LYS
38	DK	124	VAL
38	DK	142	ILE
39	DL	58	LEU
39	DL	76	VAL
39	DL	110	GLU
39	DL	113	MET
39	DL	123	LEU
40	DM	2	ARG
40	DM	91	ASP
40	DM	94	THR
40	DM	115	GLU
41	DN	58	LYS
41	DN	59	ARG
41	DN	100	LYS
42	DO	2	ARG
42	DO	14	SER
42	DO	76	VAL
43	DP	31	THR
43	DP	49	VAL
43	DP	78	VAL
44	DQ	26	VAL
44	DQ	102	GLU
45	DR	41	LYS
45	DR	51	ARG
46	DS	102	SER
47	DT	86	MET

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Mol	Chain	Res	Type
48	DU	1	MET
48	DU	3	ARG
48	DU	10	VAL
49	DV	52	LEU
49	DV	61	LYS
50	DW	7	GLU
50	DW	53	LYS
51	DX	82	ILE
52	DY	25	THR
52	DY	35	SER
53	DZ	19	LEU
53	DZ	38	GLN
54	DI	7	ASP
54	DI	16	SER
54	DI	53	ARG
54	DI	64	VAL
54	DI	117	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	18	HIS
2	AB	93	ASN
2	AB	94	HIS
2	AB	120	GLN
4	AD	136	GLN
5	AE	89	HIS
6	AF	63	ASN
7	AG	97	ASN
7	AG	142	HIS
8	AH	4	GLN
10	AJ	58	ASN
20	AT	48	GLN
20	AT	78	ASN
22	C1	6	ASN
22	C1	38	HIS
2	BB	39	HIS
2	BB	93	ASN
2	BB	94	HIS
2	BB	120	GLN
2	BB	168	HIS
4	BD	131	ASN

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Mol	Chain	Res	Type
5	BE	70	ASN
5	BE	89	HIS
5	BE	122	ASN
7	BG	97	ASN
8	BH	4	GLN
8	BH	38	ASN
17	BQ	51	ASN
20	BT	3	ASN
24	D3	26	ASN
25	D4	43	HIS
29	CC	142	HIS
29	DC	142	HIS
33	CE	115	GLN
35	CG	38	ASN
38	CK	138	GLN
43	CP	100	HIS
48	CU	28	ASN
49	CV	74	ASN
51	CX	57	HIS
53	CZ	45	GLN
49	DV	54	GLN
54	DI	122	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	239 (15%)	27 (1%)
1	BA	1529/1534 (99%)	246 (16%)	28 (1%)
28	CB	117/120 (97%)	11 (9%)	0
28	DB	119/120 (99%)	9 (7%)	0
31	CA	2892/2904 (99%)	426 (14%)	72 (2%)
55	DA	2880/2904 (99%)	367 (12%)	57 (1%)
All	All	9067/9116 (99%)	1298 (14%)	184 (2%)

All (1298) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	22	G

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Mol	Chain	Res	Type
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	69	G
1	AA	71	A
1	AA	72	A
1	AA	74	A
1	AA	80	A
1	AA	81	A
1	AA	82	G
1	AA	83	C
1	AA	85	U
1	AA	86	G
1	AA	88	U
1	AA	89	U
1	AA	90	C
1	AA	92	U
1	AA	94	G
1	AA	95	C
1	AA	108	G
1	AA	120	A
1	AA	130	A
1	AA	131	A
1	AA	137	U
1	AA	141	G
1	AA	142	G
1	AA	143	A
1	AA	144	G
1	AA	149	A
1	AA	159	G
1	AA	163	C
1	AA	168	G
1	AA	177	G
1	AA	183	C
1	AA	197	A
1	AA	205	A
1	AA	210	C
1	AA	211	G

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Mol	Chain	Res	Type
1	AA	212	G
1	AA	226	G
1	AA	240	G
1	AA	245	U
1	AA	247	G
1	AA	250	A
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	346	G
1	AA	348	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	384	G
1	AA	398	U
1	AA	406	G
1	AA	411	A
1	AA	412	A
1	AA	413	G
1	AA	414	A
1	AA	421	U
1	AA	422	C
1	AA	424	G
1	AA	429	U
1	AA	430	A
1	AA	436	C
1	AA	457	G
1	AA	458	U
1	AA	463	U
1	AA	466	A
1	AA	467	U
1	AA	468	A
1	AA	474	G

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Mol	Chain	Res	Type
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	509	A
1	AA	511	C
1	AA	527	G7M
1	AA	531	U
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	564	C
1	AA	568	G
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	615	G
1	AA	633	G
1	AA	650	G
1	AA	653	U
1	AA	661	G
1	AA	665	A
1	AA	695	A
1	AA	702	A
1	AA	703	G
1	AA	723	U
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	814	A
1	AA	815	A
1	AA	817	C
1	AA	821	G
1	AA	828	U
1	AA	836	G
1	AA	841	C
1	AA	842	U
1	AA	843	U

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Mol	Chain	Res	Type
1	AA	844	G
1	AA	845	A
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	934	C
1	AA	935	A
1	AA	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	971	G
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	987	G
1	AA	993	G
1	AA	1004	A
1	AA	1009	U
1	AA	1015	G
1	AA	1019	A
1	AA	1024	G
1	AA	1026	G
1	AA	1027	C
1	AA	1028	C
1	AA	1029	U
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	G
1	AA	1036	A
1	AA	1037	C
1	AA	1043	G
1	AA	1053	G
1	AA	1054	C
1	AA	1065	U
1	AA	1086	U
1	AA	1094	G
1	AA	1095	U
1	AA	1098	C
1	AA	1101	A
1	AA	1124	G
1	AA	1125	U

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Mol	Chain	Res	Type
1	AA	1132	C
1	AA	1133	G
1	AA	1136	C
1	AA	1137	C
1	AA	1138	G
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1142	G
1	AA	1143	G
1	AA	1145	A
1	AA	1152	A
1	AA	1159	U
1	AA	1160	G
1	AA	1168	U
1	AA	1184	G
1	AA	1196	A
1	AA	1197	A
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1236	A
1	AA	1238	A
1	AA	1239	A
1	AA	1256	A
1	AA	1257	A
1	AA	1260	G
1	AA	1280	A
1	AA	1281	C
1	AA	1286	U
1	AA	1287	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1312	G
1	AA	1317	C
1	AA	1320	C
1	AA	1346	A

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Mol	Chain	Res	Type
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1379	G
1	AA	1381	U
1	AA	1398	A
1	AA	1419	G
1	AA	1429	A
1	AA	1441	A
1	AA	1446	A
1	AA	1447	A
1	AA	1448	C
1	AA	1451	U
1	AA	1452	C
1	AA	1453	G
1	AA	1492	A
1	AA	1497	G
1	AA	1499	A
1	AA	1503	A
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1534	A
1	BA	4	U
1	BA	5	U
1	BA	9	G
1	BA	22	G
1	BA	32	A
1	BA	39	G
1	BA	47	C
1	BA	48	C
1	BA	50	A
1	BA	51	A
1	BA	52	C
1	BA	69	G
1	BA	71	A
1	BA	72	A
1	BA	74	A
1	BA	80	A
1	BA	82	G

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Mol	Chain	Res	Type
1	BA	83	C
1	BA	84	U
1	BA	85	U
1	BA	86	G
1	BA	87	C
1	BA	88	U
1	BA	89	U
1	BA	90	C
1	BA	92	U
1	BA	94	G
1	BA	95	C
1	BA	108	G
1	BA	120	A
1	BA	130	A
1	BA	131	A
1	BA	137	U
1	BA	141	G
1	BA	142	G
1	BA	143	A
1	BA	144	G
1	BA	149	A
1	BA	159	G
1	BA	163	C
1	BA	168	G
1	BA	177	G
1	BA	183	C
1	BA	197	A
1	BA	200	G
1	BA	205	A
1	BA	210	C
1	BA	211	G
1	BA	212	G
1	BA	226	G
1	BA	245	U
1	BA	247	G
1	BA	250	A
1	BA	251	G
1	BA	266	G
1	BA	267	C
1	BA	289	G
1	BA	321	A
1	BA	328	C

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Mol	Chain	Res	Type
1	BA	329	A
1	BA	330	C
1	BA	332	G
1	BA	346	G
1	BA	348	G
1	BA	352	C
1	BA	354	G
1	BA	367	U
1	BA	372	C
1	BA	373	A
1	BA	384	G
1	BA	398	U
1	BA	406	G
1	BA	412	A
1	BA	413	G
1	BA	414	A
1	BA	421	U
1	BA	422	C
1	BA	424	G
1	BA	429	U
1	BA	430	A
1	BA	436	C
1	BA	457	G
1	BA	458	U
1	BA	463	U
1	BA	467	U
1	BA	468	A
1	BA	474	G
1	BA	481	G
1	BA	484	G
1	BA	486	U
1	BA	495	A
1	BA	509	A
1	BA	511	C
1	BA	527	G7M
1	BA	531	U
1	BA	532	A
1	BA	533	A
1	BA	547	A
1	BA	559	A
1	BA	564	C
1	BA	568	G

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Mol	Chain	Res	Type
1	BA	572	A
1	BA	573	A
1	BA	576	C
1	BA	577	G
1	BA	615	G
1	BA	633	G
1	BA	650	G
1	BA	653	U
1	BA	661	G
1	BA	665	A
1	BA	695	A
1	BA	702	A
1	BA	703	G
1	BA	723	U
1	BA	734	G
1	BA	748	G
1	BA	755	G
1	BA	777	A
1	BA	793	U
1	BA	794	A
1	BA	814	A
1	BA	815	A
1	BA	817	C
1	BA	821	G
1	BA	828	U
1	BA	836	G
1	BA	839	C
1	BA	840	C
1	BA	841	C
1	BA	842	U
1	BA	843	U
1	BA	844	G
1	BA	845	A
1	BA	846	G
1	BA	914	A
1	BA	926	G
1	BA	927	G
1	BA	934	C
1	BA	935	A
1	BA	960	U
1	BA	966	2MG
1	BA	969	A

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Mol	Chain	Res	Type
1	BA	971	G
1	BA	975	A
1	BA	976	G
1	BA	977	A
1	BA	987	G
1	BA	993	G
1	BA	1004	A
1	BA	1008	U
1	BA	1009	U
1	BA	1015	G
1	BA	1019	A
1	BA	1024	G
1	BA	1026	G
1	BA	1027	C
1	BA	1028	C
1	BA	1029	U
1	BA	1030	U
1	BA	1031	C
1	BA	1032	G
1	BA	1033	G
1	BA	1036	A
1	BA	1037	C
1	BA	1043	G
1	BA	1046	A
1	BA	1053	G
1	BA	1054	C
1	BA	1065	U
1	BA	1070	U
1	BA	1086	U
1	BA	1094	G
1	BA	1095	U
1	BA	1098	C
1	BA	1101	A
1	BA	1124	G
1	BA	1125	U
1	BA	1132	C
1	BA	1133	G
1	BA	1136	C
1	BA	1137	C
1	BA	1138	G
1	BA	1139	G
1	BA	1140	C

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Mol	Chain	Res	Type
1	BA	1141	C
1	BA	1142	G
1	BA	1143	G
1	BA	1145	A
1	BA	1152	A
1	BA	1159	U
1	BA	1160	G
1	BA	1168	U
1	BA	1196	A
1	BA	1197	A
1	BA	1212	U
1	BA	1213	A
1	BA	1214	C
1	BA	1215	G
1	BA	1225	A
1	BA	1226	C
1	BA	1227	A
1	BA	1236	A
1	BA	1238	A
1	BA	1239	A
1	BA	1256	A
1	BA	1257	A
1	BA	1260	G
1	BA	1280	A
1	BA	1281	C
1	BA	1286	U
1	BA	1287	A
1	BA	1300	G
1	BA	1302	C
1	BA	1305	G
1	BA	1312	G
1	BA	1317	C
1	BA	1320	C
1	BA	1346	A
1	BA	1353	G
1	BA	1362	A
1	BA	1363	A
1	BA	1370	G
1	BA	1379	G
1	BA	1381	U
1	BA	1398	A
1	BA	1419	G

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Mol	Chain	Res	Type
1	BA	1429	A
1	BA	1441	A
1	BA	1446	A
1	BA	1447	A
1	BA	1448	C
1	BA	1451	U
1	BA	1452	C
1	BA	1453	G
1	BA	1492	A
1	BA	1493	A
1	BA	1497	G
1	BA	1499	A
1	BA	1503	A
1	BA	1506	U
1	BA	1507	A
1	BA	1517	G
1	BA	1529	G
1	BA	1530	G
1	BA	1534	A
28	CB	9	G
28	CB	25	U
28	CB	35	C
28	CB	45	A
28	CB	56	G
28	CB	57	A
28	CB	88	C
28	CB	89	U
28	CB	90	C
28	CB	99	A
28	CB	109	A
31	CA	10	A
31	CA	14	A
31	CA	34	U
31	CA	36	G
31	CA	42	A
31	CA	46	G
31	CA	49	A
31	CA	58	G
31	CA	63	A
31	CA	71	A
31	CA	74	A
31	CA	75	G

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Mol	Chain	Res	Type
31	CA	80	G
31	CA	83	A
31	CA	84	A
31	CA	101	A
31	CA	102	U
31	CA	118	A
31	CA	119	A
31	CA	120	U
31	CA	138	U
31	CA	139	U
31	CA	140	C
31	CA	141	G
31	CA	142	A
31	CA	143	C
31	CA	196	A
31	CA	199	A
31	CA	200	U
31	CA	215	G
31	CA	216	A
31	CA	221	A
31	CA	222	A
31	CA	248	G
31	CA	265	A
31	CA	266	G
31	CA	272	A
31	CA	276	U
31	CA	277	G
31	CA	278	A
31	CA	279	A
31	CA	285	G
31	CA	311	A
31	CA	329	G
31	CA	330	A
31	CA	343	C
31	CA	346	A
31	CA	352	A
31	CA	353	C
31	CA	362	A
31	CA	371	A
31	CA	372	G
31	CA	385	C
31	CA	386	G

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Mol	Chain	Res	Type
31	CA	399	U
31	CA	404	A
31	CA	405	U
31	CA	411	G
31	CA	420	C
31	CA	424	G
31	CA	425	G
31	CA	451	U
31	CA	480	A
31	CA	481	G
31	CA	491	G
31	CA	503	A
31	CA	504	A
31	CA	505	A
31	CA	508	A
31	CA	517	C
31	CA	531	C
31	CA	532	A
31	CA	543	G
31	CA	544	C
31	CA	546	U
31	CA	547	A
31	CA	549	G
31	CA	550	C
31	CA	551	G
31	CA	555	G
31	CA	556	A
31	CA	563	A
31	CA	571	U
31	CA	573	U
31	CA	575	A
31	CA	586	A
31	CA	603	A
31	CA	613	A
31	CA	614	A
31	CA	615	U
31	CA	627	A
31	CA	637	A
31	CA	645	C
31	CA	647	G
31	CA	654	A
31	CA	655	A

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Mol	Chain	Res	Type
31	CA	670	A
31	CA	684	G
31	CA	685	A
31	CA	686	U
31	CA	695	G
31	CA	717	C
31	CA	730	A
31	CA	740	C
31	CA	746	PSU
31	CA	747	5MU
31	CA	775	G
31	CA	776	G
31	CA	782	A
31	CA	784	G
31	CA	785	G
31	CA	792	A
31	CA	802	A
31	CA	805	G
31	CA	812	C
31	CA	819	A
31	CA	827	U
31	CA	828	U
31	CA	845	A
31	CA	846	U
31	CA	847	U
31	CA	858	G
31	CA	859	G
31	CA	878	A
31	CA	883	G
31	CA	896	A
31	CA	897	C
31	CA	910	A
31	CA	914	G
31	CA	915	C
31	CA	931	U
31	CA	932	U
31	CA	941	A
31	CA	946	C
31	CA	953	G
31	CA	961	C
31	CA	974	G
31	CA	983	A

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Mol	Chain	Res	Type
31	CA	984	A
31	CA	985	C
31	CA	995	C
31	CA	996	A
31	CA	1012	U
31	CA	1013	C
31	CA	1022	G
31	CA	1026	G
31	CA	1033	U
31	CA	1040	A
31	CA	1045	C
31	CA	1046	A
31	CA	1047	G
31	CA	1057	A
31	CA	1061	U
31	CA	1070	A
31	CA	1083	U
31	CA	1088	A
31	CA	1089	A
31	CA	1090	A
31	CA	1091	G
31	CA	1096	A
31	CA	1097	U
31	CA	1111	A
31	CA	1112	G
31	CA	1122	G
31	CA	1128	G
31	CA	1129	A
31	CA	1132	U
31	CA	1133	A
31	CA	1135	C
31	CA	1136	G
31	CA	1142	A
31	CA	1168	G
31	CA	1169	A
31	CA	1170	C
31	CA	1171	G
31	CA	1172	C
31	CA	1175	A
31	CA	1176	U
31	CA	1177	G
31	CA	1179	G

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Mol	Chain	Res	Type
31	CA	1180	U
31	CA	1186	G
31	CA	1210	G
31	CA	1212	G
31	CA	1236	G
31	CA	1238	G
31	CA	1253	A
31	CA	1256	G
31	CA	1266	G
31	CA	1271	G
31	CA	1272	A
31	CA	1273	U
31	CA	1300	G
31	CA	1301	A
31	CA	1313	U
31	CA	1320	C
31	CA	1321	A
31	CA	1328	A
31	CA	1352	U
31	CA	1365	A
31	CA	1376	C
31	CA	1379	U
31	CA	1380	G
31	CA	1383	A
31	CA	1391	U
31	CA	1395	A
31	CA	1416	G
31	CA	1417	C
31	CA	1419	A
31	CA	1420	A
31	CA	1428	C
31	CA	1437	C
31	CA	1452	G
31	CA	1453	A
31	CA	1460	U
31	CA	1482	G
31	CA	1490	A
31	CA	1491	G
31	CA	1493	C
31	CA	1494	A
31	CA	1497	U
31	CA	1509	A

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Mol	Chain	Res	Type
31	CA	1510	G
31	CA	1515	A
31	CA	1523	U
31	CA	1532	A
31	CA	1534	U
31	CA	1535	A
31	CA	1536	C
31	CA	1537	G
31	CA	1565	C
31	CA	1566	A
31	CA	1569	A
31	CA	1578	U
31	CA	1583	A
31	CA	1585	C
31	CA	1607	C
31	CA	1608	A
31	CA	1647	U
31	CA	1648	U
31	CA	1649	G
31	CA	1674	G
31	CA	1695	G
31	CA	1715	G
31	CA	1729	U
31	CA	1730	C
31	CA	1731	G
31	CA	1732	C
31	CA	1738	G
31	CA	1744	A
31	CA	1750	G
31	CA	1764	C
31	CA	1773	A
31	CA	1782	U
31	CA	1800	C
31	CA	1801	A
31	CA	1808	A
31	CA	1816	C
31	CA	1822	C
31	CA	1829	A
31	CA	1869	G
31	CA	1870	C
31	CA	1871	A
31	CA	1872	A

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Mol	Chain	Res	Type
31	CA	1873	G
31	CA	1900	A
31	CA	1906	G
31	CA	1907	G
31	CA	1914	C
31	CA	1929	G
31	CA	1930	G
31	CA	1931	U
31	CA	1937	A
31	CA	1938	A
31	CA	1955	U
31	CA	1967	C
31	CA	1970	A
31	CA	1972	G
31	CA	1991	U
31	CA	1993	U
31	CA	1997	C
31	CA	2022	U
31	CA	2023	C
31	CA	2031	A
31	CA	2033	A
31	CA	2036	C
31	CA	2043	C
31	CA	2055	C
31	CA	2056	G
31	CA	2060	A
31	CA	2061	G
31	CA	2062	A
31	CA	2069	G7M
31	CA	2072	C
31	CA	2080	A
31	CA	2093	G
31	CA	2095	A
31	CA	2100	G
31	CA	2102	G
31	CA	2108	A
31	CA	2110	G
31	CA	2111	U
31	CA	2112	G
31	CA	2113	U
31	CA	2115	G
31	CA	2117	A

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Mol	Chain	Res	Type
31	CA	2118	U
31	CA	2119	A
31	CA	2123	G
31	CA	2124	G
31	CA	2125	G
31	CA	2126	A
31	CA	2127	G
31	CA	2128	G
31	CA	2131	U
31	CA	2132	U
31	CA	2133	G
31	CA	2146	C
31	CA	2147	A
31	CA	2157	G
31	CA	2158	A
31	CA	2159	G
31	CA	2160	C
31	CA	2162	G
31	CA	2164	C
31	CA	2165	C
31	CA	2171	A
31	CA	2172	U
31	CA	2173	A
31	CA	2174	C
31	CA	2178	C
31	CA	2183	A
31	CA	2190	G
31	CA	2198	A
31	CA	2203	U
31	CA	2204	G
31	CA	2211	A
31	CA	2225	A
31	CA	2226	C
31	CA	2238	G
31	CA	2239	G
31	CA	2259	U
31	CA	2268	A
31	CA	2280	G
31	CA	2283	C
31	CA	2287	A
31	CA	2305	U
31	CA	2311	A

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Mol	Chain	Res	Type
31	CA	2322	A
31	CA	2326	C
31	CA	2327	A
31	CA	2333	A
31	CA	2335	A
31	CA	2345	G
31	CA	2347	C
31	CA	2350	C
31	CA	2354	C
31	CA	2361	G
31	CA	2383	G
31	CA	2385	C
31	CA	2388	A
31	CA	2402	U
31	CA	2403	C
31	CA	2406	A
31	CA	2423	U
31	CA	2424	C
31	CA	2425	A
31	CA	2426	A
31	CA	2429	G
31	CA	2430	A
31	CA	2435	A
31	CA	2441	U
31	CA	2448	A
31	CA	2465	C
31	CA	2476	A
31	CA	2491	U
31	CA	2502	G
31	CA	2505	G
31	CA	2518	A
31	CA	2529	G
31	CA	2535	G
31	CA	2547	A
31	CA	2554	U
31	CA	2556	C
31	CA	2566	A
31	CA	2567	G
31	CA	2573	C
31	CA	2578	G
31	CA	2582	G
31	CA	2585	U

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Mol	Chain	Res	Type
31	CA	2603	G
31	CA	2609	U
31	CA	2613	U
31	CA	2629	U
31	CA	2630	G
31	CA	2646	C
31	CA	2661	G
31	CA	2663	G
31	CA	2681	C
31	CA	2682	A
31	CA	2689	U
31	CA	2690	U
31	CA	2714	G
31	CA	2718	G
31	CA	2726	A
31	CA	2744	G
31	CA	2748	A
31	CA	2769	U
31	CA	2778	A
31	CA	2791	G
31	CA	2794	C
31	CA	2799	A
31	CA	2820	A
31	CA	2835	A
31	CA	2836	U
31	CA	2850	A
31	CA	2861	U
31	CA	2865	U
31	CA	2867	G
31	CA	2883	A
31	CA	2884	U
31	CA	2886	A
31	CA	2887	A
31	CA	2891	U
31	CA	2903	U
31	CA	2904	U
28	DB	25	U
28	DB	35	C
28	DB	45	A
28	DB	56	G
28	DB	57	A
28	DB	88	C

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Mol	Chain	Res	Type
28	DB	89	U
28	DB	90	C
28	DB	109	A
55	DA	10	A
55	DA	12	U
55	DA	34	U
55	DA	46	G
55	DA	63	A
55	DA	71	A
55	DA	74	A
55	DA	75	G
55	DA	80	G
55	DA	84	A
55	DA	101	A
55	DA	102	U
55	DA	118	A
55	DA	119	A
55	DA	120	U
55	DA	138	U
55	DA	139	U
55	DA	140	C
55	DA	141	G
55	DA	142	A
55	DA	143	C
55	DA	196	A
55	DA	199	A
55	DA	200	U
55	DA	215	G
55	DA	216	A
55	DA	221	A
55	DA	222	A
55	DA	248	G
55	DA	265	A
55	DA	266	G
55	DA	272	A
55	DA	276	U
55	DA	277	G
55	DA	278	A
55	DA	279	A
55	DA	285	G
55	DA	302	C
55	DA	311	A

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Mol	Chain	Res	Type
55	DA	329	G
55	DA	330	A
55	DA	343	C
55	DA	346	A
55	DA	352	A
55	DA	353	C
55	DA	362	A
55	DA	370	G
55	DA	372	G
55	DA	386	G
55	DA	399	U
55	DA	411	G
55	DA	412	A
55	DA	420	C
55	DA	424	G
55	DA	425	G
55	DA	451	U
55	DA	480	A
55	DA	481	G
55	DA	491	G
55	DA	504	A
55	DA	505	A
55	DA	508	A
55	DA	531	C
55	DA	532	A
55	DA	543	G
55	DA	544	C
55	DA	546	U
55	DA	547	A
55	DA	548	G
55	DA	549	G
55	DA	550	C
55	DA	551	G
55	DA	563	A
55	DA	573	U
55	DA	575	A
55	DA	586	A
55	DA	603	A
55	DA	613	A
55	DA	614	A
55	DA	615	U
55	DA	627	A

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Mol	Chain	Res	Type
55	DA	637	A
55	DA	645	C
55	DA	647	G
55	DA	654	A
55	DA	655	A
55	DA	686	U
55	DA	717	C
55	DA	730	A
55	DA	747	5MU
55	DA	764	A
55	DA	765	C
55	DA	775	G
55	DA	776	G
55	DA	782	A
55	DA	784	G
55	DA	785	G
55	DA	790	U
55	DA	792	A
55	DA	805	G
55	DA	812	C
55	DA	827	U
55	DA	828	U
55	DA	858	G
55	DA	859	G
55	DA	860	U
55	DA	878	A
55	DA	883	G
55	DA	885	C
55	DA	896	A
55	DA	897	C
55	DA	910	A
55	DA	914	G
55	DA	915	C
55	DA	927	A
55	DA	931	U
55	DA	932	U
55	DA	946	C
55	DA	961	C
55	DA	974	G
55	DA	983	A
55	DA	996	A
55	DA	1012	U

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Mol	Chain	Res	Type
55	DA	1013	C
55	DA	1022	G
55	DA	1026	G
55	DA	1033	U
55	DA	1040	A
55	DA	1047	G
55	DA	1057	A
55	DA	1061	U
55	DA	1070	A
55	DA	1083	U
55	DA	1088	A
55	DA	1089	A
55	DA	1090	A
55	DA	1091	G
55	DA	1096	A
55	DA	1097	U
55	DA	1112	G
55	DA	1132	U
55	DA	1133	A
55	DA	1135	C
55	DA	1136	G
55	DA	1142	A
55	DA	1168	G
55	DA	1172	C
55	DA	1174	U
55	DA	1175	A
55	DA	1176	U
55	DA	1177	G
55	DA	1180	U
55	DA	1187	G
55	DA	1237	A
55	DA	1238	G
55	DA	1253	A
55	DA	1256	G
55	DA	1271	G
55	DA	1272	A
55	DA	1273	U
55	DA	1300	G
55	DA	1301	A
55	DA	1329	U
55	DA	1352	U
55	DA	1365	A

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Mol	Chain	Res	Type
55	DA	1379	U
55	DA	1383	A
55	DA	1391	U
55	DA	1416	G
55	DA	1417	C
55	DA	1427	A
55	DA	1428	C
55	DA	1434	A
55	DA	1435	G
55	DA	1452	G
55	DA	1453	A
55	DA	1460	U
55	DA	1482	G
55	DA	1490	A
55	DA	1491	G
55	DA	1493	C
55	DA	1494	A
55	DA	1497	U
55	DA	1508	A
55	DA	1509	A
55	DA	1510	G
55	DA	1515	A
55	DA	1523	U
55	DA	1532	A
55	DA	1534	U
55	DA	1535	A
55	DA	1536	C
55	DA	1537	G
55	DA	1566	A
55	DA	1569	A
55	DA	1578	U
55	DA	1583	A
55	DA	1585	C
55	DA	1607	C
55	DA	1608	A
55	DA	1616	A
55	DA	1647	U
55	DA	1648	U
55	DA	1649	G
55	DA	1674	G
55	DA	1715	G
55	DA	1729	U

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Mol	Chain	Res	Type
55	DA	1730	C
55	DA	1731	G
55	DA	1732	C
55	DA	1738	G
55	DA	1744	A
55	DA	1764	C
55	DA	1773	A
55	DA	1782	U
55	DA	1800	C
55	DA	1801	A
55	DA	1808	A
55	DA	1816	C
55	DA	1829	A
55	DA	1869	G
55	DA	1870	C
55	DA	1871	A
55	DA	1872	A
55	DA	1873	G
55	DA	1906	G
55	DA	1907	G
55	DA	1913	A
55	DA	1914	C
55	DA	1929	G
55	DA	1930	G
55	DA	1931	U
55	DA	1937	A
55	DA	1938	A
55	DA	1955	U
55	DA	1965	C
55	DA	1967	C
55	DA	1970	A
55	DA	1972	G
55	DA	1991	U
55	DA	1993	U
55	DA	1997	C
55	DA	2023	C
55	DA	2031	A
55	DA	2033	A
55	DA	2043	C
55	DA	2055	C
55	DA	2056	G
55	DA	2060	A

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Mol	Chain	Res	Type
55	DA	2061	G
55	DA	2062	A
55	DA	2069	G7M
55	DA	2097	A
55	DA	2100	G
55	DA	2102	G
55	DA	2105	U
55	DA	2111	U
55	DA	2112	G
55	DA	2113	U
55	DA	2116	G
55	DA	2117	A
55	DA	2118	U
55	DA	2119	A
55	DA	2120	G
55	DA	2123	G
55	DA	2125	G
55	DA	2126	A
55	DA	2128	G
55	DA	2131	U
55	DA	2132	U
55	DA	2133	G
55	DA	2134	A
55	DA	2135	A
55	DA	2145	C
55	DA	2146	C
55	DA	2148	G
55	DA	2158	A
55	DA	2159	G
55	DA	2160	C
55	DA	2161	C
55	DA	2162	G
55	DA	2163	A
55	DA	2164	C
55	DA	2165	C
55	DA	2167	U
55	DA	2168	G
55	DA	2169	A
55	DA	2170	A
55	DA	2171	A
55	DA	2172	U
55	DA	2173	A

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Mol	Chain	Res	Type
55	DA	2177	C
55	DA	2178	C
55	DA	2179	C
55	DA	2181	U
55	DA	2183	A
55	DA	2185	U
55	DA	2190	G
55	DA	2198	A
55	DA	2204	G
55	DA	2211	A
55	DA	2225	A
55	DA	2238	G
55	DA	2239	G
55	DA	2268	A
55	DA	2283	C
55	DA	2286	G
55	DA	2287	A
55	DA	2305	U
55	DA	2308	G
55	DA	2312	U
55	DA	2324	U
55	DA	2325	G
55	DA	2333	A
55	DA	2335	A
55	DA	2347	C
55	DA	2383	G
55	DA	2385	C
55	DA	2402	U
55	DA	2403	C
55	DA	2406	A
55	DA	2407	A
55	DA	2423	U
55	DA	2424	C
55	DA	2425	A
55	DA	2431	U
55	DA	2435	A
55	DA	2441	U
55	DA	2448	A
55	DA	2476	A
55	DA	2491	U
55	DA	2502	G
55	DA	2505	G

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Mol	Chain	Res	Type
55	DA	2518	A
55	DA	2529	G
55	DA	2535	G
55	DA	2547	A
55	DA	2556	C
55	DA	2566	A
55	DA	2567	G
55	DA	2573	C
55	DA	2574	G
55	DA	2585	U
55	DA	2603	G
55	DA	2609	U
55	DA	2613	U
55	DA	2629	U
55	DA	2630	G
55	DA	2661	G
55	DA	2663	G
55	DA	2689	U
55	DA	2690	U
55	DA	2714	G
55	DA	2726	A
55	DA	2744	G
55	DA	2748	A
55	DA	2765	A
55	DA	2778	A
55	DA	2791	G
55	DA	2798	U
55	DA	2799	A
55	DA	2811	G
55	DA	2820	A
55	DA	2821	A
55	DA	2836	U
55	DA	2867	G
55	DA	2891	U

All (184) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	70	U
1	AA	88	U
1	AA	89	U

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Mol	Chain	Res	Type
1	AA	209	U
1	AA	413	G
1	AA	429	U
1	AA	485	U
1	AA	576	C
1	AA	653	U
1	AA	702	A
1	AA	793	U
1	AA	841	C
1	AA	842	U
1	AA	884	U
1	AA	992	U
1	AA	1086	U
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1225	A
1	AA	1281	C
1	AA	1299	A
1	AA	1397	C
1	AA	1447	A
1	AA	1452	C
1	BA	5	U
1	BA	70	U
1	BA	86	G
1	BA	89	U
1	BA	209	U
1	BA	429	U
1	BA	485	U
1	BA	576	C
1	BA	653	U
1	BA	702	A
1	BA	793	U
1	BA	842	U
1	BA	844	G
1	BA	884	U
1	BA	992	U
1	BA	1008	U
1	BA	1086	U
1	BA	1137	C
1	BA	1139	G

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Mol	Chain	Res	Type
1	BA	1140	C
1	BA	1141	C
1	BA	1225	A
1	BA	1281	C
1	BA	1299	A
1	BA	1362	A
1	BA	1397	C
1	BA	1447	A
1	BA	1452	C
31	CA	83	A
31	CA	101	A
31	CA	138	U
31	CA	141	G
31	CA	177	G
31	CA	196	A
31	CA	199	A
31	CA	221	A
31	CA	271	G
31	CA	278	A
31	CA	310	A
31	CA	345	A
31	CA	403	U
31	CA	404	A
31	CA	451	U
31	CA	503	A
31	CA	506	G
31	CA	555	G
31	CA	620	G
31	CA	764	A
31	CA	784	G
31	CA	846	U
31	CA	973	A
31	CA	984	A
31	CA	1045	C
31	CA	1046	A
31	CA	1061	U
31	CA	1069	A
31	CA	1070	A
31	CA	1088	A
31	CA	1089	A
31	CA	1128	G
31	CA	1141	U

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Mol	Chain	Res	Type
31	CA	1253	A
31	CA	1286	A
31	CA	1300	G
31	CA	1320	C
31	CA	1329	U
31	CA	1379	U
31	CA	1452	G
31	CA	1490	A
31	CA	1497	U
31	CA	1509	A
31	CA	1535	A
31	CA	1536	C
31	CA	1607	C
31	CA	1647	U
31	CA	1730	C
31	CA	1786	A
31	CA	1870	C
31	CA	1871	A
31	CA	2035	G
31	CA	2095	A
31	CA	2119	A
31	CA	2126	A
31	CA	2146	C
31	CA	2157	G
31	CA	2164	C
31	CA	2225	A
31	CA	2282	G
31	CA	2286	G
31	CA	2326	C
31	CA	2423	U
31	CA	2425	A
31	CA	2430	A
31	CA	2680	U
31	CA	2681	C
31	CA	2778	A
31	CA	2779	U
31	CA	2797	U
31	CA	2849	U
31	CA	2873	A
55	DA	138	U
55	DA	141	G
55	DA	199	A

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Mol	Chain	Res	Type
55	DA	271	G
55	DA	278	A
55	DA	370	G
55	DA	403	U
55	DA	503	A
55	DA	620	G
55	DA	764	A
55	DA	784	G
55	DA	859	G
55	DA	961	C
55	DA	984	A
55	DA	1061	U
55	DA	1069	A
55	DA	1070	A
55	DA	1087	G
55	DA	1088	A
55	DA	1089	A
55	DA	1128	G
55	DA	1141	U
55	DA	1142	A
55	DA	1175	A
55	DA	1253	A
55	DA	1286	A
55	DA	1300	G
55	DA	1320	C
55	DA	1490	A
55	DA	1497	U
55	DA	1509	A
55	DA	1535	A
55	DA	1607	C
55	DA	1647	U
55	DA	1730	C
55	DA	1870	C
55	DA	1871	A
55	DA	1936	A
55	DA	2097	A
55	DA	2119	A
55	DA	2127	G
55	DA	2146	C
55	DA	2157	G
55	DA	2158	A
55	DA	2164	C

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Mol	Chain	Res	Type
55	DA	2172	U
55	DA	2286	G
55	DA	2311	A
55	DA	2324	U
55	DA	2406	A
55	DA	2423	U
55	DA	2501	C
55	DA	2585	U
55	DA	2681	C
55	DA	2797	U
55	DA	2798	U
55	DA	2873	A

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

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	18,26,27	1.11	2 (11%)	21,38,41	2.58	4 (19%)
1	4OC	AA	1402	1	15,23,24	0.81	0	21,32,35	1.32	2 (9%)
1	5MC	AA	1407	1	14,22,23	0.87	1 (7%)	17,32,35	0.71	1 (5%)
1	UR3	AA	1498	1	13,22,23	0.83	0	18,32,35	0.64	0
1	2MG	AA	1516	1	18,26,27	1.30	2 (11%)	21,38,41	2.52	4 (19%)
1	MA6	AA	1518	1	18,26,27	0.68	0	15,38,41	0.64	0
1	MA6	AA	1519	1	18,26,27	0.63	0	15,38,41	0.55	0
1	PSU	AA	516	1,56	15,21,22	1.13	1 (6%)	16,30,33	3.47	2 (12%)
1	G7M	AA	527	1	18,26,27	1.11	1 (5%)	21,39,42	3.30	5 (23%)
1	2MG	AA	966	1	18,26,27	1.18	2 (11%)	21,38,41	2.51	3 (14%)
1	5MC	AA	967	1	14,22,23	0.84	1 (7%)	17,32,35	0.66	1 (5%)
12	D2T	AL	89	12	4,9,10	0.46	0	4,11,13	1.43	1 (25%)
1	2MG	BA	1207	1	18,26,27	1.18	2 (11%)	21,38,41	2.55	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4OC	BA	1402	1	15,23,24	0.88	0	21,32,35	1.29	2 (9%)
1	5MC	BA	1407	1	14,22,23	0.84	1 (7%)	17,32,35	0.71	1 (5%)
1	UR3	BA	1498	1	13,22,23	1.13	2 (15%)	18,32,35	0.52	0
1	2MG	BA	1516	1	18,26,27	1.21	2 (11%)	21,38,41	2.55	4 (19%)
1	MA6	BA	1518	1	18,26,27	0.67	0	15,38,41	0.62	0
1	MA6	BA	1519	1	18,26,27	0.58	0	15,38,41	0.58	0
1	PSU	BA	516	1	15,21,22	1.17	2 (13%)	16,30,33	3.49	2 (12%)
1	G7M	BA	527	1	18,26,27	1.11	1 (5%)	21,39,42	3.44	5 (23%)
1	2MG	BA	966	1	18,26,27	1.08	2 (11%)	21,38,41	2.52	4 (19%)
1	5MC	BA	967	1	14,22,23	0.83	1 (7%)	17,32,35	0.65	1 (5%)
12	D2T	BL	89	12	4,9,10	0.53	0	4,11,13	1.60	1 (25%)
31	6MZ	CA	1618	31	17,25,26	0.73	0	15,36,39	0.89	1 (6%)
31	2MG	CA	1835	31	18,26,27	1.14	1 (5%)	21,38,41	2.48	4 (19%)
31	PSU	CA	1911	31	15,21,22	1.13	1 (6%)	16,30,33	3.46	1 (6%)
31	3TD	CA	1915	31	15,22,23	1.00	2 (13%)	17,32,35	0.99	1 (5%)
31	PSU	CA	1917	31	15,21,22	1.15	2 (13%)	16,30,33	3.53	1 (6%)
31	5MU	CA	1939	31	13,22,23	1.18	1 (7%)	16,32,35	4.79	3 (18%)
31	5MC	CA	1962	31	14,22,23	0.82	1 (7%)	17,32,35	0.60	1 (5%)
31	6MZ	CA	2030	31	17,25,26	0.80	0	15,36,39	0.96	1 (6%)
31	G7M	CA	2069	31	18,26,27	0.92	1 (5%)	21,39,42	3.10	5 (23%)
31	OMG	CA	2251	31	18,26,27	1.15	2 (11%)	21,38,41	2.75	4 (19%)
31	2MG	CA	2445	31	18,26,27	1.27	2 (11%)	21,38,41	2.55	4 (19%)
31	PSU	CA	2457	31	15,21,22	1.11	2 (13%)	16,30,33	3.47	1 (6%)
31	OMC	CA	2498	31,56	15,22,23	0.89	1 (6%)	20,31,34	0.58	0
31	2MA	CA	2503	31	17,25,26	0.89	0	18,37,40	1.02	1 (5%)
31	PSU	CA	2504	31	15,21,22	1.09	2 (13%)	16,30,33	3.47	1 (6%)
31	OMU	CA	2552	31	14,22,23	1.19	2 (14%)	19,31,34	2.92	2 (10%)
31	PSU	CA	2580	31	15,21,22	1.21	2 (13%)	16,30,33	3.56	2 (12%)
31	PSU	CA	2605	31	15,21,22	1.12	2 (13%)	16,30,33	3.52	2 (12%)
31	1MG	CA	745	31	17,26,27	1.23	1 (5%)	19,39,42	1.07	2 (10%)
31	PSU	CA	746	31,56	15,21,22	1.33	3 (20%)	16,30,33	3.49	1 (6%)
31	5MU	CA	747	31	13,22,23	1.10	1 (7%)	16,32,35	4.79	3 (18%)
31	PSU	CA	955	31	15,21,22	1.15	2 (13%)	16,30,33	3.50	1 (6%)
41	4D4	CN	81	41	7,11,12	1.00	1 (14%)	5,13,15	0.80	0
55	6MZ	DA	1618	55	17,25,26	0.77	0	15,36,39	0.87	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
55	2MG	DA	1835	55	18,26,27	1.07	1 (5%)	21,38,41	2.52	4 (19%)
55	PSU	DA	1911	55	15,21,22	1.11	2 (13%)	16,30,33	3.45	1 (6%)
55	3TD	DA	1915	55	15,22,23	0.94	2 (13%)	17,32,35	1.03	1 (5%)
55	PSU	DA	1917	55	15,21,22	1.23	2 (13%)	16,30,33	3.52	1 (6%)
55	5MU	DA	1939	55	13,22,23	1.15	1 (7%)	16,32,35	4.80	3 (18%)
55	5MC	DA	1962	55	14,22,23	0.90	1 (7%)	17,32,35	0.68	0
55	6MZ	DA	2030	55	17,25,26	0.72	0	15,36,39	0.91	1 (6%)
55	G7M	DA	2069	55	18,26,27	1.00	1 (5%)	21,39,42	3.04	5 (23%)
55	OMG	DA	2251	55	18,26,27	1.00	1 (5%)	21,38,41	2.67	4 (19%)
55	2MG	DA	2445	55	18,26,27	1.18	3 (16%)	21,38,41	2.74	4 (19%)
55	H2U	DA	2449	55	17,21,22	0.56	0	23,30,33	0.64	0
55	PSU	DA	2457	55	15,21,22	1.06	2 (13%)	16,30,33	3.49	1 (6%)
55	OMC	DA	2498	55,56	15,22,23	0.84	1 (6%)	20,31,34	0.70	0
55	2MA	DA	2503	55,56	17,25,26	0.79	0	18,37,40	1.15	2 (11%)
55	PSU	DA	2504	55	15,21,22	1.21	2 (13%)	16,30,33	3.49	1 (6%)
55	OMU	DA	2552	55	14,22,23	1.12	2 (14%)	19,31,34	2.93	2 (10%)
55	PSU	DA	2580	55	15,21,22	1.42	4 (26%)	16,30,33	3.57	2 (12%)
55	PSU	DA	2604	55	15,21,22	1.25	2 (13%)	16,30,33	3.52	1 (6%)
55	PSU	DA	2605	55	15,21,22	1.10	2 (13%)	16,30,33	3.54	2 (12%)
55	1MG	DA	745	55	17,26,27	1.36	3 (17%)	19,39,42	1.18	3 (15%)
55	PSU	DA	746	55,56	15,21,22	1.70	4 (26%)	16,30,33	3.47	1 (6%)
55	5MU	DA	747	55	13,22,23	1.14	1 (7%)	16,32,35	4.73	3 (18%)
55	PSU	DA	955	55	15,21,22	1.47	3 (20%)	16,30,33	3.53	1 (6%)
32	MEQ	DD	150[A]	32	7,9,10	0.49	0	8,10,12	1.30	2 (25%)
32	MEQ	DD	150[B]	32	7,9,10	2.25	1 (14%)	8,10,12	2.19	3 (37%)
41	4D4	DN	81[A]	-	7,11,12	1.04	1 (14%)	5,13,15	0.91	0
41	4D4	DN	81[B]	-	7,11,12	0.88	0	5,13,15	0.87	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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
31	6MZ	CA	1618	31	-	0/5/27/28	0/3/3/3
31	2MG	CA	1835	31	-	0/5/27/28	0/3/3/3
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
31	5MU	CA	1939	31	-	0/3/25/26	0/2/2/2
31	5MC	CA	1962	31	-	0/3/25/26	0/2/2/2
31	6MZ	CA	2030	31	-	0/5/27/28	0/3/3/3
31	G7M	CA	2069	31	-	0/3/25/26	0/3/3/3
31	OMG	CA	2251	31	-	0/5/27/28	0/3/3/3
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
31	OMC	CA	2498	31,56	-	0/5/27/28	0/2/2/2
31	2MA	CA	2503	31	-	0/3/25/26	0/3/3/3
31	PSU	CA	2504	31	-	0/7/25/26	0/2/2/2
31	OMU	CA	2552	31	-	0/5/27/28	0/2/2/2
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
31	PSU	CA	746	31,56	-	0/7/25/26	0/2/2/2
31	5MU	CA	747	31	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
41	4D4	CN	81	41	-	0/8/12/14	0/0/0/0
55	6MZ	DA	1618	55	-	0/5/27/28	0/3/3/3
55	2MG	DA	1835	55	-	0/5/27/28	0/3/3/3
55	PSU	DA	1911	55	-	0/7/25/26	0/2/2/2
55	3TD	DA	1915	55	-	0/7/25/26	0/2/2/2
55	PSU	DA	1917	55	-	0/7/25/26	0/2/2/2
55	5MU	DA	1939	55	-	0/3/25/26	0/2/2/2
55	5MC	DA	1962	55	-	0/3/25/26	0/2/2/2
55	6MZ	DA	2030	55	-	0/5/27/28	0/3/3/3
55	G7M	DA	2069	55	-	0/3/25/26	0/3/3/3
55	OMG	DA	2251	55	-	0/5/27/28	0/3/3/3
55	2MG	DA	2445	55	-	0/5/27/28	0/3/3/3
55	H2U	DA	2449	55	-	0/7/38/39	0/2/2/2
55	PSU	DA	2457	55	-	0/7/25/26	0/2/2/2
55	OMC	DA	2498	55,56	-	0/5/27/28	0/2/2/2
55	2MA	DA	2503	55,56	-	0/3/25/26	0/3/3/3
55	PSU	DA	2504	55	-	0/7/25/26	0/2/2/2
55	OMU	DA	2552	55	-	0/5/27/28	0/2/2/2
55	PSU	DA	2580	55	-	0/7/25/26	0/2/2/2
55	PSU	DA	2604	55	-	0/7/25/26	0/2/2/2
55	PSU	DA	2605	55	-	0/7/25/26	0/2/2/2
55	1MG	DA	745	55	-	0/3/25/26	0/3/3/3
55	PSU	DA	746	55,56	-	0/7/25/26	0/2/2/2
55	5MU	DA	747	55	-	0/3/25/26	0/2/2/2
55	PSU	DA	955	55	-	0/7/25/26	0/2/2/2
32	MEQ	DD	150[A]	32	-	0/7/9/11	0/0/0/0
32	MEQ	DD	150[B]	32	-	0/7/9/11	0/0/0/0
41	4D4	DN	81[A]	-	-	0/8/12/14	0/0/0/0
41	4D4	DN	81[B]	-	-	0/8/12/14	0/0/0/0

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	746	PSU	C2'-C1'	-3.71	1.50	1.53
55	DA	955	PSU	C2'-C1'	-3.00	1.51	1.53
55	DA	746	PSU	O4'-C1'	-2.84	1.40	1.44
55	DA	2580	PSU	O4'-C1'	-2.65	1.40	1.44
31	CA	746	PSU	O4'-C1'	-2.47	1.40	1.44
55	DA	2580	PSU	C6-C5	-2.31	1.35	1.38
55	DA	2580	PSU	C5-C1'	-2.28	1.50	1.52
55	DA	745	1MG	C8-N7	-2.27	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	2457	PSU	C6-C5	-2.20	1.35	1.38
31	CA	1915	3TD	C6-C5	-2.19	1.35	1.38
55	DA	2604	PSU	C6-C5	-2.11	1.35	1.38
55	DA	1911	PSU	C6-C5	-2.10	1.35	1.38
55	DA	2445	2MG	O3'-C3'	-2.10	1.38	1.43
55	DA	746	PSU	C6-C5	-2.09	1.35	1.38
55	DA	2504	PSU	C6-C5	-2.09	1.35	1.38
31	CA	2504	PSU	C6-C5	-2.09	1.35	1.38
1	BA	516	PSU	C6-C5	-2.09	1.35	1.38
31	CA	2580	PSU	C6-C5	-2.07	1.35	1.38
31	CA	1962	5MC	C6-C5	-2.06	1.34	1.40
55	DA	1915	3TD	C6-C5	-2.06	1.35	1.38
1	AA	1407	5MC	C6-C5	-2.05	1.34	1.40
1	BA	967	5MC	C6-C5	-2.04	1.34	1.40
1	AA	967	5MC	C6-C5	-2.03	1.34	1.40
55	DA	1917	PSU	C6-C5	-2.03	1.35	1.38
1	BA	1407	5MC	C6-C5	-2.03	1.34	1.40
31	CA	746	PSU	C6-C5	-2.03	1.35	1.38
31	CA	2605	PSU	C6-C5	-2.03	1.35	1.38
55	DA	1962	5MC	C6-C5	-2.02	1.34	1.40
31	CA	955	PSU	C6-C5	-2.02	1.35	1.38
55	DA	955	PSU	C6-C5	-2.02	1.35	1.38
31	CA	2457	PSU	C6-C5	-2.01	1.35	1.38
31	CA	1917	PSU	C6-C5	-2.00	1.35	1.38
55	DA	2605	PSU	C6-C5	-2.00	1.35	1.38
55	DA	2498	OMC	O4'-C1'	2.02	1.44	1.41
55	DA	2552	OMU	C6-N1	2.15	1.38	1.35
1	BA	966	2MG	C6-C5	2.18	1.45	1.41
55	DA	1915	3TD	C4-N3	2.18	1.41	1.38
1	BA	1498	UR3	C6-N1	2.19	1.38	1.35
31	CA	2251	OMG	C6-C5	2.22	1.45	1.41
31	CA	2498	OMC	C6-N1	2.23	1.38	1.35
1	AA	1207	2MG	C6-C5	2.25	1.45	1.41
31	CA	1915	3TD	C4-N3	2.31	1.41	1.38
41	CN	81	4D4	CB-CA	2.35	1.58	1.54
55	DA	745	1MG	C6-N1	2.38	1.41	1.38
31	CA	2552	OMU	C6-N1	2.42	1.38	1.35
55	DA	2445	2MG	C6-C5	2.48	1.46	1.41
41	DN	81[A]	4D4	CB-CA	2.52	1.58	1.54
1	BA	1207	2MG	C6-C5	2.63	1.46	1.41
1	BA	1498	UR3	C4-N3	2.65	1.42	1.38
55	DA	2580	PSU	C4-N3	2.66	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	1516	2MG	C6-C5	2.69	1.46	1.41
1	AA	966	2MG	C6-C5	2.72	1.46	1.41
55	DA	2457	PSU	C4-N3	2.77	1.38	1.33
55	DA	2604	PSU	C4-N3	2.87	1.38	1.33
55	DA	2445	2MG	C6-N1	2.99	1.38	1.33
55	DA	746	PSU	C4-N3	3.04	1.38	1.33
1	BA	527	G7M	C6-N1	3.04	1.38	1.33
31	CA	2445	2MG	C6-C5	3.05	1.47	1.41
55	DA	1835	2MG	C6-N1	3.07	1.38	1.33
55	DA	747	5MU	C4-N3	3.08	1.38	1.33
55	DA	1939	5MU	C4-N3	3.10	1.38	1.33
31	CA	2552	OMU	C4-N3	3.10	1.38	1.33
1	AA	527	G7M	C6-N1	3.13	1.38	1.33
31	CA	2504	PSU	C4-N3	3.14	1.38	1.33
55	DA	2552	OMU	C4-N3	3.15	1.38	1.33
55	DA	2605	PSU	C4-N3	3.15	1.38	1.33
31	CA	2069	G7M	C6-N1	3.15	1.38	1.33
1	AA	1516	2MG	C6-C5	3.21	1.47	1.41
55	DA	1917	PSU	C4-N3	3.23	1.38	1.33
55	DA	1911	PSU	C4-N3	3.23	1.38	1.33
31	CA	2605	PSU	C4-N3	3.23	1.38	1.33
31	CA	2457	PSU	C4-N3	3.24	1.38	1.33
55	DA	2504	PSU	C4-N3	3.24	1.38	1.33
31	CA	1917	PSU	C4-N3	3.25	1.38	1.33
31	CA	2580	PSU	C4-N3	3.26	1.38	1.33
1	BA	516	PSU	C4-N3	3.26	1.38	1.33
55	DA	2069	G7M	C6-N1	3.27	1.38	1.33
1	BA	966	2MG	C6-N1	3.28	1.39	1.33
1	AA	1207	2MG	C6-N1	3.30	1.39	1.33
31	CA	747	5MU	C4-N3	3.31	1.39	1.33
31	CA	955	PSU	C4-N3	3.31	1.39	1.33
1	AA	516	PSU	C4-N3	3.31	1.39	1.33
31	CA	746	PSU	C4-N3	3.32	1.39	1.33
31	CA	1835	2MG	C6-N1	3.33	1.39	1.33
55	DA	2251	OMG	C6-N1	3.35	1.39	1.33
55	DA	955	PSU	C4-N3	3.37	1.39	1.33
31	CA	1911	PSU	C4-N3	3.37	1.39	1.33
31	CA	2251	OMG	C6-N1	3.38	1.39	1.33
55	DA	745	1MG	C6-C5	3.39	1.47	1.40
1	BA	1516	2MG	C6-N1	3.40	1.39	1.33
31	CA	1939	5MU	C4-N3	3.42	1.39	1.33
1	AA	1516	2MG	C6-N1	3.42	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	1207	2MG	C6-N1	3.43	1.39	1.33
31	CA	2445	2MG	C6-N1	3.44	1.39	1.33
1	AA	966	2MG	C6-N1	3.44	1.39	1.33
31	CA	745	1MG	C6-C5	3.85	1.48	1.40
32	DD	150[B]	MEQ	CB-CA	5.85	1.61	1.53

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	1939	5MU	C5-C4-N3	-12.10	115.19	125.35
31	CA	747	5MU	C5-C4-N3	-12.09	115.20	125.35
31	CA	1939	5MU	C5-C4-N3	-12.07	115.22	125.35
55	DA	747	5MU	C5-C4-N3	-11.94	115.33	125.35
31	CA	2069	G7M	C5-C6-N1	-10.01	110.43	123.52
1	AA	527	G7M	C5-C6-N1	-9.90	110.58	123.52
55	DA	2069	G7M	C5-C6-N1	-9.83	110.67	123.52
1	BA	527	G7M	C5-C6-N1	-9.83	110.67	123.52
55	DA	2445	2MG	C5-C6-N1	-9.08	111.65	123.52
31	CA	2445	2MG	C5-C6-N1	-8.73	112.11	123.52
1	AA	1207	2MG	C5-C6-N1	-8.69	112.16	123.52
1	AA	966	2MG	C5-C6-N1	-8.59	112.30	123.52
31	CA	2251	OMG	C5-C6-N1	-8.48	112.44	123.52
1	BA	966	2MG	C5-C6-N1	-8.47	112.45	123.52
1	BA	1207	2MG	C5-C6-N1	-8.40	112.54	123.52
31	CA	1835	2MG	C5-C6-N1	-8.30	112.67	123.52
55	DA	1835	2MG	C5-C6-N1	-8.26	112.72	123.52
1	BA	1516	2MG	C5-C6-N1	-8.25	112.73	123.52
1	AA	1516	2MG	C5-C6-N1	-8.11	112.93	123.52
55	DA	2251	OMG	C5-C6-N1	-8.09	112.94	123.52
1	BA	527	G7M	C6-C5-C4	-6.29	113.67	120.86
1	AA	527	G7M	C6-C5-C4	-5.69	114.35	120.86
31	CA	2069	G7M	C6-C5-C4	-4.37	115.86	120.86
55	DA	2069	G7M	C6-C5-C4	-4.24	116.01	120.86
55	DA	2069	G7M	N3-C2-N1	-3.89	122.27	127.56
1	AA	527	G7M	N3-C2-N1	-3.73	122.49	127.56
31	CA	2069	G7M	N3-C2-N1	-3.61	122.64	127.56
1	BA	527	G7M	N3-C2-N1	-3.58	122.68	127.56
31	CA	2552	OMU	C5-C4-N3	-3.43	114.85	123.28
55	DA	2552	OMU	C5-C4-N3	-3.42	114.89	123.28
31	CA	745	1MG	C6-C5-C4	-3.32	117.56	119.93
1	AA	1516	2MG	C6-C5-C4	-3.28	117.11	120.86
55	DA	2251	OMG	N3-C2-N1	-3.24	123.15	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	1516	2MG	C6-C5-C4	-3.12	117.30	120.86
55	DA	1915	3TD	C5-C4-N3	-3.07	116.14	118.65
31	CA	1915	3TD	C5-C4-N3	-3.03	116.18	118.65
31	CA	2251	OMG	N3-C2-N1	-2.99	123.48	127.56
55	DA	745	1MG	C6-C5-C4	-2.98	117.80	119.93
1	BA	1207	2MG	C6-C5-C4	-2.97	117.46	120.86
55	DA	2445	2MG	C6-C5-C4	-2.92	117.52	120.86
55	DA	1835	2MG	C6-C5-C4	-2.85	117.61	120.86
31	CA	2445	2MG	C6-C5-C4	-2.82	117.63	120.86
1	AA	966	2MG	C6-C5-C4	-2.80	117.66	120.86
31	CA	2251	OMG	C6-C5-C4	-2.69	117.78	120.86
1	AA	1207	2MG	C6-C5-C4	-2.68	117.79	120.86
55	DA	745	1MG	C5-C6-N1	-2.67	114.85	118.35
1	BA	966	2MG	C6-C5-C4	-2.63	117.85	120.86
32	DD	150[A]	MEQ	O-C-CA	-2.62	118.70	125.72
31	CA	745	1MG	C5-C6-N1	-2.56	115.00	118.35
31	CA	1835	2MG	C6-C5-C4	-2.52	117.98	120.86
31	CA	2605	PSU	C4-C5-C1'	-2.47	117.05	121.22
32	DD	150[A]	MEQ	CG-CB-CA	-2.38	108.62	114.03
55	DA	2251	OMG	C6-C5-C4	-2.38	118.14	120.86
55	DA	2605	PSU	C4-C5-C1'	-2.32	117.31	121.22
55	DA	745	1MG	O4'-C4'-C3'	-2.07	100.97	105.16
55	DA	2503	2MA	CM2-C2-N3	2.03	120.67	117.22
1	AA	516	PSU	O4'-C1'-C2'	2.03	106.89	104.69
55	DA	2445	2MG	N2-C2-N3	2.04	119.31	116.94
31	CA	2445	2MG	N2-C2-N3	2.05	119.31	116.94
31	CA	1962	5MC	CM5-C5-C6	2.09	122.87	118.63
1	BA	516	PSU	O4'-C1'-C2'	2.10	106.96	104.69
55	DA	1939	5MU	C5M-C5-C6	2.11	122.91	118.63
55	DA	747	5MU	C5M-C5-C6	2.15	122.98	118.63
1	BA	1407	5MC	CM5-C5-C6	2.16	123.01	118.63
1	AA	1407	5MC	CM5-C5-C6	2.17	123.02	118.63
12	AL	89	D2T	C-CA-N	2.18	114.77	109.95
1	BA	967	5MC	CM5-C5-C6	2.19	123.06	118.63
31	CA	1939	5MU	C5M-C5-C6	2.19	123.07	118.63
31	CA	747	5MU	C5M-C5-C6	2.20	123.09	118.63
1	BA	1516	2MG	N2-C2-N3	2.20	119.50	116.94
1	AA	1516	2MG	N2-C2-N3	2.20	119.50	116.94
1	AA	967	5MC	CM5-C5-C6	2.22	123.13	118.63
1	AA	1207	2MG	N2-C2-N3	2.34	119.65	116.94
1	BA	1207	2MG	N2-C2-N3	2.43	119.76	116.94
31	CA	1835	2MG	N2-C2-N3	2.43	119.76	116.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	966	2MG	N2-C2-N3	2.43	119.76	116.94
55	DA	1835	2MG	N2-C2-N3	2.46	119.80	116.94
12	BL	89	D2T	C-CA-N	2.53	115.54	109.95
55	DA	2069	G7M	O4'-C1'-N9	2.62	113.06	108.11
55	DA	1618	6MZ	C2-N1-C6	2.73	118.43	116.47
31	CA	2503	2MA	C2-N3-C4	2.80	116.64	115.29
55	DA	2580	PSU	O4'-C1'-C2'	2.89	107.82	104.69
31	CA	2069	G7M	O4'-C1'-N9	2.90	113.58	108.11
55	DA	2030	6MZ	C2-N1-C6	3.00	118.63	116.47
31	CA	2030	6MZ	C2-N1-C6	3.01	118.63	116.47
31	CA	1618	6MZ	C2-N1-C6	3.01	118.63	116.47
31	CA	2580	PSU	O4'-C1'-C2'	3.11	108.06	104.69
1	BA	1402	4OC	CM4-N4-C4	3.18	125.55	122.87
32	DD	150[B]	MEQ	CB-CA-N	3.22	119.60	110.54
55	DA	2503	2MA	C2-N3-C4	3.24	116.85	115.29
32	DD	150[B]	MEQ	CG-CB-CA	3.33	121.61	114.03
1	AA	1402	4OC	CM4-N4-C4	3.43	125.77	122.87
32	DD	150[B]	MEQ	CB-CG-CD	3.62	121.54	113.26
1	BA	1402	4OC	C2-N3-C4	4.14	120.69	115.43
1	AA	1402	4OC	C2-N3-C4	4.15	120.70	115.43
1	AA	527	G7M	O4'-C1'-N9	5.13	117.80	108.11
1	BA	527	G7M	O4'-C1'-N9	5.90	119.26	108.11
1	AA	1516	2MG	C6-N1-C2	6.30	124.27	115.24
31	CA	1835	2MG	C6-N1-C2	6.35	124.33	115.24
1	AA	966	2MG	C6-N1-C2	6.42	124.43	115.24
1	BA	1516	2MG	C6-N1-C2	6.45	124.47	115.24
31	CA	2445	2MG	C6-N1-C2	6.52	124.57	115.24
1	BA	966	2MG	C6-N1-C2	6.53	124.58	115.24
55	DA	1835	2MG	C6-N1-C2	6.53	124.60	115.24
1	BA	1207	2MG	C6-N1-C2	6.58	124.67	115.24
1	AA	1207	2MG	C6-N1-C2	6.66	124.78	115.24
1	AA	527	G7M	C6-N1-C2	7.05	124.14	115.88
55	DA	2069	G7M	C6-N1-C2	7.20	124.31	115.88
1	BA	527	G7M	C6-N1-C2	7.42	124.57	115.88
55	DA	2445	2MG	C6-N1-C2	7.46	125.92	115.24
31	CA	2069	G7M	C6-N1-C2	7.47	124.64	115.88
55	DA	2251	OMG	C6-N1-C2	7.70	124.91	115.88
31	CA	2251	OMG	C6-N1-C2	8.02	125.28	115.88
31	CA	2552	OMU	C4-N3-C2	12.10	126.96	114.21
55	DA	2552	OMU	C4-N3-C2	12.11	126.97	114.21
55	DA	2604	PSU	C4-N3-C2	13.45	126.38	115.16
55	DA	955	PSU	C4-N3-C2	13.51	126.43	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	1911	PSU	C4-N3-C2	13.51	126.43	115.16
31	CA	2605	PSU	C4-N3-C2	13.52	126.44	115.16
31	CA	955	PSU	C4-N3-C2	13.52	126.44	115.16
31	CA	1911	PSU	C4-N3-C2	13.53	126.45	115.16
31	CA	746	PSU	C4-N3-C2	13.56	126.47	115.16
31	CA	2580	PSU	C4-N3-C2	13.57	126.48	115.16
1	AA	516	PSU	C4-N3-C2	13.58	126.49	115.16
31	CA	2504	PSU	C4-N3-C2	13.60	126.50	115.16
55	DA	746	PSU	C4-N3-C2	13.60	126.51	115.16
31	CA	2457	PSU	C4-N3-C2	13.60	126.51	115.16
55	DA	2580	PSU	C4-N3-C2	13.61	126.51	115.16
55	DA	1917	PSU	C4-N3-C2	13.62	126.52	115.16
55	DA	2605	PSU	C4-N3-C2	13.63	126.53	115.16
1	BA	516	PSU	C4-N3-C2	13.68	126.57	115.16
55	DA	2504	PSU	C4-N3-C2	13.70	126.58	115.16
55	DA	2457	PSU	C4-N3-C2	13.70	126.59	115.16
31	CA	1917	PSU	C4-N3-C2	13.75	126.63	115.16
55	DA	747	5MU	C4-N3-C2	14.31	127.10	115.16
31	CA	1939	5MU	C4-N3-C2	14.54	127.29	115.16
31	CA	747	5MU	C4-N3-C2	14.54	127.29	115.16
55	DA	1939	5MU	C4-N3-C2	14.54	127.29	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1518	MA6	1	0
1	AA	1519	MA6	1	0
1	BA	1518	MA6	1	0
1	BA	1519	MA6	1	0
31	CA	2030	6MZ	2	0
31	CA	2445	2MG	1	0
31	CA	2503	2MA	1	0
31	CA	747	5MU	1	0
55	DA	2030	6MZ	1	0
55	DA	2445	2MG	1	0
55	DA	2449	H2U	1	0
55	DA	2498	OMC	1	0
55	DA	747	5MU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	DD	150[B]	MEQ	1	0
41	DN	81[B]	4D4	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
57	PG4	AA	1670	-	12,12,12	0.28	0	11,11,11	0.42	0
58	MPD	AA	1671	-	6,7,7	0.42	0	6,10,10	0.38	0
59	PUT	AA	1672	-	5,5,5	0.26	0	4,4,4	0.20	0
59	PUT	AA	1673	-	5,5,5	0.20	0	4,4,4	0.19	0
59	PUT	AA	1674	-	5,5,5	0.20	0	4,4,4	0.20	0
59	PUT	AA	1675	-	5,5,5	0.25	0	4,4,4	0.24	0
58	MPD	AA	1676	-	6,7,7	0.40	0	6,10,10	0.36	0
60	T1C	AA	1677	56	44,45,45	0.99	4 (9%)	45,72,72	1.05	3 (6%)
62	PEG	AL	201	-	6,6,6	0.26	0	5,5,5	0.10	0
57	PG4	BA	1642	-	12,12,12	0.22	0	11,11,11	0.22	0
60	T1C	BA	1643	56	44,45,45	0.96	3 (6%)	45,72,72	1.01	2 (4%)
63	EDO	D1	101	-	3,3,3	0.64	0	2,2,2	0.19	0
64	PGE	D1	102	-	9,9,9	0.31	0	8,8,8	0.28	0
62	PEG	D1	103	-	6,6,6	0.45	0	5,5,5	0.12	0
64	PGE	D3	101	-	9,9,9	0.31	0	8,8,8	0.21	0
62	PEG	D3	102	-	6,6,6	0.34	0	5,5,5	0.23	0
63	EDO	DA	3001	-	3,3,3	0.81	0	2,2,2	0.15	0
59	PUT	DA	3002	-	5,5,5	0.20	0	4,4,4	0.14	0
63	EDO	DA	3003	-	3,3,3	0.74	0	2,2,2	0.17	0
63	EDO	DA	3004	-	3,3,3	0.70	0	2,2,2	0.17	0
65	SPD	DA	3183	-	9,9,9	0.15	0	8,8,8	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
59	PUT	DA	3184	-	5,5,5	0.27	0	4,4,4	0.20	0
66	1PE	DA	3185	-	15,15,15	0.17	0	14,14,14	0.16	0
64	PGE	DA	3186	-	9,9,9	0.36	0	8,8,8	0.55	0
65	SPD	DA	3187	-	9,9,9	0.18	0	8,8,8	0.42	0
59	PUT	DA	3188	-	5,5,5	0.44	0	4,4,4	0.29	0
59	PUT	DA	3189	-	5,5,5	0.49	0	4,4,4	0.43	0
58	MPD	DA	3190	-	6,7,7	0.38	0	6,10,10	0.44	0
67	ACY	DA	3191	-	0,3,3	0.00	-	0,3,3	0.00	-
58	MPD	DA	3192	-	6,7,7	0.42	0	6,10,10	0.58	0
57	PG4	DA	3193	-	12,12,12	0.31	0	11,11,11	0.43	0
63	EDO	DA	3194	-	3,3,3	0.63	0	2,2,2	0.11	0
59	PUT	DA	3195	-	5,5,5	0.34	0	4,4,4	0.48	0
67	ACY	DA	3196	-	0,3,3	0.00	-	0,3,3	0.00	-
63	EDO	DA	3197	-	3,3,3	0.62	0	2,2,2	0.28	0
63	EDO	DA	3198	-	3,3,3	0.65	0	2,2,2	0.42	0
62	PEG	DA	3199	-	6,6,6	0.32	0	5,5,5	0.20	0
62	PEG	DA	3200	-	6,6,6	0.53	0	5,5,5	0.25	0
67	ACY	DA	3201	-	0,3,3	0.00	-	0,3,3	0.00	-
66	1PE	DA	3202	-	15,15,15	0.37	0	14,14,14	0.39	0
58	MPD	DA	3203	-	6,7,7	0.62	0	6,10,10	0.59	0
59	PUT	DA	3204	-	5,5,5	0.38	0	4,4,4	0.28	0
65	SPD	DA	3205	-	9,9,9	0.26	0	8,8,8	0.19	0
58	MPD	DA	3206	-	6,7,7	0.60	0	6,10,10	0.51	0
63	EDO	DA	3207	-	3,3,3	0.68	0	2,2,2	0.21	0
63	EDO	DA	3208	-	3,3,3	0.57	0	2,2,2	0.36	0
58	MPD	DA	3209	-	6,7,7	0.39	0	6,10,10	0.26	0
68	GUN	DA	3210	-	9,12,12	2.07	2 (22%)	7,17,17	4.82	5 (71%)
59	PUT	DA	3211	-	5,5,5	0.35	0	4,4,4	0.15	0
59	PUT	DA	3212	-	5,5,5	0.40	0	4,4,4	0.30	0
64	PGE	DA	3213	-	9,9,9	0.17	0	8,8,8	0.18	0
63	EDO	DA	3214	-	3,3,3	0.64	0	2,2,2	0.29	0
57	PG4	DA	3215	-	12,12,12	0.18	0	11,11,11	0.14	0
64	PGE	DA	3216	-	9,9,9	0.15	0	8,8,8	0.25	0
62	PEG	DA	3217	-	6,6,6	0.31	0	5,5,5	0.06	0
59	PUT	DA	3218	-	5,5,5	0.17	0	4,4,4	0.19	0
69	TRS	DA	3219	-	7,7,7	0.54	0	9,9,9	0.42	0
59	PUT	DA	3220	-	5,5,5	0.23	0	4,4,4	0.15	0
59	PUT	DA	3221	-	5,5,5	0.48	0	4,4,4	0.58	0
59	PUT	DA	3222	-	5,5,5	0.28	0	4,4,4	0.36	0
65	SPD	DA	3223	-	9,9,9	0.21	0	8,8,8	0.63	0
64	PGE	DA	3224	-	9,9,9	0.26	0	8,8,8	0.17	0
62	PEG	DA	3225	-	6,6,6	0.51	0	5,5,5	0.23	0
62	PEG	DA	3226	-	6,6,6	0.44	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
63	EDO	DB	210	-	3,3,3	0.58	0	2,2,2	0.28	0
63	EDO	DB	211	-	3,3,3	0.58	0	2,2,2	0.23	0
64	PGE	DD	301	-	9,9,9	0.30	0	8,8,8	0.32	0
58	MPD	DE	301	-	6,7,7	0.55	0	6,10,10	0.68	0
58	MPD	DE	302	-	6,7,7	0.49	0	6,10,10	0.34	0
58	MPD	DK	201	-	6,7,7	0.46	0	6,10,10	0.25	0
62	PEG	DL	201	-	6,6,6	0.15	0	5,5,5	0.13	0
58	MPD	DN	201	-	6,7,7	0.64	0	6,10,10	0.32	0
62	PEG	DP	201	-	6,6,6	0.31	0	5,5,5	0.13	0
62	PEG	DQ	201	-	6,6,6	0.23	0	5,5,5	0.14	0
57	PG4	DQ	202	-	12,12,12	0.17	0	11,11,11	0.16	0
57	PG4	DR	202	-	12,12,12	0.44	0	11,11,11	0.54	0
64	PGE	DS	201	-	9,9,9	0.49	0	8,8,8	0.48	0
57	PG4	DS	202	-	12,12,12	0.48	0	11,11,11	0.42	0
58	MPD	DS	203	-	6,7,7	0.37	0	6,10,10	0.52	0
58	MPD	DT	201	-	6,7,7	0.48	0	6,10,10	0.12	0
58	MPD	DT	202	-	6,7,7	0.42	0	6,10,10	0.44	0
64	PGE	DU	101	-	9,9,9	0.27	0	8,8,8	0.37	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
60	T1C	AA	1677	56	-	0/22/80/80	0/4/4/4
62	PEG	AL	201	-	-	0/4/4/4	0/0/0/0
57	PG4	BA	1642	-	-	0/10/10/10	0/0/0/0
60	T1C	BA	1643	56	-	0/22/80/80	0/4/4/4
63	EDO	D1	101	-	-	0/1/1/1	0/0/0/0
64	PGE	D1	102	-	-	0/7/7/7	0/0/0/0
62	PEG	D1	103	-	-	0/4/4/4	0/0/0/0
64	PGE	D3	101	-	-	0/7/7/7	0/0/0/0
62	PEG	D3	102	-	-	0/4/4/4	0/0/0/0
63	EDO	DA	3001	-	-	0/1/1/1	0/0/0/0
59	PUT	DA	3002	-	-	0/3/3/3	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	EDO	DA	3003	-	-	0/1/1/1	0/0/0/0
63	EDO	DA	3004	-	-	0/1/1/1	0/0/0/0
65	SPD	DA	3183	-	-	0/7/7/7	0/0/0/0
59	PUT	DA	3184	-	-	0/3/3/3	0/0/0/0
66	1PE	DA	3185	-	-	0/13/13/13	0/0/0/0
64	PGE	DA	3186	-	-	0/7/7/7	0/0/0/0
65	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
67	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
63	EDO	DA	3194	-	-	0/1/1/1	0/0/0/0
59	PUT	DA	3195	-	-	0/3/3/3	0/0/0/0
67	ACY	DA	3196	-	-	0/0/0/0	0/0/0/0
63	EDO	DA	3197	-	-	0/1/1/1	0/0/0/0
63	EDO	DA	3198	-	-	0/1/1/1	0/0/0/0
62	PEG	DA	3199	-	-	0/4/4/4	0/0/0/0
62	PEG	DA	3200	-	-	0/4/4/4	0/0/0/0
67	ACY	DA	3201	-	-	0/0/0/0	0/0/0/0
66	1PE	DA	3202	-	-	0/13/13/13	0/0/0/0
58	MPD	DA	3203	-	-	0/5/5/5	0/0/0/0
59	PUT	DA	3204	-	-	0/3/3/3	0/0/0/0
65	SPD	DA	3205	-	-	0/7/7/7	0/0/0/0
58	MPD	DA	3206	-	-	0/5/5/5	0/0/0/0
63	EDO	DA	3207	-	-	0/1/1/1	0/0/0/0
63	EDO	DA	3208	-	-	0/1/1/1	0/0/0/0
58	MPD	DA	3209	-	-	0/5/5/5	0/0/0/0
68	GUN	DA	3210	-	-	0/0/0/0	0/2/2/2
59	PUT	DA	3211	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3212	-	-	0/3/3/3	0/0/0/0
64	PGE	DA	3213	-	-	0/7/7/7	0/0/0/0
63	EDO	DA	3214	-	-	0/1/1/1	0/0/0/0
57	PG4	DA	3215	-	-	0/10/10/10	0/0/0/0
64	PGE	DA	3216	-	-	0/7/7/7	0/0/0/0
62	PEG	DA	3217	-	-	0/4/4/4	0/0/0/0
59	PUT	DA	3218	-	-	0/3/3/3	0/0/0/0
69	TRS	DA	3219	-	-	0/9/9/9	0/0/0/0
59	PUT	DA	3220	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3221	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3222	-	-	0/3/3/3	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
65	SPD	DA	3223	-	-	0/7/7/7	0/0/0/0
64	PGE	DA	3224	-	-	0/7/7/7	0/0/0/0
62	PEG	DA	3225	-	-	0/4/4/4	0/0/0/0
62	PEG	DA	3226	-	-	0/4/4/4	0/0/0/0
63	EDO	DB	210	-	-	0/1/1/1	0/0/0/0
63	EDO	DB	211	-	-	0/1/1/1	0/0/0/0
64	PGE	DD	301	-	-	0/7/7/7	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
62	PEG	DL	201	-	-	0/4/4/4	0/0/0/0
58	MPD	DN	201	-	-	0/5/5/5	0/0/0/0
62	PEG	DP	201	-	-	0/4/4/4	0/0/0/0
62	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
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
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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	AA	1677	T1C	C4-N4	2.15	1.51	1.47
60	BA	1643	T1C	C7-C61	2.15	1.43	1.40
60	AA	1677	T1C	C7-C61	2.24	1.43	1.40
60	AA	1677	T1C	C7-N7	2.55	1.49	1.42
60	BA	1643	T1C	C7-N7	2.62	1.49	1.42
60	AA	1677	T1C	C4-C3	2.88	1.57	1.51
60	BA	1643	T1C	C4-C3	3.28	1.58	1.51
68	DA	3210	GUN	C6-N1	3.31	1.39	1.33
68	DA	3210	GUN	C6-C5	4.52	1.50	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	DA	3210	GUN	C5-C6-N1	-8.80	112.02	123.52
60	BA	1643	T1C	C8-C9-C10	-3.97	115.88	120.54
60	AA	1677	T1C	C8-C9-C10	-3.59	116.33	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	DA	3210	GUN	C6-C5-C4	-2.99	117.44	120.86
68	DA	3210	GUN	N3-C2-N1	-2.64	123.97	127.56
68	DA	3210	GUN	C5-C4-N9	-2.54	106.62	111.12
60	BA	1643	T1C	C61-C7-N7	2.21	121.01	118.94
60	AA	1677	T1C	C5-C51-C1B	2.24	113.26	109.37
60	AA	1677	T1C	C6-C61-C1A	2.26	122.38	118.05
68	DA	3210	GUN	C6-N1-C2	7.89	125.12	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

30 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	1670	PG4	1	0
64	D1	102	PGE	2	0
62	D1	103	PEG	1	0
62	D3	102	PEG	2	0
59	DA	3189	PUT	1	0
58	DA	3190	MPD	1	0
58	DA	3192	MPD	2	0
57	DA	3193	PG4	1	0
63	DA	3194	EDO	1	0
59	DA	3195	PUT	3	0
63	DA	3197	EDO	1	0
62	DA	3200	PEG	1	0
58	DA	3203	MPD	2	0
59	DA	3212	PUT	1	0
64	DA	3213	PGE	1	0
57	DA	3215	PG4	1	0
64	DA	3216	PGE	1	0
59	DA	3218	PUT	1	0
69	DA	3219	TRS	1	0
59	DA	3221	PUT	3	0
59	DA	3222	PUT	1	0
65	DA	3223	SPD	4	0
64	DA	3224	PGE	3	0
63	DB	211	EDO	1	0
64	DD	301	PGE	2	0
58	DN	201	MPD	1	0
62	DP	201	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	DR	202	PG4	5	0
57	DS	202	PG4	1	0
64	DU	101	PGE	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1523/1534 (99%)	0.68	100 (6%) 22 11	46, 105, 241, 293	0
1	BA	1522/1534 (99%)	1.52	394 (25%) 1 1	61, 140, 279, 284	0
2	AB	224/224 (100%)	1.62	72 (32%) 1 0	83, 127, 202, 270	0
2	BB	224/224 (100%)	1.76	78 (34%) 0 0	99, 144, 211, 261	0
3	AC	206/206 (100%)	0.82	30 (14%) 3 1	80, 108, 141, 163	0
3	BC	206/206 (100%)	2.63	116 (56%) 0 0	115, 151, 190, 231	0
4	AD	205/205 (100%)	0.61	17 (8%) 14 7	64, 103, 131, 154	0
4	BD	205/205 (100%)	0.19	1 (0%) 91 81	61, 81, 107, 131	0
5	AE	155/155 (100%)	0.77	13 (8%) 14 7	67, 91, 133, 169	0
5	BE	150/155 (96%)	1.16	34 (22%) 1 1	77, 97, 144, 227	0
6	AF	106/106 (100%)	0.83	19 (17%) 2 1	82, 105, 128, 142	0
6	BF	100/106 (94%)	0.97	14 (14%) 4 2	86, 121, 146, 154	0
7	AG	151/151 (100%)	2.15	64 (42%) 0 0	107, 137, 166, 179	0
7	BG	151/151 (100%)	5.29	125 (82%) 0 0	147, 203, 218, 228	0
8	AH	129/129 (100%)	0.63	9 (6%) 19 10	71, 91, 118, 136	0
8	BH	129/129 (100%)	1.02	24 (18%) 2 1	91, 116, 150, 168	0
9	AI	127/127 (100%)	2.31	58 (45%) 0 0	96, 132, 169, 200	0
9	BI	127/127 (100%)	3.78	77 (60%) 0 0	138, 176, 209, 229	0
10	AJ	99/99 (100%)	2.03	41 (41%) 0 0	94, 121, 153, 168	0
10	BJ	98/99 (98%)	4.86	78 (79%) 0 0	141, 171, 197, 207	0
11	AK	117/117 (100%)	1.61	35 (29%) 1 0	68, 112, 147, 163	0
11	BK	117/117 (100%)	1.47	32 (27%) 1 0	83, 116, 148, 168	0
12	AL	122/123 (99%)	0.59	4 (3%) 50 31	55, 72, 104, 132	0
12	BL	122/123 (99%)	1.39	29 (23%) 1 1	79, 97, 118, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
13	AM	114/114 (100%)	2.47	57 (50%)	0	0	106, 131, 182, 202	0
13	BM	114/114 (100%)	5.54	105 (92%)	0	0	203, 237, 245, 249	0
14	AN	100/100 (100%)	1.82	37 (37%)	0	0	90, 117, 206, 215	0
14	BN	100/100 (100%)	3.86	75 (75%)	0	0	132, 181, 239, 250	0
15	AO	88/88 (100%)	0.68	10 (11%)	7	3	72, 94, 112, 132	0
15	BO	88/88 (100%)	1.25	20 (22%)	1	1	79, 112, 132, 150	0
16	AP	82/82 (100%)	1.27	21 (25%)	1	1	67, 86, 121, 139	0
16	BP	82/82 (100%)	2.79	47 (57%)	0	0	94, 111, 157, 166	0
17	AQ	80/80 (100%)	0.65	5 (6%)	23	12	70, 86, 119, 143	0
17	BQ	80/80 (100%)	2.17	35 (43%)	0	0	100, 128, 151, 156	0
18	AR	55/55 (100%)	1.21	12 (21%)	1	1	79, 99, 135, 164	0
18	BR	55/55 (100%)	1.07	6 (10%)	7	4	80, 96, 129, 157	0
19	AS	79/79 (100%)	1.55	24 (30%)	1	0	103, 119, 156, 164	0
19	BS	79/79 (100%)	5.05	66 (83%)	0	0	215, 232, 243, 251	0
20	AT	86/86 (100%)	1.04	9 (10%)	8	4	70, 85, 120, 133	0
20	BT	85/86 (98%)	3.28	53 (62%)	0	0	108, 128, 165, 179	0
21	AU	56/56 (100%)	1.60	18 (32%)	1	0	83, 123, 159, 172	0
21	BU	56/56 (100%)	1.01	8 (14%)	4	2	80, 106, 149, 160	0
22	C1	56/56 (100%)	3.34	39 (69%)	0	0	110, 150, 178, 195	0
22	D1	56/56 (100%)	0.57	0	100	100	26, 46, 71, 102	0
23	C2	50/51 (98%)	3.70	34 (68%)	0	0	133, 148, 161, 183	0
23	D2	51/51 (100%)	0.71	5 (9%)	10	5	55, 69, 95, 110	0
24	C3	46/46 (100%)	4.61	38 (82%)	0	0	108, 117, 127, 138	0
24	D3	46/46 (100%)	0.59	2 (4%)	39	23	38, 46, 61, 104	0
25	C4	64/64 (100%)	3.13	44 (68%)	0	0	112, 130, 142, 148	0
25	D4	64/64 (100%)	0.56	0	100	100	36, 44, 53, 68	0
26	C5	38/38 (100%)	2.73	23 (60%)	0	0	108, 122, 133, 143	0
26	D5	38/38 (100%)	0.63	1 (2%)	59	38	43, 54, 68, 91	0
27	C0	58/58 (100%)	3.37	40 (68%)	0	0	104, 121, 140, 143	0
27	D0	58/58 (100%)	0.51	0	100	100	33, 40, 60, 72	0
28	CB	118/120 (98%)	1.70	44 (37%)	0	0	140, 195, 250, 254	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DB	120/120 (100%)	0.29	0 100 100	33, 60, 99, 143	0
29	CC	271/272 (99%)	1.49	88 (32%) 1 0	88, 119, 152, 165	0
29	DC	271/272 (99%)	0.29	6 (2%) 65 44	31, 57, 83, 96	0
30	CD	209/209 (100%)	2.99	131 (62%) 0 0	103, 134, 170, 190	0
31	CA	2876/2904 (99%)	1.89	1013 (35%) 0 0	73, 178, 274, 295	0
32	DD	208/209 (99%)	0.14	0 100 100	22, 41, 69, 91	0
33	CE	201/201 (100%)	3.30	141 (70%) 0 0	119, 167, 201, 218	0
33	DE	201/201 (100%)	0.37	3 (1%) 76 57	31, 59, 101, 141	0
34	CF	177/178 (99%)	4.96	152 (85%) 0 0	204, 217, 226, 233	0
34	DF	177/178 (99%)	0.67	16 (9%) 12 6	58, 84, 125, 138	0
35	CG	176/176 (100%)	4.31	143 (81%) 0 0	140, 181, 219, 228	0
35	DG	176/176 (100%)	0.34	8 (4%) 37 21	49, 73, 99, 128	0
36	CH	149/149 (100%)	2.33	79 (53%) 0 0	86, 156, 175, 183	0
36	DH	149/149 (100%)	2.09	62 (41%) 0 0	79, 157, 193, 208	0
37	CJ	134/134 (100%)	7.50	127 (94%) 0 0	236, 253, 264, 272	0
37	DJ	134/134 (100%)	5.78	110 (82%) 0 0	204, 229, 238, 246	0
38	CK	142/142 (100%)	2.30	71 (50%) 0 0	105, 129, 168, 221	0
38	DK	142/142 (100%)	0.10	0 100 100	25, 37, 61, 75	0
39	CL	122/123 (99%)	1.69	43 (35%) 0 0	95, 116, 149, 167	0
39	DL	123/123 (100%)	0.08	0 100 100	30, 46, 71, 109	0
40	CM	144/144 (100%)	4.10	115 (79%) 0 0	113, 163, 214, 236	0
40	DM	144/144 (100%)	0.31	3 (2%) 67 46	21, 58, 88, 117	0
41	CN	135/136 (99%)	1.38	35 (25%) 1 1	98, 119, 150, 189	0
41	DN	135/136 (99%)	-0.04	0 100 100	29, 43, 69, 88	0
42	CO	120/125 (96%)	2.71	72 (60%) 0 0	110, 132, 155, 186	0
42	DO	125/125 (100%)	0.20	1 (0%) 87 73	29, 39, 68, 111	0
43	CP	116/117 (99%)	3.83	86 (74%) 0 0	147, 171, 185, 189	0
43	DP	117/117 (100%)	0.28	0 100 100	47, 60, 87, 97	0
44	CQ	114/114 (100%)	2.52	65 (57%) 0 0	108, 126, 156, 172	0
44	DQ	114/114 (100%)	0.13	3 (2%) 59 38	34, 52, 82, 114	0
45	CR	117/117 (100%)	2.83	70 (59%) 0 0	98, 138, 174, 199	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	DR	117/117 (100%)	0.27	1 (0%) 85 70	23, 33, 48, 70	0
46	CS	103/103 (100%)	4.13	85 (82%) 0 0	114, 143, 185, 201	0
46	DS	103/103 (100%)	0.12	1 (0%) 84 67	26, 45, 71, 93	0
47	CT	110/110 (100%)	2.50	62 (56%) 0 0	109, 137, 180, 193	0
47	DT	110/110 (100%)	0.09	1 (0%) 85 70	21, 36, 60, 118	0
48	CU	93/93 (100%)	3.95	72 (77%) 0 0	131, 156, 184, 194	0
48	DU	93/93 (100%)	0.62	5 (5%) 29 17	37, 60, 114, 130	0
49	CV	102/103 (99%)	5.47	88 (86%) 0 0	119, 167, 203, 213	0
49	DV	102/103 (99%)	0.55	11 (10%) 8 4	47, 64, 112, 144	0
50	CW	94/94 (100%)	2.59	53 (56%) 0 0	125, 145, 165, 170	0
50	DW	94/94 (100%)	0.05	0 100 100	38, 56, 80, 92	0
51	CX	75/76 (98%)	2.92	38 (50%) 0 0	111, 134, 148, 178	0
51	DX	76/76 (100%)	0.07	1 (1%) 79 61	31, 45, 69, 107	0
52	CY	77/77 (100%)	1.91	32 (41%) 0 0	103, 122, 147, 168	0
52	DY	77/77 (100%)	0.29	1 (1%) 79 61	37, 59, 92, 108	0
53	CZ	62/62 (100%)	4.43	49 (79%) 0 0	134, 171, 184, 195	0
53	DZ	62/62 (100%)	0.77	6 (9%) 10 5	52, 75, 111, 132	0
54	DI	135/135 (100%)	2.39	71 (52%) 0 0	82, 158, 202, 211	1 (0%)
55	DA	2873/2904 (98%)	0.62	134 (4%) 35 20	22, 48, 215, 300	0
All	All	20634/20751 (99%)	1.60	5696 (27%) 1 0	21, 116, 247, 300	1 (0%)

All (5696) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	DJ	54	PRO	42.6
37	DJ	76	ALA	22.9
9	BI	128	SER	22.8
37	CJ	13	VAL	22.7
37	DJ	55	ILE	22.0
37	CJ	69	PHE	21.4
37	DJ	53	LEU	21.3
37	CJ	76	ALA	20.6
34	CF	128	TYR	18.3
37	CJ	14	ALA	18.3
37	DJ	114	ALA	17.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
37	CJ	11	LEU	17.7
37	CJ	12	GLN	17.7
9	BI	16	ALA	17.3
37	DJ	79	LEU	16.3
51	CX	54	GLY	16.2
9	BI	31	ASN	16.2
49	CV	80	ALA	16.1
10	BJ	41	PRO	16.0
49	CV	31	SER	15.6
31	CA	2172	U	15.3
9	AI	130	ARG	15.3
10	BJ	74	VAL	15.2
10	BJ	8	ILE	15.1
37	CJ	54	PRO	15.0
7	BG	62	PHE	14.9
55	DA	2120	G	14.8
7	BG	65	ALA	14.7
20	BT	4	ILE	14.6
34	CF	85	ILE	14.6
37	DJ	80	LEU	14.6
40	CM	114	GLY	14.5
37	CJ	138	LEU	14.5
49	CV	20	GLY	14.3
13	BM	45	ILE	14.3
46	CS	96	VAL	14.1
1	BA	211	G	14.0
9	BI	130	ARG	13.9
31	CA	1067	A	13.9
49	CV	13	VAL	13.8
37	CJ	55	ILE	13.8
37	CJ	57	VAL	13.7
7	BG	52	GLN	13.7
37	DJ	78	VAL	13.7
37	DJ	96	ASP	13.6
10	BJ	42	LEU	13.6
33	CE	55	SER	13.5
10	BJ	73	LEU	13.5
37	DJ	135	SER	13.4
37	CJ	80	LEU	13.3
19	BS	48	THR	13.3
37	CJ	82	LYS	13.2
19	BS	66	MET	13.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
40	CM	80	SER	13.1
31	CA	1068	G	13.1
9	BI	17	ALA	13.1
34	CF	156	ILE	13.0
14	BN	60	GLN	13.0
49	CV	36	VAL	13.0
53	CZ	45	GLN	13.0
37	DJ	13	VAL	13.0
37	CJ	17	MET	12.9
7	BG	49	THR	12.8
54	DI	131	THR	12.8
7	BG	111	ARG	12.8
37	CJ	129	ILE	12.8
1	BA	1307	U	12.6
37	CJ	20	PRO	12.6
24	C3	1	MET	12.6
30	CD	4	LEU	12.5
37	CJ	21	SER	12.5
37	CJ	56	PRO	12.5
37	DJ	88	SER	12.5
19	BS	29	LYS	12.5
37	CJ	99	GLY	12.5
37	DJ	67	PHE	12.4
34	CF	76	GLY	12.4
30	CD	6	GLY	12.4
34	CF	157	THR	12.4
1	BA	1302	C	12.3
7	BG	42	ILE	12.3
1	AA	86	G	12.3
33	CE	172	ALA	12.3
48	CU	83	ALA	12.3
53	CZ	32	ALA	12.3
34	CF	40	VAL	12.2
48	CU	43	ILE	12.2
13	BM	105	ASN	12.2
1	BA	1242	G	12.2
1	BA	983	A	12.2
13	BM	46	SER	12.1
40	CM	101	ILE	12.1
13	BM	10	PRO	12.1
7	BG	133	THR	12.1
46	CS	50	GLY	12.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
22	C1	5	GLN	12.0
49	CV	33	LYS	12.0
7	BG	75	VAL	12.0
37	CJ	23	PRO	11.9
9	BI	67	VAL	11.9
48	CU	60	THR	11.9
35	CG	32	GLU	11.9
48	CU	59	ASN	11.8
46	CS	27	ILE	11.7
55	DA	2163	A	11.7
1	BA	1030	U	11.7
31	CA	2174	C	11.7
1	BA	1024	G	11.7
35	CG	40	ALA	11.6
35	CG	108	GLY	11.6
23	C2	24	THR	11.5
1	BA	1020	G	11.5
7	BG	116	MET	11.5
37	CJ	42	PHE	11.5
37	CJ	51	LYS	11.5
34	CF	154	ILE	11.4
9	BI	126	GLN	11.4
49	CV	39	ILE	11.3
46	CS	32	THR	11.3
13	BM	95	LEU	11.3
37	CJ	139	VAL	11.3
37	CJ	126	THR	11.3
37	CJ	59	ILE	11.2
31	CA	931	U	11.1
40	CM	100	ILE	11.1
31	CA	2110	G	11.1
31	CA	2126	A	11.1
31	CA	331	C	11.1
13	BM	84	GLY	11.0
40	CM	81	ASP	11.0
1	AA	1030	U	11.0
37	CJ	38	PHE	11.0
7	BG	134	ALA	11.0
49	CV	78	GLY	11.0
34	CF	97	TRP	11.0
13	BM	32	ALA	11.0
1	BA	209	U	10.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	BM	22	ILE	10.9
50	CW	57	TYR	10.8
40	CM	79	LEU	10.8
14	BN	4	GLN	10.8
34	CF	65	PRO	10.7
31	CA	1537	G	10.7
1	BA	1022	A	10.7
37	CJ	121	ASP	10.7
23	C2	47	VAL	10.6
20	BT	3	ASN	10.6
14	BN	36	ALA	10.6
40	CM	92	LEU	10.6
37	CJ	120	ALA	10.6
13	BM	23	TYR	10.6
53	CZ	15	ASN	10.6
35	CG	33	LEU	10.5
30	CD	26	VAL	10.5
37	DJ	12	GLN	10.5
37	CJ	97	LYS	10.5
37	DJ	23	PRO	10.5
49	CV	35	ILE	10.4
49	CV	50	PRO	10.4
1	BA	1021	A	10.4
35	CG	103	ILE	10.4
37	CJ	22	PRO	10.4
37	CJ	132	THR	10.4
22	C1	3	VAL	10.4
37	CJ	78	VAL	10.4
35	CG	148	LEU	10.3
7	BG	43	VAL	10.3
43	CP	117	PHE	10.3
37	DJ	24	VAL	10.3
34	CF	106	ILE	10.3
31	CA	1103	A	10.3
9	BI	11	ARG	10.2
37	DJ	138	LEU	10.2
35	CG	62	TRP	10.1
35	CG	105	LEU	10.1
35	CG	157	TYR	10.1
37	CJ	87	LYS	10.1
7	BG	73	VAL	10.0
1	BA	1025	U	10.0

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Mol	Chain	Res	Type	RSRZ
3	BC	196	ILE	10.0
37	CJ	130	GLU	10.0
34	CF	155	THR	10.0
37	CJ	68	THR	10.0
19	BS	14	HIS	10.0
37	CJ	43	ASN	10.0
23	C2	21	TYR	10.0
34	CF	35	THR	9.9
31	CA	1087	G	9.9
10	BJ	26	VAL	9.9
7	BG	103	TRP	9.9
7	BG	91	VAL	9.9
37	CJ	94	ASN	9.9
31	CA	2125	G	9.9
54	DI	128	THR	9.9
24	C3	42	LEU	9.8
1	BA	1305	G	9.8
55	DA	2121	G	9.8
1	BA	1016	A	9.8
34	CF	86	GLY	9.8
7	BG	66	LEU	9.8
13	BM	5	ALA	9.8
7	BG	69	VAL	9.8
7	BG	77	SER	9.7
22	C1	2	ALA	9.7
7	BG	151	PHE	9.7
37	CJ	96	ASP	9.7
30	CD	10	GLY	9.7
34	CF	129	SER	9.7
13	BM	83	LEU	9.6
9	AI	20	PHE	9.6
22	C1	6	ASN	9.6
31	CA	1084	A	9.6
13	BM	33	ILE	9.6
19	BS	38	SER	9.6
13	BM	39	ILE	9.6
31	CA	1086	A	9.6
37	CJ	98	VAL	9.6
37	CJ	89	GLY	9.5
13	BM	96	PRO	9.5
44	CQ	85	SER	9.5
19	BS	49	ILE	9.5

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Mol	Chain	Res	Type	RSRZ
40	CM	82	LEU	9.5
10	BJ	40	ILE	9.4
24	C3	35	ARG	9.4
1	BA	204	G	9.4
37	CJ	28	LEU	9.4
9	BI	32	GLN	9.4
1	AA	87	C	9.4
49	CV	87	PHE	9.4
34	CF	105	THR	9.3
51	CX	53	CYS	9.3
37	CJ	61	VAL	9.3
53	CZ	29	ARG	9.3
13	BM	19	LEU	9.3
16	BP	57	ILE	9.3
3	BC	155	GLY	9.3
43	CP	64	TYR	9.3
1	BA	985	C	9.3
43	CP	63	LYS	9.3
43	CP	40	ILE	9.2
1	BA	1274	A	9.2
37	DJ	94	ASN	9.2
10	BJ	90	LEU	9.2
55	DA	2124	G	9.2
7	BG	71	PRO	9.2
1	BA	1222	G	9.2
46	CS	63	VAL	9.1
10	BJ	76	ILE	9.1
37	DJ	36	MET	9.1
46	CS	88	GLY	9.1
19	BS	28	LYS	9.1
7	BG	112	GLY	9.1
34	CF	117	LEU	9.1
18	BR	20	GLU	9.1
10	BJ	87	LEU	9.1
3	BC	193	TYR	9.1
7	BG	137	LYS	9.0
49	CV	19	LYS	9.0
37	CJ	71	THR	9.0
3	BC	197	GLY	9.0
31	CA	2666	C	9.0
48	CU	47	VAL	9.0
37	DJ	133	ALA	9.0

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Mol	Chain	Res	Type	RSRZ
31	CA	329	G	9.0
7	BG	46	ALA	9.0
14	BN	72	GLY	9.0
20	BT	60	ARG	9.0
24	C3	17	GLY	9.0
31	CA	1066	U	8.9
13	BM	48	LEU	8.9
49	CV	89	ASP	8.9
55	DA	2110	G	8.9
37	CJ	90	SER	8.9
46	CS	20	VAL	8.9
7	BG	53	ARG	8.9
34	CF	131	GLY	8.9
34	CF	153	ASP	8.9
31	CA	613	A	8.9
53	CZ	17	GLU	8.9
49	CV	75	ALA	8.9
9	BI	66	THR	8.9
1	BA	1032	G	8.8
1	BA	958	A	8.8
19	BS	31	LEU	8.8
48	CU	72	GLN	8.8
40	CM	89	VAL	8.8
16	BP	17	TYR	8.8
49	CV	79	LYS	8.8
19	BS	63	THR	8.8
49	CV	14	LEU	8.8
49	CV	29	LEU	8.8
9	BI	18	ARG	8.7
13	BM	64	VAL	8.7
48	CU	55	VAL	8.7
34	CF	126	GLY	8.7
49	CV	3	ALA	8.7
27	C0	56	LYS	8.7
10	BJ	72	ARG	8.7
24	C3	18	PHE	8.7
29	CC	239	ASN	8.7
29	CC	241	GLY	8.7
1	BA	1243	C	8.7
37	DJ	116	ASP	8.7
10	BJ	12	ALA	8.7
37	CJ	47	ASP	8.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	BA	1271	A	8.6
34	CF	23	ASN	8.6
10	BJ	77	VAL	8.6
31	CA	1175	A	8.6
34	CF	132	VAL	8.6
37	CJ	75	PRO	8.6
31	CA	2665	A	8.6
37	DJ	69	PHE	8.6
35	CG	43	VAL	8.6
40	CM	78	ARG	8.6
37	DJ	115	ALA	8.6
33	CE	33	VAL	8.6
19	BS	37	ARG	8.6
34	CF	130	MET	8.6
48	CU	10	VAL	8.6
54	DI	130	PRO	8.6
13	AM	30	SER	8.6
31	CA	1211	C	8.6
37	CJ	60	THR	8.6
1	BA	1026	G	8.6
24	C3	7	PRO	8.6
34	CF	176	PRO	8.6
34	CF	95	ARG	8.5
3	BC	71	ALA	8.5
31	CA	2123	G	8.5
34	CF	147	ASP	8.5
14	AN	21	PHE	8.5
37	DJ	59	ILE	8.5
9	AI	21	ILE	8.5
14	BN	20	TYR	8.5
7	BG	106	GLU	8.5
49	CV	98	SER	8.5
35	CG	52	PHE	8.5
37	DJ	20	PRO	8.5
1	BA	1296	C	8.5
7	BG	17	LYS	8.5
3	BC	195	VAL	8.5
31	CA	1083	U	8.4
7	BG	45	SER	8.4
9	BI	68	LYS	8.4
13	BM	40	ALA	8.4
7	BG	148	ASN	8.4

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Mol	Chain	Res	Type	RSRZ
49	CV	32	GLY	8.4
37	DJ	89	GLY	8.4
33	CE	143	LEU	8.4
37	DJ	68	THR	8.4
34	CF	144	ASP	8.4
19	BS	60	VAL	8.4
45	CR	106	PHE	8.3
53	CZ	33	ALA	8.3
7	BG	132	GLY	8.3
40	CM	20	GLY	8.3
48	CU	42	GLU	8.3
10	BJ	7	ARG	8.3
49	CV	48	PRO	8.3
49	CV	81	ASP	8.3
19	BS	5	LEU	8.3
37	CJ	9	VAL	8.3
17	BQ	70	THR	8.3
23	C2	36	LEU	8.3
7	BG	39	ALA	8.3
48	CU	15	HIS	8.3
7	BG	79	ARG	8.3
1	BA	984	C	8.2
24	C3	30	VAL	8.2
19	BS	24	GLU	8.2
35	CG	172	LYS	8.2
34	CF	80	ARG	8.2
1	BA	942	G	8.2
43	CP	99	TYR	8.2
13	BM	2	ALA	8.2
7	BG	4	ARG	8.2
50	CW	94	ALA	8.2
55	DA	2125	G	8.2
40	CM	71	ALA	8.2
43	CP	24	THR	8.2
1	BA	948	C	8.2
2	BB	34	ALA	8.2
10	BJ	86	ALA	8.2
31	CA	1085	A	8.2
33	CE	104	ALA	8.2
51	CX	33	ALA	8.2
14	BN	35	ASN	8.1
9	BI	40	GLY	8.1

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Mol	Chain	Res	Type	RSRZ
7	BG	109	ARG	8.1
43	CP	51	ALA	8.1
7	BG	141	VAL	8.1
37	CJ	83	ALA	8.1
42	CO	111	ALA	8.1
9	BI	127	PHE	8.1
23	C2	52	ALA	8.1
19	BS	74	PHE	8.1
44	CQ	84	ILE	8.1
3	BC	119	SER	8.1
55	DA	1067	A	8.1
10	BJ	71	LEU	8.0
35	CG	151	TYR	8.0
37	DJ	137	GLY	8.0
13	BM	55	THR	8.0
1	BA	1241	G	8.0
31	CA	75	G	8.0
19	BS	32	ARG	8.0
10	BJ	94	ALA	8.0
11	BK	47	ALA	8.0
48	CU	46	ALA	8.0
37	CJ	33	VAL	8.0
40	CM	8	PRO	8.0
1	BA	1017	U	8.0
49	CV	88	GLU	8.0
33	CE	173	THR	8.0
55	DA	2174	C	8.0
2	AB	6	MET	8.0
55	DA	2116	G	8.0
55	DA	896	A	8.0
2	AB	136	MET	8.0
35	CG	171	THR	7.9
31	CA	2124	G	7.9
2	AB	14	VAL	7.9
16	BP	80	LYS	7.9
1	BA	82	G	7.9
19	BS	39	THR	7.9
33	CE	150	THR	7.9
14	AN	31	ILE	7.9
42	CO	28	LEU	7.9
48	CU	61	LEU	7.9
14	AN	23	LYS	7.9

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Mol	Chain	Res	Type	RSRZ
31	CA	330	A	7.9
20	BT	72	ALA	7.9
35	CG	111	HIS	7.9
24	C3	36	ALA	7.9
33	CE	23	PHE	7.9
19	BS	76	PRO	7.9
24	C3	33	ARG	7.9
40	CM	130	GLY	7.8
7	BG	144	MET	7.8
37	CJ	133	ALA	7.8
1	BA	80	A	7.8
31	CA	1078	U	7.8
40	CM	10	GLU	7.8
1	AA	1031	C	7.8
1	AA	1032	G	7.8
13	BM	47	GLU	7.8
36	DH	137	GLU	7.8
7	BG	54	SER	7.8
9	BI	14	SER	7.8
43	CP	54	VAL	7.8
16	BP	52	LEU	7.8
3	BC	198	VAL	7.7
22	C1	4	GLN	7.7
24	C3	27	GLY	7.7
55	DA	138	U	7.7
13	AM	33	ILE	7.7
45	CR	74	ILE	7.7
34	CF	31	VAL	7.7
13	BM	25	VAL	7.7
31	CA	1167	C	7.7
13	AM	43	VAL	7.7
35	CG	26	ILE	7.7
43	CP	65	THR	7.7
36	CH	140	ALA	7.7
33	CE	47	LYS	7.7
7	BG	41	SER	7.7
34	CF	93	GLY	7.7
35	CG	169	VAL	7.7
37	CJ	119	GLY	7.7
10	BJ	22	THR	7.7
40	CM	120	VAL	7.6
14	BN	54	ASP	7.6

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Mol	Chain	Res	Type	RSRZ
30	CD	186	LEU	7.6
37	CJ	29	GLY	7.6
10	BJ	75	ASP	7.6
13	BM	29	ARG	7.6
13	BM	85	CYS	7.6
55	DA	2175	C	7.6
14	BN	2	ALA	7.6
37	CJ	31	GLN	7.6
1	BA	1031	C	7.6
2	AB	135	LEU	7.6
7	AG	62	PHE	7.6
33	CE	201	ALA	7.6
3	BC	192	THR	7.6
50	CW	6	ALA	7.6
31	CA	2171	A	7.6
51	CX	63	ALA	7.6
7	BG	87	VAL	7.6
34	CF	34	ILE	7.5
35	CG	106	SER	7.5
43	CP	38	GLN	7.5
1	BA	1028	C	7.5
7	BG	15	ASP	7.5
29	CC	27	GLY	7.5
46	CS	59	ILE	7.5
37	DJ	66	SER	7.5
16	BP	41	PRO	7.5
36	CH	11	ASN	7.5
7	BG	105	VAL	7.5
37	CJ	24	VAL	7.5
2	BB	135	LEU	7.5
34	CF	152	LEU	7.5
31	CA	1077	A	7.5
43	CP	29	HIS	7.5
10	BJ	95	GLY	7.5
34	CF	113	ASP	7.5
35	CG	83	PHE	7.5
53	CZ	14	LEU	7.5
53	CZ	37	LEU	7.5
53	CZ	49	ASP	7.5
55	DA	2172	U	7.5
33	CE	119	ILE	7.5
40	CM	77	ILE	7.5

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Mol	Chain	Res	Type	RSRZ
35	CG	2	SER	7.4
1	BA	953	G	7.4
9	BI	64	TYR	7.4
34	CF	28	VAL	7.4
31	CA	2402	U	7.4
25	C4	43	HIS	7.4
1	BA	949	A	7.4
1	BA	959	A	7.4
47	CT	84	ARG	7.4
55	DA	1065	U	7.4
31	CA	312	G	7.4
31	CA	2802	G	7.4
37	CJ	74	PRO	7.4
42	CO	116	VAL	7.4
26	C5	10	LEU	7.4
1	BA	1275	A	7.4
31	CA	1069	A	7.4
29	CC	233	GLY	7.4
40	CM	102	GLY	7.4
1	BA	1314	C	7.4
25	C4	37	ALA	7.4
13	BM	24	GLY	7.4
31	CA	1065	U	7.4
20	BT	79	LEU	7.4
37	CJ	73	THR	7.4
31	CA	1075	C	7.4
9	BI	44	ALA	7.3
49	CV	83	VAL	7.3
34	CF	83	TYR	7.3
37	DJ	77	ALA	7.3
10	BJ	101	SER	7.3
53	CZ	31	GLN	7.3
31	CA	2163	A	7.3
55	DA	1172	C	7.3
1	AA	88	U	7.3
47	CT	5	ALA	7.3
38	CK	22	GLY	7.3
31	CA	2173	A	7.3
34	CF	39	GLY	7.3
19	BS	30	PRO	7.3
37	CJ	86	ILE	7.3
48	CU	8	LEU	7.3

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Mol	Chain	Res	Type	RSRZ
46	CS	35	PHE	7.3
9	BI	5	GLN	7.3
31	CA	2300	C	7.3
46	CS	103	ALA	7.3
34	CF	151	GLY	7.3
50	CW	27	PRO	7.3
2	BB	14	VAL	7.3
33	CE	164	LEU	7.3
31	CA	289	G	7.3
53	CZ	59	GLU	7.3
41	CN	136	MET	7.2
46	CS	14	VAL	7.2
7	BG	16	PRO	7.2
3	BC	156	ARG	7.2
7	BG	108	ALA	7.2
27	C0	29	LEU	7.2
49	CV	52	LEU	7.2
33	CE	144	GLU	7.2
7	BG	150	ALA	7.2
53	CZ	42	LEU	7.2
43	CP	115	LEU	7.2
40	CM	142	ILE	7.2
1	BA	954	G	7.2
37	DJ	134	ARG	7.2
10	BJ	10	LEU	7.2
33	CE	200	LEU	7.2
34	CF	173	PHE	7.2
14	BN	68	GLY	7.2
31	CA	2891	U	7.2
13	BM	101	ARG	7.2
49	CV	30	SER	7.2
1	BA	94	G	7.2
35	CG	10	VAL	7.2
37	DJ	84	ALA	7.2
9	BI	4	ASN	7.2
1	BA	1050	G	7.2
24	C3	32	ALA	7.2
48	CU	87	LEU	7.1
1	BA	1218	C	7.1
31	CA	2797	U	7.1
26	C5	32	LYS	7.1
25	C4	28	ASN	7.1

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Mol	Chain	Res	Type	RSRZ
31	CA	2169	A	7.1
23	C2	37	LYS	7.1
35	CG	86	LYS	7.1
37	CJ	95	LYS	7.1
49	CV	12	ILE	7.1
37	CJ	85	GLY	7.1
37	DJ	52	GLY	7.1
34	CF	102	ARG	7.1
31	CA	1057	A	7.1
37	CJ	18	ALA	7.1
55	DA	2118	U	7.1
19	BS	61	PHE	7.1
43	CP	108	ASP	7.1
44	CQ	97	LEU	7.1
1	BA	1303	C	7.1
10	AJ	6	ILE	7.1
49	CV	5	ILE	7.1
31	CA	2127	G	7.1
1	AA	81	A	7.1
31	CA	878	A	7.1
49	CV	26	LYS	7.1
44	CQ	95	ALA	7.1
55	DA	2111	U	7.1
37	DJ	28	LEU	7.1
23	C2	23	THR	7.1
53	CZ	41	HIS	7.0
35	CG	9	VAL	7.0
39	CL	110	GLU	7.0
7	BG	18	PHE	7.0
55	DA	2167	U	7.0
20	BT	75	HIS	7.0
3	BC	79	LYS	7.0
31	CA	2175	C	7.0
31	CA	2667	C	7.0
14	BN	61	ARG	7.0
37	DJ	87	LYS	7.0
40	CM	28	GLY	7.0
10	BJ	91	ASP	7.0
31	CA	2121	G	7.0
55	DA	2178	C	7.0
7	BG	129	GLU	7.0
49	CV	77	THR	7.0

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Mol	Chain	Res	Type	RSRZ
10	BJ	11	LYS	7.0
34	CF	174	ASP	7.0
13	BM	109	ARG	7.0
33	CE	118	LEU	7.0
3	BC	159	GLY	7.0
33	CE	183	PHE	7.0
43	CP	39	VAL	7.0
55	DA	2166	U	7.0
7	BG	47	LEU	7.0
46	CS	98	ILE	7.0
34	CF	158	THR	7.0
13	BM	94	GLY	7.0
51	CX	52	GLY	6.9
40	CM	90	VAL	6.9
14	BN	53	ARG	6.9
1	BA	203	G	6.9
10	AJ	42	LEU	6.9
27	C0	24	LEU	6.9
30	CD	44	GLY	6.9
49	CV	38	GLY	6.9
19	BS	41	PHE	6.9
37	CJ	50	GLU	6.9
35	CG	45	HIS	6.9
7	BG	48	GLU	6.9
10	BJ	98	VAL	6.9
26	C5	38	GLY	6.9
54	DI	134	GLU	6.9
31	CA	316	C	6.9
1	BA	1304	G	6.9
9	AI	90	TYR	6.9
34	CF	175	PHE	6.9
48	CU	57	VAL	6.9
1	BA	79	G	6.9
31	CA	1536	C	6.9
34	CF	121	SER	6.9
30	CD	8	LYS	6.9
31	CA	1168	G	6.9
31	CA	1185	G	6.9
31	CA	1095	A	6.8
37	CJ	8	TYR	6.8
35	CG	41	VAL	6.8
31	CA	549	G	6.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
37	CJ	113	LYS	6.8
37	CJ	93	PRO	6.8
27	C0	43	ALA	6.8
46	CS	28	ALA	6.8
30	CD	166	GLY	6.8
7	BG	30	LEU	6.8
31	CA	2120	G	6.8
2	AB	123	ASP	6.8
46	CS	101	ILE	6.8
16	BP	60	TRP	6.8
19	BS	72	GLY	6.8
40	CM	75	ALA	6.8
43	CP	107	ALA	6.8
13	BM	28	THR	6.8
31	CA	1210	G	6.8
25	C4	4	ILE	6.8
54	DI	2	ALA	6.8
35	CG	30	ASN	6.8
47	CT	97	LEU	6.8
31	CA	2168	G	6.8
55	DA	2176	A	6.8
10	BJ	102	LEU	6.8
14	BN	16	LEU	6.8
36	DH	66	ASN	6.8
37	CJ	123	GLU	6.8
35	CG	92	VAL	6.8
55	DA	2123	G	6.8
31	CA	1076	C	6.8
31	CA	1104	C	6.8
13	BM	63	PHE	6.8
33	CE	75	SER	6.8
1	BA	1023	U	6.8
31	CA	2119	A	6.8
2	BB	186	ILE	6.8
25	C4	40	ARG	6.7
55	DA	2127	G	6.7
31	CA	2170	A	6.7
2	BB	201	PRO	6.7
19	BS	80	TYR	6.7
49	CV	28	VAL	6.7
13	BM	56	LEU	6.7
10	BJ	6	ILE	6.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	BM	51	GLY	6.7
31	CA	311	A	6.7
9	BI	7	TYR	6.7
35	CG	51	THR	6.7
7	BG	107	ALA	6.7
37	CJ	44	ALA	6.7
53	CZ	22	LEU	6.7
31	CA	877	A	6.7
34	CF	75	ALA	6.7
37	CJ	62	TYR	6.7
11	AK	82	LEU	6.7
13	AM	19	LEU	6.7
13	BM	31	LYS	6.7
33	CE	24	ASN	6.7
49	DV	56	GLY	6.7
34	CF	107	ALA	6.7
47	CT	86	MET	6.7
30	CD	38	LYS	6.7
20	BT	76	LYS	6.7
42	CO	120	GLU	6.7
46	CS	78	ARG	6.7
20	BT	56	PRO	6.7
10	BJ	9	ARG	6.7
31	CA	12	U	6.7
31	CA	2108	A	6.7
19	BS	40	ILE	6.7
1	BA	1217	C	6.7
3	BC	53	SER	6.7
49	CV	69	ASN	6.7
46	CS	87	GLN	6.6
10	AJ	74	VAL	6.6
53	CZ	40	SER	6.6
2	BB	35	ARG	6.6
7	BG	123	GLU	6.6
53	CZ	24	GLU	6.6
23	C2	49	TYR	6.6
14	BN	31	ILE	6.6
37	DJ	73	THR	6.6
44	CQ	110	ILE	6.6
20	BT	24	ARG	6.6
7	BG	101	MET	6.6
42	CO	24	MET	6.6

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Mol	Chain	Res	Type	RSRZ
31	CA	356	G	6.6
31	CA	1105	U	6.6
35	CG	84	THR	6.6
13	BM	6	GLY	6.6
30	CD	96	ILE	6.6
10	BJ	82	LYS	6.6
14	BN	27	LEU	6.6
35	CG	58	TYR	6.6
31	CA	267	C	6.6
34	CF	55	ALA	6.6
1	BA	1049	U	6.6
13	BM	12	HIS	6.6
14	BN	52	PRO	6.6
37	DJ	22	PRO	6.6
33	CE	54	GLY	6.6
49	CV	95	PHE	6.6
9	AI	17	ALA	6.6
27	C0	23	THR	6.6
31	CA	2128	G	6.6
1	BA	1004	A	6.6
30	CD	154	LYS	6.6
37	CJ	122	ILE	6.5
1	BA	1331	G	6.5
35	CG	69	ARG	6.5
35	CG	102	VAL	6.5
54	DI	132	TYR	6.5
9	AI	129	LYS	6.5
35	CG	27	LYS	6.5
13	BM	35	ALA	6.5
1	BA	1236	A	6.5
31	CA	1535	A	6.5
7	AG	4	ARG	6.5
45	CR	90	ILE	6.5
30	CD	201	LEU	6.5
3	BC	154	SER	6.5
21	AU	2	PRO	6.5
9	BI	38	TYR	6.5
17	BQ	45	HIS	6.5
10	BJ	100	ILE	6.5
35	CG	112	PRO	6.5
31	CA	846	U	6.5
43	CP	103	VAL	6.5

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Mol	Chain	Res	Type	RSRZ
51	CX	26	PHE	6.5
1	BA	1018	G	6.5
31	CA	1213	A	6.5
36	CH	132	PHE	6.5
40	CM	85	VAL	6.5
42	CO	29	VAL	6.5
54	DI	121	SER	6.5
3	BC	43	LEU	6.5
37	DJ	14	ALA	6.5
38	CK	35	ARG	6.5
36	CH	136	SER	6.5
17	BQ	73	TRP	6.5
31	CA	2161	C	6.5
31	CA	1082	U	6.5
43	CP	25	ARG	6.5
13	BM	21	SER	6.5
1	AA	1026	G	6.5
1	BA	1276	G	6.5
31	CA	409	G	6.5
35	CG	7	ALA	6.5
1	BA	78	A	6.4
31	CA	1169	A	6.4
7	BG	8	GLY	6.4
10	BJ	38	GLY	6.4
37	CJ	131	GLY	6.4
37	DJ	99	GLY	6.4
1	BA	85	U	6.4
9	BI	9	THR	6.4
16	BP	81	ALA	6.4
25	C4	41	LYS	6.4
10	BJ	25	ILE	6.4
8	BH	55	THR	6.4
33	CE	193	VAL	6.4
7	BG	38	THR	6.4
34	CF	136	ILE	6.4
43	CP	92	PHE	6.4
19	BS	12	ASP	6.4
37	CJ	84	ALA	6.4
51	CX	59	LEU	6.4
12	AL	124	ALA	6.4
34	CF	122	PHE	6.4
13	BM	79	ARG	6.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
47	CT	105	VAL	6.4
34	CF	41	GLY	6.4
43	CP	46	GLU	6.4
54	DI	96	PHE	6.4
13	BM	108	THR	6.4
24	C3	31	LEU	6.4
31	CA	1238	G	6.4
37	CJ	79	LEU	6.4
37	DJ	11	LEU	6.4
47	CT	47	VAL	6.4
14	BN	22	ALA	6.4
27	C0	8	THR	6.3
35	CG	17	VAL	6.3
34	CF	84	PRO	6.3
37	CJ	81	LYS	6.3
2	BB	12	ALA	6.3
31	CA	2803	G	6.3
33	CE	128	ALA	6.3
9	AI	128	SER	6.3
1	BA	989	U	6.3
13	BM	98	ARG	6.3
34	CF	69	LYS	6.3
31	CA	885	C	6.3
31	CA	1870	C	6.3
35	CG	80	THR	6.3
55	DA	1062	G	6.3
14	AN	47	LYS	6.3
25	C4	36	LYS	6.3
42	CO	118	ARG	6.3
45	CR	98	ILE	6.3
7	AG	66	LEU	6.3
34	CF	92	ARG	6.3
44	CQ	22	PRO	6.3
22	C1	46	ASP	6.3
37	DJ	19	ASN	6.3
31	CA	81	G	6.3
7	BG	115	SER	6.3
43	CP	52	SER	6.3
27	C0	34	HIS	6.3
2	AB	74	ARG	6.3
35	CG	107	LEU	6.3
9	AI	6	TYR	6.3

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Mol	Chain	Res	Type	RSRZ
15	BO	17	ARG	6.3
30	CD	77	ARG	6.3
43	CP	66	GLY	6.3
49	CV	40	ASN	6.3
13	BM	93	ARG	6.3
34	CF	143	TYR	6.3
7	BG	145	ALA	6.3
1	AA	844	G	6.3
36	CH	72	ILE	6.2
37	CJ	46	THR	6.2
31	CA	1094	U	6.2
7	BG	35	LYS	6.2
13	BM	103	LYS	6.2
13	BM	65	VAL	6.2
31	CA	930	G	6.2
37	CJ	58	VAL	6.2
55	DA	1064	C	6.2
1	AA	85	U	6.2
1	BA	1321	U	6.2
31	CA	2860	A	6.2
40	CM	113	ALA	6.2
37	DJ	74	PRO	6.2
40	CM	88	GLY	6.2
49	CV	4	LYS	6.2
7	AG	42	ILE	6.2
30	CD	97	SER	6.2
37	CJ	32	GLY	6.2
40	CM	126	ARG	6.2
34	CF	94	GLU	6.2
43	CP	27	VAL	6.2
2	BB	20	THR	6.2
37	CJ	19	ASN	6.2
37	CJ	77	ALA	6.2
53	CZ	18	LEU	6.2
23	C2	43	VAL	6.2
37	CJ	67	PHE	6.2
10	BJ	80	THR	6.2
35	CG	174	ALA	6.2
37	DJ	117	MET	6.2
33	CE	154	ASP	6.2
13	BM	43	VAL	6.2
31	CA	1107	G	6.2

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Mol	Chain	Res	Type	RSRZ
55	DA	883	G	6.2
13	AM	99	GLY	6.2
13	BM	41	GLU	6.2
40	CM	117	THR	6.2
40	CM	19	LEU	6.2
53	CZ	56	LEU	6.2
2	BB	21	ARG	6.1
33	CE	89	PRO	6.1
14	BN	18	ASP	6.1
34	CF	60	ILE	6.1
50	CW	89	ILE	6.1
45	CR	73	GLY	6.1
14	BN	8	ALA	6.1
20	BT	34	LYS	6.1
51	CX	62	LYS	6.1
51	CX	32	LEU	6.1
23	C2	45	GLN	6.1
37	CJ	70	VAL	6.1
30	CD	74	GLU	6.1
7	AG	79	ARG	6.1
13	BM	36	ALA	6.1
2	BB	67	ILE	6.1
40	CM	107	PHE	6.1
13	BM	99	GLY	6.1
24	C3	28	ARG	6.1
38	CK	93	ILE	6.1
10	AJ	35	GLN	6.1
7	BG	72	THR	6.1
13	BM	54	ASP	6.1
55	DA	884	U	6.1
24	C3	26	ASN	6.1
19	BS	21	LYS	6.1
49	CV	51	ALA	6.1
7	BG	50	LEU	6.1
44	CQ	27	GLU	6.1
16	BP	20	VAL	6.1
30	CD	9	VAL	6.1
18	BR	51	TYR	6.1
33	CE	131	THR	6.1
37	CJ	118	THR	6.1
40	CM	133	ALA	6.1
10	AJ	73	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
37	CJ	30	GLN	6.1
43	CP	106	LEU	6.1
1	BA	1270	G	6.1
43	CP	78	VAL	6.1
29	CC	234	GLY	6.0
46	CS	18	GLN	6.0
1	BA	1019	A	6.0
13	BM	30	SER	6.0
54	DI	38	MET	6.0
10	BJ	21	ALA	6.0
20	BT	63	ALA	6.0
31	CA	1217	U	6.0
43	CP	41	ALA	6.0
40	CM	135	ILE	6.0
55	DA	2122	U	6.0
49	CV	25	VAL	6.0
34	CF	164	GLU	6.0
1	BA	1005	A	6.0
16	BP	54	LEU	6.0
43	CP	105	ALA	6.0
31	CA	1106	G	6.0
43	CP	87	ILE	6.0
27	C0	55	VAL	6.0
14	BN	55	SER	6.0
1	BA	1280	A	6.0
31	CA	344	A	6.0
31	CA	476	G	6.0
36	CH	130	VAL	6.0
37	DJ	98	VAL	6.0
25	C4	61	CYS	6.0
46	CS	61	ALA	6.0
7	BG	58	GLU	6.0
23	C2	18	GLY	6.0
35	CG	82	GLY	6.0
46	CS	22	LEU	6.0
1	BA	208	U	6.0
29	CC	242	LYS	6.0
1	BA	1306	A	6.0
19	BS	52	HIS	6.0
31	CA	2892	G	6.0
17	BQ	63	GLU	6.0
37	CJ	53	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
2	BB	40	ILE	6.0
9	BI	90	TYR	6.0
38	CK	119	PHE	6.0
35	CG	152	ARG	5.9
35	CG	8	PRO	5.9
22	C1	35	GLY	5.9
46	CS	55	ASP	5.9
7	BG	99	LEU	5.9
45	CR	71	GLN	5.9
45	CR	29	SER	5.9
3	BC	126	ARG	5.9
7	AG	109	ARG	5.9
49	CV	6	ARG	5.9
46	CS	31	GLU	5.9
31	CA	2107	G	5.9
23	C2	15	ALA	5.9
15	BO	89	ARG	5.9
37	CJ	27	ALA	5.9
1	BA	1201	A	5.9
22	C1	34	SER	5.9
19	BS	6	LYS	5.9
16	BP	16	PHE	5.9
20	BT	73	ALA	5.9
1	BA	950	U	5.9
1	BA	1235	U	5.9
23	C2	53	LYS	5.9
29	CC	245	VAL	5.9
31	CA	345	A	5.9
31	CA	2150	C	5.9
48	CU	85	VAL	5.9
10	AJ	75	ASP	5.9
19	BS	77	THR	5.9
31	CA	1088	A	5.9
45	CR	33	ARG	5.9
52	CY	49	LEU	5.9
25	C4	27	ALA	5.9
37	CJ	41	ALA	5.9
46	CS	62	GLU	5.9
47	CT	101	SER	5.9
37	CJ	91	GLY	5.9
55	DA	2115	G	5.9
34	CF	165	GLU	5.8

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Mol	Chain	Res	Type	RSRZ
35	CG	56	ASP	5.8
30	CD	82	PHE	5.8
51	CX	55	ARG	5.8
2	AB	131	LYS	5.8
13	BM	86	TYR	5.8
43	CP	62	LEU	5.8
52	CY	78	TYR	5.8
31	CA	896	A	5.8
35	CG	31	GLY	5.8
10	BJ	19	ASP	5.8
45	CR	91	ASP	5.8
31	CA	1064	C	5.8
7	BG	152	ALA	5.8
35	CG	121	ILE	5.8
9	AI	19	VAL	5.8
29	CC	244	PRO	5.8
31	CA	2118	U	5.8
9	BI	81	HIS	5.8
55	DA	1068	G	5.8
14	BN	37	SER	5.8
19	BS	27	ASP	5.8
37	DJ	38	PHE	5.8
7	BG	60	GLU	5.8
44	CQ	9	GLU	5.8
25	C4	2	PRO	5.8
41	CN	16	ARG	5.8
30	CD	185	ASN	5.8
47	CT	43	ALA	5.8
36	DH	70	GLU	5.8
2	AB	4	VAL	5.8
2	BB	187	VAL	5.8
9	AI	104	VAL	5.8
31	CA	1215	G	5.8
47	CT	82	MET	5.8
30	CD	30	GLU	5.8
44	CQ	115	ASN	5.8
43	CP	26	LEU	5.8
54	DI	129	LEU	5.8
11	BK	55	SER	5.8
55	DA	879	G	5.8
13	AM	16	VAL	5.8
35	CG	162	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
48	CU	34	VAL	5.8
36	CH	15	LEU	5.8
49	CV	73	PHE	5.8
20	BT	49	LYS	5.7
2	AB	46	THR	5.7
10	BJ	89	ARG	5.7
46	CS	49	ILE	5.7
42	CO	119	SER	5.7
30	CD	76	GLY	5.7
37	DJ	85	GLY	5.7
43	CP	67	ASN	5.7
34	CF	135	GLN	5.7
34	CF	170	LEU	5.7
29	CC	249	GLY	5.7
36	DH	74	ALA	5.7
49	CV	64	ALA	5.7
7	BG	88	PRO	5.7
9	BI	125	PRO	5.7
55	DA	2165	C	5.7
1	BA	1240	U	5.7
37	DJ	100	LYS	5.7
1	BA	213	G	5.7
17	BQ	17	MET	5.7
50	CW	1	MET	5.7
33	CE	138	LEU	5.7
31	CA	2162	G	5.7
37	DJ	110	ALA	5.7
35	CG	4	VAL	5.7
49	CV	70	VAL	5.7
37	DJ	71	THR	5.7
31	CA	1214	A	5.7
7	BG	140	ASP	5.7
37	CJ	125	MET	5.7
31	CA	1049	C	5.7
37	DJ	103	ARG	5.7
1	BA	987	G	5.7
31	CA	317	G	5.7
33	CE	17	THR	5.7
35	CG	54	PRO	5.7
30	CD	3	GLY	5.7
37	DJ	50	GLU	5.7
49	DV	53	ASN	5.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
48	CU	1	MET	5.7
3	BC	106	VAL	5.7
33	CE	178	VAL	5.7
53	CZ	11	VAL	5.7
1	BA	1126	U	5.7
51	CX	60	PHE	5.7
35	CG	104	ASN	5.7
34	CF	110	ARG	5.7
39	CL	68	GLY	5.7
37	CJ	45	LYS	5.6
49	CV	71	ALA	5.6
25	C4	64	TYR	5.6
35	CG	110	SER	5.6
37	CJ	135	SER	5.6
27	C0	9	GLN	5.6
34	CF	79	ILE	5.6
30	CD	203	VAL	5.6
31	CA	646	U	5.6
31	CA	1606	C	5.6
44	CQ	8	LEU	5.6
13	BM	14	HIS	5.6
30	CD	43	ASP	5.6
30	CD	200	ASP	5.6
37	CJ	124	ALA	5.6
13	AM	64	VAL	5.6
19	BS	71	LEU	5.6
1	BA	1029	U	5.6
33	CE	98	LYS	5.6
9	BI	15	SER	5.6
10	BJ	39	PRO	5.6
47	CT	103	ILE	5.6
34	CF	43	ALA	5.6
30	CD	5	VAL	5.6
27	C0	27	LEU	5.6
35	CG	78	GLY	5.6
1	BA	196	A	5.6
35	CG	35	ARG	5.6
51	CX	61	ALA	5.6
30	CD	151	THR	5.6
35	CG	67	THR	5.6
1	BA	102	G	5.6
31	CA	2628	C	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
33	CE	101	TYR	5.6
36	DH	94	ILE	5.6
7	BG	83	SER	5.6
31	CA	1046	A	5.6
45	CR	118	ALA	5.6
25	C4	22	PHE	5.6
31	CA	1174	U	5.6
55	DA	2109	U	5.6
24	C3	37	LYS	5.6
1	BA	90	C	5.6
37	DJ	8	TYR	5.6
19	BS	59	PRO	5.6
31	CA	514	A	5.6
7	AG	82	GLY	5.6
11	AK	19	GLY	5.6
35	CG	117	LEU	5.6
31	CA	328	U	5.6
45	CR	6	ARG	5.6
34	CF	32	GLU	5.6
1	BA	81	A	5.6
46	CS	94	THR	5.6
31	CA	546	U	5.6
3	BC	206	GLU	5.6
29	CC	240	PHE	5.5
36	DH	63	ALA	5.5
37	DJ	27	ALA	5.5
7	BG	76	LYS	5.5
50	CW	42	LEU	5.5
1	AA	82	G	5.5
1	BA	1221	G	5.5
48	CU	35	ALA	5.5
14	BN	11	VAL	5.5
29	CC	48	ARG	5.5
35	CG	57	GLY	5.5
1	BA	202	G	5.5
31	CA	45	G	5.5
3	BC	39	VAL	5.5
24	C3	16	HIS	5.5
10	BJ	27	GLU	5.5
9	BI	30	ILE	5.5
27	C0	48	ILE	5.5
31	CA	291	G	5.5

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Mol	Chain	Res	Type	RSRZ
37	CJ	15	ALA	5.5
14	BN	45	VAL	5.5
13	BM	76	SER	5.5
23	C2	44	ARG	5.5
34	CF	99	PHE	5.5
3	BC	76	VAL	5.5
35	CG	160	LYS	5.5
42	CO	56	LYS	5.5
51	CX	56	ASP	5.5
2	BB	37	LYS	5.5
31	CA	1872	A	5.5
38	CK	139	VAL	5.5
55	DA	1098	A	5.5
7	BG	5	ARG	5.5
34	CF	37	ASN	5.5
41	CN	17	ASN	5.5
1	BA	1237	C	5.5
49	CV	66	GLN	5.5
10	AJ	76	ILE	5.5
22	C1	27	SER	5.5
31	CA	327	G	5.5
9	BI	10	GLY	5.5
9	BI	58	VAL	5.5
30	CD	180	VAL	5.5
34	CF	18	THR	5.5
23	C2	46	HIS	5.5
44	CQ	12	GLN	5.5
1	BA	1333	A	5.5
3	BC	120	ILE	5.5
31	CA	355	U	5.5
1	BA	844	G	5.5
46	CS	25	LEU	5.4
13	AM	44	LYS	5.4
1	BA	4	U	5.4
31	CA	1089	A	5.4
37	CJ	128	SER	5.4
31	CA	1518	C	5.4
7	BG	89	VAL	5.4
31	CA	1212	G	5.4
36	CH	142	VAL	5.4
7	BG	130	ASN	5.4
37	CJ	52	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
53	CZ	47	ARG	5.4
2	BB	82	ASP	5.4
49	CV	18	ASP	5.4
33	CE	142	ALA	5.4
40	CM	131	ALA	5.4
45	CR	99	ALA	5.4
1	AA	1027	C	5.4
31	CA	2801	G	5.4
40	CM	45	GLY	5.4
42	CO	62	ASN	5.4
31	CA	892	A	5.4
31	CA	335	C	5.4
42	CO	63	ARG	5.4
31	CA	548	G	5.4
1	BA	955	U	5.4
10	BJ	93	ALA	5.4
13	BM	74	SER	5.4
30	CD	41	ALA	5.4
10	BJ	99	GLN	5.4
1	BA	1245	C	5.4
51	CX	57	HIS	5.4
7	BG	118	LEU	5.4
12	BL	124	ALA	5.4
7	BG	119	ARG	5.4
1	BA	1273	C	5.4
9	AI	127	PHE	5.4
50	CW	29	ILE	5.4
10	BJ	81	GLU	5.4
3	BC	111	LEU	5.4
43	CP	110	ALA	5.4
31	CA	879	G	5.4
38	CK	97	PRO	5.4
31	CA	626	A	5.4
31	CA	1048	A	5.4
35	CG	109	PHE	5.4
55	DA	1077	A	5.4
49	CV	43	LYS	5.4
43	CP	69	ASP	5.4
13	AM	32	ALA	5.4
37	DJ	104	ALA	5.4
36	DH	138	VAL	5.4
49	CV	49	VAL	5.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
34	CF	77	PHE	5.4
19	AS	55	ARG	5.4
39	CL	37	ASP	5.4
34	CF	74	VAL	5.3
14	BN	5	SER	5.3
1	AA	1020	G	5.3
1	BA	1297	G	5.3
9	BI	20	PHE	5.3
27	C0	7	ILE	5.3
30	CD	46	ARG	5.3
31	CA	183	C	5.3
54	DI	84	TYR	5.3
1	BA	974	A	5.3
31	CA	74	A	5.3
34	CF	25	VAL	5.3
36	DH	139	PHE	5.3
7	AG	69	VAL	5.3
35	CG	132	VAL	5.3
37	DJ	43	ASN	5.3
48	CU	58	VAL	5.3
19	BS	68	GLY	5.3
33	CE	197	GLU	5.3
37	DJ	48	SER	5.3
14	BN	49	GLN	5.3
36	CH	133	GLN	5.3
13	AM	5	ALA	5.3
55	DA	882	G	5.3
9	AI	5	GLN	5.3
10	BJ	37	ARG	5.3
1	BA	1244	G	5.3
27	C0	10	THR	5.3
34	CF	177	PHE	5.3
34	CF	26	MET	5.3
47	CT	85	ILE	5.3
1	BA	1148	U	5.3
35	CG	161	GLY	5.3
27	C0	44	ILE	5.3
31	CA	1216	G	5.3
37	CJ	136	MET	5.3
33	CE	72	SER	5.3
42	CO	83	LEU	5.3
34	CF	119	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
46	CS	33	VAL	5.3
45	CR	81	ASN	5.3
1	BA	1015	G	5.3
31	CA	1873	G	5.3
55	DA	1061	U	5.3
46	CS	54	VAL	5.3
31	CA	420	C	5.3
13	AM	11	ASP	5.3
7	BG	110	LYS	5.2
35	CG	131	ILE	5.2
40	CM	115	GLU	5.2
48	CU	36	LYS	5.2
14	BN	6	MET	5.2
13	BM	34	LEU	5.2
13	BM	58	ASP	5.2
19	BS	58	VAL	5.2
33	CE	88	ARG	5.2
1	BA	101	A	5.2
1	BA	988	G	5.2
14	BN	43	ASN	5.2
20	BT	38	ALA	5.2
30	CD	31	ALA	5.2
35	CG	59	ALA	5.2
35	CG	81	GLU	5.2
16	BP	42	ILE	5.2
49	CV	15	THR	5.2
37	DJ	10	LYS	5.2
21	AU	11	PRO	5.2
36	CH	74	ALA	5.2
48	CU	37	ASP	5.2
23	C2	39	PHE	5.2
50	CW	69	GLU	5.2
13	AM	7	ILE	5.2
14	BN	13	ARG	5.2
34	CF	81	GLN	5.2
38	CK	142	ILE	5.2
31	CA	138	U	5.2
48	CU	16	VAL	5.2
55	DA	2168	G	5.2
37	DJ	132	THR	5.2
13	BM	77	ILE	5.2
9	BI	8	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
12	BL	70	GLU	5.2
20	BT	53	GLU	5.2
31	CA	268	C	5.2
3	BC	77	ILE	5.2
53	CZ	21	LEU	5.2
7	BG	113	ASP	5.2
10	BJ	85	ASP	5.2
15	AO	17	ARG	5.2
27	C0	53	PHE	5.2
33	CE	124	PHE	5.2
14	BN	58	SER	5.2
31	CA	1166	G	5.2
52	CY	35	SER	5.2
6	AF	61	LEU	5.2
40	CM	35	HIS	5.2
13	BM	113	ARG	5.2
43	CP	30	ARG	5.2
30	CD	153	GLY	5.1
31	CA	2651	C	5.1
3	BC	124	LEU	5.1
37	DJ	51	LYS	5.1
53	CZ	28	LEU	5.1
9	BI	41	ARG	5.1
31	CA	408	G	5.1
31	CA	1171	G	5.1
34	CF	56	ASP	5.1
55	DA	2106	U	5.1
31	CA	893	C	5.1
24	C3	34	ARG	5.1
7	BG	80	VAL	5.1
31	CA	1047	G	5.1
37	DJ	131	GLY	5.1
1	BA	207	C	5.1
1	BA	977	A	5.1
39	CL	33	ALA	5.1
31	CA	1271	G	5.1
46	CS	100	GLY	5.1
44	CQ	4	ILE	5.1
51	CX	58	THR	5.1
7	BG	131	LYS	5.1
9	BI	103	PHE	5.1
46	CS	83	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
50	CW	91	PHE	5.1
19	BS	50	ALA	5.1
9	BI	37	GLN	5.1
13	AM	4	ILE	5.1
34	CF	67	ILE	5.1
7	AG	151	PHE	5.1
1	BA	1336	C	5.1
13	BM	104	THR	5.1
14	BN	9	ARG	5.1
26	C5	20	ASP	5.1
30	CD	133	THR	5.1
40	CM	74	THR	5.1
48	CU	84	TYR	5.1
17	BQ	50	ASN	5.1
30	CD	152	PRO	5.1
17	BQ	44	LEU	5.1
34	CF	91	LEU	5.1
44	CQ	74	PHE	5.1
33	CE	48	THR	5.1
34	CF	68	THR	5.1
37	DJ	60	THR	5.1
52	CY	34	HIS	5.1
3	BC	103	ILE	5.1
14	BN	30	ILE	5.1
35	CG	141	ILE	5.1
7	AG	53	ARG	5.1
40	CM	144	GLU	5.1
10	BJ	34	ALA	5.1
36	CH	67	ALA	5.1
49	CV	84	GLY	5.1
1	BA	1312	G	5.1
33	CE	157	LEU	5.0
37	DJ	106	LEU	5.0
20	BT	64	LYS	5.0
36	DH	132	PHE	5.0
48	CU	75	GLY	5.0
48	CU	24	MET	5.0
54	DI	124	ASP	5.0
16	BP	50	THR	5.0
31	CA	2177	C	5.0
33	CE	73	ILE	5.0
37	DJ	49	ILE	5.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
11	AK	81	ASN	5.0
51	CX	83	GLU	5.0
52	CY	45	ARG	5.0
13	AM	25	VAL	5.0
36	DH	65	ALA	5.0
45	CR	113	ALA	5.0
49	CV	76	ALA	5.0
7	BG	102	ARG	5.0
19	BS	42	PRO	5.0
38	CK	128	ASN	5.0
20	BT	50	ALA	5.0
31	CA	332	A	5.0
22	C1	36	GLU	5.0
31	CA	2904	U	5.0
7	BG	68	ASN	5.0
20	BT	46	ALA	5.0
31	CA	501	A	5.0
13	BM	4	ILE	5.0
34	CF	4	LEU	5.0
37	DJ	42	PHE	5.0
7	AG	5	ARG	5.0
47	CT	6	LYS	5.0
51	CX	25	ARG	5.0
34	CF	38	MET	5.0
19	BS	57	HIS	5.0
31	CA	513	A	5.0
7	BG	82	GLY	5.0
1	BA	83	C	5.0
24	C3	12	ARG	5.0
44	CQ	111	LYS	5.0
54	DI	40	GLU	5.0
34	CF	172	ALA	5.0
2	BB	9	MET	5.0
13	BM	81	MET	5.0
43	CP	88	LYS	5.0
53	CZ	54	LYS	5.0
55	DA	2141	G	5.0
3	BC	73	PRO	5.0
8	AH	2	SER	5.0
14	BN	24	ARG	5.0
19	BS	25	SER	5.0
30	CD	25	THR	5.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	BA	222	C	5.0
7	AG	134	ALA	5.0
27	C0	2	ALA	5.0
43	CP	93	ASP	5.0
7	AG	59	LEU	5.0
44	CQ	59	PHE	5.0
7	AG	58	GLU	5.0
35	CG	25	THR	5.0
40	CM	108	ALA	5.0
53	CZ	63	ALA	5.0
38	CK	136	GLN	4.9
42	CO	36	THR	4.9
13	BM	11	ASP	4.9
33	CE	11	ALA	4.9
45	CR	94	ILE	4.9
51	CX	34	GLY	4.9
9	AI	32	GLN	4.9
33	CE	32	VAL	4.9
13	AM	36	ALA	4.9
48	CU	12	ARG	4.9
1	BA	962	C	4.9
9	BI	92	GLU	4.9
22	C1	55	ILE	4.9
30	CD	199	SER	4.9
50	CW	58	SER	4.9
46	CS	26	ASP	4.9
19	AS	39	THR	4.9
31	CA	103	A	4.9
31	CA	2800	A	4.9
55	DA	654	A	4.9
1	BA	1309	G	4.9
16	BP	39	PHE	4.9
41	CN	79	ALA	4.9
49	CV	47	LYS	4.9
1	AA	1025	U	4.9
13	AM	45	ILE	4.9
30	CD	48	ILE	4.9
53	CZ	6	LEU	4.9
1	BA	1034	G	4.9
53	CZ	36	GLN	4.9
2	BB	39	HIS	4.9
27	C0	42	PRO	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
30	CD	47	ALA	4.9
31	CA	369	U	4.9
45	CR	26	GLY	4.9
48	CU	2	ILE	4.9
2	AB	139	ARG	4.9
37	CJ	92	LYS	4.9
17	BQ	46	VAL	4.9
31	CA	1056	G	4.9
48	CU	31	VAL	4.9
11	BK	21	ALA	4.9
14	BN	40	ASP	4.9
31	CA	431	U	4.9
37	DJ	113	LYS	4.9
55	DA	885	C	4.9
31	CA	262	A	4.9
14	BN	33	ASP	4.9
31	CA	1235	G	4.9
49	CV	82	ARG	4.9
3	BC	144	LEU	4.9
35	CG	77	ILE	4.9
55	DA	1094	U	4.9
11	BK	64	GLN	4.9
9	AI	55	VAL	4.9
17	BQ	78	VAL	4.9
42	CO	93	GLY	4.9
20	BT	67	ILE	4.9
34	CF	47	LYS	4.9
36	CH	58	LEU	4.9
55	DA	1066	U	4.9
35	CG	127	THR	4.8
10	AJ	36	VAL	4.8
17	BQ	6	ARG	4.8
3	BC	80	LYS	4.8
9	AI	22	LYS	4.8
31	CA	357	C	4.8
46	CS	13	ARG	4.8
30	CD	132	ALA	4.8
38	CK	47	HIS	4.8
37	CJ	37	GLU	4.8
3	BC	107	ARG	4.8
19	BS	55	ARG	4.8
3	BC	42	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
6	BF	39	LEU	4.8
30	CD	101	PHE	4.8
43	CP	58	ILE	4.8
34	CF	30	ARG	4.8
19	BS	34	TRP	4.8
31	CA	2808	G	4.8
33	CE	186	VAL	4.8
36	DH	107	GLY	4.8
7	AG	106	GLU	4.8
13	BM	80	LEU	4.8
31	CA	1234	U	4.8
31	CA	2180	U	4.8
7	BG	122	ASN	4.8
26	C5	1	MET	4.8
40	CM	132	ARG	4.8
31	CA	505	A	4.8
16	BP	19	VAL	4.8
36	DH	96	THR	4.8
13	BM	61	ALA	4.8
31	CA	882	G	4.8
37	DJ	75	PRO	4.8
18	AR	51	TYR	4.8
27	C0	32	ILE	4.8
35	CG	94	TYR	4.8
10	BJ	35	GLN	4.8
40	CM	21	ARG	4.8
55	DA	892	A	4.8
10	AJ	7	ARG	4.8
16	BP	53	ASP	4.8
40	CM	70	LYS	4.8
16	BP	9	HIS	4.8
30	CD	45	TYR	4.8
31	CA	315	G	4.8
13	BM	13	LYS	4.8
45	CR	95	LEU	4.8
52	CY	46	PHE	4.8
30	CD	35	THR	4.8
13	BM	52	GLN	4.8
1	BA	1209	C	4.8
31	CA	1863	G	4.8
35	CG	175	LYS	4.8
54	DI	101	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
30	CD	60	VAL	4.8
37	CJ	88	SER	4.8
7	AG	65	ALA	4.8
45	CR	38	ALA	4.8
1	AA	1022	A	4.8
41	CN	72	PRO	4.8
55	DA	2126	A	4.8
55	DA	2132	U	4.8
31	CA	343	C	4.8
34	CF	42	GLU	4.8
14	BN	32	SER	4.8
25	C4	14	PHE	4.8
1	BA	1219	A	4.8
31	CA	101	A	4.8
37	DJ	40	LYS	4.8
38	CK	21	THR	4.8
47	CT	83	LYS	4.8
31	CA	2106	U	4.8
54	DI	114	GLU	4.8
31	CA	1547	C	4.7
3	BC	203	PHE	4.7
9	BI	107	ASP	4.7
34	CF	10	ASP	4.7
31	CA	895	U	4.7
1	BA	1340	A	4.7
31	CA	336	C	4.7
55	DA	2177	C	4.7
13	AM	40	ALA	4.7
41	CN	41	LEU	4.7
43	CP	59	ALA	4.7
7	AG	7	ILE	4.7
31	CA	2877	G	4.7
49	CV	55	PRO	4.7
2	AB	210	VAL	4.7
13	BM	69	LEU	4.7
30	CD	187	LEU	4.7
36	DH	56	ALA	4.7
30	CD	83	ARG	4.7
31	CA	214	G	4.7
2	AB	44	GLU	4.7
19	BS	3	ARG	4.7
33	CE	22	ASP	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
35	CG	24	ILE	4.7
1	BA	981	U	4.7
34	CF	8	TYR	4.7
41	CN	80	VAL	4.7
39	CL	3	GLN	4.7
40	CM	72	ALA	4.7
20	BT	8	LYS	4.7
47	CT	4	ILE	4.7
1	BA	1341	U	4.7
14	BN	34	VAL	4.7
35	CG	44	LYS	4.7
48	CU	81	LYS	4.7
55	DA	2164	C	4.7
34	CF	150	ARG	4.7
11	BK	30	THR	4.7
43	CP	53	THR	4.7
53	CZ	35	GLY	4.7
31	CA	313	G	4.7
31	CA	2627	G	4.7
7	BG	78	ARG	4.7
55	DA	2117	A	4.7
30	CD	1	MET	4.7
30	CD	29	VAL	4.7
40	CM	127	VAL	4.7
9	BI	43	THR	4.7
7	AG	68	ASN	4.7
36	CH	137	GLU	4.7
1	BA	1534	A	4.7
24	C3	22	MET	4.6
2	BB	10	LEU	4.6
10	BJ	92	LEU	4.6
29	CC	232	HIS	4.6
36	CH	135	HIS	4.6
2	BB	32	PHE	4.6
30	CD	90	PHE	4.6
31	CA	318	C	4.6
43	CP	36	TYR	4.6
13	AM	26	GLY	4.6
45	CR	7	GLY	4.6
21	AU	9	ASN	4.6
1	BA	1224	U	4.6
14	BN	21	PHE	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
35	CG	126	PRO	4.6
49	CV	11	VAL	4.6
51	CX	23	VAL	4.6
2	AB	117	LEU	4.6
1	BA	1033	G	4.6
1	BA	1231	G	4.6
13	BM	50	GLU	4.6
47	CT	94	ASP	4.6
24	C3	43	THR	4.6
25	C4	46	PRO	4.6
31	CA	850	U	4.6
33	CE	177	PRO	4.6
55	DA	1060	U	4.6
14	AN	100	SER	4.6
43	CP	33	ARG	4.6
21	AU	16	LEU	4.6
48	CU	62	VAL	4.6
2	BB	33	GLY	4.6
7	BG	63	GLU	4.6
40	CM	76	GLU	4.6
55	DA	1089	A	4.6
22	C1	44	THR	4.6
31	CA	1534	U	4.6
47	CT	92	ARG	4.6
54	DI	94	ARG	4.6
27	C0	12	SER	4.6
50	CW	67	GLY	4.6
11	AK	18	ASP	4.6
39	CL	111	LYS	4.6
36	DH	124	THR	4.6
36	DH	87	GLU	4.6
43	CP	49	VAL	4.6
51	CX	42	GLY	4.6
39	CL	38	ILE	4.6
40	CM	137	ALA	4.6
43	CP	109	ALA	4.6
45	CR	17	ILE	4.6
13	BM	42	ASP	4.6
31	CA	2122	U	4.6
37	DJ	37	GLU	4.6
1	BA	68	G	4.6
1	BA	951	G	4.6

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Mol	Chain	Res	Type	RSRZ
11	AK	43	GLY	4.6
29	CC	47	GLY	4.6
31	CA	1530	G	4.6
36	CH	61	VAL	4.6
33	CE	100	MET	4.6
7	BG	98	ALA	4.6
31	CA	1868	C	4.6
33	CE	127	GLU	4.6
45	CR	37	GLN	4.6
17	BQ	8	LEU	4.6
35	CG	6	LYS	4.6
36	DH	125	THR	4.6
22	C1	15	MET	4.6
31	CA	880	G	4.6
38	CK	42	ALA	4.6
31	CA	314	C	4.6
7	AG	6	VAL	4.5
25	C4	38	THR	4.5
31	CA	44	A	4.5
48	CU	76	ARG	4.5
38	CK	55	ILE	4.5
44	CQ	13	MET	4.5
7	AG	54	SER	4.5
36	DH	136	SER	4.5
31	CA	1074	G	4.5
31	CA	2116	G	4.5
31	CA	2630	G	4.5
55	DA	1063	G	4.5
1	BA	972	C	4.5
7	AG	26	PHE	4.5
13	BM	70	ARG	4.5
33	CE	134	LEU	4.5
3	BC	109	PRO	4.5
38	CK	137	PRO	4.5
1	BA	205	A	4.5
42	CO	114	GLU	4.5
2	BB	16	PHE	4.5
20	BT	31	PHE	4.5
1	BA	1027	C	4.5
31	CA	88	G	4.5
37	DJ	107	GLN	4.5
39	CL	69	VAL	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	DI	135	ALA	4.5
33	CE	15	SER	4.5
16	BP	56	ARG	4.5
26	C5	33	HIS	4.5
3	BC	78	GLY	4.5
33	CE	103	GLY	4.5
43	CP	104	GLN	4.5
33	CE	43	THR	4.5
37	CJ	64	ASP	4.5
1	AA	78	A	4.5
1	BA	89	U	4.5
9	AI	63	LEU	4.5
47	CT	48	LYS	4.5
54	DI	133	GLU	4.5
2	BB	206	ALA	4.5
50	CW	48	MET	4.5
55	DA	881	G	4.5
43	CP	97	PHE	4.5
17	BQ	72	SER	4.5
1	BA	946	A	4.5
7	AG	141	VAL	4.5
34	CF	49	LEU	4.5
19	BS	11	ILE	4.5
35	CG	75	MET	4.5
47	CT	54	ALA	4.5
48	DU	1	MET	4.5
16	AP	16	PHE	4.5
31	CA	1059	G	4.5
30	CD	73	VAL	4.5
33	CE	199	MET	4.5
5	BE	140	THR	4.5
40	CM	121	THR	4.5
9	BI	98	LEU	4.5
13	AM	48	LEU	4.5
26	C5	12	ARG	4.5
31	CA	2181	U	4.5
35	CG	76	VAL	4.5
49	CV	42	VAL	4.5
13	AM	39	ILE	4.5
54	DI	136	ILE	4.5
31	CA	281	C	4.5
31	CA	816	C	4.5

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Mol	Chain	Res	Type	RSRZ
31	CA	1233	C	4.5
7	AG	8	GLY	4.5
26	C5	19	ARG	4.5
33	CE	49	ARG	4.5
35	CG	129	THR	4.5
38	CK	40	HIS	4.5
42	CO	113	ILE	4.4
13	AM	115	PRO	4.4
7	AG	52	GLN	4.4
14	BN	73	PHE	4.4
27	C0	39	GLU	4.4
33	CE	42	GLY	4.4
37	CJ	25	GLY	4.4
40	CM	124	GLY	4.4
55	DA	2161	C	4.4
33	CE	180	LEU	4.4
1	BA	842	U	4.4
42	CO	76	VAL	4.4
46	CS	15	SER	4.4
1	BA	941	G	4.4
15	BO	19	ALA	4.4
31	CA	1407	G	4.4
16	BP	51	ARG	4.4
31	CA	876	C	4.4
37	DJ	127	ARG	4.4
31	CA	1061	U	4.4
37	DJ	33	VAL	4.4
50	CW	64	VAL	4.4
14	BN	63	ARG	4.4
34	CF	14	LYS	4.4
34	CF	100	PHE	4.4
19	BS	44	MET	4.4
42	CO	79	LEU	4.4
1	BA	1125	U	4.4
36	CH	110	VAL	4.4
46	CS	29	THR	4.4
7	BG	90	GLU	4.4
13	BM	49	SER	4.4
38	CK	98	GLU	4.4
31	CA	1093	G	4.4
31	CA	1984	G	4.4
9	BI	129	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
43	CP	56	LYS	4.4
2	AB	7	ARG	4.4
10	BJ	32	THR	4.4
44	CQ	50	ILE	4.4
34	CF	27	GLN	4.4
40	CM	7	SER	4.4
9	BI	79	ILE	4.4
31	CA	1090	A	4.4
31	CA	2799	A	4.4
51	CX	37	ILE	4.4
2	AB	9	MET	4.4
40	CM	91	ASP	4.4
49	CV	21	LYS	4.4
35	CG	38	ASN	4.4
49	CV	67	VAL	4.4
31	CA	413	C	4.4
1	BA	1003	G	4.4
2	BB	213	TYR	4.4
7	BG	86	GLN	4.4
49	CV	63	ALA	4.4
20	BT	9	LYS	4.4
35	CG	156	PRO	4.4
51	CX	64	ASP	4.4
34	CF	112	ARG	4.4
11	AK	97	ILE	4.4
31	CA	2178	C	4.4
41	CN	73	ILE	4.4
19	BS	56	GLN	4.4
13	BM	75	MET	4.4
30	CD	184	ARG	4.4
12	BL	81	LEU	4.4
14	BN	10	GLU	4.4
40	CM	122	VAL	4.4
30	CD	55	LYS	4.4
36	CH	94	ILE	4.4
37	DJ	92	LYS	4.4
40	CM	139	GLY	4.4
15	BO	15	PHE	4.3
1	AA	1001	C	4.3
19	AS	56	GLN	4.3
55	DA	897	C	4.3
33	CE	122	GLU	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
43	CP	32	PRO	4.3
45	CR	117	LEU	4.3
35	CG	113	VAL	4.3
2	BB	164	ILE	4.3
3	BC	102	ASN	4.3
17	BQ	21	ILE	4.3
33	CE	175	ILE	4.3
35	CG	48	ASN	4.3
49	CV	72	ILE	4.3
14	AN	25	ALA	4.3
37	CJ	127	ARG	4.3
20	BT	68	HIS	4.3
34	CF	11	GLU	4.3
34	CF	22	TYR	4.3
12	BL	108	LYS	4.3
40	CM	30	THR	4.3
49	DV	52	LEU	4.3
28	CB	24	G	4.3
49	CV	56	GLY	4.3
11	BK	110	ILE	4.3
46	CS	6	GLN	4.3
9	AI	59	GLU	4.3
2	AB	37	LYS	4.3
55	DA	893	C	4.3
7	BG	120	LEU	4.3
8	AH	121	LEU	4.3
13	BM	111	GLY	4.3
51	CX	41	ARG	4.3
7	BG	9	GLN	4.3
19	BS	43	ASN	4.3
31	CA	124	G	4.3
31	CA	2668	G	4.3
31	CA	475	C	4.3
31	CA	1079	C	4.3
54	DI	72	LEU	4.3
22	C1	8	PRO	4.3
23	C2	22	THR	4.3
37	DJ	97	LYS	4.3
40	CM	38	GLN	4.3
1	BA	1239	A	4.3
8	BH	130	ALA	4.3
33	CE	147	LEU	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
25	C4	45	ARG	4.3
41	CN	12	MET	4.3
10	BJ	96	VAL	4.3
19	BS	23	VAL	4.3
52	CY	47	VAL	4.3
40	CM	50	PHE	4.3
1	BA	1150	A	4.3
10	AJ	102	LEU	4.3
20	BT	59	ASP	4.3
30	CD	84	LEU	4.3
2	AB	27	MET	4.3
2	BB	131	LYS	4.3
13	BM	62	LYS	4.3
31	CA	2693	G	4.3
36	DH	89	LYS	4.3
9	AI	89	GLU	4.3
30	CD	50	VAL	4.3
34	CF	101	GLU	4.3
55	DA	2146	C	4.3
3	BC	50	ALA	4.3
27	C0	25	LEU	4.3
35	CG	166	ASP	4.3
20	BT	36	TYR	4.3
38	CK	118	MET	4.3
40	CM	119	PRO	4.3
42	CO	94	TYR	4.3
31	CA	1015	U	4.3
25	C4	25	LYS	4.3
45	CR	30	ARG	4.3
19	BS	13	LEU	4.3
51	CX	85	GLU	4.3
1	BA	1035	A	4.3
14	BN	71	HIS	4.3
15	BO	75	VAL	4.3
50	CW	2	PHE	4.3
1	AA	1033	G	4.3
1	BA	1013	G	4.3
49	DV	51	ALA	4.2
49	DV	49	VAL	4.2
31	CA	1073	A	4.2
46	CS	60	LYS	4.2
47	CT	95	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	BA	1281	C	4.2
1	BA	1272	G	4.2
35	CG	21	GLY	4.2
46	CS	30	GLY	4.2
16	AP	39	PHE	4.2
36	CH	139	PHE	4.2
45	CR	101	PHE	4.2
31	CA	2657	A	4.2
31	CA	810	U	4.2
31	CA	2164	C	4.2
34	CF	171	ALA	4.2
3	BC	112	ASP	4.2
17	BQ	74	THR	4.2
20	AT	80	THR	4.2
13	BM	90	ARG	4.2
31	CA	1279	G	4.2
7	BG	44	TYR	4.2
31	CA	884	U	4.2
8	BH	122	GLY	4.2
11	BK	67	ALA	4.2
31	CA	1548	A	4.2
6	BF	97	THR	4.2
9	BI	48	VAL	4.2
33	CE	126	VAL	4.2
6	AF	37	HIS	4.2
11	AK	110	ILE	4.2
1	BA	952	U	4.2
25	C4	35	LYS	4.2
48	CU	33	LYS	4.2
1	BA	250	A	4.2
7	AG	23	LEU	4.2
34	CF	36	LEU	4.2
24	C3	5	PHE	4.2
37	DJ	57	VAL	4.2
49	CV	85	PHE	4.2
9	AI	88	MET	4.2
35	CG	173	GLU	4.2
37	CJ	117	MET	4.2
42	CO	1	MET	4.2
9	BI	21	ILE	4.2
19	AS	49	ILE	4.2
36	DH	99	ILE	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
35	CG	125	CYS	4.2
45	CR	25	TYR	4.2
31	CA	280	U	4.2
9	BI	94	LEU	4.2
45	CR	18	LEU	4.2
54	DI	3	LEU	4.2
15	BO	21	ASP	4.2
31	CA	2165	C	4.2
13	BM	44	LYS	4.2
33	CE	121	VAL	4.2
37	CJ	36	MET	4.2
1	BA	1007	U	4.2
31	CA	1112	G	4.2
37	CJ	115	ALA	4.2
40	CM	83	ALA	4.2
55	DA	2105	U	4.2
1	BA	1310	G	4.2
13	AM	13	LYS	4.2
48	CU	44	LYS	4.2
28	CB	63	C	4.2
24	C3	13	ASN	4.2
33	CE	28	VAL	4.2
35	CG	90	VAL	4.2
30	CD	121	THR	4.2
49	CV	65	ILE	4.2
37	CJ	16	GLY	4.2
36	DH	67	ALA	4.2
43	CP	70	ALA	4.2
46	CS	92	TRP	4.2
49	CV	2	ALA	4.2
3	BC	108	LYS	4.2
37	DJ	81	LYS	4.2
9	AI	97	GLU	4.2
11	BK	68	GLU	4.2
19	BS	65	GLU	4.2
31	CA	180	G	4.2
31	CA	1444	G	4.2
34	CF	114	PHE	4.2
1	BA	1230	C	4.2
10	AJ	45	ARG	4.2
30	CD	59	ARG	4.2
31	CA	1874	C	4.2

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Mol	Chain	Res	Type	RSRZ
5	BE	80	THR	4.2
44	CQ	5	ILE	4.2
34	CF	139	PRO	4.2
34	CF	64	LYS	4.2
46	CS	82	HIS	4.2
5	BE	120	VAL	4.1
14	AN	37	SER	4.1
1	AA	1277	C	4.1
37	CJ	34	ASN	4.1
7	AG	110	LYS	4.1
13	BM	102	THR	4.1
40	CM	5	THR	4.1
1	AA	1000	A	4.1
53	CZ	48	ARG	4.1
38	CK	54	ILE	4.1
46	CS	24	LYS	4.1
1	BA	1001	C	4.1
31	CA	2032	G	4.1
1	BA	982	U	4.1
49	CV	62	GLU	4.1
3	BC	179	ARG	4.1
9	BI	33	ARG	4.1
13	AM	35	ALA	4.1
55	DA	2171	A	4.1
7	BG	26	PHE	4.1
38	CK	141	ASP	4.1
7	AG	64	VAL	4.1
9	BI	117	GLY	4.1
13	BM	38	GLY	4.1
37	CJ	35	ILE	4.1
16	AP	47	GLU	4.1
21	AU	36	GLU	4.1
31	CA	1533	C	4.1
46	CS	37	GLU	4.1
34	CF	29	PRO	4.1
8	BH	121	LEU	4.1
45	CR	92	ARG	4.1
2	AB	132	LYS	4.1
40	CM	84	LYS	4.1
8	BH	90	ASP	4.1
4	AD	39	GLY	4.1
33	CE	10	SER	4.1

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Mol	Chain	Res	Type	RSRZ
12	BL	50	ARG	4.1
1	BA	1210	C	4.1
28	CB	22	U	4.1
2	AB	16	PHE	4.1
9	AI	39	PHE	4.1
33	CE	35	TYR	4.1
31	CA	799	G	4.1
31	CA	1041	G	4.1
33	CE	176	ASP	4.1
1	AA	1036	A	4.1
31	CA	2835	A	4.1
14	BN	39	GLU	4.1
22	C1	51	GLY	4.1
7	AG	50	LEU	4.1
9	BI	121	ALA	4.1
41	CN	78	LEU	4.1
1	AA	1037	C	4.1
28	CB	97	C	4.1
30	CD	39	ASP	4.1
17	BQ	23	VAL	4.1
33	CE	196	VAL	4.1
36	CH	134	VAL	4.1
46	CS	46	GLU	4.1
13	BM	53	ILE	4.1
1	AA	89	U	4.1
40	CM	138	ALA	4.1
45	CR	35	ALA	4.1
54	DI	106	PHE	4.1
33	CE	140	ASP	4.1
37	CJ	137	GLY	4.1
54	DI	66	GLY	4.1
11	AK	100	LEU	4.1
13	AM	34	LEU	4.1
35	CG	50	LEU	4.1
48	CU	80	TRP	4.1
14	BN	15	ALA	4.1
39	CL	89	ASN	4.1
35	CG	158	LYS	4.1
43	CP	102	ARG	4.1
47	CT	99	ARG	4.1
31	CA	1531	C	4.1
10	AJ	8	ILE	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	DI	123	ILE	4.1
2	AB	214	LEU	4.1
1	BA	1048	G	4.1
9	BI	124	ARG	4.0
14	BN	47	LYS	4.1
31	CA	638	G	4.1
31	CA	801	G	4.1
31	CA	2111	U	4.1
40	CM	52	GLY	4.0
31	CA	1044	C	4.0
34	CF	141	ILE	4.0
45	CR	65	ILE	4.0
14	AN	27	LEU	4.0
31	CA	1325	U	4.0
33	CE	50	ALA	4.0
41	CN	116	ALA	4.0
30	CD	80	TRP	4.0
31	CA	1142	A	4.0
35	CG	154	PRO	4.0
31	CA	85	G	4.0
33	CE	64	GLY	4.0
55	DA	277	G	4.0
13	BM	16	VAL	4.0
45	CR	39	VAL	4.0
17	BQ	61	ILE	4.0
31	CA	1732	C	4.0
3	BC	172	ARG	4.0
7	AG	116	MET	4.0
36	CH	122	LEU	4.0
36	DH	127	GLU	4.0
31	CA	545	U	4.0
44	CQ	91	ALA	4.0
2	AB	36	ASN	4.0
3	BC	194	GLY	4.0
37	CJ	66	SER	4.0
50	CW	37	PRO	4.0
1	AA	412	A	4.0
31	CA	477	A	4.0
31	CA	866	A	4.0
31	CA	2872	A	4.0
1	BA	945	G	4.0
3	BC	200	VAL	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	BC	204	LYS	4.0
7	AG	105	VAL	4.0
11	AK	84	VAL	4.0
44	CQ	26	VAL	4.0
46	CS	51	VAL	4.0
19	BS	81	ARG	4.0
35	CG	49	THR	4.0
31	CA	2167	U	4.0
23	C2	31	PRO	4.0
3	BC	118	ASP	4.0
14	BN	3	LYS	4.0
30	CD	95	SER	4.0
49	CV	27	ASN	4.0
16	AP	4	ILE	4.0
44	CQ	72	ARG	4.0
48	CU	30	ILE	4.0
1	AA	1276	G	4.0
2	AB	10	LEU	4.0
43	CP	61	GLN	4.0
2	BB	134	ALA	4.0
19	BS	75	ALA	4.0
35	CG	91	GLY	4.0
43	CP	22	GLY	4.0
29	CC	101	ARG	4.0
33	CE	67	ARG	4.0
37	DJ	61	VAL	4.0
6	AF	36	ILE	4.0
45	CR	45	TYR	4.0
55	DA	1847	A	4.0
7	AG	49	THR	4.0
29	CC	225	MET	4.0
42	CO	20	MET	4.0
46	CS	99	THR	4.0
9	AI	16	ALA	4.0
19	BS	26	GLY	4.0
31	CA	2367	G	4.0
37	CJ	104	ALA	4.0
31	CA	290	U	4.0
33	CE	76	PRO	4.0
49	CV	22	ARG	4.0
49	DV	55	PRO	4.0
20	BT	35	VAL	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	DI	88	HIS	4.0
44	CQ	99	TYR	4.0
7	BG	51	ALA	4.0
28	CB	37	C	4.0
31	CA	1018	U	4.0
36	DH	123	ARG	4.0
40	CM	34	GLY	4.0
42	CO	101	GLY	4.0
31	CA	2819	G	4.0
34	CF	98	GLU	4.0
35	CG	73	ASN	4.0
44	CQ	92	VAL	4.0
47	CT	98	LYS	4.0
33	CE	12	LEU	4.0
14	BN	59	ARG	4.0
1	BA	174	A	4.0
11	AK	21	ALA	4.0
23	C2	29	THR	4.0
30	CD	75	ALA	4.0
31	CA	603	A	4.0
31	CA	1143	A	4.0
36	CH	127	GLU	4.0
14	BN	7	LYS	4.0
33	CE	171	ASP	4.0
31	CA	2383	G	4.0
34	CF	149	VAL	4.0
36	DH	142	VAL	4.0
34	CF	127	ASN	4.0
37	DJ	21	SER	4.0
2	AB	49	MET	4.0
20	BT	45	ALA	4.0
50	CW	28	ALA	4.0
1	BA	194	C	3.9
1	BA	1226	C	3.9
13	AM	31	LYS	3.9
31	CA	224	U	3.9
31	CA	1406	U	3.9
43	CP	60	GLU	4.0
53	CZ	5	GLU	4.0
55	DA	2114	A	3.9
1	BA	944	G	3.9
31	CA	989	G	3.9

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Mol	Chain	Res	Type	RSRZ
22	C1	37	LYS	3.9
22	C1	33	THR	3.9
27	C0	41	THR	3.9
1	BA	460	A	3.9
13	BM	100	GLN	3.9
7	AG	48	GLU	3.9
1	BA	1127	G	3.9
15	AO	69	TYR	3.9
31	CA	361	G	3.9
35	CG	96	ALA	3.9
46	CS	1	MET	3.9
23	C2	40	ASP	3.9
26	C5	25	VAL	3.9
36	CH	68	ARG	3.9
49	CV	86	ARG	3.9
1	BA	1038	C	3.9
7	BG	23	LEU	3.9
31	CA	222	A	3.9
48	CU	82	LYS	3.9
36	CH	70	GLU	3.9
38	CK	94	ALA	3.9
53	DZ	63	ALA	3.9
1	BA	976	G	3.9
31	CA	259	G	3.9
31	CA	2895	G	3.9
36	CH	108	VAL	3.9
2	AB	85	LEU	3.9
30	CD	188	LEU	3.9
13	BM	106	ALA	3.9
49	CV	94	ARG	3.9
47	CT	16	LYS	3.9
1	BA	1041	G	3.9
31	CA	1017	G	3.9
14	BN	50	THR	3.9
16	AP	45	GLU	3.9
29	CC	236	GLU	3.9
1	BA	1277	C	3.9
3	BC	171	GLY	3.9
16	BP	58	ALA	3.9
55	DA	2119	A	3.9
31	CA	2833	U	3.9
21	AU	13	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
48	CU	56	GLU	3.9
1	BA	1253	G	3.9
22	C1	26	THR	3.9
31	CA	1202	G	3.9
1	BA	325	A	3.9
3	BC	56	VAL	3.9
8	BH	110	VAL	3.9
27	C0	57	VAL	3.9
30	CD	86	GLU	3.9
37	CJ	116	ASP	3.9
13	AM	24	GLY	3.9
43	CP	101	GLY	3.9
2	BB	212	LEU	3.9
3	BC	54	ARG	3.9
20	BT	5	LYS	3.9
38	CK	23	LYS	3.9
1	BA	1214	C	3.9
31	CA	805	G	3.9
33	CE	26	ALA	3.9
35	CG	20	ASN	3.9
47	CT	40	ASN	3.9
14	AN	5	SER	3.9
1	AA	80	A	3.9
1	AA	1004	A	3.9
31	CA	423	A	3.9
49	DV	54	GLN	3.9
26	C5	2	LYS	3.9
40	CM	65	GLY	3.9
39	CL	48	PRO	3.9
40	CM	3	LEU	3.9
52	CY	18	ARG	3.9
7	BG	121	ALA	3.9
31	CA	2129	C	3.9
42	CO	107	ASN	3.9
50	CW	7	GLU	3.9
31	CA	1731	G	3.9
55	DA	2128	G	3.9
3	BC	116	VAL	3.8
7	BG	149	LYS	3.8
17	BQ	5	ILE	3.8
29	CC	172	VAL	3.8
34	CF	142	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
50	CW	45	ASP	3.8
31	CA	2176	A	3.8
9	AI	51	PRO	3.8
46	CS	52	PRO	3.8
1	BA	175	C	3.8
2	AB	42	ASN	3.8
10	BJ	23	ALA	3.8
33	CE	135	ALA	3.8
31	CA	1043	C	3.8
34	CF	12	VAL	3.8
28	CB	23	G	3.8
31	CA	2876	G	3.8
55	DA	2162	G	3.8
35	CG	37	LEU	3.8
1	AA	1019	A	3.8
1	BA	1254	A	3.8
31	CA	213	A	3.8
31	CA	1395	A	3.8
31	CA	2309	A	3.8
20	AT	87	ALA	3.8
38	CK	78	THR	3.8
40	CM	118	THR	3.8
45	CR	42	ALA	3.8
30	CD	42	ASN	3.8
31	CA	1599	U	3.8
2	AB	41	ILE	3.8
38	CK	64	VAL	3.8
30	CD	68	PHE	3.8
1	BA	108	G	3.8
2	AB	12	ALA	3.8
3	BC	117	ALA	3.8
7	BG	127	ALA	3.8
24	C3	14	ARG	3.8
2	BB	36	ASN	3.8
1	BA	1364	U	3.8
6	AF	62	MET	3.8
25	C4	26	HIS	3.8
53	CZ	25	GLN	3.8
3	BC	122	SER	3.8
7	BG	57	SER	3.8
31	CA	76	C	3.8
33	CE	168	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
38	CK	60	ASP	3.8
46	CS	64	VAL	3.8
10	AJ	10	LEU	3.8
53	CZ	44	LYS	3.8
3	BC	127	ARG	3.8
1	AA	1002	G	3.8
1	AA	1024	G	3.8
2	BB	89	GLN	3.8
7	BG	84	THR	3.8
30	CD	2	ILE	3.8
45	CR	14	HIS	3.8
51	CX	51	VAL	3.8
7	BG	59	LEU	3.8
16	BP	77	GLU	3.8
10	AJ	39	PRO	3.8
35	CG	68	ALA	3.8
10	BJ	33	GLY	3.8
28	CB	98	G	3.8
31	CA	474	G	3.8
31	CA	1341	G	3.8
34	CF	120	LYS	3.8
35	CG	66	GLY	3.8
48	CU	71	GLY	3.8
17	BQ	29	VAL	3.8
36	DH	11	ASN	3.8
46	CS	19	THR	3.8
30	CD	49	GLN	3.8
2	AB	8	ASP	3.8
14	BN	69	ARG	3.8
31	CA	2491	U	3.8
33	CE	148	ILE	3.8
38	CK	1	MET	3.8
44	CQ	86	VAL	3.8
3	AC	168	TYR	3.8
31	CA	2045	C	3.8
2	AB	30	PHE	3.8
10	AJ	5	ARG	3.8
53	CZ	8	GLU	3.8
11	BK	65	VAL	3.8
42	CO	52	ILE	3.8
54	DI	55	VAL	3.8
20	BT	70	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
30	CD	149	ASN	3.8
1	BA	1002	G	3.8
26	C5	8	LYS	3.8
31	CA	270	A	3.8
31	CA	308	G	3.8
31	CA	1328	A	3.8
31	CA	1524	G	3.8
1	BA	1267	C	3.8
22	C1	18	SER	3.8
37	CJ	26	PRO	3.8
16	AP	43	ALA	3.8
19	BS	22	ALA	3.8
38	CK	66	GLY	3.8
3	BC	181	ASP	3.7
7	BG	104	ILE	3.8
38	CK	17	VAL	3.8
46	CS	58	VAL	3.8
36	CH	77	THR	3.7
1	BA	172	A	3.7
1	BA	165	G	3.7
42	CO	6	SER	3.7
55	DA	880	G	3.7
7	AG	39	ALA	3.7
14	BN	12	LYS	3.7
16	BP	36	VAL	3.7
29	CC	5	LYS	3.7
41	CN	84	LYS	3.7
1	BA	121	U	3.7
7	BG	85	TYR	3.7
31	CA	412	A	3.7
33	CE	37	ALA	3.7
33	CE	129	PRO	3.7
1	BA	100	G	3.7
1	BA	1320	C	3.7
28	CB	51	G	3.7
31	CA	2890	G	3.7
38	CK	89	PHE	3.7
33	CE	14	VAL	3.7
45	CR	8	VAL	3.7
14	BN	62	ASN	3.7
22	C1	19	HIS	3.7
47	CT	11	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
50	CW	79	ARG	3.7
25	C4	15	LYS	3.7
38	CK	53	TYR	3.7
30	CD	102	ALA	3.7
37	DJ	124	ALA	3.7
1	BA	1265	C	3.7
31	CA	228	C	3.7
31	CA	233	A	3.7
31	CA	611	C	3.7
10	AJ	77	VAL	3.7
49	CV	93	VAL	3.7
31	CA	295	G	3.7
31	CA	377	G	3.7
31	CA	1653	G	3.7
43	CP	89	ASP	3.7
55	DA	2133	G	3.7
2	BB	44	GLU	3.7
22	C1	57	LYS	3.7
46	CS	12	HIS	3.7
2	AB	134	ALA	3.7
8	BH	2	SER	3.7
37	DJ	128	SER	3.7
46	CS	42	ALA	3.7
46	CS	75	VAL	3.7
51	CX	38	VAL	3.7
33	CE	188	MET	3.7
33	DE	7	ASP	3.7
35	CG	167	GLU	3.7
42	CO	117	ASP	3.7
31	CA	1245	G	3.7
26	C5	13	ASN	3.7
42	CO	7	GLY	3.7
27	C0	20	HIS	3.7
12	BL	117	TYR	3.7
14	AN	66	GLN	3.7
13	AM	10	PRO	3.7
13	BM	37	ALA	3.7
37	DJ	83	ALA	3.7
40	CM	15	ALA	3.7
13	BM	97	VAL	3.7
38	CK	95	ARG	3.7
44	CQ	93	ARG	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
45	CR	64	ARG	3.7
15	BO	26	GLU	3.7
40	CM	95	LEU	3.7
31	CA	2629	U	3.7
10	BJ	20	GLN	3.7
14	BN	99	ALA	3.7
30	CD	206	ALA	3.7
36	CH	91	PHE	3.7
40	CM	141	LYS	3.7
37	CJ	112	THR	3.7
2	AB	186	ILE	3.7
36	CH	143	ILE	3.7
2	BB	123	ASP	3.7
9	BI	91	ASP	3.7
31	CA	1045	C	3.7
31	CA	2796	U	3.7
33	CE	7	ASP	3.7
46	CS	95	ASP	3.7
31	CA	53	A	3.7
55	DA	2147	A	3.7
37	CJ	134	ARG	3.7
10	BJ	24	GLU	3.7
31	CA	117	G	3.7
33	CE	190	ALA	3.7
2	AB	47	VAL	3.7
2	BB	41	ILE	3.7
30	CD	100	LEU	3.7
38	CK	140	LEU	3.7
11	BK	85	MET	3.7
28	CB	19	C	3.7
31	CA	353	C	3.7
31	CA	1289	C	3.7
18	BR	48	ARG	3.7
15	BO	20	ASN	3.7
13	AM	15	ALA	3.7
46	CS	36	ALA	3.7
54	DI	104	ALA	3.7
1	BA	212	G	3.7
13	AM	56	LEU	3.7
37	DJ	58	VAL	3.7
45	CR	34	VAL	3.7
31	CA	30	G	3.7

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Mol	Chain	Res	Type	RSRZ
31	CA	495	G	3.7
33	CE	13	THR	3.7
37	CJ	48	SER	3.7
1	BA	1313	U	3.6
2	BB	6	MET	3.6
5	BE	91	GLY	3.6
1	BA	1037	C	3.6
1	BA	1132	C	3.6
29	CC	251	GLN	3.6
33	CE	30	GLN	3.6
42	CO	103	ARG	3.6
4	AD	113	GLU	3.6
3	BC	160	ALA	3.6
16	BP	38	PHE	3.6
19	BS	69	HIS	3.6
31	CA	666	A	3.6
31	CA	1608	A	3.6
31	CA	2614	A	3.6
47	CT	7	HIS	3.6
52	CY	20	HIS	3.6
9	BI	19	VAL	3.6
30	CD	27	ILE	3.6
30	CD	34	VAL	3.6
2	AB	5	SER	3.6
24	C3	24	THR	3.6
33	CE	179	SER	3.6
35	CG	74	SER	3.6
36	CH	14	SER	3.6
39	CL	21	CYS	3.6
40	CM	18	ARG	3.6
35	CG	22	GLN	3.6
1	BA	63	C	3.6
31	CA	680	C	3.6
33	CE	16	GLU	3.6
7	BG	61	ALA	3.6
10	AJ	34	ALA	3.6
11	AK	66	ALA	3.6
19	AS	57	HIS	3.6
47	CT	44	ALA	3.6
53	CZ	58	ASN	3.6
9	AI	83	ILE	3.6
6	AF	97	THR	3.6

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Mol	Chain	Res	Type	RSRZ
46	CS	45	GLU	3.6
1	BA	1266	G	3.6
31	CA	1309	G	3.6
1	AA	1281	C	3.6
31	CA	1207	C	3.6
37	CJ	100	LYS	3.6
2	BB	31	ILE	3.6
11	AK	56	ARG	3.6
13	BM	57	ARG	3.6
42	CO	105	GLY	3.6
1	BA	1036	A	3.6
1	BA	986	U	3.6
31	CA	1060	U	3.6
3	BC	70	THR	3.6
20	BT	80	THR	3.6
36	CH	89	LYS	3.6
9	BI	39	PHE	3.6
31	CA	1236	G	3.6
35	CG	133	LEU	3.6
40	CM	27	LEU	3.6
54	DI	126	LEU	3.6
18	AR	23	TYR	3.6
40	CM	62	PRO	3.6
1	AA	121	U	3.6
10	BJ	88	MET	3.6
31	CA	849	A	3.6
13	BM	3	ARG	3.6
1	BA	210	C	3.6
2	AB	15	HIS	3.6
2	BB	13	GLY	3.6
4	AD	21	LEU	3.6
9	AI	87	LEU	3.6
11	BK	86	VAL	3.6
14	BN	51	LEU	3.6
31	CA	1278	C	3.6
37	CJ	49	ILE	3.6
38	CK	56	VAL	3.6
39	CL	99	ILE	3.6
54	DI	59	LEU	3.6
7	AG	74	GLU	3.6
14	AN	101	TRP	3.6
33	CE	132	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
7	AG	18	PHE	3.6
55	DA	2108	A	3.6
9	AI	94	LEU	3.6
1	BA	980	C	3.6
11	AK	129	VAL	3.6
13	BM	66	GLU	3.6
14	BN	23	LYS	3.6
22	C1	42	HIS	3.6
36	CH	109	GLU	3.6
43	CP	20	GLU	3.6
1	BA	1347	G	3.6
31	CA	767	U	3.6
31	CA	1475	G	3.6
35	CG	128	GLN	3.6
2	BB	139	ARG	3.6
34	CF	96	MET	3.6
13	BM	15	ALA	3.6
35	CG	5	ALA	3.6
47	CT	3	THR	3.6
48	CU	29	THR	3.6
2	AB	221	VAL	3.6
4	AD	117	LEU	3.6
14	BN	79	LEU	3.6
21	AU	3	VAL	3.6
33	CE	77	ILE	3.6
40	CM	116	VAL	3.6
41	CN	126	ILE	3.6
28	CB	110	C	3.6
31	CA	1647	U	3.6
36	CH	27	ARG	3.6
44	CQ	24	ASP	3.6
3	BC	129	MET	3.6
1	AA	1015	G	3.6
17	BQ	53	CYS	3.6
29	CC	30	PHE	3.6
14	AN	67	THR	3.6
33	CE	36	ALA	3.6
36	CH	60	GLU	3.6
31	CA	2117	A	3.6
37	DJ	129	ILE	3.6
39	CL	2	ILE	3.6
10	BJ	15	HIS	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
31	CA	1320	C	3.5
31	CA	2109	U	3.5
31	CA	2305	U	3.5
1	BA	1323	G	3.5
7	BG	125	SER	3.5
31	CA	512	G	3.5
30	CD	146	ILE	3.5
33	CE	4	VAL	3.5
34	DF	176	PRO	3.5
31	CA	11	C	3.5
31	CA	565	C	3.5
12	BL	69	GLY	3.5
33	CE	34	ALA	3.5
34	CF	62	GLY	3.5
7	AG	57	SER	3.5
18	AR	48	ARG	3.5
16	AP	71	VAL	3.5
30	CD	91	THR	3.5
55	DA	1059	G	3.5
1	BA	195	A	3.5
9	AI	31	ASN	3.5
10	AJ	55	PRO	3.5
31	CA	1322	A	3.5
31	CA	2792	A	3.5
36	CH	128	HIS	3.5
2	AB	32	PHE	3.5
16	BP	45	GLU	3.5
31	CA	2364	C	3.5
40	CM	106	GLU	3.5
2	BB	7	ARG	3.5
43	CP	111	ARG	3.5
6	AF	39	LEU	3.5
7	BG	37	SER	3.5
19	BS	4	SER	3.5
19	BS	35	SER	3.5
35	DG	17	VAL	3.5
31	CA	7	G	3.5
31	CA	619	G	3.5
35	CG	130	GLU	3.5
42	CO	11	ASN	3.5
45	CR	57	PHE	3.5
48	DU	92	ASN	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	BA	1325	C	3.5
46	CS	79	ARG	3.5
25	C4	29	LEU	3.5
36	DH	105	ALA	3.5
46	CS	39	LEU	3.5
3	AC	195	VAL	3.5
13	BM	73	ILE	3.5
19	BS	51	VAL	3.5
43	CP	28	VAL	3.5
7	BG	74	GLU	3.5
10	BJ	28	THR	3.5
13	AM	42	ASP	3.5
20	BT	71	LYS	3.5
34	DF	80	ARG	3.5
46	CS	81	LYS	3.5
48	CU	6	ARG	3.5
1	BA	1252	A	3.5
13	BM	67	GLY	3.5
28	CB	21	G	3.5
34	CF	7	TYR	3.5
1	BA	979	C	3.5
30	CD	156	PHE	3.5
45	CR	11	ARG	3.5
1	BA	216	U	3.5
31	CA	1201	U	3.5
41	CN	99	GLY	3.5
48	CU	28	ASN	3.5
1	BA	223	A	3.5
1	BA	1327	C	3.5
31	CA	2654	A	3.5
39	CL	103	VAL	3.5
50	CW	63	ILE	3.5
50	CW	12	GLN	3.5
53	CZ	38	GLN	3.5
9	AI	85	ARG	3.5
33	CE	21	ARG	3.5
10	BJ	97	ASP	3.5
34	CF	24	SER	3.5
1	BA	1295	U	3.5
31	CA	2783	U	3.5
31	CA	2861	U	3.5
36	DH	126	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
55	DA	546	U	3.5
47	CT	9	HIS	3.5
34	CF	137	ILE	3.5
43	CP	82	ALA	3.5
1	BA	1006	G	3.5
1	BA	1208	C	3.5
2	BB	11	LYS	3.5
4	AD	31	LYS	3.5
50	CW	11	GLU	3.5
28	CB	117	G	3.5
31	CA	126	A	3.5
31	CA	508	A	3.5
31	CA	2502	G	3.5
5	BE	109	GLY	3.5
14	BN	70	PRO	3.5
27	C0	17	LEU	3.5
48	CU	4	GLU	3.5
49	CV	92	LYS	3.5
27	C0	14	ILE	3.5
36	DH	108	VAL	3.5
31	CA	2047	C	3.5
20	BT	51	PHE	3.5
31	CA	1026	G	3.5
45	CR	102	ASP	3.5
10	AJ	33	GLY	3.4
1	BA	957	U	3.4
31	CA	1864	U	3.4
49	CV	44	LYS	3.4
11	AK	111	THR	3.4
30	CD	167	ASN	3.4
47	CT	39	THR	3.4
13	BM	60	VAL	3.4
40	CM	26	GLY	3.4
40	CM	42	SER	3.4
12	BL	114	ARG	3.4
26	C5	36	ARG	3.4
31	CA	808	G	3.4
31	CA	881	G	3.4
47	CT	87	PRO	3.4
55	DA	1093	G	3.4
11	AK	47	ALA	3.4
37	DJ	46	THR	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	DI	120	ALA	3.4
7	AG	43	VAL	3.4
34	DF	74	VAL	3.4
35	CG	79	VAL	3.4
22	C1	32	LYS	3.4
14	AN	54	ASP	3.4
36	DH	95	GLY	3.4
2	BB	208	ARG	3.4
1	BA	975	A	3.4
7	BG	2	PRO	3.4
10	AJ	43	PRO	3.4
13	BM	112	PRO	3.4
37	DJ	93	PRO	3.4
12	BL	24	LEU	3.4
37	CJ	101	ILE	3.4
45	DR	118	ALA	3.4
30	CD	98	VAL	3.4
7	BG	70	ARG	3.4
9	AI	24	GLY	3.4
44	CQ	35	GLY	3.4
1	AA	1029	U	3.4
1	BA	88	U	3.4
31	CA	817	C	3.4
9	AI	54	LEU	3.4
30	CD	36	GLN	3.4
31	CA	422	A	3.4
35	CG	136	ALA	3.4
40	CM	1	MET	3.4
1	BA	1356	G	3.4
2	AB	213	TYR	3.4
41	CN	36	VAL	3.4
31	CA	1250	G	3.4
31	CA	1734	G	3.4
31	CA	1869	G	3.4
31	CA	2238	G	3.4
40	CM	24	GLY	3.4
42	CO	2	ARG	3.4
44	CQ	43	PHE	3.4
30	CD	28	GLU	3.4
54	DI	36	ASP	3.4
1	BA	206	C	3.4
28	CB	118	C	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
31	CA	405	U	3.4
31	CA	1052	C	3.4
31	CA	2650	U	3.4
36	CH	75	LEU	3.4
2	BB	166	ALA	3.4
31	CA	1551	A	3.4
48	CU	67	VAL	3.4
2	BB	145	GLU	3.4
21	AU	17	ARG	3.4
34	CF	133	ARG	3.4
12	BL	71	GLY	3.4
36	DH	77	THR	3.4
38	CK	65	THR	3.4
44	CQ	11	GLU	3.4
31	CA	406	G	3.4
31	CA	407	G	3.4
31	CA	1332	G	3.4
31	CA	1622	G	3.4
40	CM	13	LYS	3.4
48	CU	68	LYS	3.4
1	BA	473	U	3.4
31	CA	334	C	3.4
2	AB	35	ARG	3.4
35	CG	65	ALA	3.4
5	BE	123	VAL	3.4
7	AG	123	GLU	3.4
13	AM	23	TYR	3.4
40	CM	140	GLY	3.4
14	BN	67	THR	3.4
17	BQ	69	LYS	3.4
37	CJ	72	LYS	3.4
40	CM	128	THR	3.4
31	CA	2405	G	3.4
1	AA	83	C	3.4
2	AB	225	ARG	3.4
7	BG	143	ARG	3.4
13	AM	57	ARG	3.4
13	BM	71	ARG	3.4
31	CA	510	C	3.4
31	CA	2310	C	3.4
5	BE	46	VAL	3.4
14	BN	97	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
24	C3	11	LYS	3.4
29	CC	235	GLY	3.4
29	DC	240	PHE	3.4
47	CT	49	LYS	3.4
29	CC	213	TRP	3.4
50	CW	43	ASP	3.4
1	BA	218	U	3.4
1	BA	956	U	3.4
1	BA	1330	U	3.4
3	BC	164	ARG	3.4
36	CH	117	LEU	3.4
1	BA	1039	G	3.4
16	BP	11	ALA	3.4
31	CA	539	G	3.4
31	CA	1875	G	3.4
33	CE	63	LYS	3.4
36	CH	144	VAL	3.4
34	CF	138	PHE	3.4
6	AF	63	ASN	3.4
1	BA	532	A	3.3
31	CA	309	A	3.3
31	CA	478	A	3.3
1	BA	1308	U	3.3
5	BE	23	LYS	3.3
36	CH	141	LYS	3.3
41	CN	11	LYS	3.3
5	AE	111	MET	3.3
34	CF	59	ALA	3.3
39	CL	83	ALA	3.3
1	BA	1454	G	3.3
31	CA	1042	G	3.3
33	CE	158	PHE	3.3
37	DJ	90	SER	3.3
15	AO	89	ARG	3.3
34	CF	33	LYS	3.3
37	CJ	39	CYS	3.3
1	BA	1211	U	3.3
5	BE	36	LEU	3.3
1	BA	969	A	3.3
31	CA	241	A	3.3
31	CA	279	A	3.3
31	CA	911	A	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
31	CA	1609	A	3.3
38	CK	105	VAL	3.3
45	CR	27	ALA	3.3
46	CS	7	SER	3.3
1	BA	1187	G	3.3
7	AG	140	ASP	3.3
35	CG	99	LYS	3.3
51	CX	68	LYS	3.3
54	DI	47	GLU	3.3
31	CA	1539	U	3.3
17	BQ	64	CYS	3.3
3	BC	37	PHE	3.3
14	AN	99	ALA	3.3
30	CD	162	ALA	3.3
42	CO	84	GLY	3.3
43	CP	44	GLY	3.3
45	CR	82	GLY	3.3
39	CL	35	VAL	3.3
9	BI	85	ARG	3.3
38	CK	34	ARG	3.3
47	CT	8	ARG	3.3
7	AG	41	SER	3.3
29	CC	230	HIS	3.3
3	BC	170	GLU	3.3
31	CA	2691	C	3.3
36	DH	86	ASP	3.3
1	BA	1334	G	3.3
20	BT	13	GLN	3.3
25	C4	44	LEU	3.3
31	CA	266	G	3.3
35	CG	116	GLN	3.3
31	CA	139	U	3.3
9	BI	95	ARG	3.3
10	AJ	37	ARG	3.3
11	BK	45	ALA	3.3
33	CE	151	GLY	3.3
39	CL	112	PHE	3.3
44	CQ	30	VAL	3.3
44	CQ	33	VAL	3.3
49	CV	97	LYS	3.3
1	BA	978	A	3.3
1	BA	153	C	3.3

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Mol	Chain	Res	Type	RSRZ
31	CA	57	C	3.3
31	CA	1880	U	3.3
1	BA	933	G	3.3
1	BA	1139	G	3.3
2	AB	69	PHE	3.3
10	AJ	25	ILE	3.3
55	DA	141	G	3.3
33	CE	182	ALA	3.3
1	AA	1028	C	3.3
1	BA	87	C	3.3
10	BJ	45	ARG	3.3
25	C4	3	LYS	3.3
31	CA	31	C	3.3
31	CA	1607	C	3.3
44	CQ	101	ARG	3.3
11	AK	102	ALA	3.3
37	CJ	110	ALA	3.3
45	CR	68	ALA	3.3
1	BA	847	G	3.3
31	CA	2455	G	3.3
34	CF	134	GLU	3.3
3	BC	167	TRP	3.3
37	DJ	136	MET	3.3
1	BA	1014	A	3.3
2	BB	15	HIS	3.3
33	CE	165	HIS	3.3
40	CM	129	LYS	3.3
10	AJ	31	ARG	3.3
1	BA	330	C	3.3
3	AC	155	GLY	3.3
17	AQ	53	CYS	3.3
31	CA	150	U	3.3
31	CA	1600	C	3.3
30	CD	202	ILE	3.3
7	BG	117	ALA	3.3
12	BL	93	VAL	3.3
37	CJ	140	VAL	3.3
40	CM	143	GLU	3.3
54	DI	98	GLU	3.3
10	BJ	43	PRO	3.3
30	CD	197	THR	3.3
1	BA	275	G	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
30	CD	204	LYS	3.3
31	CA	914	G	3.3
31	CA	2159	G	3.3
36	CH	83	LYS	3.3
15	BO	18	ASP	3.3
25	C4	57	LEU	3.3
40	CM	61	LEU	3.3
43	CP	34	HIS	3.3
48	CU	32	LEU	3.3
1	BA	1269	A	3.3
25	C4	9	GLY	3.3
31	CA	1205	A	3.3
36	DH	92	GLY	3.3
1	BA	1247	U	3.3
37	DJ	62	TYR	3.3
7	BG	7	ILE	3.3
31	CA	1986	C	3.3
53	CZ	13	GLU	3.3
12	BL	23	ALA	3.3
15	BO	12	VAL	3.3
23	C2	12	VAL	3.3
46	CS	38	VAL	3.3
8	BH	89	LYS	3.3
3	BC	26	THR	3.3
1	AA	1034	G	3.3
7	BG	55	GLY	3.3
31	CA	1239	G	3.3
31	CA	2004	G	3.3
31	CA	2363	G	3.3
16	AP	17	TYR	3.2
49	CV	53	ASN	3.2
49	CV	60	GLU	3.2
49	CV	101	GLU	3.2
31	CA	1373	A	3.2
36	DH	143	ILE	3.2
11	AK	99	ALA	3.2
36	CH	65	ALA	3.2
53	CZ	2	LYS	3.2
55	DA	1057	A	3.2
55	DA	1088	A	3.2
13	AM	101	ARG	3.2
3	BC	145	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
3	BC	190	HIS	3.2
1	BA	86	G	3.2
23	C2	20	PHE	3.2
31	CA	271	G	3.2
31	CA	1022	G	3.2
31	CA	1277	G	3.2
31	CA	1326	U	3.2
31	CA	2152	G	3.2
37	DJ	34	ASN	3.2
48	CU	92	ASN	3.2
1	BA	186	C	3.2
31	CA	1764	C	3.2
36	CH	123	ARG	3.2
41	CN	40	ARG	3.2
55	DA	1070	A	3.2
25	C4	49	MET	3.2
38	CK	92	MET	3.2
3	BC	183	ASP	3.2
11	BK	43	GLY	3.2
21	BU	16	LEU	3.2
34	DF	39	GLY	3.2
42	CO	100	CYS	3.2
43	CP	75	GLY	3.2
44	CQ	40	LEU	3.2
25	C4	24	HIS	3.2
24	C3	41	ARG	3.2
2	BB	210	VAL	3.2
11	AK	32	VAL	3.2
43	CP	74	VAL	3.2
1	BA	1355	G	3.2
28	CB	56	G	3.2
31	CA	375	G	3.2
35	CG	138	LYS	3.2
50	CW	50	MET	3.2
53	CZ	30	MET	3.2
5	BE	103	THR	3.2
11	AK	42	LEU	3.2
38	CK	15	TRP	3.2
48	CU	74	ILE	3.2
10	BJ	36	VAL	3.2
36	DH	147	VAL	3.2
45	CR	10	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
47	CT	56	ALA	3.2
52	CY	44	LYS	3.2
3	BC	85	GLU	3.2
7	BG	14	PRO	3.2
30	CD	148	GLN	3.2
31	CA	2862	G	3.2
47	CT	2	GLU	3.2
1	BA	1362	A	3.2
31	CA	515	A	3.2
31	CA	1285	A	3.2
31	CA	2412	A	3.2
55	DA	2170	A	3.2
2	AB	211	THR	3.2
25	C4	42	ARG	3.2
33	CE	102	ARG	3.2
47	CT	110	ARG	3.2
50	CW	56	PHE	3.2
31	CA	894	U	3.2
31	CA	1173	U	3.2
21	AU	26	ALA	3.2
39	CL	24	VAL	3.2
43	CP	90	VAL	3.2
46	CS	34	GLU	3.2
16	AP	74	LEU	3.2
31	CA	550	C	3.2
31	CA	1730	C	3.2
33	CE	56	GLY	3.2
1	AA	1127	G	3.2
19	AS	27	ASP	3.2
31	CA	2525	G	3.2
2	AB	60	ILE	3.2
20	BT	12	ILE	3.2
21	AU	4	ILE	3.2
35	CG	176	LYS	3.2
45	CR	93	LYS	3.2
52	CY	54	LYS	3.2
52	CY	77	LYS	3.2
31	CA	929	U	3.2
36	DH	135	HIS	3.2
37	DJ	70	VAL	3.2
3	AC	82	GLU	3.2
24	C3	15	SER	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
14	AN	63	ARG	3.2
24	C3	21	ARG	3.2
53	DZ	39	GLN	3.2
5	BE	144	LEU	3.2
46	CS	76	LYS	3.2
1	AA	1332	A	3.2
1	BA	1145	A	3.2
13	AM	17	ILE	3.2
31	CA	182	A	3.2
31	CA	1133	A	3.2
31	CA	1253	A	3.2
31	CA	1643	G	3.2
43	CP	35	ILE	3.2
52	CY	48	THR	3.2
55	DA	613	A	3.2
11	BK	102	ALA	3.2
9	AI	64	TYR	3.2
45	CR	44	GLN	3.2
34	CF	169	LEU	3.2
50	CW	68	LYS	3.2
50	CW	71	LYS	3.2
53	CZ	60	LYS	3.2
1	AA	984	C	3.2
21	AU	19	PHE	3.2
31	CA	421	C	3.2
51	CX	36	ILE	3.2
1	BA	91	U	3.2
1	AA	1170	A	3.2
2	BB	199	VAL	3.2
31	CA	2807	U	3.2
43	CP	50	ALA	3.2
31	CA	535	G	3.2
31	CA	2732	G	3.2
31	CA	2782	G	3.2
7	AG	77	SER	3.2
24	C3	8	SER	3.2
27	C0	33	GLY	3.2
44	CQ	3	ASN	3.2
35	CG	16	ASP	3.2
39	CL	56	ASP	3.2
44	CQ	16	ASP	3.2
31	CA	2815	C	3.2

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Mol	Chain	Res	Type	RSRZ
45	CR	89	GLU	3.2
30	CD	179	ARG	3.1
17	BQ	42	THR	3.1
31	CA	29	U	3.1
33	CE	8	ALA	3.1
35	CG	63	ALA	3.1
35	CG	145	ALA	3.1
36	CH	9	VAL	3.1
55	DA	2131	U	3.1
33	CE	62	GLN	3.1
36	DH	128	HIS	3.1
31	CA	1596	A	3.1
1	AA	79	G	3.1
20	BT	21	ASN	3.1
31	CA	1037	G	3.1
31	CA	1538	G	3.1
3	AC	105	GLU	3.1
13	AM	29	ARG	3.1
1	AA	1282	C	3.1
1	BA	1383	C	3.1
28	CB	4	C	3.1
28	CB	49	C	3.1
37	DJ	95	LYS	3.1
54	DI	11	ILE	3.1
38	CK	124	VAL	3.1
40	CM	134	ALA	3.1
45	CR	110	VAL	3.1
10	AJ	56	HIS	3.1
41	CN	24	THR	3.1
41	CN	74	THR	3.1
1	BA	1151	A	3.1
31	CA	2639	A	3.1
42	CO	23	ASN	3.1
44	DQ	2	SER	3.1
1	BA	1144	G	3.1
30	CD	88	GLU	3.1
34	CF	163	ASP	3.1
42	CO	39	PRO	3.1
46	CS	93	PHE	3.1
48	CU	69	ARG	3.1
55	DA	2140	G	3.1
44	CQ	31	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
30	CD	14	ILE	3.1
38	CK	81	ILE	3.1
1	BA	999	C	3.1
2	AB	53	ALA	3.1
7	AG	61	ALA	3.1
11	AK	45	ALA	3.1
31	CA	587	C	3.1
31	CA	1172	C	3.1
48	CU	91	GLN	3.1
23	C2	19	HIS	3.1
7	BG	124	LEU	3.1
36	CH	6	LEU	3.1
36	DH	90	LEU	3.1
41	CN	88	ASN	3.1
54	DI	5	LEU	3.1
30	CD	7	LYS	3.1
31	CA	1525	A	3.1
13	BM	9	ILE	3.1
31	CA	597	G	3.1
31	CA	2410	G	3.1
14	BN	17	ALA	3.1
16	BP	10	GLY	3.1
21	AU	14	VAL	3.1
31	CA	596	U	3.1
36	CH	63	ALA	3.1
36	CH	78	VAL	3.1
1	BA	1141	C	3.1
1	BA	1262	C	3.1
1	BA	1317	C	3.1
31	CA	2260	C	3.1
3	AC	190	HIS	3.1
12	AL	108	LYS	3.1
12	BL	97	THR	3.1
18	AR	55	LEU	3.1
25	C4	39	LYS	3.1
21	BU	2	PRO	3.1
39	CL	109	SER	3.1
43	CP	2	ASP	3.1
1	BA	1000	A	3.1
31	CA	1321	A	3.1
5	AE	137	VAL	3.1
1	BA	1215	G	3.1

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Mol	Chain	Res	Type	RSRZ
12	BL	113	ALA	3.1
13	AM	38	GLY	3.1
31	CA	288	U	3.1
16	BP	35	ARG	3.1
53	CZ	7	ARG	3.1
34	CF	5	HIS	3.1
37	DJ	118	THR	3.1
38	CK	125	TYR	3.1
3	BC	180	ALA	3.1
12	BL	119	VAL	3.1
21	BU	6	VAL	3.1
4	AD	154	ARG	3.1
19	BS	73	GLU	3.1
37	CJ	108	GLU	3.1
1	BA	177	G	3.1
3	AC	43	LEU	3.1
31	CA	1138	G	3.1
36	CH	90	LEU	3.1
21	AU	37	PHE	3.1
4	AD	30	THR	3.1
34	DF	83	TYR	3.1
46	CS	43	ASN	3.1
10	AJ	100	ILE	3.1
12	BL	67	ILE	3.1
53	CZ	4	LYS	3.1
2	AB	208	ARG	3.1
26	D5	38	GLY	3.1
7	BG	64	VAL	3.1
20	BT	48	GLN	3.1
41	CN	56	ALA	3.1
44	CQ	73	VAL	3.1
31	CA	2786	U	3.1
31	CA	2346	A	3.1
55	DA	1175	A	3.1
1	BA	1149	C	3.1
1	BA	1263	C	3.1
1	BA	1342	C	3.1
31	CA	1092	C	3.1
3	BC	36	ASP	3.1
29	CC	26	LYS	3.1
31	CA	2325	G	3.1
34	CF	51	ASP	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	BC	72	ARG	3.1
23	C2	6	ARG	3.1
29	CC	237	GLY	3.1
6	BF	10	VAL	3.1
9	BI	75	GLN	3.1
1	AA	84	U	3.1
31	CA	2245	U	3.1
42	CO	91	ALA	3.1
1	BA	1368	A	3.1
13	BM	78	LYS	3.1
31	CA	2814	A	3.1
34	CF	9	LYS	3.1
36	DH	15	LEU	3.1
46	CS	5	PHE	3.1
55	DA	878	A	3.1
1	BA	1322	C	3.1
28	CB	27	C	3.1
31	CA	544	C	3.1
1	BA	354	G	3.1
13	AM	96	PRO	3.1
31	CA	1024	G	3.1
31	CA	1071	G	3.1
34	CF	44	ILE	3.1
37	DJ	86	ILE	3.1
55	DA	2156	G	3.1
11	AK	86	VAL	3.0
13	AM	21	SER	3.0
22	C1	54	VAL	3.0
53	CZ	10	SER	3.0
31	CA	615	U	3.0
36	DH	100	ALA	3.0
44	CQ	42	ALA	3.0
40	CM	64	PHE	3.0
1	AA	1492	A	3.0
31	CA	1260	A	3.0
31	CA	2311	A	3.0
55	DA	2169	A	3.0
31	CA	61	C	3.0
31	CA	2313	C	3.0
38	CK	67	ASN	3.0
38	CK	138	GLN	3.0
41	CN	77	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
44	CQ	17	VAL	3.0
31	CA	1016	G	3.0
31	CA	1225	G	3.0
31	CA	2526	G	3.0
42	CO	25	ALA	3.0
9	AI	95	ARG	3.0
2	AB	40	ILE	3.0
28	CB	119	A	3.0
31	CA	443	A	3.0
49	CV	9	ASP	3.0
14	BN	57	PRO	3.0
30	CD	94	GLN	3.0
5	BE	75	ALA	3.0
10	BJ	83	THR	3.0
31	CA	1438	U	3.0
31	CA	2299	U	3.0
22	C1	16	ARG	3.0
25	C4	8	ARG	3.0
1	BA	993	G	3.0
1	BA	1370	G	3.0
2	AB	129	LEU	3.0
28	CB	7	G	3.0
31	CA	376	G	3.0
31	CA	748	G	3.0
31	CA	1517	G	3.0
31	CA	2115	G	3.0
36	CH	47	PHE	3.0
9	AI	79	ILE	3.0
30	CD	134	HIS	3.0
44	CQ	23	GLY	3.0
46	CS	66	HIS	3.0
14	BN	66	GLN	3.0
9	BI	6	TYR	3.0
11	BK	84	VAL	3.0
29	CC	37	ASN	3.0
31	CA	151	C	3.0
31	CA	257	C	3.0
31	CA	2052	A	3.0
36	DH	25	TYR	3.0
1	BA	96	U	3.0
31	CA	1108	U	3.0
54	DI	80	THR	3.0

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Mol	Chain	Res	Type	RSRZ
21	BU	19	PHE	3.0
1	BA	104	G	3.0
31	CA	1186	G	3.0
30	CD	150	GLN	3.0
43	CP	100	HIS	3.0
53	DZ	38	GLN	3.0
7	AG	73	VAL	3.0
9	BI	123	ARG	3.0
39	CL	32	TYR	3.0
42	CO	96	ARG	3.0
45	CR	53	ARG	3.0
1	BA	352	C	3.0
1	BA	1204	A	3.0
5	AE	19	ASN	3.0
9	BI	86	ALA	3.0
12	BL	48	ALA	3.0
31	CA	609	A	3.0
31	CA	1319	C	3.0
31	CA	1958	C	3.0
31	CA	2248	C	3.0
31	CA	2362	C	3.0
31	CA	2632	A	3.0
42	CO	66	ALA	3.0
43	CP	79	ALA	3.0
47	CT	93	ALA	3.0
13	AM	46	SER	3.0
14	BN	19	LYS	3.0
30	CD	118	PHE	3.0
36	DH	12	LEU	3.0
43	CP	68	LYS	3.0
1	AA	1187	G	3.0
1	BA	378	G	3.0
1	BA	1220	G	3.0
10	BJ	70	HIS	3.0
28	CB	20	G	3.0
31	CA	1252	G	3.0
42	CO	33	ILE	3.0
49	CV	58	ILE	3.0
7	AG	71	PRO	3.0
43	CP	47	VAL	3.0
36	CH	36	ALA	3.0
36	DH	64	ALA	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
31	CA	1460	U	3.0
1	AA	77	A	3.0
15	BO	22	THR	3.0
31	CA	310	A	3.0
31	CA	502	A	3.0
36	DH	88	GLY	3.0
42	CO	46	ARG	3.0
44	CQ	109	ARG	3.0
7	BG	6	VAL	3.0
20	BT	16	LYS	3.0
25	C4	47	LYS	3.0
31	CA	2633	G	3.0
34	CF	19	GLU	3.0
44	CQ	34	GLU	3.0
1	AA	1023	U	3.0
3	BC	157	LEU	3.0
44	CQ	100	LEU	3.0
31	CA	236	C	3.0
3	BC	158	GLY	3.0
7	AG	133	THR	3.0
29	CC	223	THR	3.0
31	CA	504	A	3.0
31	CA	1532	A	3.0
31	CA	2660	A	3.0
36	CH	13	GLY	3.0
42	CO	26	GLY	3.0
3	BC	132	ARG	3.0
35	CG	3	ARG	3.0
46	CS	84	ARG	3.0
29	CC	97	LYS	3.0
37	DJ	47	ASP	3.0
40	DM	104	GLN	3.0
2	BB	217	VAL	3.0
51	CX	67	VAL	3.0
24	C3	23	ALA	3.0
38	CK	126	ALA	3.0
44	CQ	108	ALA	3.0
31	CA	1468	U	3.0
1	BA	470	C	3.0
7	AG	132	GLY	3.0
31	CA	1983	G	3.0
35	CG	159	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
36	CH	16	GLY	3.0
40	CM	41	ARG	3.0
39	CL	65	THR	3.0
49	CV	17	LYS	3.0
31	CA	1652	A	3.0
37	DJ	31	GLN	3.0
49	CV	46	GLN	3.0
12	AL	70	GLU	3.0
16	AP	21	VAL	3.0
30	CD	155	VAL	3.0
40	CM	110	VAL	3.0
1	BA	1008	U	2.9
1	BA	1212	U	2.9
31	CA	665	U	2.9
11	AK	80	LYS	2.9
17	AQ	4	LYS	2.9
19	BS	18	LYS	2.9
29	CC	28	LYS	2.9
30	CD	56	LYS	2.9
49	CV	90	GLY	2.9
52	CY	55	GLY	2.9
1	BA	176	C	2.9
1	BA	963	G	2.9
31	CA	184	C	2.9
31	CA	245	G	2.9
31	CA	411	G	2.9
31	CA	902	C	2.9
31	CA	2000	C	2.9
31	CA	2078	C	2.9
31	CA	2112	G	2.9
54	DI	67	THR	2.9
7	BG	29	ILE	2.9
9	AI	62	ASP	2.9
31	CA	2453	A	2.9
3	AC	189	ALA	2.9
1	BA	632	U	2.9
18	AR	29	LEU	2.9
29	CC	270	ARG	2.9
34	CF	20	PHE	2.9
45	CR	70	ARG	2.9
50	CW	26	PHE	2.9
51	CX	84	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
50	CW	46	LYS	2.9
16	BP	18	GLN	2.9
1	BA	1129	C	2.9
13	BM	17	ILE	2.9
22	C1	11	SER	2.9
31	CA	32	C	2.9
31	CA	540	C	2.9
31	CA	1295	C	2.9
31	CA	2616	C	2.9
31	CA	2896	C	2.9
1	BA	1337	G	2.9
28	CB	96	G	2.9
31	CA	1228	G	2.9
3	AC	66	VAL	2.9
6	AF	96	VAL	2.9
9	BI	122	ARG	2.9
14	BN	41	ARG	2.9
36	DH	103	VAL	2.9
37	DJ	140	VAL	2.9
42	CO	45	ARG	2.9
49	CV	34	VAL	2.9
29	CC	243	HIS	2.9
34	CF	45	ALA	2.9
48	CU	45	ALA	2.9
38	CK	79	GLY	2.9
54	DI	119	PRO	2.9
42	CO	112	TYR	2.9
9	AI	92	GLU	2.9
18	AR	20	GLU	2.9
45	CR	59	GLN	2.9
1	BA	54	C	2.9
3	AC	68	ILE	2.9
31	CA	1985	C	2.9
50	CW	3	THR	2.9
52	CY	61	LYS	2.9
2	BB	80	VAL	2.9
30	CD	24	VAL	2.9
36	DH	110	VAL	2.9
1	BA	198	G	2.9
3	BC	104	ALA	2.9
10	AJ	12	ALA	2.9
31	CA	494	G	2.9

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Mol	Chain	Res	Type	RSRZ
1	AA	1021	A	2.9
1	BA	468	A	2.9
1	BA	1339	A	2.9
31	CA	1237	A	2.9
40	CM	87	GLY	2.9
49	DV	48	PRO	2.9
7	BG	139	GLU	2.9
9	AI	28	ILE	2.9
10	BJ	16	ARG	2.9
13	AM	20	THR	2.9
36	CH	21	VAL	2.9
36	CH	125	THR	2.9
42	CO	21	PHE	2.9
5	BE	108	GLY	2.9
7	AG	47	LEU	2.9
17	BQ	67	LEU	2.9
19	AS	47	LEU	2.9
47	CT	58	ALA	2.9
10	BJ	56	HIS	2.9
21	AU	39	GLU	2.9
29	CC	227	PRO	2.9
31	CA	1224	U	2.9
1	BA	1227	A	2.9
7	AG	137	LYS	2.9
22	C1	53	LYS	2.9
31	CA	71	A	2.9
31	CA	127	A	2.9
31	CA	1521	G	2.9
39	CL	49	ARG	2.9
36	CH	4	ILE	2.9
1	AA	1302	C	2.9
1	BA	1369	C	2.9
3	AC	39	VAL	2.9
7	BG	27	VAL	2.9
10	AJ	101	SER	2.9
26	C5	3	VAL	2.9
41	CN	101	VAL	2.9
42	CO	70	THR	2.9
50	CW	77	VAL	2.9
53	CZ	55	THR	2.9
54	DI	76	PHE	2.9
9	AI	82	GLY	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
9	BI	63	LEU	2.9
13	AM	37	ALA	2.9
19	BS	47	LEU	2.9
22	C1	45	ALA	2.9
29	CC	210	ALA	2.9
34	CF	168	ALA	2.9
36	CH	126	GLY	2.9
50	CW	74	ALA	2.9
54	DI	127	ALA	2.9
24	D3	46	LYS	2.9
33	CE	99	LYS	2.9
55	DA	2113	U	2.9
37	CJ	65	ARG	2.9
1	BA	134	G	2.9
1	BA	1248	A	2.9
31	CA	70	G	2.9
31	CA	272	A	2.9
31	CA	326	G	2.9
31	CA	1244	A	2.9
31	CA	2365	G	2.9
31	CA	2694	G	2.9
55	DA	1090	A	2.9
2	BB	93	ASN	2.9
7	BG	126	ASP	2.9
29	CC	46	ASN	2.9
50	CW	5	ASN	2.9
6	BF	8	PHE	2.9
14	AN	32	SER	2.9
30	CD	183	GLU	2.9
35	CG	42	GLU	2.9
40	CM	29	LYS	2.9
52	CY	15	GLY	2.9
6	AF	42	TRP	2.9
31	CA	1100	C	2.9
1	BA	1205	U	2.9
6	BF	38	ARG	2.9
9	AI	18	ARG	2.9
9	AI	33	ARG	2.9
24	C3	39	ARG	2.9
31	CA	598	U	2.9
31	CA	2878	U	2.9
1	AA	963	G	2.9

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Mol	Chain	Res	Type	RSRZ
1	BA	105	G	2.9
1	BA	1361	G	2.9
1	BA	1375	A	2.9
13	BM	82	ASP	2.9
16	BP	40	ASN	2.9
31	CA	1529	G	2.9
31	CA	1583	A	2.9
31	CA	1616	A	2.9
31	CA	2778	A	2.9
47	CT	66	ILE	2.9
31	CA	86	G	2.9
21	AU	8	GLU	2.9
26	C5	21	GLY	2.9
36	CH	107	GLY	2.9
6	AF	66	ALA	2.9
7	BG	13	LEU	2.9
38	CK	20	ALA	2.9
48	CU	21	SER	2.9
1	AA	1320	C	2.9
34	CF	109	PRO	2.9
35	CG	64	GLN	2.9
43	CP	98	GLN	2.9
46	CS	11	GLN	2.9
55	DA	1058	U	2.9
21	BU	4	ILE	2.9
40	CM	111	ILE	2.9
5	BE	78	ASN	2.9
1	BA	1363	A	2.9
17	AQ	83	VAL	2.9
31	CA	883	G	2.9
38	CK	108	MET	2.9
3	BC	51	SER	2.8
39	CL	28	SER	2.8
19	BS	33	THR	2.8
31	CA	1113	U	2.8
31	CA	1729	U	2.8
31	CA	2050	C	2.8
50	CW	84	PRO	2.8
55	DA	2153	C	2.8
55	DA	2180	U	2.8
13	AM	114	LYS	2.8
29	DC	243	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
38	CK	75	TYR	2.8
24	C3	9	VAL	2.8
30	CD	135	GLY	2.8
42	CO	12	ARG	2.8
14	AN	36	ALA	2.8
30	CD	138	LEU	2.8
31	CA	196	A	2.8
31	CA	941	A	2.8
31	CA	2158	A	2.8
31	CA	2358	A	2.8
36	DH	6	LEU	2.8
1	AA	1125	U	2.8
1	AA	1148	U	2.8
1	BA	1343	G	2.8
14	BN	76	LYS	2.8
31	CA	261	G	2.8
31	CA	612	G	2.8
31	CA	1523	U	2.8
31	CA	1862	G	2.8
31	CA	2157	G	2.8
46	CS	102	SER	2.8
31	CA	2302	U	2.8
1	BA	1228	C	2.8
31	CA	623	C	2.8
31	CA	815	C	2.8
30	CD	176	ASP	2.8
21	AU	12	PHE	2.8
2	AB	57	LEU	2.8
40	CM	112	LEU	2.8
1	AA	959	A	2.8
1	BA	263	A	2.8
20	AT	55	GLN	2.8
1	AA	1286	U	2.8
31	CA	653	U	2.8
31	CA	2903	U	2.8
51	CX	35	SER	2.8
1	BA	201	G	2.8
1	BA	1140	C	2.8
10	BJ	50	THR	2.8
33	CE	2	GLU	2.8
35	CG	124	GLU	2.8
42	CO	85	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
12	BL	82	ILE	2.8
34	CF	87	CYS	2.8
33	CE	96	VAL	2.8
35	CG	15	VAL	2.8
40	CM	109	LYS	2.8
41	CN	26	VAL	2.8
45	CR	88	VAL	2.8
54	DI	35	VAL	2.8
47	CT	69	LEU	2.8
20	BT	11	ALA	2.8
25	C4	60	ALA	2.8
33	CE	39	ALA	2.8
43	CP	37	ALA	2.8
43	CP	77	ALA	2.8
1	BA	961	U	2.8
10	BJ	31	ARG	2.8
11	BK	98	ARG	2.8
30	CD	145	SER	2.8
31	CA	2847	U	2.8
31	CA	1275	A	2.8
36	DH	82	SER	2.8
29	CC	231	PRO	2.8
3	BC	74	GLY	2.8
22	C1	7	LYS	2.8
25	C4	21	GLY	2.8
31	CA	2830	C	2.8
47	CT	55	ILE	2.8
31	CA	215	G	2.8
55	DA	2107	G	2.8
55	DA	2159	G	2.8
10	BJ	51	VAL	2.8
44	CQ	32	VAL	2.8
14	BN	46	LEU	2.8
33	CE	153	LEU	2.8
2	BB	84	ALA	2.8
20	BT	61	GLN	2.8
25	C4	65	ALA	2.8
11	AK	98	ARG	2.8
31	CA	87	U	2.8
31	CA	1542	U	2.8
29	CC	18	LYS	2.8
36	DH	141	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
46	CS	48	LYS	2.8
31	CA	616	A	2.8
31	CA	1420	A	2.8
15	AO	21	ASP	2.8
48	CU	79	ASP	2.8
21	AU	38	TYR	2.8
34	CF	13	VAL	2.8
38	CK	74	TYR	2.8
3	BC	65	ARG	2.8
3	BC	161	GLU	2.8
17	BQ	60	GLU	2.8
31	CA	307	G	2.8
31	CA	561	G	2.8
23	D2	45	GLN	2.8
27	C0	54	MET	2.8
16	BP	12	LYS	2.8
31	CA	1176	U	2.8
34	CF	72	LYS	2.8
9	BI	69	GLY	2.8
18	AR	59	ILE	2.8
19	AS	25	SER	2.8
35	CG	19	ILE	2.8
39	CL	15	GLY	2.8
47	CT	96	ILE	2.8
50	CW	40	ILE	2.8
2	BB	91	PHE	2.8
1	AA	1441	A	2.8
1	BA	1238	A	2.8
2	AB	82	ASP	2.8
8	AH	54	ASP	2.8
13	AM	104	THR	2.8
45	CR	49	ASP	2.8
5	BE	124	LEU	2.8
14	BN	14	VAL	2.8
18	BR	40	VAL	2.8
27	C0	45	ARG	2.8
31	CA	128	C	2.8
3	BC	123	GLN	2.8
5	BE	148	ASN	2.8
7	AG	103	TRP	2.8
33	CE	60	TRP	2.8
45	CR	116	ALA	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	BA	1278	G	2.8
31	CA	2621	G	2.8
31	CA	2677	G	2.8
31	CA	2816	G	2.8
52	CY	56	MET	2.8
3	BC	205	GLY	2.8
20	BT	32	ILE	2.8
34	CF	82	GLY	2.8
44	CQ	25	THR	2.8
44	CQ	103	ARG	2.8
54	DI	7	ASP	2.8
36	CH	138	VAL	2.8
46	CS	4	VAL	2.8
46	CS	23	GLU	2.8
50	CW	14	LYS	2.8
51	DX	10	THR	2.8
1	BA	1044	A	2.8
31	CA	1909	C	2.8
53	CZ	9	LYS	2.8
45	CR	96	ALA	2.8
12	AL	73	ASN	2.8
31	CA	273	G	2.8
31	CA	390	U	2.8
31	CA	1324	G	2.8
31	CA	1807	G	2.8
40	CM	11	GLY	2.8
11	AK	34	ILE	2.8
35	CG	12	PRO	2.8
5	AE	10	GLU	2.8
16	BP	76	LYS	2.8
40	CM	25	SER	2.8
47	CT	68	ASP	2.8
50	CW	10	LYS	2.8
3	BC	87	LEU	2.8
7	AG	144	MET	2.7
20	BT	78	ASN	2.7
31	CA	6	A	2.7
31	CA	240	C	2.8
31	CA	440	C	2.8
31	CA	854	C	2.8
31	CA	1135	C	2.8
31	CA	1708	C	2.8

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Mol	Chain	Res	Type	RSRZ
31	CA	2147	A	2.7
31	CA	2716	C	2.8
50	CW	54	ALA	2.8
31	CA	2749	A	2.7
33	CE	156	ASN	2.7
1	BA	1264	U	2.7
3	AC	81	GLY	2.7
31	CA	235	U	2.7
31	CA	2149	U	2.7
9	BI	45	ARG	2.7
11	AK	31	ILE	2.7
16	BP	5	ARG	2.7
29	CC	238	ARG	2.7
33	CE	114	ARG	2.7
34	CF	71	ARG	2.7
46	CS	21	ARG	2.7
1	BA	1186	G	2.7
31	CA	168	G	2.7
31	CA	263	G	2.7
10	AJ	98	VAL	2.7
3	AC	104	ALA	2.7
22	C1	48	TYR	2.7
42	CO	77	ALA	2.7
31	CA	867	C	2.7
31	CA	1330	C	2.7
1	BA	109	A	2.7
30	CD	19	GLY	2.7
31	CA	244	A	2.7
31	CA	2376	A	2.7
41	CN	23	GLY	2.7
31	CA	1467	U	2.7
51	CX	66	LYS	2.7
23	C2	35	GLU	2.7
34	CF	6	ASP	2.7
54	DI	33	VAL	2.7
31	CA	178	G	2.7
31	CA	367	G	2.7
31	CA	488	G	2.7
31	CA	551	G	2.7
31	CA	2618	G	2.7
11	AK	33	THR	2.7
25	C4	6	THR	2.7

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Mol	Chain	Res	Type	RSRZ
31	CA	1658	C	2.7
34	DF	38	MET	2.7
37	DJ	72	LYS	2.7
13	AM	51	GLY	2.7
30	CD	126	ASN	2.7
31	CA	264	C	2.7
31	CA	394	C	2.7
37	DJ	25	GLY	2.7
31	CA	1004	U	2.7
31	CA	1340	U	2.7
37	DJ	108	GLU	2.7
31	CA	1080	A	2.7
16	BP	15	PRO	2.7
9	AI	58	VAL	2.7
29	CC	202	LEU	2.7
38	CK	71	ASP	2.7
33	CE	195	GLN	2.7
42	CO	18	GLN	2.7
42	CO	115	LEU	2.7
5	BE	149	SER	2.7
5	BE	118	ALA	2.7
25	C4	23	LYS	2.7
1	BA	377	G	2.7
4	AD	160	GLU	2.7
9	AI	9	THR	2.7
31	CA	1063	G	2.7
31	CA	1311	G	2.7
46	CS	56	GLY	2.7
55	DA	2148	G	2.7
1	AA	962	C	2.7
13	AM	63	PHE	2.7
20	BT	52	ASN	2.7
31	CA	1963	U	2.7
28	CB	50	A	2.7
31	CA	52	A	2.7
31	CA	227	A	2.7
31	CA	368	A	2.7
31	CA	1111	A	2.7
31	CA	1871	A	2.7
6	AF	89	VAL	2.7
15	BO	29	VAL	2.7
26	C5	15	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
3	BC	69	HIS	2.7
9	BI	34	SER	2.7
19	AS	78	ARG	2.7
30	CD	71	ALA	2.7
8	BH	123	GLY	2.7
14	BN	95	GLY	2.7
16	BP	62	GLY	2.7
2	BB	46	THR	2.7
35	CG	122	THR	2.7
3	AC	103	ILE	2.7
28	CB	102	G	2.7
29	CC	86	ASN	2.7
31	CA	43	G	2.7
31	CA	77	G	2.7
31	CA	248	G	2.7
31	CA	536	G	2.7
31	CA	1633	G	2.7
31	CA	2334	U	2.7
55	DA	1087	G	2.7
27	C0	19	LYS	2.7
31	CA	584	C	2.7
48	CU	9	LYS	2.7
1	BA	478	A	2.7
11	BK	13	ARG	2.7
20	BT	29	ARG	2.7
22	C1	30	VAL	2.7
23	C2	42	VAL	2.7
25	C4	30	ARG	2.7
27	C0	36	VAL	2.7
34	DF	40	VAL	2.7
36	CH	12	LEU	2.7
36	DH	117	LEU	2.7
40	CM	123	ARG	2.7
42	CO	30	ARG	2.7
54	DI	29	ASP	2.7
31	CA	256	A	2.7
10	BJ	54	SER	2.7
35	CG	28	GLY	2.7
36	DH	106	ALA	2.7
38	CK	134	ALA	2.7
40	CM	136	GLU	2.7
52	CY	21	ALA	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
37	DJ	17	MET	2.7
1	BA	157	U	2.7
3	BC	202	ILE	2.7
16	BP	4	ILE	2.7
31	CA	113	U	2.7
31	CA	2259	U	2.7
34	DF	77	PHE	2.7
38	CK	131	ASN	2.7
31	CA	26	G	2.7
31	CA	237	C	2.7
31	CA	333	G	2.7
31	CA	2179	C	2.7
31	CA	2793	C	2.7
5	BE	150	PRO	2.7
42	CO	106	ASP	2.7
54	DI	27	VAL	2.7
1	BA	71	A	2.7
1	BA	845	A	2.7
31	CA	89	A	2.7
55	DA	1848	A	2.7
29	CC	6	CYS	2.7
39	CL	84	CYS	2.7
40	CM	40	SER	2.7
44	CQ	2	SER	2.7
2	BB	69	PHE	2.7
1	BA	943	U	2.7
10	AJ	62	ARG	2.7
14	AN	53	ARG	2.7
2	BB	42	ASN	2.7
35	CG	36	THR	2.7
2	AB	142	GLU	2.7
16	BP	6	LEU	2.7
27	C0	51	VAL	2.7
29	CC	3	VAL	2.7
30	CD	37	VAL	2.7
31	CA	269	C	2.7
31	CA	1251	C	2.7
1	BA	1057	G	2.7
31	CA	93	G	2.7
31	CA	953	G	2.7
16	BP	27	ALA	2.7
33	CE	161	ALA	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
40	CM	98	ALA	2.7
46	CS	69	GLY	2.7
1	BA	1188	A	2.7
40	CM	68	SER	2.7
45	CR	75	SER	2.7
39	CL	1	MET	2.7
9	BI	65	ILE	2.7
31	CA	932	U	2.7
31	CA	1183	U	2.7
40	CM	73	ILE	2.7
55	DA	1078	U	2.7
16	BP	47	GLU	2.7
38	CK	3	THR	2.7
40	CM	4	ASN	2.7
2	BB	163	VAL	2.7
3	BC	31	ASP	2.7
29	CC	228	VAL	2.7
1	BA	1136	C	2.7
3	AC	89	LYS	2.7
3	BC	91	VAL	2.7
48	CU	50	LEU	2.7
35	CG	85	LYS	2.7
43	CP	85	LYS	2.7
45	CR	78	LYS	2.7
2	AB	65	GLY	2.7
16	BP	30	GLY	2.7
40	CM	22	GLY	2.7
10	BJ	29	ALA	2.7
20	BT	7	ALA	2.7
29	CC	2	ALA	2.7
7	BG	10	ARG	2.7
10	AJ	9	ARG	2.7
24	C3	3	ARG	2.7
29	CC	203	ARG	2.7
31	CA	1193	G	2.7
26	C5	6	SER	2.6
27	C0	52	SER	2.6
29	CC	266	PHE	2.6
45	CR	28	ARG	2.7
1	AA	1035	A	2.6
1	BA	1213	A	2.6
1	BA	1257	A	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	AD	178	MET	2.6
33	CE	107	SER	2.6
42	CO	59	SER	2.6
31	CA	10	A	2.6
1	AA	1126	U	2.6
3	BC	75	ILE	2.6
3	BC	168	TYR	2.6
31	CA	1070	A	2.6
31	CA	1272	A	2.6
8	BH	99	LEU	2.6
14	AN	3	LYS	2.6
16	BP	3	THR	2.6
18	AR	47	THR	2.6
29	CC	257	THR	2.6
30	CD	32	ASN	2.6
34	DF	117	LEU	2.6
44	CQ	94	LYS	2.6
38	CK	50	THR	2.6
45	CR	66	ASN	2.6
50	CW	20	LEU	2.6
3	AC	50	ALA	2.6
31	CA	1117	C	2.6
31	CA	1323	C	2.6
35	CG	97	ALA	2.6
39	CL	16	ALA	2.6
50	CW	44	HIS	2.6
11	BK	44	TRP	2.6
1	BA	252	U	2.6
14	BN	28	LYS	2.6
20	AT	76	LYS	2.6
20	BT	57	ILE	2.6
29	CC	74	ILE	2.6
29	CC	180	GLU	2.6
31	CA	277	G	2.6
31	CA	1137	G	2.6
31	CA	1715	G	2.6
31	CA	72	U	2.6
31	CA	511	U	2.6
31	CA	2166	U	2.6
54	DI	118	ILE	2.6
55	DA	895	U	2.6
1	BA	1357	A	2.6

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Mol	Chain	Res	Type	RSRZ
16	BP	74	LEU	2.6
31	CA	2003	A	2.6
55	DA	2173	A	2.6
9	AI	47	VAL	2.6
2	AB	17	GLY	2.6
11	AK	30	THR	2.6
13	AM	8	ASN	2.6
14	BN	38	ASP	2.6
15	AO	27	VAL	2.6
30	CD	87	GLY	2.6
44	DQ	115	ASN	2.6
48	CU	86	THR	2.6
46	CS	80	ARG	2.6
31	CA	610	C	2.6
31	CA	640	C	2.6
42	CO	68	ALA	2.6
43	CP	6	ALA	2.6
55	DA	1072	C	2.6
55	DA	2143	C	2.6
11	AK	61	PHE	2.6
3	BC	105	GLU	2.6
18	AR	24	LYS	2.6
43	CP	76	LYS	2.6
6	AF	88	MET	2.6
1	BA	92	U	2.6
1	BA	1301	U	2.6
31	CA	2743	U	2.6
40	CM	103	ILE	2.6
1	BA	191	G	2.6
2	AB	114	LEU	2.6
9	AI	98	LEU	2.6
10	AJ	71	LEU	2.6
28	CB	2	G	2.6
31	CA	2859	G	2.6
35	CG	71	LEU	2.6
1	AA	1171	A	2.6
1	BA	1146	A	2.6
2	BB	205	ASP	2.6
19	AS	32	ARG	2.6
29	CC	12	GLY	2.6
30	CD	198	GLY	2.6
31	CA	608	A	2.6

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Mol	Chain	Res	Type	RSRZ
31	CA	633	A	2.6
31	CA	1614	A	2.6
31	CA	1635	A	2.6
35	CG	53	GLY	2.6
37	DJ	29	GLY	2.6
41	CN	15	GLY	2.6
3	BC	7	PRO	2.6
9	AI	66	THR	2.6
33	CE	65	THR	2.6
44	CQ	18	PRO	2.6
3	BC	110	GLU	2.6
13	AM	41	GLU	2.6
50	CW	35	GLU	2.6
51	CX	17	GLU	2.6
50	CW	4	ILE	2.6
1	BA	103	U	2.6
31	CA	102	U	2.6
31	CA	2151	U	2.6
36	CH	131	SER	2.6
42	CO	8	ARG	2.6
8	AH	110	VAL	2.6
19	AS	67	VAL	2.6
42	CO	72	ASP	2.6
1	AA	1166	G	2.6
3	BC	147	LYS	2.6
28	CB	116	G	2.6
31	CA	216	A	2.6
31	CA	841	G	2.6
31	CA	1134	A	2.6
31	CA	1179	G	2.6
31	CA	1496	A	2.6
3	AC	133	ALA	2.6
29	CC	246	THR	2.6
34	CF	54	ALA	2.6
46	CS	77	PHE	2.6
8	BH	36	ILE	2.6
36	DH	72	ILE	2.6
1	BA	992	U	2.6
1	BA	1189	U	2.6
27	C0	31	ARG	2.6
31	CA	2690	U	2.6
40	CM	60	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
7	AG	30	LEU	2.6
30	CD	113	SER	2.6
4	AD	174	ASP	2.6
42	CO	40	LYS	2.6
45	CR	85	LYS	2.6
9	AI	23	PRO	2.6
29	CC	194	GLU	2.6
43	CP	71	ALA	2.6
1	BA	609	A	2.6
19	AS	74	PHE	2.6
31	CA	631	A	2.6
31	CA	1021	A	2.6
55	DA	2154	A	2.6
1	BA	1223	C	2.6
1	BA	1121	U	2.6
23	C2	38	LYS	2.6
24	C3	29	GLN	2.6
36	CH	41	LYS	2.6
41	CN	124	LEU	2.6
16	AP	78	VAL	2.6
22	C1	29	SER	2.6
11	AK	70	CYS	2.6
33	CE	198	GLU	2.6
48	CU	54	GLU	2.6
17	BQ	82	ALA	2.6
23	C2	41	PRO	2.6
43	CP	57	ALA	2.6
47	CT	10	ALA	2.6
52	CY	73	ALA	2.6
1	BA	107	G	2.6
1	BA	139	A	2.6
31	CA	528	A	2.6
31	CA	1354	A	2.6
53	CZ	16	THR	2.6
11	AK	107	ILE	2.6
31	CA	583	G	2.6
35	CG	18	LYS	2.6
37	CJ	10	LYS	2.6
43	CP	19	GLN	2.6
48	CU	49	LYS	2.6
55	DA	1731	G	2.6
8	BH	120	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
30	CD	120	GLY	2.6
31	CA	667	U	2.6
31	CA	1454	C	2.6
31	CA	2871	U	2.6
44	CQ	114	LEU	2.6
6	BF	96	VAL	2.6
8	BH	86	TYR	2.6
29	CC	250	VAL	2.6
29	DC	272	SER	2.6
33	CE	116	ASP	2.6
44	CQ	19	SER	2.6
46	CS	2	TYR	2.6
3	AC	107	ARG	2.6
5	BE	112	ARG	2.6
25	C4	48	ALA	2.6
7	BG	36	LYS	2.6
26	C5	24	ARG	2.6
38	CK	63	ALA	2.6
52	CY	39	TRP	2.6
41	CN	71	LYS	2.6
48	CU	14	PRO	2.6
23	D2	5	ILE	2.6
5	AE	115	LEU	2.6
30	CD	158	GLY	2.6
31	CA	1276	A	2.6
31	CA	1141	U	2.6
40	CM	53	GLY	2.6
1	AA	1347	G	2.6
31	CA	68	G	2.6
31	CA	389	G	2.6
7	AG	87	VAL	2.6
9	BI	42	GLU	2.6
31	CA	624	C	2.6
31	CA	1615	C	2.6
31	CA	2275	C	2.6
31	CA	2791	G	2.6
31	CA	2857	G	2.6
10	AJ	60	ASP	2.6
13	BM	68	ASP	2.6
29	CC	98	ASP	2.6
14	AN	55	SER	2.6
14	BN	80	SER	2.6

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Mol	Chain	Res	Type	RSRZ
20	BT	85	LYS	2.6
33	CE	79	ARG	2.6
35	CG	149	ARG	2.6
35	CG	170	ARG	2.6
37	DJ	44	ALA	2.6
10	AJ	58	ASN	2.6
3	AC	64	ILE	2.5
36	CH	80	ILE	2.5
10	BJ	66	GLU	2.5
17	BQ	54	GLY	2.5
29	CC	181	MET	2.5
30	CD	89	GLU	2.5
10	BJ	57	VAL	2.5
31	CA	374	A	2.5
1	BA	148	G	2.5
1	BA	187	G	2.5
13	AM	3	ARG	2.5
31	CA	1208	C	2.5
34	CF	89	VAL	2.5
36	CH	22	LYS	2.5
39	CL	108	ARG	2.5
42	CO	22	ARG	2.5
50	CW	60	VAL	2.5
31	CA	386	G	2.5
31	CA	1867	G	2.5
29	CC	259	SER	2.5
34	CF	162	SER	2.5
17	BQ	66	PRO	2.5
2	AB	67	ILE	2.5
14	AN	4	GLN	2.5
26	C5	35	GLN	2.5
13	AM	111	GLY	2.5
19	AS	54	GLY	2.5
7	AG	99	LEU	2.5
34	DF	152	LEU	2.5
40	CM	51	GLU	2.5
48	CU	93	LEU	2.5
7	AG	75	VAL	2.5
10	BJ	62	ARG	2.5
31	CA	906	U	2.5
33	CE	61	ARG	2.5
41	CN	14	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
12	BL	107	VAL	2.5
17	BQ	47	HIS	2.5
1	BA	135	C	2.5
1	BA	935	A	2.5
1	BA	1441	A	2.5
31	CA	246	C	2.5
31	CA	800	A	2.5
31	CA	2054	A	2.5
2	BB	191	SER	2.5
17	BQ	20	SER	2.5
24	C3	45	SER	2.5
1	BA	251	G	2.5
1	BA	351	G	2.5
31	CA	27	G	2.5
31	CA	2046	G	2.5
31	CA	2242	G	2.5
31	CA	2844	G	2.5
50	CW	23	ALA	2.5
20	BT	82	GLN	2.5
4	AD	170	TRP	2.5
7	BG	19	GLY	2.5
9	AI	8	GLY	2.5
29	CC	49	ILE	2.5
37	CJ	141	GLU	2.5
40	CM	49	GLY	2.5
1	BA	467	U	2.5
29	DC	252	THR	2.5
31	CA	1058	U	2.5
31	CA	1443	U	2.5
12	BL	72	HIS	2.5
35	CG	137	ASP	2.5
1	BA	1045	C	2.5
31	CA	975	A	2.5
31	CA	1053	C	2.5
31	CA	1270	C	2.5
31	CA	2212	A	2.5
36	CH	102	ALA	2.5
37	DJ	15	ALA	2.5
50	CW	16	ALA	2.5
55	DA	898	C	2.5
1	BA	380	G	2.5
1	BA	1190	G	2.5

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Mol	Chain	Res	Type	RSRZ
16	BP	29	ASN	2.5
23	C2	48	ILE	2.5
31	CA	776	G	2.5
31	CA	1811	G	2.5
31	CA	2053	G	2.5
2	AB	212	LEU	2.5
8	AH	32	LEU	2.5
1	BA	84	U	2.5
3	BC	128	VAL	2.5
5	AE	120	VAL	2.5
23	D2	42	VAL	2.5
34	CF	159	THR	2.5
11	AK	75	LYS	2.5
13	AM	62	LYS	2.5
1	AA	1128	C	2.5
1	AA	1140	C	2.5
1	BA	379	C	2.5
14	AN	22	ALA	2.5
31	CA	2374	C	2.5
31	CA	2527	C	2.5
34	CF	140	GLU	2.5
36	DH	84	ALA	2.5
38	CK	129	GLU	2.5
5	AE	92	SER	2.5
14	BN	100	SER	2.5
31	CA	1008	A	2.5
31	CA	2274	A	2.5
33	CE	170	ARG	2.5
47	CT	15	GLN	2.5
9	AI	125	PRO	2.5
48	CU	77	ARG	2.5
35	CG	89	LEU	2.5
36	CH	5	LEU	2.5
1	AA	4	U	2.5
1	BA	326	G	2.5
1	BA	1255	G	2.5
31	CA	1	G	2.5
31	CA	489	G	2.5
31	CA	1038	G	2.5
31	CA	1124	G	2.5
31	CA	1361	G	2.5
31	CA	1543	G	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
30	CD	104	VAL	2.5
30	CD	122	VAL	2.5
31	CA	2321	U	2.5
33	CE	187	VAL	2.5
44	CQ	47	VAL	2.5
9	BI	13	LYS	2.5
30	CD	52	THR	2.5
30	CD	103	ASP	2.5
52	CY	36	HIS	2.5
19	BS	36	ARG	2.5
1	BA	381	C	2.5
29	DC	241	GLY	2.5
31	CA	581	C	2.5
31	CA	838	C	2.5
1	BA	461	A	2.5
3	BC	207	ILE	2.5
53	CZ	34	SER	2.5
2	BB	129	LEU	2.5
21	BU	9	ASN	2.5
31	CA	1522	A	2.5
31	CA	1722	A	2.5
34	CF	50	LEU	2.5
47	CT	19	LEU	2.5
5	BE	114	VAL	2.5
29	CC	59	LYS	2.5
34	CF	78	LYS	2.5
38	CK	48	VAL	2.5
1	AA	971	G	2.5
1	AA	1260	G	2.5
31	CA	467	G	2.5
31	CA	537	G	2.5
44	CQ	20	PHE	2.5
55	DA	1071	G	2.5
7	BG	92	ARG	2.5
33	CE	84	THR	2.5
38	CK	120	ARG	2.5
3	AC	71	ALA	2.5
11	BK	71	ALA	2.5
9	AI	126	GLN	2.5
36	CH	92	GLY	2.5
2	AB	43	LEU	2.5
2	BB	57	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
13	AM	22	ILE	2.5
31	CA	198	C	2.5
10	AJ	11	LYS	2.5
51	CX	24	LYS	2.5
1	AA	205	A	2.5
1	AA	1016	A	2.5
31	CA	429	A	2.5
31	CA	482	A	2.5
3	BC	84	VAL	2.5
8	BH	91	GLU	2.5
13	BM	59	GLU	2.5
33	CE	169	VAL	2.5
39	CL	57	VAL	2.5
55	DA	2130	U	2.5
55	DA	2151	U	2.5
27	C0	30	ARG	2.5
9	BI	108	ALA	2.5
23	C2	16	GLY	2.5
28	CB	79	G	2.5
31	CA	48	G	2.5
31	CA	54	G	2.5
31	CA	242	G	2.5
31	CA	1055	G	2.5
31	CA	1296	G	2.5
31	CA	1645	G	2.5
48	CU	39	THR	2.5
55	DA	2138	G	2.5
12	BL	80	ILE	2.5
42	CO	99	LYS	2.5
46	CS	73	LYS	2.5
1	BA	1112	C	2.5
28	CB	62	C	2.5
31	CA	645	C	2.5
37	DJ	26	PRO	2.5
39	CL	75	SER	2.5
55	DA	2179	C	2.5
30	CD	33	ARG	2.5
30	CD	99	GLU	2.5
1	AA	1368	A	2.5
1	BA	1311	A	2.5
2	AB	50	PHE	2.5
25	C4	54	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
31	CA	1039	A	2.5
31	CA	1654	A	2.5
31	CA	2837	A	2.5
2	AB	39	HIS	2.5
2	BB	216	ALA	2.5
7	BG	34	GLY	2.5
14	AN	8	ALA	2.5
14	BN	101	TRP	2.5
15	AO	22	THR	2.5
16	AP	80	LYS	2.5
37	CJ	40	LYS	2.5
49	CV	16	GLY	2.5
50	CW	33	GLY	2.5
38	CK	24	THR	2.5
17	BQ	75	LEU	2.5
31	CA	618	G	2.5
31	CA	1619	G	2.5
31	CA	2414	G	2.5
37	DJ	122	ILE	2.5
42	CO	98	LEU	2.5
52	CY	64	ILE	2.5
55	DA	2152	G	2.5
4	AD	172	GLU	2.4
23	C2	32	GLU	2.4
31	CA	1170	C	2.4
38	CK	73	VAL	2.4
52	CY	51	VAL	2.4
2	AB	64	LYS	2.4
28	CB	45	A	2.4
31	CA	1302	A	2.4
34	CF	145	LYS	2.4
43	CP	23	ALA	2.4
43	CP	72	ALA	2.4
2	BB	189	THR	2.4
47	CT	100	THR	2.4
30	CD	40	LEU	2.4
40	CM	33	ARG	2.4
53	DZ	28	LEU	2.4
1	AA	1138	G	2.4
31	CA	1131	G	2.4
31	CA	1182	G	2.4
1	BA	215	C	2.4

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Mol	Chain	Res	Type	RSRZ
2	AB	187	VAL	2.4
8	AH	111	MET	2.4
54	DI	4	ASN	2.4
55	DA	2137	U	2.4
13	AM	58	ASP	2.4
30	CD	209	ALA	2.4
37	CJ	105	GLN	2.4
37	DJ	120	ALA	2.4
44	CQ	41	GLN	2.4
31	CA	342	A	2.4
31	CA	432	A	2.4
31	CA	1359	A	2.4
31	CA	2287	A	2.4
31	CA	2298	A	2.4
19	AS	5	LEU	2.4
42	CO	97	ILE	2.4
44	CQ	76	THR	2.4
48	CU	18	GLU	2.4
22	C1	49	TYR	2.4
45	CR	32	TYR	2.4
2	BB	29	PRO	2.4
2	BB	182	PRO	2.4
9	BI	114	LYS	2.4
50	CW	34	LYS	2.4
3	BC	151	VAL	2.4
31	CA	1091	G	2.4
31	CA	1102	C	2.4
31	CA	1779	U	2.4
31	CA	2296	U	2.4
31	CA	2427	C	2.4
31	CA	2462	C	2.4
31	CA	2473	U	2.4
47	CT	20	VAL	2.4
3	BC	8	ASN	2.4
28	CB	3	C	2.4
31	CA	491	G	2.4
31	CA	2742	G	2.4
39	CL	7	MET	2.4
33	CE	90	GLN	2.4
34	CF	116	GLY	2.4
51	CX	65	GLY	2.4
55	DA	1727	C	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	BB	76	ALA	2.4
19	AS	3	ARG	2.4
30	CD	124	ARG	2.4
54	DI	31	ARG	2.4
18	BR	74	HIS	2.4
36	DH	76	GLU	2.4
44	CQ	44	GLU	2.4
50	CW	59	GLU	2.4
1	BA	459	A	2.4
8	BH	59	LEU	2.4
10	BJ	17	LEU	2.4
29	CC	33	LEU	2.4
30	CD	79	LEU	2.4
31	CA	104	A	2.4
31	CA	190	A	2.4
31	CA	294	A	2.4
31	CA	1165	A	2.4
31	CA	2602	A	2.4
31	CA	2820	A	2.4
44	CQ	14	LYS	2.4
15	BO	79	THR	2.4
19	AS	77	THR	2.4
4	AD	38	PRO	2.4
29	CC	248	TRP	2.4
30	CD	129	THR	2.4
38	CK	8	PRO	2.4
39	CL	120	PRO	2.4
39	CL	62	VAL	2.4
46	CS	47	VAL	2.4
53	CZ	26	PHE	2.4
53	CZ	46	VAL	2.4
28	CB	82	U	2.4
31	CA	112	U	2.4
31	CA	686	U	2.4
10	BJ	60	ASP	2.4
1	BA	67	C	2.4
1	BA	848	C	2.4
31	CA	433	C	2.4
31	CA	435	C	2.4
1	AA	413	G	2.4
2	BB	64	LYS	2.4
13	AM	47	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
15	BO	14	GLU	2.4
31	CA	2318	G	2.4
31	CA	2391	G	2.4
31	CA	2623	G	2.4
35	CG	165	ALA	2.4
41	CN	8	LYS	2.4
47	CT	90	LYS	2.4
26	C5	23	ILE	2.4
29	CC	104	ILE	2.4
34	CF	103	LEU	2.4
1	AA	1169	A	2.4
31	CA	2882	A	2.4
8	BH	71	VAL	2.4
10	BJ	49	PHE	2.4
30	CD	142	VAL	2.4
35	CG	118	PRO	2.4
2	BB	74	ARG	2.4
2	BB	136	MET	2.4
9	BI	80	ARG	2.4
9	BI	82	GLY	2.4
20	BT	65	GLY	2.4
31	CA	358	U	2.4
30	CD	161	MET	2.4
19	BS	17	LYS	2.4
29	CC	100	GLU	2.4
35	DG	177	LYS	2.4
36	CH	76	GLU	2.4
45	CR	54	LYS	2.4
51	CX	78	LYS	2.4
54	DI	122	GLN	2.4
31	CA	853	C	2.4
31	CA	2347	C	2.4
31	CA	674	G	2.4
31	CA	1358	G	2.4
31	CA	1540	G	2.4
33	CE	108	ILE	2.4
34	CF	111	ILE	2.4
36	DH	5	LEU	2.4
47	CT	36	LEU	2.4
4	AD	182	PHE	2.4
31	CA	1284	A	2.4
35	CG	11	VAL	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
48	CU	51	PHE	2.4
1	BA	55	A	2.4
1	BA	1202	U	2.4
16	BP	13	LYS	2.4
28	CB	74	U	2.4
30	CD	159	LYS	2.4
31	CA	675	A	2.4
50	CW	65	VAL	2.4
55	DA	139	U	2.4
35	CG	101	ASN	2.4
8	BH	116	ALA	2.4
20	BT	47	ALA	2.4
31	CA	115	C	2.4
6	BF	74	LEU	2.4
34	DF	85	ILE	2.4
44	CQ	48	ILE	2.4
3	BC	136	ARG	2.4
13	BM	72	GLU	2.4
37	DJ	9	VAL	2.4
17	BQ	7	THR	2.4
31	CA	1709	U	2.4
33	CE	53	THR	2.4
46	CS	16	GLU	2.4
1	AA	1236	A	2.4
27	C0	47	MET	2.4
31	CA	575	A	2.4
31	CA	1254	A	2.4
55	DA	1073	A	2.4
16	AP	79	ASN	2.4
23	C2	34	LEU	2.4
31	CA	2795	C	2.4
24	C3	25	LYS	2.4
3	BC	60	PRO	2.4
16	BP	61	VAL	2.4
17	BQ	22	VAL	2.4
20	BT	55	GLN	2.4
31	CA	1355	G	2.4
31	CA	2250	G	2.4
31	CA	2744	G	2.4
31	CA	2838	G	2.4
41	CN	7	THR	2.4
1	BA	151	A	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	BA	1046	A	2.4
14	AN	2	ALA	2.4
14	BN	42	TRP	2.4
22	C1	21	ALA	2.4
28	CB	52	A	2.4
31	CA	167	A	2.4
31	CA	1144	A	2.4
31	CA	1477	A	2.4
31	CA	1528	A	2.4
31	CA	1650	A	2.4
33	CE	86	ALA	2.4
49	CV	74	ASN	2.4
49	CV	99	ASN	2.4
52	CY	17	ASN	2.4
2	AB	45	LYS	2.4
3	BC	14	ILE	2.4
6	AF	38	ARG	2.4
13	AM	113	ARG	2.4
18	AR	21	ILE	2.4
29	CC	135	ILE	2.4
33	CE	105	LEU	2.4
44	CQ	6	LYS	2.4
48	CU	11	LEU	2.4
52	CY	3	ARG	2.4
2	BB	162	PHE	2.3
15	AO	16	GLY	2.3
20	AT	20	HIS	2.3
33	CE	29	HIS	2.3
47	CT	52	GLU	2.3
48	DU	70	HIS	2.3
29	CC	19	VAL	2.3
1	BA	224	U	2.3
12	BL	38	TYR	2.3
28	CB	32	U	2.3
54	DI	6	GLN	2.3
55	DA	1729	U	2.3
2	AB	137	ARG	2.3
17	BQ	40	ARG	2.3
25	C4	5	LYS	2.3
31	CA	1651	G	2.3
1	BA	1042	A	2.3
1	BA	1360	A	2.3

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Mol	Chain	Res	Type	RSRZ
3	AC	77	ILE	2.3
3	BC	115	LEU	2.3
6	AF	6	ILE	2.3
31	CA	1129	A	2.3
31	CA	1810	A	2.3
31	CA	2868	A	2.3
31	CA	2883	A	2.3
44	DQ	114	LEU	2.3
28	CB	28	C	2.3
31	CA	16	C	2.3
31	CA	179	C	2.3
31	CA	2368	C	2.3
3	BC	173	VAL	2.3
20	AT	85	LYS	2.3
29	CC	265	LYS	2.3
31	CA	1487	U	2.3
36	CH	69	ALA	2.3
29	CC	95	LEU	2.3
1	AA	1185	G	2.3
1	BA	1453	G	2.3
5	BE	92	SER	2.3
10	AJ	54	SER	2.3
28	CB	67	G	2.3
31	CA	1546	G	2.3
31	CA	2599	G	2.3
33	CE	78	TRP	2.3
36	CH	119	ASN	2.3
43	CP	45	SER	2.3
50	CW	24	ASN	2.3
52	CY	16	ASN	2.3
6	AF	8	PHE	2.3
28	CB	99	A	2.3
31	CA	788	A	2.3
31	CA	1735	A	2.3
38	CK	83	GLY	2.3
1	AA	470	C	2.3
1	BA	110	C	2.3
3	AC	151	VAL	2.3
8	BH	104	VAL	2.3
24	C3	2	LYS	2.3
31	CA	393	C	2.3
35	CG	134	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
47	CT	42	LYS	2.3
54	DI	12	VAL	2.3
1	BA	843	U	2.3
31	CA	1184	U	2.3
31	CA	1396	U	2.3
33	CE	40	ARG	2.3
54	DI	102	ALA	2.3
2	BB	111	ILE	2.3
6	BF	92	THR	2.3
9	BI	72	ILE	2.3
11	BK	100	LEU	2.3
22	C1	9	THR	2.3
37	DJ	141	GLU	2.3
3	BC	187	SER	2.3
2	BB	90	PHE	2.3
1	BA	76	G	2.3
1	BA	143	A	2.3
31	CA	496	G	2.3
31	CA	829	A	2.3
31	CA	1385	A	2.3
31	CA	1439	A	2.3
31	CA	2671	G	2.3
31	CA	2822	G	2.3
54	DI	105	LYS	2.3
11	AK	38	GLN	2.3
31	CA	1646	C	2.3
31	CA	2215	C	2.3
31	CA	2863	C	2.3
1	BA	1183	U	2.3
6	AF	9	MET	2.3
18	AR	32	TYR	2.3
38	CK	49	ASP	2.3
48	CU	5	GLU	2.3
5	BE	81	LEU	2.3
5	AE	31	PHE	2.3
5	BE	135	ASN	2.3
33	DE	6	LYS	2.3
35	CG	29	LYS	2.3
44	CQ	63	LYS	2.3
35	CG	61	GLY	2.3
45	CR	72	ASN	2.3
29	CC	52	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
4	AD	25	VAL	2.3
4	AD	40	GLN	2.3
5	BE	82	GLN	2.3
7	AG	3	ARG	2.3
34	CF	63	GLN	2.3
1	AA	1237	C	2.3
1	BA	221	C	2.3
1	BA	1365	G	2.3
3	AC	176	HIS	2.3
31	CA	547	A	2.3
31	CA	957	C	2.3
31	CA	2154	A	2.3
9	AI	91	ASP	2.3
12	BL	109	ASP	2.3
31	CA	395	U	2.3
36	DH	98	ASP	2.3
36	CH	64	ALA	2.3
40	DM	95	LEU	2.3
45	CR	22	LYS	2.3
11	BK	107	ILE	2.3
38	CK	38	GLY	2.3
7	AG	45	SER	2.3
12	BL	96	HIS	2.3
1	AA	1188	A	2.3
14	AN	28	LYS	2.3
19	AS	21	LYS	2.3
19	BS	70	LYS	2.3
43	CP	80	GLU	2.3
49	CV	37	GLU	2.3
28	CB	64	G	2.3
28	CB	90	C	2.3
31	CA	254	G	2.3
31	CA	324	A	2.3
31	CA	466	A	2.3
31	CA	503	A	2.3
31	CA	577	G	2.3
31	CA	671	C	2.3
31	CA	1040	A	2.3
31	CA	1116	G	2.3
31	CA	1469	A	2.3
31	CA	1655	A	2.3
31	CA	1721	G	2.3

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Mol	Chain	Res	Type	RSRZ
31	CA	1861	G	2.3
31	CA	2753	A	2.3
3	BC	175	LEU	2.3
6	AF	90	MET	2.3
7	AG	101	MET	2.3
9	BI	87	LEU	2.3
29	CC	93	LEU	2.3
36	CH	56	ALA	2.3
36	DH	59	ALA	2.3
45	CR	21	ALA	2.3
2	BB	202	GLY	2.3
11	BK	23	ILE	2.3
36	DH	68	ARG	2.3
3	BC	29	PHE	2.3
11	BK	27	PHE	2.3
38	CK	115	GLY	2.3
11	BK	29	ASN	2.3
29	CC	50	THR	2.3
35	DG	101	ASN	2.3
42	CO	13	ASN	2.3
11	BK	20	VAL	2.3
36	CH	103	VAL	2.3
40	CM	46	VAL	2.3
42	CO	27	SER	2.3
52	CY	40	VAL	2.3
3	BC	28	GLU	2.3
9	AI	53	GLU	2.3
48	CU	19	LYS	2.3
1	BA	1232	U	2.3
1	BA	1315	U	2.3
30	CD	23	PRO	2.3
31	CA	1865	U	2.3
31	CA	2585	U	2.3
31	CA	2784	U	2.3
55	DA	2797	U	2.3
1	BA	274	A	2.3
10	AJ	72	ARG	2.3
14	BN	81	ARG	2.3
19	AS	22	ALA	2.3
20	BT	54	MET	2.3
31	CA	865	C	2.3
47	CT	88	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
54	DI	100	ALA	2.3
29	CC	64	ILE	2.3
31	CA	125	A	2.3
31	CA	677	A	2.3
31	CA	1156	A	2.3
31	CA	446	G	2.3
31	CA	1136	G	2.3
31	CA	1449	G	2.3
31	CA	1455	G	2.3
31	CA	2056	G	2.3
31	CA	2230	G	2.3
31	CA	2488	G	2.3
31	CA	2894	G	2.3
11	BK	70	CYS	2.3
41	CN	9	PHE	2.3
9	AI	27	LYS	2.3
14	AN	35	ASN	2.3
30	CD	58	ASN	2.3
34	DF	72	LYS	2.3
36	CH	31	VAL	2.3
49	CV	68	SER	2.3
31	CA	2818	U	2.3
33	CE	69	ARG	2.3
11	BK	62	ALA	2.3
14	AN	15	ALA	2.3
40	DM	102	GLY	2.3
48	DU	32	LEU	2.3
1	AA	90	C	2.3
1	BA	322	C	2.3
1	BA	1366	C	2.3
9	AI	7	TYR	2.3
16	BP	32	PHE	2.3
31	CA	414	C	2.3
35	CG	164	TYR	2.3
54	DI	52	MET	2.3
31	CA	73	A	2.3
31	CA	900	A	2.3
31	CA	1508	A	2.3
33	CE	74	LYS	2.3
44	CQ	96	LYS	2.3
45	CR	41	LYS	2.3
1	AA	201	G	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	AA	1003	G	2.3
9	AI	110	GLN	2.3
12	BL	29	GLN	2.3
14	AN	11	VAL	2.2
26	C5	22	VAL	2.2
5	BE	157	ARG	2.2
31	CA	1765	U	2.2
5	AE	110	ALA	2.2
9	BI	71	GLY	2.2
19	BS	15	LEU	2.2
29	CC	41	GLY	2.2
30	CD	93	GLY	2.2
34	CF	16	LEU	2.2
34	DF	116	GLY	2.2
38	CK	6	ALA	2.2
39	CL	107	LEU	2.2
52	CY	31	PRO	2.2
54	DI	73	LYS	2.2
54	DI	90	GLY	2.2
21	BU	37	PHE	2.2
14	AN	26	GLU	2.2
31	CA	238	C	2.2
33	CE	85	PHE	2.2
1	AA	468	A	2.2
31	CA	2060	A	2.2
31	CA	2317	A	2.2
55	DA	1084	A	2.2
1	AA	951	G	2.2
1	AA	1190	G	2.2
1	AA	1370	G	2.2
1	BA	1385	G	2.2
31	CA	1401	G	2.2
31	CA	1719	G	2.2
31	CA	2294	G	2.2
43	CP	91	SER	2.2
55	DA	2112	G	2.2
2	BB	45	LYS	2.2
2	AB	68	LEU	2.2
3	BC	146	ALA	2.2
14	AN	71	HIS	2.2
31	CA	67	U	2.2
31	CA	2615	U	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
48	CU	88	LYS	2.2
15	BO	3	LEU	2.2
19	AS	50	ALA	2.2
34	CF	2	ALA	2.2
54	DI	91	ALA	2.2
15	AO	43	PHE	2.2
44	CQ	112	GLU	2.2
31	CA	385	C	2.2
31	CA	1161	C	2.2
46	CS	86	GLN	2.2
16	AP	14	ARG	2.2
21	BU	18	ARG	2.2
35	CG	98	VAL	2.2
1	BA	389	A	2.2
9	BI	100	LYS	2.2
31	CA	2059	A	2.2
31	CA	2077	A	2.2
39	CL	82	ASN	2.2
42	DO	121	LYS	2.2
1	BA	75	G	2.2
1	BA	249	U	2.2
3	BC	81	GLY	2.2
3	BC	174	PRO	2.2
4	AD	9	LEU	2.2
6	BF	66	ALA	2.2
10	BJ	52	LEU	2.2
19	AS	31	LEU	2.2
31	CA	1115	G	2.2
31	CA	1163	G	2.2
31	CA	2624	G	2.2
46	CS	67	GLY	2.2
47	CT	26	GLY	2.2
48	CU	38	ALA	2.2
53	DZ	37	LEU	2.2
2	AB	151	ILE	2.2
3	AC	149	ILE	2.2
9	BI	112	GLU	2.2
39	CL	115	ILE	2.2
54	DI	92	ALA	2.2
14	AN	6	MET	2.2
30	CD	127	PHE	2.2
5	BE	93	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
6	BF	4	TYR	2.2
27	C0	38	ARG	2.2
43	CP	116	GLN	2.2
5	BE	159	LYS	2.2
7	AG	80	VAL	2.2
31	CA	903	C	2.2
31	CA	1488	C	2.2
33	CE	120	VAL	2.2
50	CW	49	ASN	2.2
1	BA	65	A	2.2
1	BA	1067	A	2.2
1	BA	1319	A	2.2
7	AG	129	GLU	2.2
9	AI	52	LEU	2.2
12	BL	64	THR	2.2
12	BL	68	GLY	2.2
31	CA	149	A	2.2
31	CA	2020	A	2.2
31	CA	2088	A	2.2
15	BO	67	LEU	2.2
28	CB	111	U	2.2
39	CL	104	THR	2.2
47	CT	34	ASP	2.2
42	CO	19	ALA	2.2
43	CP	112	GLU	2.2
55	DA	1083	U	2.2
10	AJ	40	ILE	2.2
17	AQ	21	ILE	2.2
35	DG	111	HIS	2.2
47	CT	32	ALA	2.2
53	DZ	3	ALA	2.2
1	BA	113	G	2.2
1	BA	973	G	2.2
1	BA	1455	G	2.2
3	BC	131	ARG	2.2
13	BM	87	ARG	2.2
16	BP	8	ARG	2.2
31	CA	60	G	2.2
31	CA	185	G	2.2
31	CA	469	G	2.2
31	CA	1248	G	2.2
31	CA	1374	G	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
31	CA	1382	G	2.2
44	CQ	98	TYR	2.2
45	CR	84	LYS	2.2
1	BA	214	C	2.2
1	BA	995	C	2.2
1	BA	1203	C	2.2
1	BA	1452	C	2.2
2	AB	217	VAL	2.2
11	AK	113	VAL	2.2
31	CA	143	C	2.2
31	CA	509	C	2.2
31	CA	672	C	2.2
41	CN	135	VAL	2.2
3	BC	125	GLU	2.2
31	CA	2522	U	2.2
36	CH	86	ASP	2.2
46	CS	57	GLY	2.2
1	BA	630	A	2.2
1	BA	1170	A	2.2
8	BH	107	SER	2.2
15	BO	56	LEU	2.2
29	CC	176	LEU	2.2
14	AN	81	ARG	2.2
23	D2	39	PHE	2.2
31	CA	2033	A	2.2
38	CK	45	THR	2.2
40	CM	69	ARG	2.2
42	CO	87	PHE	2.2
55	DA	1095	A	2.2
27	C0	18	PRO	2.2
29	CC	247	PRO	2.2
38	CK	123	LYS	2.2
49	DV	50	PRO	2.2
54	DI	79	PRO	2.2
1	BA	457	G	2.2
31	CA	1206	G	2.2
31	CA	2631	G	2.2
50	CW	82	TYR	2.2
55	DA	2144	G	2.2
5	BE	153	VAL	2.2
19	AS	58	VAL	2.2
29	CC	78	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
6	AF	98	GLU	2.2
14	AN	64	CYS	2.2
31	CA	1005	C	2.2
31	CA	1472	C	2.2
2	BB	146	ASN	2.2
16	AP	40	ASN	2.2
36	DH	73	ASN	2.2
1	BA	219	U	2.2
49	CV	96	PHE	2.2
52	CY	62	LYS	2.2
55	DA	653	U	2.2
55	DA	2139	U	2.2
2	AB	200	ILE	2.2
8	BH	126	ILE	2.2
13	AM	12	HIS	2.2
13	AM	55	THR	2.2
29	DC	247	PRO	2.2
31	CA	223	A	2.2
31	CA	430	A	2.2
31	CA	927	A	2.2
31	CA	1027	A	2.2
31	CA	2758	A	2.2
33	CE	141	MET	2.2
37	DJ	105	GLN	2.2
42	CO	110	MET	2.2
3	AC	153	VAL	2.2
20	AT	35	VAL	2.2
51	CX	31	VAL	2.2
1	BA	350	G	2.2
9	BI	59	GLU	2.2
19	AS	24	GLU	2.2
2	AB	124	GLY	2.2
31	CA	400	G	2.2
31	CA	1910	G	2.2
31	CA	2209	G	2.2
31	CA	2828	G	2.2
33	CE	51	GLU	2.2
34	CF	48	LYS	2.2
40	CM	43	GLY	2.2
46	CS	85	LYS	2.2
49	DV	57	GLY	2.2
1	BA	106	C	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
31	CA	33	C	2.2
54	DI	8	LYS	2.2
1	AA	1364	U	2.2
2	AB	203	ASN	2.2
12	BL	74	LEU	2.2
35	DG	114	ASP	2.2
31	CA	1203	U	2.2
31	CA	2493	U	2.2
36	CH	54	LEU	2.2
52	CY	33	LEU	2.2
6	BF	32	ALA	2.2
20	BT	41	ALA	2.2
35	DG	13	ALA	2.2
24	D3	1	MET	2.2
33	CE	41	GLN	2.2
40	CM	56	PRO	2.2
40	CM	94	THR	2.2
1	BA	383	A	2.2
1	BA	1332	A	2.2
31	CA	1808	A	2.2
31	CA	2662	A	2.2
55	DA	2101	A	2.2
55	DA	2886[A]	A	2.2
29	CC	268	VAL	2.2
36	CH	35	LYS	2.2
36	CH	45	GLU	2.2
7	AG	112	GLY	2.2
23	D2	18	GLY	2.2
25	C4	56	GLY	2.2
54	DI	56	ARG	2.2
1	BA	1134	G	2.2
31	CA	692	C	2.2
31	CA	1519	G	2.2
31	CA	1675	C	2.2
31	CA	1812	U	2.2
31	CA	1957	C	2.2
31	CA	2016	U	2.2
31	CA	2389	G	2.2
31	CA	2408	U	2.2
31	CA	2532	G	2.2
31	CA	2661	G	2.2
54	DI	60	LEU	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	BA	1335	U	2.2
54	DI	103	ASN	2.2
55	DA	414	C	2.2
55	DA	1091	G	2.2
55	DA	1733	G	2.2
47	CT	89	ALA	2.2
36	DH	93	SER	2.2
13	AM	108	THR	2.2
18	AR	45	THR	2.2
36	DH	104	THR	2.2
7	AG	76	LYS	2.2
12	BL	14	ARG	2.2
29	CC	255	LYS	2.2
1	AA	1346	A	2.2
1	BA	353	A	2.2
1	BA	1012	A	2.2
14	AN	34	VAL	2.2
11	BK	48	GLY	2.1
31	CA	574	A	2.2
31	CA	1287	A	2.2
31	CA	1353	A	2.2
31	CA	2377	A	2.2
48	CU	53	VAL	2.2
49	CV	57	GLY	2.1
2	BB	167	ASP	2.1
2	BB	188	ASP	2.1
14	BN	96	LEU	2.1
1	AA	183	C	2.1
1	BA	180	U	2.1
1	BA	217	C	2.1
1	BA	472	U	2.1
3	BC	163	ALA	2.1
15	AO	11	ILE	2.1
31	CA	157	C	2.1
31	CA	286	U	2.1
31	CA	1019	U	2.1
31	CA	1209	U	2.1
31	CA	1748	C	2.1
31	CA	2798	U	2.1
33	DE	11	ALA	2.1
34	CF	52	ASN	2.1
1	AA	1371	G	2.1

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Mol	Chain	Res	Type	RSRZ
3	AC	80	LYS	2.1
3	BC	114	LYS	2.1
31	CA	518	G	2.1
31	CA	625	G	2.1
31	CA	2494	G	2.1
31	CA	2583	G	2.1
36	CH	71	LYS	2.1
47	CT	73	LYS	2.1
55	DA	1074	G	2.1
3	BC	142	MET	2.1
8	BH	3	MET	2.1
9	AI	11	ARG	2.1
29	CC	94	VAL	2.1
33	CE	174	GLY	2.1
36	CH	121	VAL	2.1
53	CZ	50	VAL	2.1
54	DI	71	CYS	2.1
31	CA	354	A	2.1
31	CA	391	A	2.1
31	CA	1854	A	2.1
31	CA	2388	A	2.1
19	BS	64	ASP	2.1
34	CF	57	LEU	2.1
40	CM	125	LEU	2.1
47	CT	109	ASP	2.1
1	AA	1321	U	2.1
13	BM	110	LYS	2.1
20	BT	19	LYS	2.1
29	CC	253	LYS	2.1
31	CA	296	U	2.1
31	CA	1294	U	2.1
1	BA	1051	C	2.1
1	BA	1448	C	2.1
2	BB	96	TRP	2.1
34	DF	106	ILE	2.1
11	AK	94	GLU	2.1
24	C3	19	ARG	2.1
29	CC	221	ARG	2.1
31	CA	915	C	2.1
31	CA	1229	C	2.1
31	CA	2055	C	2.1
31	CA	2456	C	2.1

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Mol	Chain	Res	Type	RSRZ
40	CM	86	GLU	2.1
42	CO	32	GLU	2.1
54	DI	62	ARG	2.1
26	C5	31	PRO	2.1
1	BA	1064	G	2.1
31	CA	24	G	2.1
31	CA	1149	G	2.1
31	CA	2010	G	2.1
31	CA	2029	G	2.1
31	CA	2144	G	2.1
31	CA	2349	G	2.1
31	CA	2409	G	2.1
31	CA	2415	G	2.1
31	CA	2692	G	2.1
55	DA	1171	G	2.1
3	AC	2	GLY	2.1
3	BC	15	VAL	2.1
3	BC	67	THR	2.1
8	AH	55	THR	2.1
29	CC	119	GLY	2.1
37	DJ	139	VAL	2.1
47	CT	50	VAL	2.1
18	BR	23	TYR	2.1
2	AB	205	ASP	2.1
25	C4	33	LEU	2.1
34	DF	145	LYS	2.1
45	CR	60	LEU	2.1
31	CA	1307	A	2.1
31	CA	1387	A	2.1
31	CA	2406	A	2.1
31	CA	2435	A	2.1
52	CY	29	PHE	2.1
52	CY	38	PHE	2.1
3	AC	188	GLU	2.1
8	AH	130	ALA	2.1
9	AI	86	ALA	2.1
22	C1	52	ARG	2.1
25	C4	13	ARG	2.1
31	CA	234	U	2.1
31	CA	1621	U	2.1
37	CJ	63	ALA	2.1
27	C0	49	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
28	CB	114	C	2.1
31	CA	105	C	2.1
31	CA	1006	C	2.1
31	CA	2153	C	2.1
2	BB	226	SER	2.1
1	BA	324	G	2.1
28	CB	18	G	2.1
31	CA	604	G	2.1
31	CA	1601	G	2.1
31	CA	1992	G	2.1
31	CA	2834	G	2.1
38	CK	30	THR	2.1
54	DI	86	THR	2.1
29	CC	205	LEU	2.1
16	BP	48	GLU	2.1
19	AS	40	ILE	2.1
1	BA	1446	A	2.1
2	AB	34	ALA	2.1
10	AJ	24	GLU	2.1
10	BJ	78	GLU	2.1
31	CA	1372	U	2.1
31	CA	2449	U	2.1
35	DG	173	GLU	2.1
31	CA	764	A	2.1
46	CS	65	ALA	2.1
31	CA	806	C	2.1
31	CA	1150	C	2.1
31	CA	2824	C	2.1
51	CX	27	GLY	2.1
55	DA	143	C	2.1
2	BB	86	SER	2.1
3	BC	153	VAL	2.1
9	BI	47	VAL	2.1
13	BM	91	HIS	2.1
29	CC	220	VAL	2.1
7	AG	38	THR	2.1
33	CE	44	ARG	2.1
34	DF	128	TYR	2.1
1	BA	454	G	2.1
22	C1	31	ASP	2.1
28	CB	6	G	2.1
31	CA	15	G	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
31	CA	2027	G	2.1
31	CA	2428	G	2.1
26	C5	26	ILE	2.1
33	CE	136	GLN	2.1
48	DU	91	GLN	2.1
31	CA	1409	U	2.1
31	CA	1742	U	2.1
43	CP	113	ALA	2.1
1	BA	66	A	2.1
1	BA	253	A	2.1
1	BA	1251	A	2.1
29	CC	256	LYS	2.1
9	BI	102	GLY	2.1
14	AN	68	GLY	2.1
31	CA	278	A	2.1
54	DI	89	PRO	2.1
1	BA	316	C	2.1
19	BS	62	VAL	2.1
20	AT	58	VAL	2.1
31	CA	351	C	2.1
31	CA	2755	C	2.1
31	CA	2888	C	2.1
55	DA	2150	C	2.1
42	CO	4	ARG	2.1
7	BG	67	GLU	2.1
15	AO	25	THR	2.1
33	CE	19	PHE	2.1
10	BJ	64	GLN	2.1
47	CT	31	GLN	2.1
5	AE	141	ILE	2.1
2	AB	11	LYS	2.1
9	BI	78	ALA	2.1
14	BN	44	ALA	2.1
16	BP	7	ALA	2.1
25	C4	16	LYS	2.1
29	CC	61	ALA	2.1
31	CA	25	U	2.1
31	CA	2155	U	2.1
31	CA	2312	U	2.1
33	CE	149	ILE	2.1
36	CH	84	ALA	2.1
28	CB	100	G	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	809	G	2.1
31	CA	1555	G	2.1
31	CA	2351	G	2.1
31	CA	2659	G	2.1
48	CU	64	LYS	2.1
2	BB	65	GLY	2.1
6	AF	64	VAL	2.1
8	BH	39	VAL	2.1
29	CC	216	VAL	2.1
31	CA	2005	A	2.1
34	CF	148	ARG	2.1
48	CU	63	VAL	2.1
1	AA	1096	C	2.1
7	BG	20	SER	2.1
31	CA	366	C	2.1
31	CA	812	C	2.1
31	CA	897	C	2.1
31	CA	1644	C	2.1
31	CA	2214	C	2.1
47	CT	59	GLU	2.1
54	DI	95	LEU	2.1
3	BC	3	GLN	2.1
4	BD	40	GLN	2.1
23	C2	17	THR	2.1
1	AA	218	U	2.1
3	BC	162	ILE	2.1
7	AG	29	ILE	2.1
40	CM	58	TYR	2.1
31	CA	1255	U	2.1
31	CA	2845	U	2.1
42	CO	88	ALA	2.1
54	DI	83	ALA	2.1
13	BM	26	GLY	2.1
19	AS	46	GLY	2.1
1	AA	1186	G	2.1
1	BA	1386	G	2.1
6	BF	91	ARG	2.1
21	AU	34	ARG	2.1
30	CD	165	MET	2.1
31	CA	258	G	2.1
31	CA	396	G	2.1
31	CA	585	G	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	855	G	2.1
31	CA	954	G	2.1
31	CA	1339	G	2.1
31	CA	2304	G	2.1
31	CA	2674	G	2.1
31	CA	2825	G	2.1
41	CN	59	ARG	2.1
55	DA	2136	G	2.1
1	BA	1216	A	2.1
9	AI	103	PHE	2.1
11	BK	82	LEU	2.1
31	CA	1656	C	2.1
31	CA	2013	A	2.1
31	CA	2670	A	2.1
55	DA	1728	C	2.1
11	AK	79	ILE	2.1
15	BO	7	ALA	2.1
22	C1	43	ILE	2.1
30	CD	12	THR	2.1
35	DG	121	ILE	2.1
38	CK	101	ILE	2.1
31	CA	1758	U	2.1
49	DV	2	ALA	2.1
2	BB	17	GLY	2.1
3	AC	179	ARG	2.1
7	AG	81	GLY	2.1
7	BG	138	ARG	2.1
29	CC	209	GLY	2.1
5	BE	74	VAL	2.1
6	BF	64	VAL	2.1
11	BK	94	GLU	2.1
10	BJ	58	ASN	2.1
29	CC	132	MET	2.1
38	CK	61	LYS	2.1
39	CL	20	MET	2.1
1	BA	184	G	2.1
1	BA	260	G	2.1
19	BS	10	PHE	2.1
31	CA	774	G	2.1
31	CA	1300	G	2.1
36	DH	54	LEU	2.0
1	BA	1246	A	2.0

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Mol	Chain	Res	Type	RSRZ
8	AH	107	SER	2.0
23	C2	13	SER	2.0
31	CA	384	A	2.0
31	CA	582	A	2.0
31	CA	632	A	2.0
31	CA	898	C	2.0
31	CA	910	A	2.0
31	CA	2051	A	2.0
31	CA	2433	A	2.0
41	CN	22	GLN	2.0
5	BE	72	ILE	2.0
31	CA	1602	U	2.0
33	CE	87	ALA	2.0
42	CO	34	ILE	2.0
45	CR	62	ILE	2.0
1	AA	961	U	2.0
5	BE	34	THR	2.0
13	BM	20	THR	2.0
36	CH	79	THR	2.0
53	CZ	62	GLY	2.0
3	BC	62	LYS	2.0
45	CR	15	LYS	2.0
2	AB	201	PRO	2.0
5	BE	85	VAL	2.0
14	AN	94	PRO	2.0
36	DH	115	VAL	2.0
11	BK	52	PHE	2.0
35	CG	87	LEU	2.0
1	AA	200	G	2.0
1	AA	838	G	2.0
1	AA	979	C	2.0
1	BA	633	G	2.0
1	BA	1316	G	2.0
28	CB	73	A	2.0
31	CA	560	C	2.0
31	CA	620	G	2.0
31	CA	664	G	2.0
31	CA	795	C	2.0
31	CA	1356	G	2.0
31	CA	804	A	2.0
31	CA	1908	C	2.0
39	CL	14	SER	2.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
46	DS	26	ASP	2.0
30	CD	85	ALA	2.0
31	CA	118	A	2.0
16	AP	76	LYS	2.0
17	BQ	43	LYS	2.0
31	CA	588	U	2.0
31	CA	2249	U	2.0
36	CH	59	ALA	2.0
39	CL	60	ALA	2.0
6	BF	62	MET	2.0
17	AQ	58	VAL	2.0
3	AC	157	LEU	2.0
5	AE	144	LEU	2.0
15	BO	87	LEU	2.0
29	CC	174	LEU	2.0
35	CG	72	LEU	2.0
38	CK	122	LEU	2.0
11	BK	22	HIS	2.0
13	BM	92	ARG	2.0
22	C1	38	HIS	2.0
34	CF	115	ARG	2.0
8	BH	14	ILE	2.0
33	CE	181	ILE	2.0
16	AP	7	ALA	2.0
1	AA	1124	G	2.0
1	AA	1220	G	2.0
1	BA	259	G	2.0
1	BA	970	C	2.0
7	BG	147	ALA	2.0
10	AJ	29	ALA	2.0
30	CD	125	TRP	2.0
31	CA	58	G	2.0
31	CA	82	U	2.0
31	CA	175	G	2.0
31	CA	181	A	2.0
31	CA	287	G	2.0
31	CA	416	U	2.0
31	CA	662	G	2.0
31	CA	669	G	2.0
31	CA	1033	U	2.0
31	CA	1363	C	2.0
31	CA	899	A	2.0

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Mol	Chain	Res	Type	RSRZ
31	CA	926	G	2.0
31	CA	1598	A	2.0
31	CA	1642	G	2.0
31	CA	2048	G	2.0
31	CA	2160	C	2.0
31	CA	2382	G	2.0
31	CA	2695	U	2.0
31	CA	2712	C	2.0
55	DA	2104	C	2.0
31	CA	2682	A	2.0
2	BB	4	VAL	2.0
16	AP	19	VAL	2.0
8	BH	93	PRO	2.0
16	AP	6	LEU	2.0
20	AT	56	PRO	2.0
27	C0	11	ARG	2.0
39	CL	87	LEU	2.0
52	DY	77	LYS	2.0
9	AI	81	HIS	2.0
10	AJ	63	ASP	2.0
2	AB	75	ALA	2.0
3	BC	61	ALA	2.0
15	BO	16	GLY	2.0
37	DJ	64	ASP	2.0
54	DI	82	ILE	2.0
1	BA	70	U	2.0
31	CA	225	C	2.0
31	CA	1164	C	2.0
31	CA	2143	C	2.0
31	CA	2244	U	2.0
31	CA	2306	C	2.0
31	CA	2350	C	2.0
31	CA	2779	U	2.0
1	BA	74	A	2.0
1	BA	846	G	2.0
5	AE	74	VAL	2.0
5	BE	24	THR	2.0
16	AP	50	THR	2.0
31	CA	17	G	2.0
31	CA	497	A	2.0
31	CA	1452	G	2.0
31	CA	2444	G	2.0

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Mol	Chain	Res	Type	RSRZ
31	CA	2850	A	2.0
16	AP	38	PHE	2.0
17	BQ	37	PHE	2.0
29	CC	175	ARG	2.0
39	CL	98	ARG	2.0
44	CQ	46	VAL	2.0
45	CR	58	ARG	2.0
47	CT	106	VAL	2.0
47	DT	110	ARG	2.0
5	AE	81	LEU	2.0
10	AJ	41	PRO	2.0
14	AN	51	LEU	2.0
33	CE	9	GLN	2.0
36	DH	75	LEU	2.0
42	CO	65	LEU	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	5MC	AA	1407	21/22	0.97	0.15	-	60,61,63,64	0
55	2MG	DA	2445	24/25	0.99	0.21	-	25,29,33,34	0
12	D2T	AL	89	10/11	0.91	0.27	-	66,71,78,78	0
1	2MG	BA	1207	24/25	0.80	0.29	-	158,161,165,168	0
1	MA6	BA	1518	24/25	0.92	0.25	-	84,88,95,96	0
31	PSU	CA	2605	20/21	0.92	0.22	-	82,84,86,87	0
32	MEQ	DD	150[A]	10/11	0.96	0.24	-	14,23,32,32	10
31	G7M	CA	2069	24/25	0.87	0.26	-	109,112,115,116	0
1	MA6	BA	1519	24/25	0.93	0.26	-	84,87,91,92	0
55	1MG	DA	745	24/25	0.99	0.20	-	28,31,33,38	0
1	PSU	AA	516	20/21	0.94	0.16	-	88,92,97,97	0
31	2MG	CA	1835	24/25	0.92	0.18	-	74,76,78,78	0
31	PSU	CA	955	20/21	0.86	0.26	-	107,112,115,115	0
1	2MG	AA	1207	24/25	0.91	0.16	-	114,118,121,124	0
55	6MZ	DA	1618	23/24	0.99	0.20	-	25,30,32,35	0
55	2MA	DA	2503	23/24	0.99	0.20	-	33,36,39,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	PSU	DA	746	20/21	0.99	0.19	-	28,32,36,38	0
31	6MZ	CA	2030	23/24	0.85	0.24	-	108,114,116,117	0
55	2MG	DA	1835	24/25	0.96	0.23	-	49,55,56,56	0
1	MA6	AA	1518	24/25	0.97	0.16	-	60,61,62,64	0
1	2MG	BA	966	24/25	0.75	0.36	-	153,160,171,171	0
41	4D4	CN	81	12/13	0.90	0.34	-	112,122,143,143	0
1	UR3	AA	1498	21/22	0.95	0.19	-	64,68,72,73	0
31	3TD	CA	1915	21/22	0.86	0.28	-	150,155,157,157	0
55	5MU	DA	1939	21/22	0.98	0.22	-	35,38,40,43	0
55	PSU	DA	2604	20/21	0.97	0.19	-	37,42,54,55	0
31	6MZ	CA	1618	23/24	0.91	0.30	-	136,143,148,149	0
1	2MG	AA	966	24/25	0.91	0.19	-	95,98,107,108	0
31	2MA	CA	2503	23/24	0.84	0.26	-	110,115,118,118	0
1	2MG	AA	1516	24/25	0.96	0.17	-	58,61,62,63	0
31	5MC	CA	1962	21/22	0.93	0.16	-	72,78,79,82	0
55	5MC	DA	1962	21/22	0.96	0.22	-	43,46,50,52	0
55	PSU	DA	2580	20/21	0.99	0.21	-	25,30,33,35	0
31	2MG	CA	2445	24/25	0.87	0.31	-	105,110,112,113	0
55	OMU	DA	2552	21/22	0.98	0.22	-	33,37,39,43	0
55	6MZ	DA	2030	23/24	0.99	0.22	-	24,28,32,39	0
31	1MG	CA	745	24/25	0.90	0.25	-	106,113,118,121	0
31	PSU	CA	2580	20/21	0.87	0.22	-	102,105,109,109	0
55	PSU	DA	1917	20/21	0.94	0.17	-	74,82,90,90	0
1	5MC	BA	967	21/22	0.67	0.39	-	153,164,167,167	0
55	G7M	DA	2069	24/25	0.99	0.20	-	26,35,36,37	0
55	OMG	DA	2251	24/25	0.98	0.21	-	29,33,35,39	0
31	PSU	CA	1917	20/21	0.81	0.21	-	119,125,134,135	0
1	PSU	BA	516	20/21	0.85	0.16	-	88,99,102,104	0
1	G7M	BA	527	24/25	0.96	0.15	-	75,80,83,84	0
1	4OC	BA	1402	22/23	0.93	0.17	-	78,81,84,85	0
1	MA6	AA	1519	24/25	0.96	0.19	-	61,62,70,71	0
1	2MG	BA	1516	24/25	0.89	0.21	-	82,90,99,100	0
31	PSU	CA	2504	20/21	0.86	0.24	-	98,108,110,111	0
31	OMU	CA	2552	21/22	0.85	0.44	-	91,96,100,101	0
41	4D4	DN	81[A]	12/13	0.96	0.24	-	33,38,53,55	9
31	OMG	CA	2251	24/25	0.89	0.26	-	90,95,100,101	0
41	4D4	DN	81[B]	12/13	0.96	0.24	-	27,32,34,35	9
1	G7M	AA	527	24/25	0.96	0.17	-	63,67,73,74	0
31	PSU	CA	2457	20/21	0.89	0.25	-	106,107,108,109	0
31	PSU	CA	1911	20/21	0.86	0.24	-	123,137,138,139	0
55	PSU	DA	2504	20/21	0.98	0.20	-	33,41,49,52	0
32	MEQ	DD	150[B]	10/11	0.96	0.24	-	27,32,45,50	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	5MC	AA	967	21/22	0.88	0.20	-	90,106,107,108	0
1	4OC	AA	1402	22/23	0.96	0.18	-	61,68,72,73	0
1	UR3	BA	1498	21/22	0.92	0.18	-	89,93,97,98	0
55	PSU	DA	955	20/21	0.99	0.21	-	27,28,32,35	0
31	5MU	CA	1939	21/22	0.93	0.19	-	75,79,81,82	0
55	OMC	DA	2498	21/22	0.99	0.21	-	20,27,31,37	0
12	D2T	BL	89	10/11	0.91	0.28	-	86,88,94,95	0
31	PSU	CA	746	20/21	0.87	0.25	-	120,123,126,127	0
55	H2U	DA	2449	20/21	0.99	0.22	-	27,30,36,39	0
1	5MC	BA	1407	21/22	0.89	0.21	-	100,109,114,117	0
31	OMC	CA	2498	21/22	0.92	0.28	-	97,102,104,106	0
55	PSU	DA	1911	20/21	0.91	0.18	-	78,88,91,91	0
55	3TD	DA	1915	21/22	0.91	0.22	-	103,106,112,113	0
55	5MU	DA	747	21/22	0.99	0.20	-	28,31,37,38	0
55	PSU	DA	2605	20/21	0.98	0.19	-	35,41,43,44	0
31	5MU	CA	747	21/22	0.88	0.28	-	126,128,130,131	0
55	PSU	DA	2457	20/21	0.99	0.18	-	25,29,31,35	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
62	PEG	DA	3217	7/7	0.71	0.55	78.73	89,93,98,99	0
59	PUT	AA	1674	6/6	0.72	0.73	52.39	98,99,100,100	0
64	PGE	DA	3213	10/10	0.85	0.49	47.16	84,86,90,90	0
58	MPD	DA	3203	8/8	0.76	0.74	39.61	96,99,102,104	0
56	MG	DA	3182	1/1	0.58	0.53	36.01	73,73,73,73	0
56	MG	CA	3003	1/1	0.36	2.63	28.81	284,284,284,284	0
56	MG	DA	3128	1/1	0.85	0.47	27.76	78,78,78,78	0
59	PUT	DA	3195	6/6	0.82	0.54	25.50	51,53,62,65	0
58	MPD	AA	1676	8/8	0.90	0.57	24.35	97,100,100,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	PUT	DA	3212	6/6	0.83	0.45	21.94	55,57,64,66	0
56	MG	DA	3123	1/1	0.84	0.51	21.46	77,77,77,77	0
56	MG	CA	3133	1/1	0.45	0.63	21.12	140,140,140,140	0
62	PEG	D3	102	7/7	0.75	1.24	20.87	72,74,83,84	0
62	PEG	DA	3200	7/7	0.80	0.52	20.51	55,58,65,65	0
56	MG	AA	1607	1/1	0.90	0.61	19.15	92,92,92,92	0
56	MG	AA	1612	1/1	0.65	0.72	18.98	81,81,81,81	0
65	SPD	DA	3183	10/10	0.86	0.44	18.88	57,63,66,66	0
59	PUT	DA	3218	6/6	0.77	0.42	17.34	75,77,80,81	0
62	PEG	DQ	201	7/7	0.48	1.03	16.27	107,109,110,110	0
57	PG4	DA	3193	13/13	0.85	0.87	16.18	63,65,76,77	0
67	ACY	DA	3201	4/4	0.84	0.33	15.73	60,64,64,66	0
59	PUT	AA	1673	6/6	0.78	0.49	15.33	125,126,127,128	0
64	PGE	D3	101	10/10	0.76	0.67	15.28	87,88,88,88	0
56	MG	DA	3127	1/1	0.95	0.43	14.38	62,62,62,62	0
65	SPD	DA	3205	10/10	0.70	0.38	13.81	75,81,84,85	0
57	PG4	DA	3215	13/13	0.76	0.43	13.49	95,103,104,104	0
59	PUT	DA	3220	6/6	0.85	0.36	13.47	92,92,94,95	0
66	1PE	DA	3202	16/16	0.84	0.37	13.30	60,63,65,65	0
59	PUT	AA	1672	6/6	0.73	0.65	12.34	110,112,114,114	0
56	MG	CA	3026	1/1	0.79	1.01	11.89	197,197,197,197	0
56	MG	DA	3163	1/1	0.51	0.36	11.79	84,84,84,84	0
63	EDO	DA	3001	4/4	0.88	0.36	11.67	72,73,75,77	0
58	MPD	DA	3192	8/8	0.89	0.59	11.40	79,79,82,83	0
56	MG	CA	3131	1/1	0.59	0.58	11.30	111,111,111,111	0
58	MPD	DE	302	8/8	0.76	0.57	11.02	96,97,98,98	0
64	PGE	D1	102	10/10	0.71	0.59	10.77	95,96,100,100	0
59	PUT	DA	3189	6/6	0.81	0.38	10.61	47,48,49,49	0
56	MG	DA	3125	1/1	0.71	0.42	9.99	83,83,83,83	0
56	MG	AA	1642	1/1	0.27	0.51	9.70	165,165,165,165	0
66	1PE	DA	3185	16/16	0.89	0.31	9.63	44,53,71,72	0
62	PEG	D1	103	7/7	0.77	0.47	9.59	56,60,61,62	0
59	PUT	DA	3221	6/6	0.89	0.33	9.30	44,48,50,50	0
58	MPD	DA	3206	8/8	0.79	0.51	9.13	89,93,94,94	0
59	PUT	DA	3204	6/6	0.82	0.43	8.85	66,66,70,71	0
56	MG	DA	3172	1/1	0.84	0.38	8.75	89,89,89,89	0
56	MG	CA	3147	1/1	0.80	0.40	8.49	91,91,91,91	1
56	MG	CA	3110	1/1	0.35	0.83	8.38	188,188,188,188	0
56	MG	DA	3133	1/1	0.83	0.41	8.26	78,78,78,78	0
64	PGE	DD	301	10/10	0.87	0.37	7.76	63,67,72,73	0
63	EDO	DA	3198	4/4	0.92	0.35	7.61	56,57,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3137	1/1	0.72	0.59	7.28	168,168,168,168	0
59	PUT	DA	3211	6/6	0.79	0.34	6.66	65,66,72,74	0
65	SPD	DA	3223	10/10	0.91	0.26	6.58	40,44,54,55	0
57	PG4	BA	1642	13/13	0.81	0.42	6.41	96,102,107,107	0
64	PGE	DU	101	10/10	0.87	0.50	6.21	64,72,83,83	0
62	PEG	AL	201	7/7	0.85	0.39	5.89	74,78,85,85	0
68	GUN	DA	3210	11/11	0.77	0.38	5.83	71,73,74,74	0
56	MG	DA	3148	1/1	0.86	0.24	5.73	115,115,115,115	0
56	MG	AA	1633	1/1	0.94	0.29	5.62	101,101,101,101	0
63	EDO	D1	101	4/4	0.84	0.34	5.61	67,67,68,68	0
64	PGE	DA	3224	10/10	0.78	0.33	5.38	74,81,83,83	0
57	PG4	AA	1670	13/13	0.78	0.30	5.31	80,92,101,102	0
58	MPD	DE	301	8/8	0.80	0.61	4.93	102,104,107,109	0
63	EDO	DA	3197	4/4	0.92	0.25	4.86	68,68,69,69	0
57	PG4	DS	202	13/13	0.87	0.34	4.45	43,51,59,61	0
56	MG	CA	3151	1/1	0.77	0.36	3.80	84,84,84,84	0
56	MG	BA	1612	1/1	0.83	0.26	3.68	137,137,137,137	0
62	PEG	DL	201	7/7	0.88	0.28	3.45	65,69,76,78	0
58	MPD	AA	1671	8/8	0.92	0.53	3.36	101,103,104,106	0
56	MG	DA	3038	1/1	0.93	0.22	3.07	29,29,29,29	0
56	MG	BA	1626	1/1	0.71	0.32	3.01	111,111,111,111	0
56	MG	CA	3100	1/1	0.91	0.31	2.94	110,110,110,110	0
56	MG	CA	3022	1/1	0.83	0.72	2.94	188,188,188,188	0
56	MG	AA	1661	1/1	0.63	0.33	2.12	190,190,190,190	0
65	SPD	DA	3187	10/10	0.94	0.24	2.09	38,40,48,50	0
56	MG	AA	1657	1/1	0.85	0.49	2.03	162,162,162,162	0
64	PGE	DS	201	10/10	0.84	0.37	1.93	56,66,68,69	0
56	MG	CA	3037	1/1	0.96	0.42	1.92	235,235,235,235	0
64	PGE	DA	3186	10/10	0.92	0.21	1.86	39,46,49,50	0
57	PG4	DQ	202	13/13	0.83	0.30	1.74	64,66,71,72	0
56	MG	CA	3032	1/1	0.73	0.54	1.73	269,269,269,269	0
56	MG	DA	3023	1/1	0.98	0.21	1.45	34,34,34,34	0
60	T1C	AA	1677	42/42	0.92	0.25	1.35	89,96,109,110	0
56	MG	DA	3032	1/1	0.98	0.23	1.08	42,42,42,42	0
56	MG	CA	3136	1/1	0.91	0.34	0.96	105,105,105,105	0
56	MG	DA	3018	1/1	0.97	0.25	0.93	29,29,29,29	0
56	MG	CA	3105	1/1	0.69	0.40	0.84	254,254,254,254	0
56	MG	AA	1611	1/1	0.72	0.26	0.83	113,113,113,113	0
59	PUT	DA	3002	6/6	0.92	0.23	0.72	45,52,54,55	0
56	MG	DA	3014	1/1	0.99	0.24	0.41	19,19,19,19	0
56	MG	DA	3091	1/1	0.95	0.23	0.24	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	1614	1/1	0.75	0.17	0.20	147,147,147,147	0
56	MG	DA	3025	1/1	0.99	0.23	0.16	25,25,25,25	0
61	ZN	AB	301	1/1	0.92	0.30	-0.10	209,209,209,209	0
56	MG	CA	3033	1/1	-0.13	0.30	-0.14	200,200,200,200	0
60	T1C	BA	1643	42/42	0.78	0.23	-0.22	169,175,185,185	0
56	MG	DA	3094	1/1	0.93	0.21	-0.26	35,35,35,35	0
56	MG	CA	3054	1/1	0.59	0.21	-0.46	140,140,140,140	0
56	MG	CA	3102	1/1	0.93	0.27	-0.48	114,114,114,114	0
56	MG	BA	1601	1/1	0.85	0.17	-0.52	95,95,95,95	0
56	MG	AA	1662	1/1	0.98	0.22	-0.70	110,110,110,110	0
56	MG	CA	3061	1/1	0.21	0.21	-0.88	274,274,274,274	0
56	MG	CA	3153	1/1	0.89	0.22	-0.91	90,90,90,90	0
56	MG	BA	1624	1/1	0.67	0.26	-0.97	275,275,275,275	0
56	MG	DA	3067	1/1	0.98	0.19	-0.97	55,55,55,55	0
56	MG	CA	3089	1/1	0.91	0.22	-1.02	95,95,95,95	0
56	MG	CA	3011	1/1	0.92	0.28	-1.02	117,117,117,117	0
56	MG	AA	1679	1/1	0.74	0.24	-1.04	189,189,189,189	0
58	MPD	DS	203	8/8	0.98	0.21	-1.14	37,40,44,47	0
56	MG	DA	3024	1/1	0.99	0.20	-1.26	32,32,32,32	0
56	MG	BA	1620	1/1	0.97	0.17	-1.28	97,97,97,97	0
61	ZN	D5	101	1/1	0.95	0.15	-1.31	60,60,60,60	0
56	MG	CA	3095	1/1	0.91	0.18	-1.33	81,81,81,81	0
56	MG	DA	3011	1/1	1.00	0.17	-1.39	28,28,28,28	0
56	MG	CA	3018	1/1	0.65	0.16	-1.43	133,133,133,133	0
56	MG	CA	3099	1/1	0.72	0.28	-1.50	235,235,235,235	0
61	ZN	C5	101	1/1	0.82	0.06	-1.57	148,148,148,148	0
56	MG	CA	3103	1/1	0.92	0.15	-1.65	120,120,120,120	0
56	MG	CA	3094	1/1	0.86	0.26	-1.84	159,159,159,159	0
56	MG	DA	3177	1/1	0.95	0.18	-1.91	68,68,68,68	0
56	MG	DA	3113	1/1	1.00	0.22	-1.92	18,18,18,18	0
56	MG	AA	1647	1/1	0.90	0.13	-1.94	202,202,202,202	0
56	MG	CA	3019	1/1	0.89	0.10	-1.97	79,79,79,79	0
56	MG	CA	3063	1/1	0.78	0.24	-2.01	207,207,207,207	0
56	MG	CA	3052	1/1	0.88	0.13	-2.27	97,97,97,97	0
56	MG	CA	3031	1/1	0.67	0.23	-2.28	127,127,127,127	0
56	MG	BA	1622	1/1	0.83	0.12	-2.40	95,95,95,95	0
56	MG	CA	3009	1/1	0.81	0.16	-2.42	248,248,248,248	0
56	MG	CB	201	1/1	0.78	0.10	-2.46	166,166,166,166	0
56	MG	DA	3010	1/1	0.98	0.14	-2.49	34,34,34,34	0
56	MG	CA	3079	1/1	0.65	0.16	-2.52	143,143,143,143	0
56	MG	AA	1663	1/1	0.77	0.19	-2.59	110,110,110,110	0
56	MG	DA	3095	1/1	0.88	0.17	-2.60	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1644	1/1	0.82	0.14	-2.68	94,94,94,94	0
56	MG	DA	3047	1/1	0.99	0.19	-2.71	27,27,27,27	0
56	MG	BA	1617	1/1	0.90	0.14	-2.77	126,126,126,126	0
56	MG	BA	1613	1/1	0.95	0.17	-2.86	78,78,78,78	0
56	MG	DB	201	1/1	0.94	0.14	-2.90	64,64,64,64	0
56	MG	DA	3065	1/1	0.85	0.17	-2.94	71,71,71,71	0
56	MG	AA	1637	1/1	0.97	0.08	-3.08	57,57,57,57	0
56	MG	CA	3006	1/1	0.78	0.19	-3.14	227,227,227,227	0
56	MG	BA	1610	1/1	0.84	0.08	-3.22	109,109,109,109	0
56	MG	AA	1656	1/1	0.90	0.16	-3.22	149,149,149,149	0
56	MG	CA	3051	1/1	0.85	0.13	-3.26	109,109,109,109	0
56	MG	CA	3101	1/1	0.90	0.11	-3.31	149,149,149,149	0
56	MG	CA	3024	1/1	0.97	0.17	-3.39	141,141,141,141	0
56	MG	DA	3027	1/1	0.97	0.15	-3.41	71,71,71,71	0
56	MG	DA	3007	1/1	0.85	0.12	-3.42	112,112,112,112	0
56	MG	CA	3144	1/1	0.90	0.13	-3.54	83,83,83,83	0
56	MG	AA	1629	1/1	0.96	0.14	-3.57	83,83,83,83	0
56	MG	BA	1632	1/1	0.91	0.12	-3.61	72,72,72,72	0
56	MG	CA	3044	1/1	0.81	0.18	-3.71	84,84,84,84	0
56	MG	CA	3088	1/1	0.87	0.10	-3.71	88,88,88,88	0
56	MG	AA	1659	1/1	0.83	0.09	-3.72	97,97,97,97	0
56	MG	BA	1615	1/1	0.94	0.08	-3.72	76,76,76,76	0
56	MG	CA	3020	1/1	0.87	0.11	-3.73	103,103,103,103	0
56	MG	DA	3085	1/1	0.98	0.14	-3.74	41,41,41,41	0
56	MG	BA	1608	1/1	0.73	0.13	-3.89	122,122,122,122	0
56	MG	DA	3098	1/1	0.96	0.09	-4.05	29,29,29,29	0
56	MG	DA	3059	1/1	1.00	0.15	-4.08	37,37,37,37	0
56	MG	DD	302	1/1	0.97	0.13	-4.20	48,48,48,48	0
56	MG	CA	3040	1/1	0.85	0.09	-4.43	126,126,126,126	0
56	MG	CA	3086	1/1	0.86	0.16	-4.47	97,97,97,97	0
56	MG	DA	3111	1/1	0.98	0.15	-4.57	32,32,32,32	0
56	MG	DA	3015	1/1	0.98	0.18	-4.67	18,18,18,18	0
56	MG	DA	3136	1/1	0.76	0.12	-4.87	92,92,92,92	0
56	MG	DA	3030	1/1	0.99	0.14	-4.89	25,25,25,25	0
56	MG	DA	3104	1/1	0.99	0.08	-4.96	42,42,42,42	0
56	MG	AA	1668	1/1	0.99	0.11	-4.96	54,54,54,54	0
56	MG	AA	1631	1/1	0.98	0.06	-5.07	56,56,56,56	0
56	MG	DA	3048	1/1	0.99	0.13	-5.30	42,42,42,42	0
56	MG	DA	3096	1/1	0.99	0.11	-5.37	61,61,61,61	0
56	MG	CA	3013	1/1	0.70	0.18	-5.54	135,135,135,135	0
56	MG	BA	1605	1/1	0.97	0.09	-5.59	125,125,125,125	0
56	MG	DA	3019	1/1	0.99	0.10	-5.69	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3060	1/1	0.99	0.10	-5.78	16,16,16,16	0
56	MG	DA	3005	1/1	0.94	0.10	-5.85	81,81,81,81	0
56	MG	BA	1602	1/1	0.88	0.07	-6.10	100,100,100,100	0
56	MG	DA	3151	1/1	0.84	0.10	-6.24	58,58,58,58	0
56	MG	DA	3044	1/1	0.92	0.15	-6.35	36,36,36,36	0
56	MG	DA	3072	1/1	0.99	0.09	-6.62	47,47,47,47	0
56	MG	DA	3227	1/1	0.96	0.14	-6.70	45,45,45,45	0
56	MG	AA	1639	1/1	0.85	0.09	-6.72	132,132,132,132	0
56	MG	AA	1643	1/1	0.95	0.14	-7.21	78,78,78,78	0
56	MG	DA	3051	1/1	1.00	0.14	-7.37	17,17,17,17	0
56	MG	DA	3036	1/1	0.98	0.16	-7.60	34,34,34,34	0
56	MG	DA	3064	1/1	0.99	0.08	-7.86	59,59,59,59	0
56	MG	AA	1648	1/1	0.99	0.09	-7.91	76,76,76,76	0
56	MG	DA	3028	1/1	0.97	0.14	-7.93	38,38,38,38	0
56	MG	DA	3093	1/1	0.98	0.14	-8.45	36,36,36,36	0
56	MG	DA	3100	1/1	0.97	0.14	-9.22	30,30,30,30	0
56	MG	DA	3102	1/1	0.97	0.14	-9.64	56,56,56,56	0
56	MG	DA	3008	1/1	0.96	0.05	-11.37	82,82,82,82	0
56	MG	AA	1653	1/1	0.95	0.04	-12.90	75,75,75,75	0
56	MG	DA	3103	1/1	0.91	0.12	-14.07	44,44,44,44	0
56	MG	AA	1646	1/1	0.98	0.08	-18.09	65,65,65,65	0
56	MG	DA	3110	1/1	0.99	0.18	-18.97	19,19,19,19	0
56	MG	CA	3129	1/1	0.69	0.23	-	141,141,141,141	0
56	MG	DA	3147	1/1	0.61	0.42	-	89,89,89,89	0
56	MG	DA	3022	1/1	0.96	0.15	-	43,43,43,43	0
56	MG	DA	3171	1/1	0.79	0.57	-	82,82,82,82	0
56	MG	AA	1652	1/1	0.97	0.28	-	57,57,57,57	0
56	MG	DA	3145	1/1	0.40	0.75	-	101,101,101,101	0
56	MG	CA	3075	1/1	0.56	1.37	-	253,253,253,253	0
56	MG	DA	3118	1/1	0.93	0.34	-	76,76,76,76	0
56	MG	AA	1620	1/1	0.76	0.45	-	83,83,83,83	0
56	MG	AA	1613	1/1	0.71	1.49	-	85,85,85,85	0
63	EDO	DA	3207	4/4	0.88	0.26	-	58,60,62,63	0
58	MPD	DT	202	8/8	0.73	0.41	-	87,88,89,91	0
56	MG	CA	3039	1/1	0.53	0.35	-	153,153,153,153	0
56	MG	AA	1624	1/1	0.63	0.80	-	93,93,93,93	0
56	MG	CA	3036	1/1	0.88	0.33	-	203,203,203,203	0
56	MG	CA	3078	1/1	0.66	0.19	-	195,195,195,195	0
56	MG	DA	3078	1/1	0.97	0.09	-	38,38,38,38	0
56	MG	AA	1627	1/1	0.62	0.55	-	99,99,99,99	0
56	MG	AA	1669	1/1	0.93	0.41	-	118,118,118,118	0
58	MPD	DT	201	8/8	0.72	0.41	-	73,82,84,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3057	1/1	0.98	0.23	-	57,57,57,57	0
56	MG	BA	1604	1/1	0.70	0.19	-	182,182,182,182	0
56	MG	DA	3161	1/1	0.74	0.43	-	78,78,78,78	0
56	MG	DA	3043	1/1	0.96	0.08	-	31,31,31,31	0
56	MG	DA	3099	1/1	0.96	0.13	-	78,78,78,78	0
56	MG	DA	3026	1/1	0.98	0.10	-	40,40,40,40	0
56	MG	BA	1606	1/1	0.72	0.21	-	251,251,251,251	0
56	MG	CA	3087	1/1	0.93	0.07	-	97,97,97,97	0
56	MG	DR	203	1/1	0.92	0.42	-	111,111,111,111	0
56	MG	DA	3135	1/1	0.95	0.27	-	72,72,72,72	0
56	MG	CA	3055	1/1	0.72	0.10	-	195,195,195,195	0
56	MG	CA	3139	1/1	0.19	1.21	-	139,139,139,139	0
56	MG	AA	1616	1/1	0.52	0.92	-	88,88,88,88	0
56	MG	DM	201	1/1	0.96	0.06	-	62,62,62,62	0
56	MG	DA	3040	1/1	0.98	0.14	-	26,26,26,26	0
56	MG	CA	3126	1/1	0.61	0.38	-	136,136,136,136	0
56	MG	DA	3142	1/1	0.90	0.27	-	79,79,79,79	0
56	MG	CA	3021	1/1	0.87	1.09	-	278,278,278,278	0
56	MG	DA	3071	1/1	0.98	0.06	-	91,91,91,91	0
56	MG	DA	3157	1/1	0.69	0.52	-	73,73,73,73	0
56	MG	DA	3120	1/1	0.90	0.36	-	55,55,55,55	0
56	MG	AA	1625	1/1	0.82	0.30	-	78,78,78,78	0
56	MG	CA	3007	1/1	0.66	0.46	-	257,257,257,257	0
56	MG	CA	3074	1/1	0.93	0.27	-	206,206,206,206	0
56	MG	AA	1610	1/1	0.89	0.40	-	99,99,99,99	0
56	MG	CA	3010	1/1	0.77	0.52	-	231,231,231,231	0
56	MG	DA	3088	1/1	0.96	0.17	-	45,45,45,45	0
56	MG	CA	3005	1/1	0.44	1.14	-	253,253,253,253	0
56	MG	CA	3071	1/1	0.62	0.20	-	207,207,207,207	0
56	MG	CA	3085	1/1	0.95	0.11	-	89,89,89,89	0
56	MG	CA	3117	1/1	0.90	0.77	-	109,109,109,109	0
56	MG	DA	3124	1/1	0.84	0.39	-	114,114,114,114	0
56	MG	DA	3069	1/1	0.95	0.17	-	44,44,44,44	0
56	MG	AA	1630	1/1	0.91	0.15	-	134,134,134,134	0
56	MG	CA	3145	1/1	0.79	0.38	-	75,75,75,75	0
56	MG	BA	1619	1/1	0.95	0.19	-	107,107,107,107	0
56	MG	CA	3135	1/1	0.65	0.54	-	104,104,104,104	0
56	MG	CA	3069	1/1	0.80	0.21	-	115,115,115,115	0
56	MG	CA	3143	1/1	0.87	0.50	-	107,107,107,107	0
56	MG	AA	1649	1/1	0.88	0.12	-	77,77,77,77	0
56	MG	CA	3106	1/1	0.73	0.59	-	103,103,103,103	0
63	EDO	DA	3208	4/4	0.75	0.48	-	98,99,100,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	CA	3148	1/1	0.77	0.79	-	86,86,86,86	1
56	MG	DA	3041	1/1	0.98	0.09	-	58,58,58,58	0
56	MG	DA	3080	1/1	0.94	0.10	-	109,109,109,109	0
56	MG	DA	3165	1/1	0.86	0.45	-	69,69,69,69	0
58	MPD	DA	3190	8/8	0.85	0.34	-	91,92,93,94	0
56	MG	DA	3159	1/1	0.75	0.44	-	80,80,80,80	0
56	MG	BA	1645	1/1	0.92	0.05	-	98,98,98,98	0
56	MG	CA	3059	1/1	0.84	0.36	-	147,147,147,147	0
56	MG	DA	3152	1/1	0.94	0.23	-	47,47,47,47	0
56	MG	CA	3128	1/1	0.79	0.42	-	87,87,87,87	0
56	MG	DA	3101	1/1	0.98	0.22	-	30,30,30,30	0
56	MG	AA	1654	1/1	0.83	0.47	-	252,252,252,252	0
56	MG	CA	3073	1/1	0.95	0.28	-	260,260,260,260	0
56	MG	DA	3049	1/1	0.96	0.17	-	33,33,33,33	0
56	MG	AA	1608	1/1	0.66	0.49	-	119,119,119,119	0
56	MG	DA	3029	1/1	0.96	0.14	-	61,61,61,61	0
63	EDO	DB	210	4/4	0.78	0.43	-	85,85,85,86	0
59	PUT	DA	3222	6/6	0.94	0.24	-	50,54,55,55	0
56	MG	AA	1665	1/1	0.85	0.43	-	168,168,168,168	0
56	MG	DA	3162	1/1	0.89	0.25	-	64,64,64,64	0
56	MG	CA	3034	1/1	0.62	0.17	-	256,256,256,256	0
56	MG	AA	1678	1/1	0.95	0.16	-	74,74,74,74	0
56	MG	DA	3106	1/1	0.98	0.20	-	31,31,31,31	0
56	MG	CA	3053	1/1	0.86	0.22	-	108,108,108,108	0
56	MG	AA	1609	1/1	0.86	0.38	-	107,107,107,107	0
56	MG	CA	3121	1/1	0.73	0.50	-	101,101,101,101	0
56	MG	AA	1635	1/1	0.91	0.10	-	100,100,100,100	0
56	MG	CA	3111	1/1	0.75	0.99	-	159,159,159,159	0
62	PEG	DA	3199	7/7	0.87	0.44	-	60,64,69,70	0
56	MG	AA	1604	1/1	0.27	0.84	-	82,82,82,82	0
56	MG	BA	1637	1/1	0.65	0.59	-	93,93,93,93	0
56	MG	AA	1650	1/1	0.95	0.09	-	87,87,87,87	0
56	MG	CB	202	1/1	0.85	0.12	-	139,139,139,139	0
56	MG	CA	3154	1/1	0.57	0.44	-	155,155,155,155	0
56	MG	DA	3070	1/1	0.95	0.15	-	61,61,61,61	0
56	MG	DD	303	1/1	0.85	0.35	-	66,66,66,66	0
56	MG	CA	3120	1/1	0.78	0.25	-	195,195,195,195	0
56	MG	CA	3096	1/1	0.86	0.13	-	116,116,116,116	0
56	MG	CA	3118	1/1	0.92	0.44	-	90,90,90,90	0
56	MG	DA	3006	1/1	0.96	0.10	-	68,68,68,68	0
56	MG	AA	1628	1/1	0.30	0.97	-	142,142,142,142	0
56	MG	DA	3166	1/1	0.90	0.86	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3082	1/1	0.95	0.08	-	55,55,55,55	0
56	MG	DA	3173	1/1	0.79	0.56	-	81,81,81,81	0
56	MG	CA	3004	1/1	0.87	0.23	-	223,223,223,223	0
56	MG	DA	3138	1/1	0.34	0.38	-	89,89,89,89	0
56	MG	DA	3116	1/1	0.98	0.13	-	28,28,28,28	0
56	MG	DA	3084	1/1	0.94	0.08	-	57,57,57,57	0
56	MG	CA	3119	1/1	0.82	0.72	-	134,134,134,134	0
56	MG	DA	3146	1/1	0.95	0.15	-	72,72,72,72	0
56	MG	CA	3049	1/1	0.74	0.24	-	100,100,100,100	0
56	MG	DA	3132	1/1	0.94	0.52	-	77,77,77,77	0
56	MG	CA	3012	1/1	0.87	0.27	-	130,130,130,130	0
56	MG	AA	1660	1/1	0.88	0.29	-	286,286,286,286	0
56	MG	CA	3138	1/1	0.94	0.15	-	103,103,103,103	0
56	MG	CA	3065	1/1	0.80	0.24	-	122,122,122,122	0
56	MG	DA	3230	1/1	0.97	0.35	-	45,45,45,45	0
56	MG	DA	3130	1/1	0.54	0.35	-	87,87,87,87	0
62	PEG	DP	201	7/7	0.78	0.53	-	94,94,99,100	0
63	EDO	DA	3214	4/4	0.85	0.31	-	77,78,79,79	0
59	PUT	AA	1675	6/6	0.64	0.62	-	90,92,93,93	0
56	MG	AA	1621	1/1	0.66	0.44	-	83,83,83,83	0
56	MG	CA	3109	1/1	0.77	0.58	-	93,93,93,93	0
56	MG	AA	1618	1/1	0.74	0.82	-	91,91,91,91	0
56	MG	DA	3140	1/1	0.95	0.19	-	57,57,57,57	0
56	MG	BA	1639	1/1	0.62	0.63	-	106,106,106,106	0
56	MG	DA	3083	1/1	0.97	0.08	-	69,69,69,69	0
56	MG	CA	3050	1/1	0.86	0.13	-	91,91,91,91	0
56	MG	CA	3123	1/1	-0.03	0.99	-	188,188,188,188	0
56	MG	DA	3121	1/1	0.94	0.37	-	91,91,91,91	0
56	MG	DA	3079	1/1	0.97	0.07	-	63,63,63,63	0
56	MG	BA	1640	1/1	0.91	0.81	-	156,156,156,156	0
56	MG	AA	1606	1/1	0.47	0.48	-	120,120,120,120	0
56	MG	DA	3045	1/1	0.89	0.09	-	85,85,85,85	0
56	MG	BA	1609	1/1	0.91	0.16	-	194,194,194,194	0
58	MPD	DN	201	8/8	0.83	0.41	-	87,89,92,93	0
56	MG	AA	1623	1/1	0.88	0.36	-	85,85,85,85	0
56	MG	AA	1640	1/1	0.84	0.13	-	62,62,62,62	0
56	MG	CA	3081	1/1	0.93	0.17	-	134,134,134,134	0
56	MG	CA	3107	1/1	0.80	0.71	-	106,106,106,106	0
56	MG	CA	3015	1/1	0.93	0.26	-	83,83,83,83	0
56	MG	DA	3081	1/1	0.95	0.17	-	94,94,94,94	0
56	MG	DA	3168	1/1	0.27	0.49	-	108,108,108,108	0
56	MG	DA	3228	1/1	0.98	0.09	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3143	1/1	0.80	0.45	-	95,95,95,95	0
56	MG	CA	3038	1/1	-0.03	0.22	-	268,268,268,268	0
56	MG	CA	3060	1/1	0.75	0.38	-	242,242,242,242	0
56	MG	DA	3075	1/1	0.97	0.07	-	49,49,49,49	0
56	MG	DA	3141	1/1	0.98	0.22	-	66,66,66,66	0
56	MG	DA	3126	1/1	0.78	0.36	-	76,76,76,76	0
56	MG	AA	1651	1/1	0.92	0.13	-	70,70,70,70	0
56	MG	CA	3014	1/1	0.72	0.18	-	262,262,262,262	0
56	MG	DA	3108	1/1	0.95	0.18	-	36,36,36,36	0
56	MG	DA	3178	1/1	0.55	0.67	-	101,101,101,101	0
64	PGE	DA	3216	10/10	0.87	0.39	-	62,64,65,65	0
56	MG	DA	3061	1/1	0.99	0.15	-	19,19,19,19	0
56	MG	CA	3001	1/1	0.77	0.38	-	299,299,299,299	0
56	MG	CA	3017	1/1	0.87	0.10	-	106,106,106,106	0
56	MG	CA	3083	1/1	0.81	0.34	-	241,241,241,241	0
56	MG	AA	1636	1/1	0.91	0.28	-	97,97,97,97	0
56	MG	CA	3149	1/1	0.10	1.20	-	92,92,92,92	0
56	MG	DA	3087	1/1	0.99	0.16	-	48,48,48,48	0
56	MG	DA	3097	1/1	0.95	0.14	-	45,45,45,45	0
56	MG	DR	201	1/1	0.92	0.59	-	44,44,44,44	0
56	MG	DA	3020	1/1	0.96	0.32	-	33,33,33,33	0
56	MG	CA	3070	1/1	0.93	0.08	-	112,112,112,112	0
56	MG	CA	3084	1/1	0.91	0.34	-	208,208,208,208	0
56	MG	CA	3098	1/1	0.85	0.13	-	110,110,110,110	0
56	MG	DA	3034	1/1	0.98	0.17	-	28,28,28,28	0
56	MG	CA	3091	1/1	0.94	0.10	-	96,96,96,96	0
56	MG	BA	1623	1/1	0.67	1.44	-	235,235,235,235	0
56	MG	DA	3164	1/1	0.94	0.31	-	72,72,72,72	0
56	MG	CA	3155	1/1	0.82	0.31	-	204,204,204,204	0
56	MG	CA	3048	1/1	0.83	0.17	-	107,107,107,107	0
56	MG	AA	1645	1/1	0.98	0.12	-	61,61,61,61	0
56	MG	DB	202	1/1	0.97	0.13	-	29,29,29,29	0
56	MG	CA	3132	1/1	0.62	0.75	-	152,152,152,152	0
56	MG	DA	3174	1/1	0.86	0.30	-	78,78,78,78	0
56	MG	DA	3180	1/1	0.15	1.25	-	97,97,97,97	0
56	MG	AA	1622	1/1	-0.16	1.83	-	130,130,130,130	0
56	MG	DA	3139	1/1	0.95	0.39	-	64,64,64,64	1
56	MG	DA	3056	1/1	0.99	0.17	-	22,22,22,22	0
56	MG	AA	1601	1/1	0.87	1.42	-	104,104,104,104	0
56	MG	CA	3097	1/1	0.55	0.16	-	125,125,125,125	0
56	MG	DA	3129	1/1	0.88	1.12	-	60,60,60,60	0
56	MG	DA	3077	1/1	0.97	0.18	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DB	207	1/1	0.48	0.78	-	105,105,105,105	0
56	MG	DA	3131	1/1	0.33	0.76	-	87,87,87,87	0
59	PUT	DA	3188	6/6	0.94	0.22	-	32,35,40,41	0
56	MG	CA	3064	1/1	0.87	0.57	-	267,267,267,267	0
56	MG	DA	3016	1/1	0.93	0.11	-	44,44,44,44	0
56	MG	CA	3029	1/1	0.90	0.36	-	177,177,177,177	0
56	MG	CA	3067	1/1	0.82	0.45	-	289,289,289,289	0
63	EDO	DA	3003	4/4	0.88	0.53	-	64,64,66,67	0
56	MG	DA	3137	1/1	0.96	0.25	-	47,47,47,47	0
56	MG	BA	1635	1/1	0.92	0.10	-	111,111,111,111	0
56	MG	CA	3104	1/1	0.13	0.32	-	263,263,263,263	0
56	MG	BA	1636	1/1	0.89	0.64	-	172,172,172,172	0
56	MG	CA	3023	1/1	0.82	0.14	-	150,150,150,150	0
56	MG	AA	1638	1/1	0.97	0.09	-	103,103,103,103	0
56	MG	CA	3035	1/1	0.89	0.27	-	158,158,158,158	0
56	MG	DA	3117	1/1	0.96	0.11	-	41,41,41,41	0
56	MG	CA	3008	1/1	0.82	0.10	-	179,179,179,179	0
56	MG	CA	3076	1/1	0.69	0.22	-	213,213,213,213	0
56	MG	CA	3141	1/1	0.20	0.60	-	109,109,109,109	0
59	PUT	DA	3184	6/6	0.85	0.37	-	42,48,50,51	0
56	MG	CA	3130	1/1	0.18	1.10	-	141,141,141,141	0
56	MG	AA	1615	1/1	0.67	0.55	-	90,90,90,90	0
56	MG	DA	3050	1/1	0.96	0.12	-	43,43,43,43	0
56	MG	BA	1638	1/1	0.59	0.93	-	110,110,110,110	0
56	MG	CA	3142	1/1	0.04	0.56	-	133,133,133,133	0
56	MG	DA	3089	1/1	0.98	0.08	-	36,36,36,36	0
56	MG	CA	3152	1/1	0.88	0.45	-	215,215,215,215	0
56	MG	CA	3057	1/1	0.81	0.16	-	132,132,132,132	0
56	MG	DA	3176	1/1	0.83	0.32	-	93,93,93,93	0
63	EDO	DA	3194	4/4	0.84	0.30	-	51,56,59,60	0
56	MG	CA	3066	1/1	0.82	0.14	-	125,125,125,125	0
56	MG	CA	3116	1/1	0.90	0.80	-	89,89,89,89	0
56	MG	DA	3033	1/1	0.99	0.19	-	26,26,26,26	0
56	MG	DA	3021	1/1	0.94	0.07	-	48,48,48,48	0
56	MG	DA	3066	1/1	0.98	0.19	-	29,29,29,29	0
56	MG	BA	1616	1/1	0.97	0.17	-	149,149,149,149	0
56	MG	DA	3122	1/1	0.92	0.32	-	80,80,80,80	0
56	MG	BA	1607	1/1	0.86	0.38	-	162,162,162,162	0
56	MG	AA	1664	1/1	0.87	0.36	-	186,186,186,186	0
63	EDO	DA	3004	4/4	0.76	0.45	-	107,107,108,109	0
56	MG	DA	3107	1/1	0.98	0.17	-	47,47,47,47	0
56	MG	DA	3154	1/1	0.87	0.46	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DB	209	1/1	0.96	0.50	-	80,80,80,80	0
56	MG	CA	3043	1/1	0.92	0.14	-	101,101,101,101	0
56	MG	DA	3119	1/1	0.94	0.11	-	63,63,63,63	0
56	MG	AA	1603	1/1	0.21	1.09	-	119,119,119,119	0
56	MG	DA	3068	1/1	0.98	0.11	-	62,62,62,62	0
56	MG	DA	3052	1/1	0.99	0.14	-	36,36,36,36	0
56	MG	CA	3125	1/1	0.85	0.27	-	141,141,141,141	0
56	MG	DA	3170	1/1	0.76	0.40	-	73,73,73,73	0
56	MG	AA	1619	1/1	0.90	0.27	-	92,92,92,92	0
56	MG	CA	3068	1/1	0.53	0.43	-	253,253,253,253	0
56	MG	BA	1633	1/1	0.90	0.28	-	235,235,235,235	0
56	MG	BA	1630	1/1	0.29	0.14	-	221,221,221,221	0
56	MG	BA	1634	1/1	0.90	0.07	-	116,116,116,116	0
56	MG	CA	3058	1/1	0.85	0.40	-	135,135,135,135	0
56	MG	DA	3013	1/1	0.96	0.13	-	71,71,71,71	0
56	MG	DA	3105	1/1	0.96	0.19	-	39,39,39,39	0
56	MG	DA	3156	1/1	0.89	0.34	-	74,74,74,74	0
67	ACY	DA	3191	4/4	0.95	0.27	-	56,57,58,59	0
56	MG	CA	3127	1/1	0.90	0.11	-	85,85,85,85	0
56	MG	DA	3179	1/1	0.35	0.48	-	102,102,102,102	0
56	MG	DB	203	1/1	0.97	0.05	-	39,39,39,39	0
56	MG	DB	204	1/1	0.99	0.15	-	56,56,56,56	0
56	MG	DA	3062	1/1	0.98	0.15	-	37,37,37,37	0
56	MG	CA	3134	1/1	0.54	0.52	-	204,204,204,204	0
56	MG	DA	3158	1/1	0.96	0.17	-	71,71,71,71	0
56	MG	CA	3093	1/1	0.79	0.23	-	123,123,123,123	0
56	MG	CA	3115	1/1	0.64	0.46	-	108,108,108,108	0
56	MG	CA	3112	1/1	0.82	0.33	-	110,110,110,110	0
62	PEG	DA	3225	7/7	0.76	0.39	-	62,65,70,70	0
56	MG	CA	3113	1/1	0.30	0.77	-	94,94,94,94	0
56	MG	DA	3167	1/1	0.73	0.39	-	75,75,75,75	0
56	MG	DA	3169	1/1	0.85	0.33	-	73,73,73,73	0
56	MG	AA	1617	1/1	0.68	0.36	-	98,98,98,98	0
56	MG	DA	3155	1/1	0.73	0.57	-	74,74,74,74	0
56	MG	CA	3122	1/1	0.61	0.78	-	136,136,136,136	0
56	MG	CA	3077	1/1	0.00	0.48	-	252,252,252,252	0
56	MG	DA	3031	1/1	0.97	0.21	-	46,46,46,46	0
56	MG	DA	3153	1/1	0.82	0.32	-	100,100,100,100	0
56	MG	BA	1631	1/1	0.79	0.07	-	71,71,71,71	0
56	MG	DA	3175	1/1	0.87	0.50	-	75,75,75,75	0
56	MG	DA	3160	1/1	0.93	0.11	-	72,72,72,72	0
57	PG4	DR	202	13/13	0.84	0.46	-	61,63,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1667	1/1	0.97	0.12	-	49,49,49,49	0
56	MG	AA	1666	1/1	0.96	0.05	-	67,67,67,67	0
56	MG	CA	3042	1/1	0.93	0.12	-	91,91,91,91	0
56	MG	DA	3181	1/1	0.83	0.69	-	91,91,91,91	0
56	MG	CA	3027	1/1	0.63	0.31	-	137,137,137,137	0
56	MG	DA	3012	1/1	1.00	0.09	-	29,29,29,29	0
56	MG	DA	3144	1/1	0.95	0.36	-	65,65,65,65	0
56	MG	CA	3072	1/1	0.83	0.88	-	272,272,272,272	0
56	MG	CA	3062	1/1	0.87	0.18	-	237,237,237,237	0
56	MG	AA	1655	1/1	0.81	0.16	-	115,115,115,115	0
56	MG	DA	3053	1/1	0.93	0.12	-	78,78,78,78	0
56	MG	DA	3086	1/1	0.98	0.11	-	39,39,39,39	0
56	MG	DA	3090	1/1	0.96	0.18	-	26,26,26,26	0
56	MG	AA	1626	1/1	0.04	1.42	-	111,111,111,111	0
56	MG	CA	3002	1/1	0.38	0.32	-	259,259,259,259	0
56	MG	AA	1614	1/1	0.35	0.20	-	131,131,131,131	0
56	MG	BA	1618	1/1	0.82	0.19	-	106,106,106,106	0
56	MG	AA	1658	1/1	0.93	0.10	-	100,100,100,100	0
56	MG	BA	1621	1/1	0.95	0.19	-	42,42,42,42	0
56	MG	CA	3156	1/1	0.10	0.18	-	246,246,246,246	0
58	MPD	DA	3209	8/8	0.88	0.31	-	68,70,70,71	0
56	MG	CA	3140	1/1	-0.34	0.60	-	147,147,147,147	0
56	MG	DA	3134	1/1	0.62	0.37	-	78,78,78,78	0
56	MG	DA	3076	1/1	0.95	0.19	-	38,38,38,38	0
56	MG	DA	3039	1/1	0.98	0.12	-	20,20,20,20	0
56	MG	BA	1641	1/1	0.59	0.94	-	140,140,140,140	0
56	MG	CA	3030	1/1	0.87	0.15	-	124,124,124,124	0
56	MG	DA	3150	1/1	0.95	0.18	-	59,59,59,59	0
56	MG	CA	3090	1/1	0.59	0.57	-	215,215,215,215	0
56	MG	BA	1603	1/1	0.81	0.69	-	261,261,261,261	0
56	MG	CA	3092	1/1	0.50	0.23	-	202,202,202,202	0
56	MG	BA	1644	1/1	0.91	0.12	-	97,97,97,97	0
56	MG	DB	208	1/1	0.95	0.26	-	64,64,64,64	0
56	MG	AA	1632	1/1	0.64	0.08	-	124,124,124,124	0
56	MG	CA	3108	1/1	0.68	0.52	-	109,109,109,109	0
56	MG	DA	3112	1/1	0.84	0.44	-	293,293,293,293	0
56	MG	CA	3041	1/1	0.94	0.19	-	71,71,71,71	0
62	PEG	DA	3226	7/7	0.86	0.33	-	58,59,65,67	0
56	MG	AA	1605	1/1	0.58	0.71	-	99,99,99,99	0
56	MG	CA	3025	1/1	0.98	0.28	-	105,105,105,105	0
56	MG	DA	3017	1/1	0.97	0.12	-	56,56,56,56	0
56	MG	CA	3028	1/1	0.14	0.75	-	283,283,283,283	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CB	203	1/1	0.71	0.11	-	155,155,155,155	0
56	MG	DB	205	1/1	0.95	0.17	-	49,49,49,49	0
56	MG	CA	3114	1/1	0.95	0.47	-	62,62,62,62	0
56	MG	DA	3114	1/1	0.97	0.11	-	62,62,62,62	0
56	MG	DA	3149	1/1	0.90	0.27	-	77,77,77,77	0
56	MG	BA	1628	1/1	0.92	0.18	-	111,111,111,111	0
56	MG	DA	3229	1/1	0.94	0.13	-	55,55,55,55	0
56	MG	DA	3054	1/1	0.98	0.09	-	57,57,57,57	0
56	MG	CA	3150	1/1	0.90	0.50	-	82,82,82,82	0
63	EDO	DB	211	4/4	0.90	0.23	-	73,73,74,75	0
56	MG	BA	1627	1/1	0.84	0.77	-	129,129,129,129	0
56	MG	DA	3074	1/1	0.98	0.15	-	33,33,33,33	0
56	MG	DA	3092	1/1	0.99	0.17	-	31,31,31,31	0
56	MG	DA	3055	1/1	0.98	0.08	-	49,49,49,49	0
56	MG	DA	3009	1/1	0.95	0.12	-	102,102,102,102	0
69	TRS	DA	3219	8/8	0.76	0.56	-	98,99,102,104	0
56	MG	CA	3056	1/1	0.35	0.72	-	100,100,100,100	0
56	MG	AA	1641	1/1	0.96	0.08	-	92,92,92,92	0
56	MG	CA	3045	1/1	0.90	0.08	-	93,93,93,93	0
56	MG	DA	3035	1/1	1.00	0.18	-	24,24,24,24	0
56	MG	BA	1611	1/1	0.98	0.11	-	66,66,66,66	0
56	MG	CA	3016	1/1	0.74	0.33	-	148,148,148,148	0
56	MG	CA	3082	1/1	0.78	0.45	-	160,160,160,160	0
56	MG	CA	3124	1/1	0.35	0.52	-	202,202,202,202	0
58	MPD	DK	201	8/8	0.82	0.27	-	93,94,95,95	0
56	MG	CA	3146	1/1	0.25	0.37	-	247,247,247,247	0
56	MG	DB	206	1/1	0.56	0.47	-	102,102,102,102	0
56	MG	DA	3046	1/1	0.97	0.08	-	47,47,47,47	0
56	MG	BA	1629	1/1	0.52	0.58	-	157,157,157,157	0
56	MG	DA	3063	1/1	0.85	0.13	-	222,222,222,222	0
56	MG	DA	3058	1/1	0.99	0.07	-	31,31,31,31	0
56	MG	DA	3109	1/1	0.97	0.10	-	29,29,29,29	0
56	MG	DA	3073	1/1	0.98	0.14	-	47,47,47,47	0
56	MG	DA	3115	1/1	0.96	0.15	-	49,49,49,49	0
56	MG	CA	3080	1/1	0.85	0.34	-	186,186,186,186	0
56	MG	DA	3042	1/1	0.99	0.16	-	20,20,20,20	0
56	MG	AA	1634	1/1	0.91	0.19	-	108,108,108,108	0
67	ACY	DA	3196	4/4	0.77	0.32	-	75,79,79,80	0
56	MG	DA	3037	1/1	0.98	0.23	-	31,31,31,31	0
56	MG	BA	1625	1/1	0.76	0.39	-	274,274,274,274	0
56	MG	AA	1602	1/1	0.64	0.54	-	88,88,88,88	0
56	MG	CA	3046	1/1	0.97	0.14	-	143,143,143,143	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3047	1/1	0.59	1.50	-	240,240,240,240	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.