



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 27, 2016 – 09:06 AM EDT

PDB ID : 5J7L
Title : Structure of the 70S E coli ribosome with the U1052G mutation in the 16S rRNA bound to tetracycline
Authors : Cocozaki, A.; Ferguson, A.
Deposited on : 2016-04-06
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (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

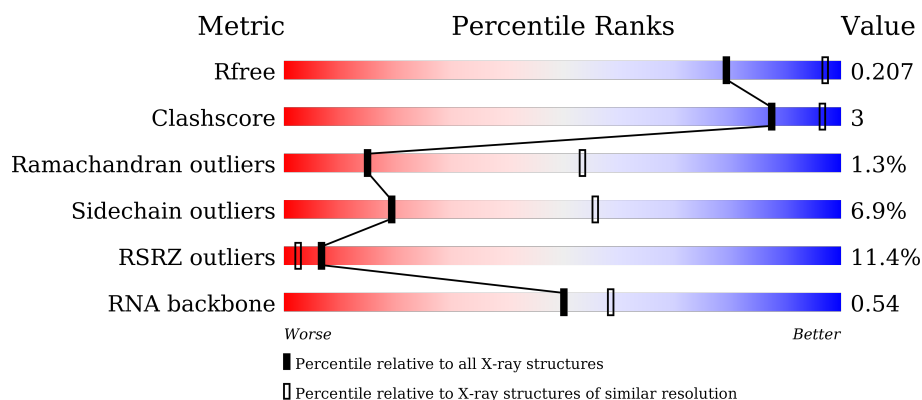
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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

Mol	Chain	Length	Quality of chain
1	AA	1534	<div> <div>2%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
1	BA	1534	<div> <div>11%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>
2	AB	224	<div> <div>13%</div> <div>88%</div> <div>12%</div> <div>.</div> </div>
2	BB	224	<div> <div>16%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AC	206	% 84% 15%
3	BC	206	19% 81% 19%
4	AD	205	89% 10% .
4	BD	205	86% 12% .
5	AE	155	78% 19% .
5	BE	155	% 65% 26% 5% . .
6	AF	106	2% 81% 19%
6	BF	106	2% 69% 24% . 6%
7	AG	151	20% 83% 16% .
7	BG	151	50% 83% 17%
8	AH	129	% 83% 16% .
8	BH	129	3% 83% 17%
9	AI	127	21% 87% 13% .
9	BI	127	39% 87% 12% .
10	AJ	99	11% 77% 21% .
10	BJ	99	60% 74% 21% . .
11	AK	117	4% 83% 16% .
11	BK	117	3% 76% 23% .
12	AL	123	% 89% 10% .
12	BL	123	3% 84% 13% .
13	AM	114	29% 80% 18% .
13	BM	114	76% 72% 25% .
14	AN	100	16% 87% 12% .
14	BN	100	52% 89% 11%
15	AO	88	% 92% 8%

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
41	CO	125	<div> <div>22%</div> <div>82%</div> <div>12%</div> <div>.</div> <div>.</div> </div>
41	DO	125	<div> <div>91%</div> <div>6%</div> <div>.</div> </div>
42	CP	117	<div> <div>40%</div> <div>87%</div> <div>10%</div> <div>.</div> <div>.</div> </div>
42	DP	117	<div> <div>85%</div> <div>12%</div> <div>.</div> </div>
43	CQ	114	<div> <div>19%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
43	DQ	114	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
44	CR	117	<div> <div>16%</div> <div>87%</div> <div>13%</div> </div>
44	DR	117	<div> <div>%</div> <div>89%</div> <div>11%</div> </div>
45	CS	103	<div> <div>32%</div> <div>80%</div> <div>17%</div> <div>.</div> <div>.</div> </div>
45	DS	103	<div> <div>90%</div> <div>10%</div> </div>
46	CT	110	<div> <div>14%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
46	DT	110	<div> <div>85%</div> <div>15%</div> </div>
47	CU	93	<div> <div>32%</div> <div>80%</div> <div>16%</div> <div>.</div> </div>
47	DU	93	<div> <div>2%</div> <div>87%</div> <div>13%</div> </div>
48	CV	102	<div> <div>57%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
48	DV	102	<div> <div>2%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
49	CW	94	<div> <div>31%</div> <div>86%</div> <div>14%</div> </div>
49	DW	94	<div> <div>89%</div> <div>11%</div> </div>
50	CX	76	<div> <div>30%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
50	DX	76	<div> <div>%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>
51	CY	77	<div> <div>4%</div> <div>82%</div> <div>18%</div> </div>
51	DY	77	<div> <div>91%</div> <div>9%</div> </div>
52	CZ	62	<div> <div>53%</div> <div>82%</div> <div>18%</div> </div>
52	DZ	62	<div> <div>2%</div> <div>92%</div> <div>8%</div> </div>
53	DI	135	<div> <div>21%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	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
55	MG	AA	1608	-	-	-	X
55	MG	AA	1612	-	-	-	X
55	MG	BA	1601	-	-	-	X
55	MG	BA	1612	-	-	-	X
55	MG	BA	1646	-	-	-	X
55	MG	CA	3003	-	-	-	X
55	MG	CA	3026	-	-	-	X
55	MG	CA	3105	-	-	-	X
55	MG	CA	3122	-	-	-	X
55	MG	CA	3123	-	-	-	X
55	MG	CA	3130	-	-	-	X
55	MG	CA	3133	-	-	-	X
55	MG	CA	3137	-	-	-	X
55	MG	CA	3147	-	-	-	X
55	MG	CA	3151	-	-	-	X
55	MG	DA	3037	-	-	-	X
55	MG	DA	3124	-	-	-	X
55	MG	DA	3126	-	-	-	X
55	MG	DA	3127	-	-	-	X
55	MG	DA	3172	-	-	-	X
56	PG4	AA	1670	-	-	-	X
56	PG4	BA	1642	-	-	-	X
56	PG4	DA	3193	-	-	-	X
56	PG4	DA	3216	-	-	-	X
56	PG4	DS	202	-	-	-	X
57	MPD	AA	1671	-	-	-	X
57	MPD	AA	1676	-	-	-	X
57	MPD	DA	3192	-	-	-	X
57	MPD	DA	3204	-	-	-	X
57	MPD	DA	3207	-	-	-	X
57	MPD	DE	301	-	-	-	X
58	PUT	AA	1672	-	-	-	X
58	PUT	AA	1673	-	-	-	X
58	PUT	AA	1674	-	-	-	X
58	PUT	DA	3184	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	PUT	DA	3189	-	-	-	X
58	PUT	DA	3195	-	-	-	X
58	PUT	DA	3205	-	-	-	X
58	PUT	DA	3213	-	-	-	X
58	PUT	DA	3219	-	-	-	X
58	PUT	DA	3222	-	-	-	X
59	TAC	BA	1644	-	-	-	X
61	PEG	D1	103	-	-	-	X
61	PEG	D3	101	-	-	-	X
61	PEG	DA	3200	-	-	-	X
61	PEG	DA	3218	-	-	-	X
61	PEG	DA	3226	-	-	-	X
61	PEG	DL	201	-	-	-	X
61	PEG	DQ	201	-	-	-	X
62	EDO	D1	101	-	-	-	X
62	EDO	DA	3197	-	-	-	X
62	EDO	DA	3198	-	-	-	X
62	EDO	DA	3209	-	-	-	X
62	EDO	DB	201	-	-	-	X
63	PGE	D1	102	-	-	-	X
63	PGE	DA	3001	-	-	-	X
63	PGE	DA	3203	-	-	-	X
63	PGE	DA	3214	-	-	-	X
63	PGE	DA	3217	-	-	-	X
63	PGE	DA	3225	-	-	-	X
63	PGE	DS	201	-	-	-	X
63	PGE	DU	101	-	-	-	X
64	SPD	DA	3183	-	-	-	X
64	SPD	DA	3187	-	-	-	X
64	SPD	DA	3206	-	-	-	X
64	SPD	DA	3224	-	-	-	X
65	1PE	DA	3185	-	-	-	X
65	1PE	DA	3202	-	-	-	X
66	ACY	DA	3201	-	-	-	X
67	GUN	DA	3211	-	-	-	X

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295261 atoms, of which 2 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
			32933	14695	6044	10660	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32911	14685	6039	10654	1533			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1052	G	U	engineered mutation	GB 595593103
BA	1052	G	U	engineered mutation	GB 595593103

- 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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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 50S ribosomal protein L1.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
30	DD	209	Total	C	N	O	S	0	1	0
			1576	986	290	296	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 L4.

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

- Molecule 33 is a protein called 50S ribosomal protein L5.

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

- Molecule 34 is a protein called 50S ribosomal protein L6.

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

- Molecule 35 is a protein called 50S ribosomal protein L9.

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

- Molecule 36 is a protein called 50S ribosomal protein L11.

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

- Molecule 37 is a protein called 50S ribosomal protein L13.

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

- Molecule 38 is a protein called 50S ribosomal protein L14.

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

- Molecule 39 is a protein called 50S ribosomal protein L15.

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

- Molecule 40 is a protein called 50S ribosomal protein L16.

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

- Molecule 41 is a protein called 50S ribosomal protein L17.

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

- Molecule 42 is a protein called 50S ribosomal protein L18.

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

- Molecule 43 is a protein called 50S ribosomal protein L19.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called 50S ribosomal protein L21.

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

- Molecule 46 is a protein called 50S ribosomal protein L22.

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

- Molecule 47 is a protein called 50S ribosomal protein L23.

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

Continued on next page...

Continued from previous page...

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

- Molecule 48 is a protein called 50S ribosomal protein L24.

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

- Molecule 49 is a protein called 50S ribosomal protein L25.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

- Molecule 52 is a protein called 50S ribosomal protein L29.

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

- Molecule 53 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	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

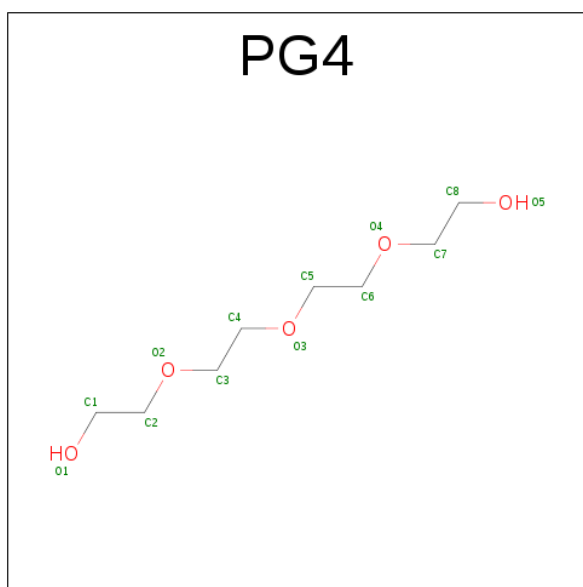
- Molecule 54 is a RNA chain called 23S rRNA.

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

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

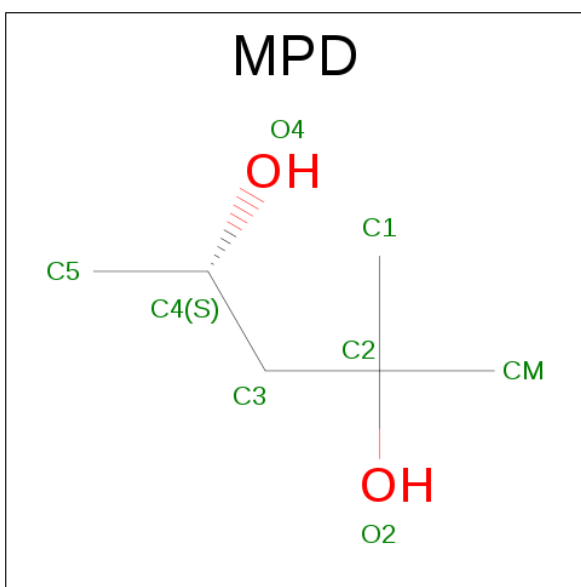
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BA	45	Total	Mg	0	0
			45	45		
55	CA	156	Total	Mg	0	0
			156	156		
55	CB	3	Total	Mg	0	0
			3	3		
55	DM	1	Total	Mg	0	0
			1	1		
55	DR	2	Total	Mg	0	0
			2	2		
55	AA	72	Total	Mg	0	0
			72	72		
55	DA	183	Total	Mg	0	0
			183	183		
55	DB	9	Total	Mg	0	0
			9	9		
55	DD	1	Total	Mg	0	0
			1	1		

- Molecule 56 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



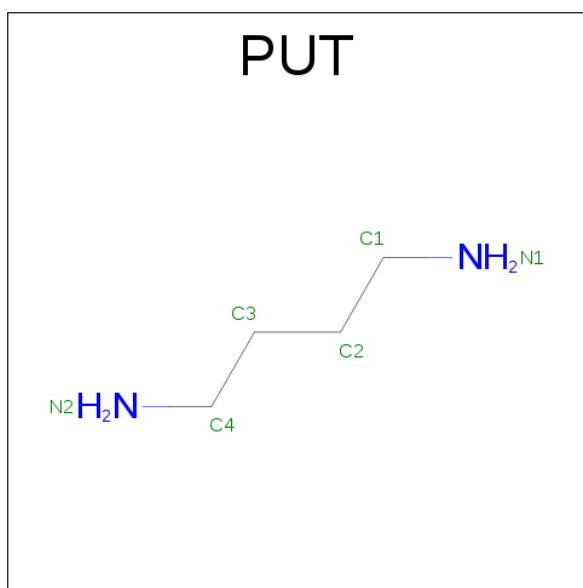
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	C	O	0	0
			13	8	5		
56	BA	1	Total	C	O	0	0
			13	8	5		
56	DQ	1	Total	C	O	0	0
			13	8	5		
56	DR	1	Total	C	O	0	0
			13	8	5		
56	DS	1	Total	C	O	0	0
			13	8	5		
56	DA	1	Total	C	O	0	0
			13	8	5		
56	DA	1	Total	C	O	0	0
			13	8	5		

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 58 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula: C₄H₁₂N₂).



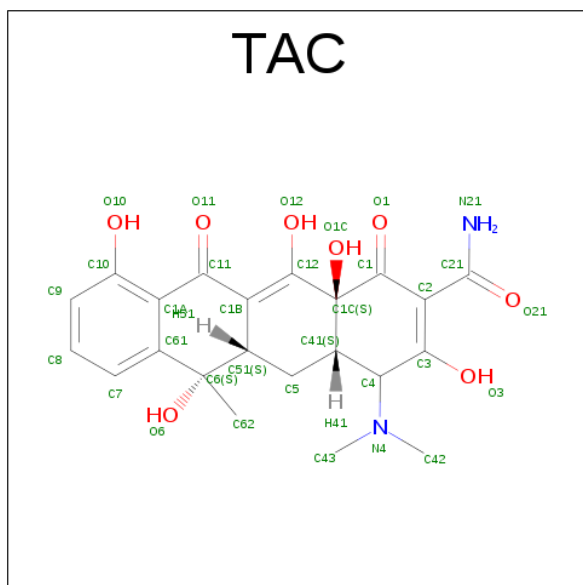
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AA	1	Total	C	N	0	0
			6	4	2		
58	AA	1	Total	C	N	0	0
			6	4	2		
58	AA	1	Total	C	N	0	0
			6	4	2		
58	AA	1	Total	C	N	0	0
			6	4	2		
58	DM	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6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

Continued on next page...

Continued from previous page...

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

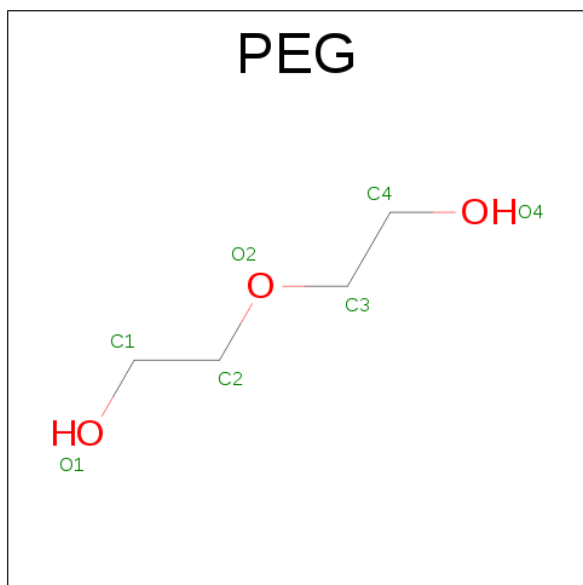
- Molecule 59 is TETRACYCLINE (three-letter code: TAC) (formula: $C_{22}H_{24}N_2O_8$).



Continued from previous page...

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

- Molecule 61 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



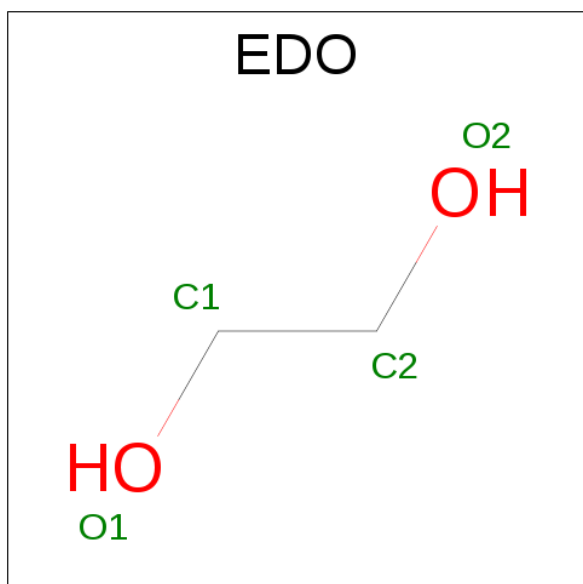
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	D1	1	Total	C	O	0	0
			7	4	3		
61	D3	1	Total	C	O	0	0
			7	4	3		
61	DL	1	Total	C	O	0	0
			7	4	3		
61	DP	1	Total	C	O	0	0
			7	4	3		
61	DQ	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7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

Continued on next page...

Continued from previous page...

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

- Molecule 62 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



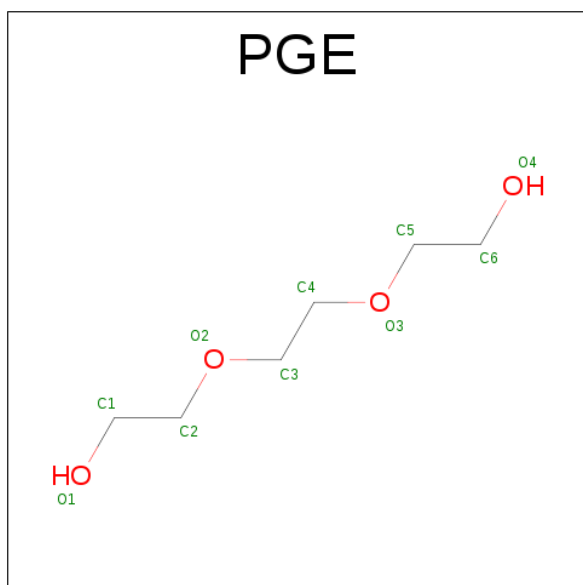
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	D1	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4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

Continued on next page...

Continued from previous page...

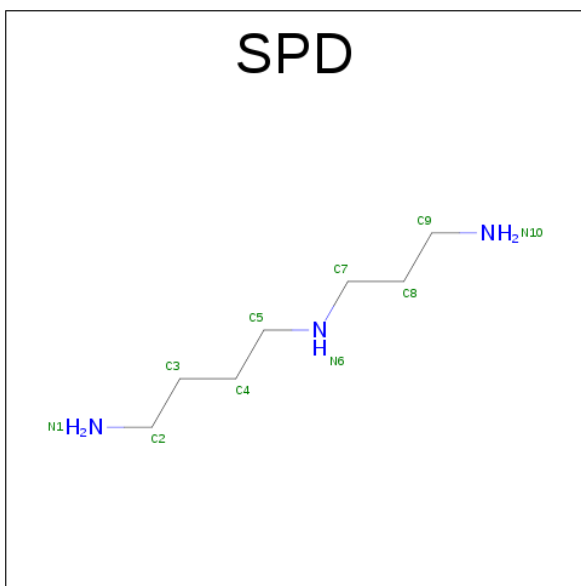
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 63 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



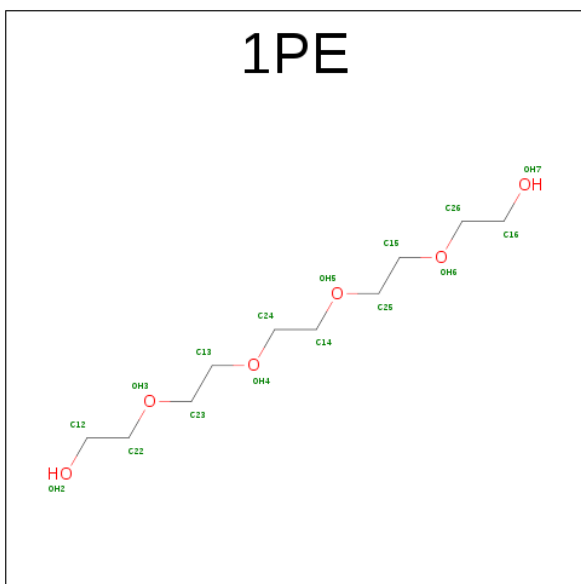
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			10	6	4		
63	DS	1	Total	C	O	0	0
			10	6	4		
63	DU	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0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

- Molecule 64 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



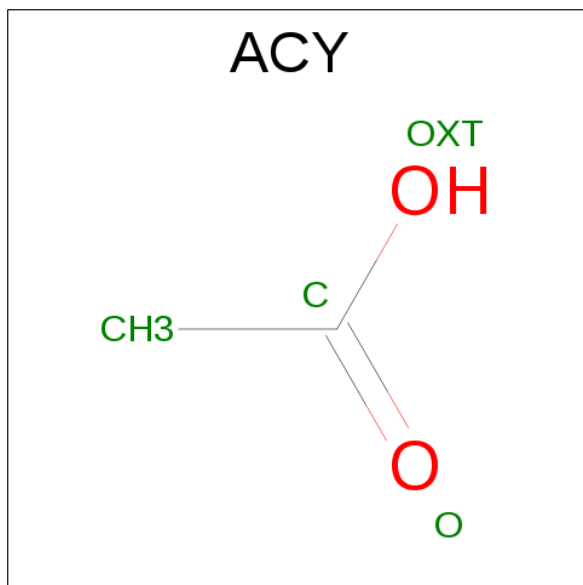
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		

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



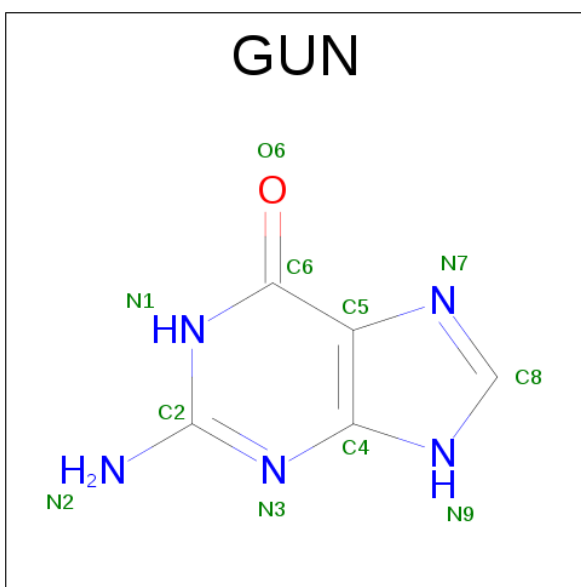
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
65	DA	1	Total	C	O	0	0
			16	10	6		
65	DA	1	Total	C	O	0	0
			16	10	6		

- Molecule 66 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



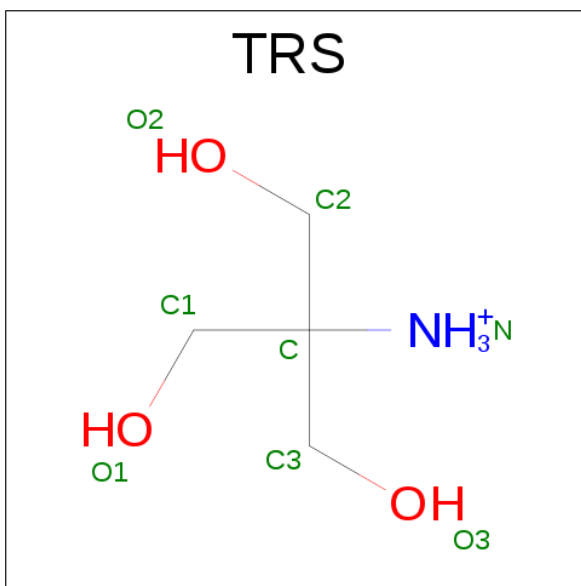
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 67 is GUANINE (three-letter code: GUN) (formula: C₅H₅N₅O).



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

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



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

- Molecule 69 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AA	501	Total 501	O 501	0	0
69	AC	4	Total 4	O 4	0	0
69	AD	2	Total 2	O 2	0	0
69	AE	5	Total 5	O 5	0	0
69	AG	1	Total 1	O 1	0	0
69	AH	1	Total 1	O 1	0	0
69	AJ	2	Total 2	O 2	0	0
69	AK	6	Total 6	O 6	0	0
69	AL	10	Total 10	O 10	0	0
69	AM	5	Total 5	O 5	0	0
69	AN	6	Total 6	O 6	0	0
69	AO	2	Total 2	O 2	0	0
69	AP	2	Total 2	O 2	0	0
69	AR	1	Total 1	O 1	0	0
69	AT	3	Total 3	O 3	0	0
69	AU	3	Total 3	O 3	0	0
69	C3	4	Total 4	O 4	0	0
69	C4	1	Total 1	O 1	0	0
69	BA	287	Total 287	O 287	0	0
69	BD	13	Total 13	O 13	0	0
69	BE	1	Total 1	O 1	0	0
69	BF	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	BK	2	Total 2	O 2	0	0
69	BL	4	Total 4	O 4	0	0
69	BN	2	Total 2	O 2	0	0
69	BO	1	Total 1	O 1	0	0
69	BP	3	Total 3	O 3	0	0
69	BT	2	Total 2	O 2	0	0
69	BU	2	Total 2	O 2	0	0
69	D1	43	Total 43	O 43	0	0
69	D2	6	Total 6	O 6	0	0
69	D3	22	Total 22	O 22	0	0
69	D4	39	Total 39	O 39	0	0
69	D5	8	Total 8	O 8	0	0
69	D0	24	Total 24	O 24	0	0
69	CB	13	Total 13	O 13	0	0
69	CC	10	Total 10	O 10	0	0
69	CD	6	Total 6	O 6	0	0
69	CA	691	Total 691	O 691	0	0
69	DC	100	Total 100	O 100	0	0
69	DD	98	Total 98	O 98	0	0
69	CE	5	Total 5	O 5	0	0
69	CL	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	CM	4	Total 4	O 4	0	0
69	CO	2	Total 2	O 2	0	0
69	CU	3	Total 3	O 3	0	0
69	CV	1	Total 1	O 1	0	0
69	CW	1	Total 1	O 1	0	0
69	CY	1	Total 1	O 1	0	0
69	DE	61	Total 61	O 61	0	0
69	DF	15	Total 15	O 15	0	0
69	DG	6	Total 6	O 6	0	0
69	DH	2	Total 2	O 2	0	0
69	DK	65	Total 65	O 65	0	0
69	DL	52	Total 52	O 52	0	0
69	DM	63	Total 63	O 63	0	0
69	DN	72	Total 72	O 72	0	0
69	DO	44	Total 44	O 44	0	0
69	DP	38	Total 38	O 38	0	0
69	DQ	33	Total 33	O 33	0	0
69	DR	62	Total 62	O 62	0	0
69	DS	46	Total 46	O 46	0	0
69	DT	69	Total 69	O 69	0	0
69	DU	18	Total 18	O 18	0	0

Continued on next page...

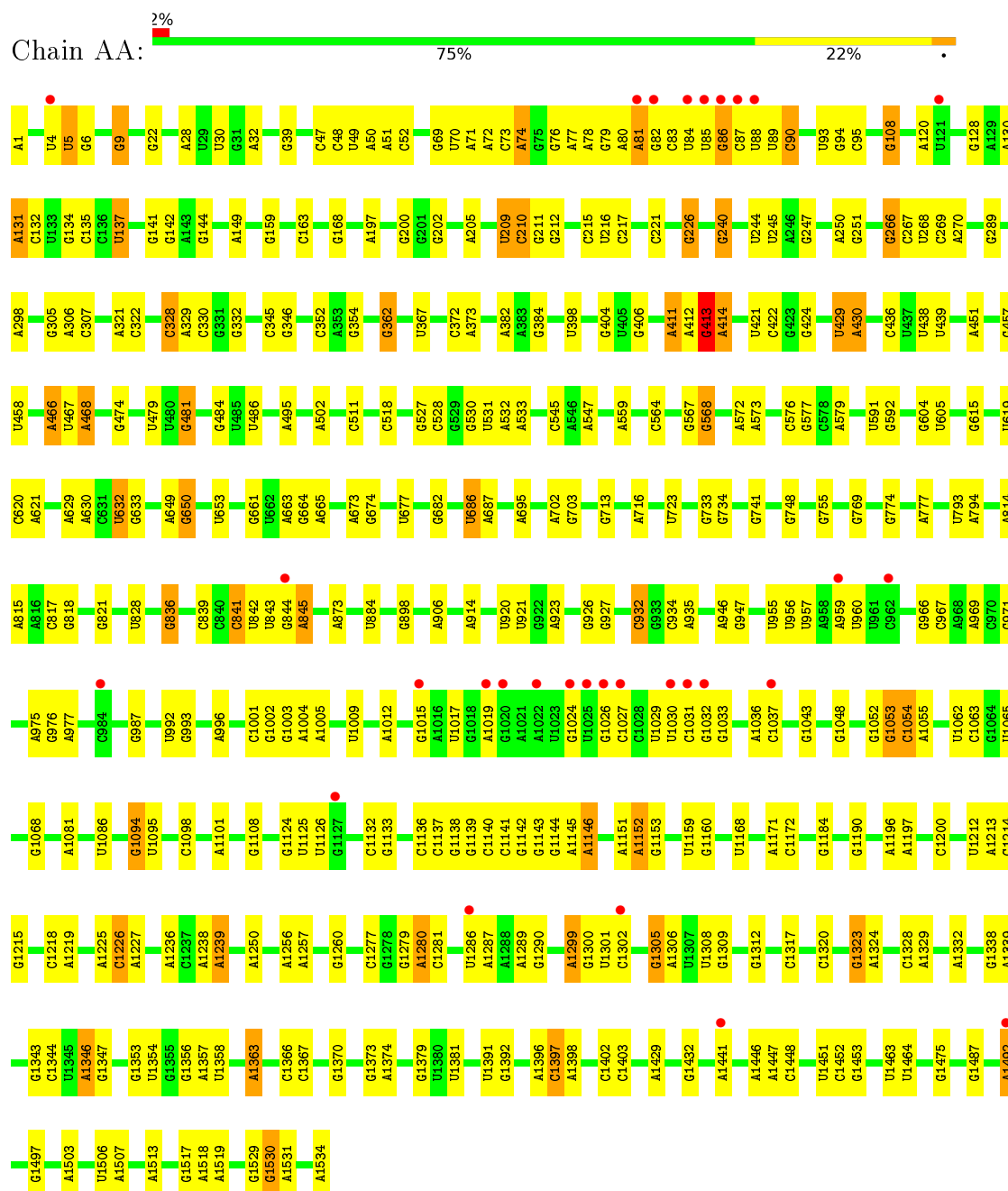
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DV	20	Total 20	O 20	0	0
69	DW	31	Total 31	O 31	0	0
69	DX	25	Total 25	O 25	0	0
69	DY	9	Total 9	O 9	0	0
69	DZ	8	Total 8	O 8	0	0
69	DB	209	Total 209	O 209	0	0
69	DA	4840	Total 4840	O 4840	0	0

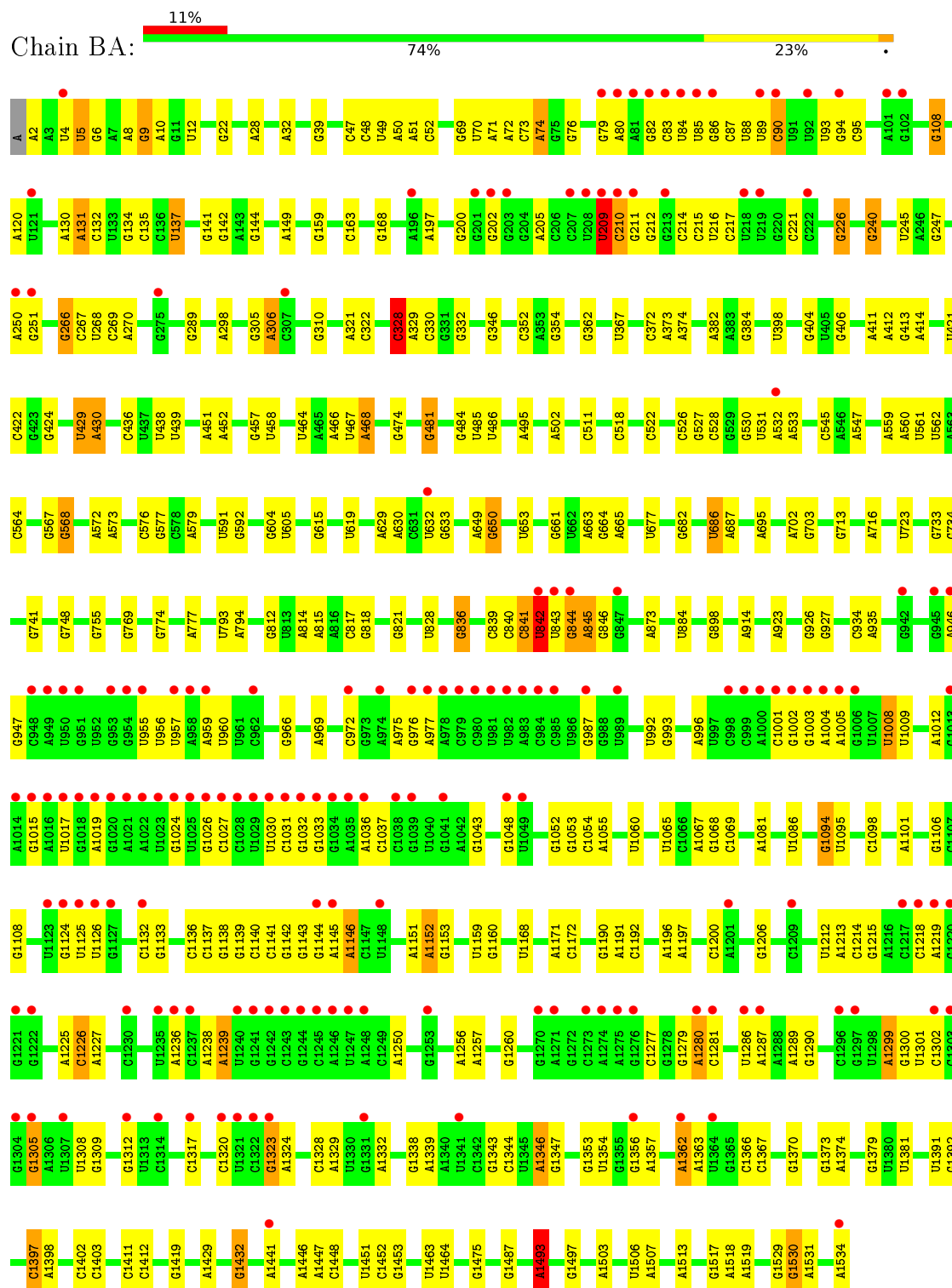
3 Residue-property plots

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.

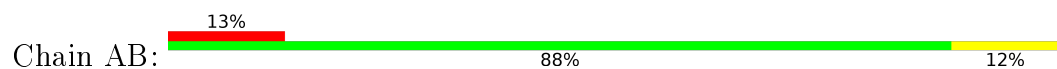
• Molecule 1: 16S rRNA

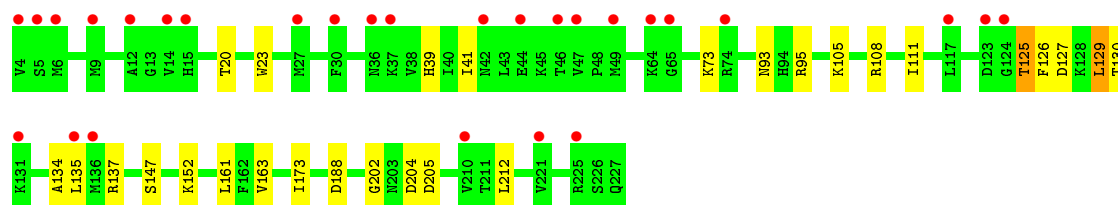


- Molecule 1: 16S rRNA

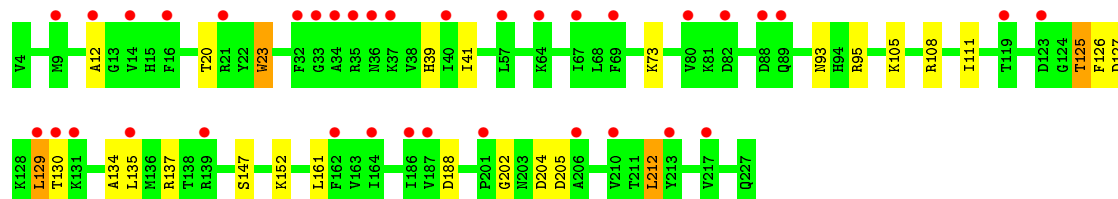
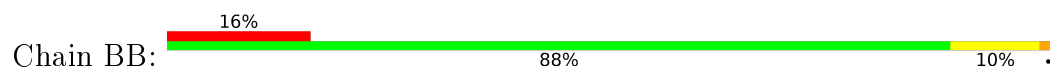


- Molecule 2: 30S ribosomal protein S2

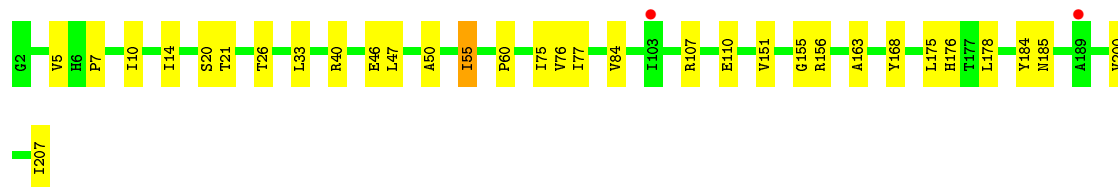
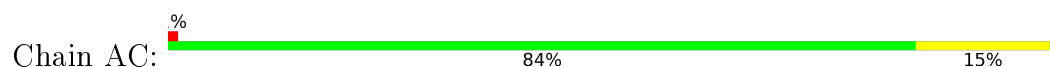




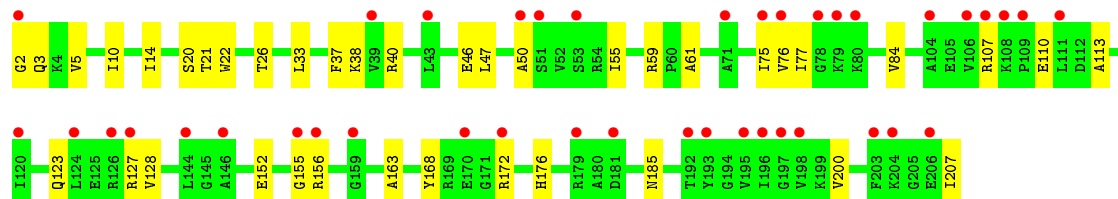
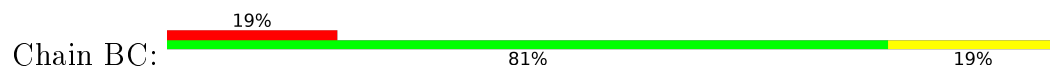
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3



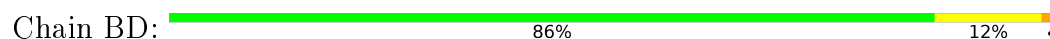
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4





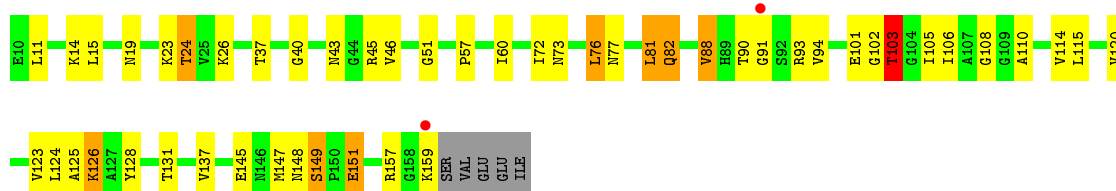
- Molecule 5: 30S ribosomal protein S5

Chain AE: 78% 19% .



- Molecule 5: 30S ribosomal protein S5

Chain BE: 65% 26% 5% . .



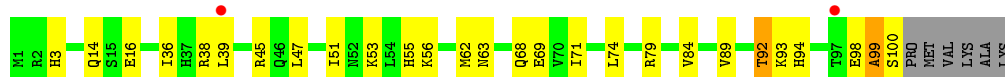
- Molecule 6: 30S ribosomal protein S6

Chain AF: 81% 19%



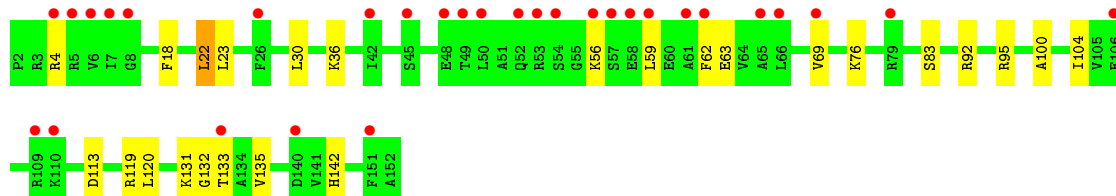
- Molecule 6: 30S ribosomal protein S6

Chain BF: 69% 24% 6%



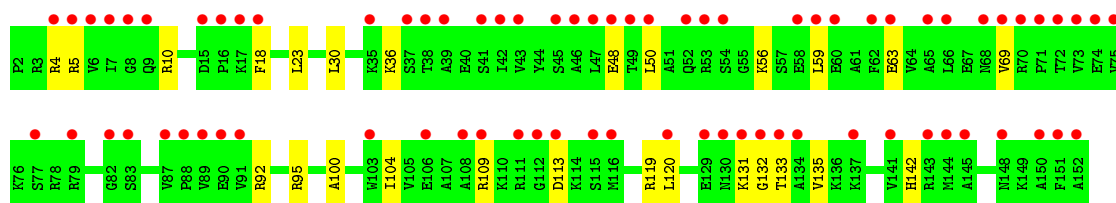
- Molecule 7: 30S ribosomal protein S7

Chain AG: 20% 83% 16% .

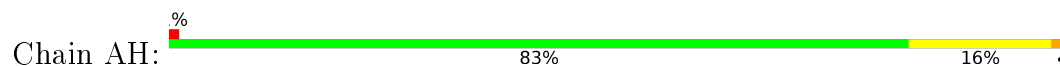


- Molecule 7: 30S ribosomal protein S7

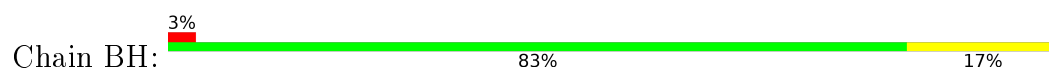
Chain BG: 50% 83% 17%



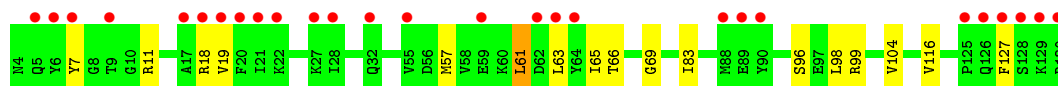
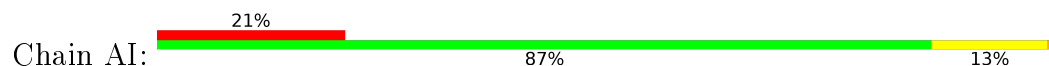
- Molecule 8: 30S ribosomal protein S8



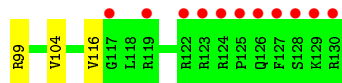
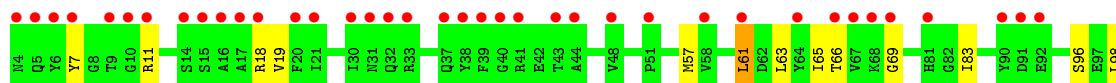
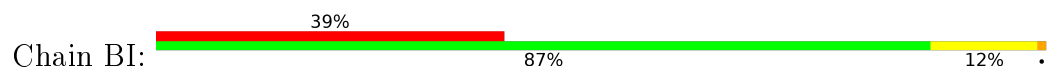
- Molecule 8: 30S ribosomal protein S8



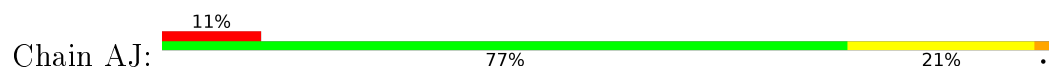
- Molecule 9: 30S ribosomal protein S9



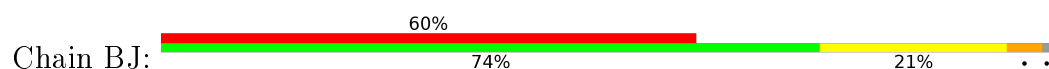
- Molecule 9: 30S ribosomal protein S9

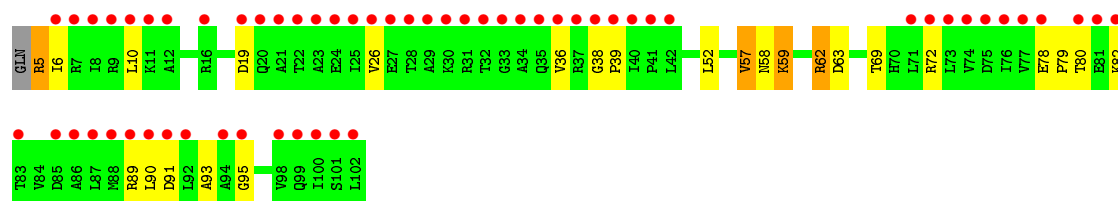


- Molecule 10: 30S ribosomal protein S10

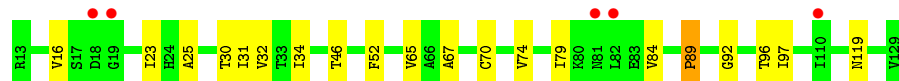
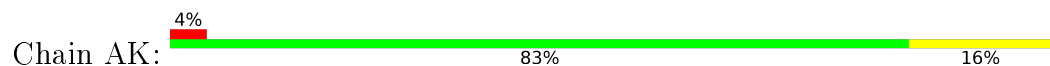


- Molecule 10: 30S ribosomal protein S10

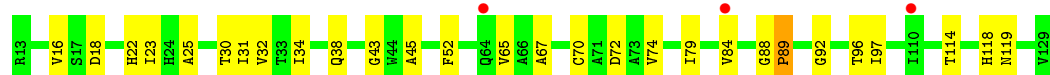
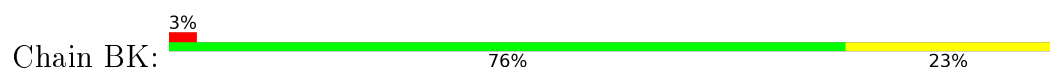




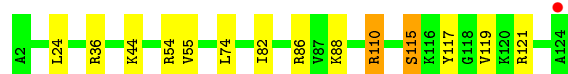
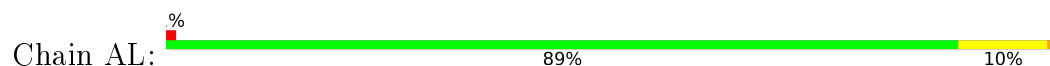
- Molecule 11: 30S ribosomal protein S11



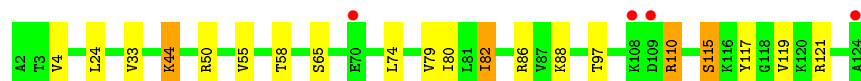
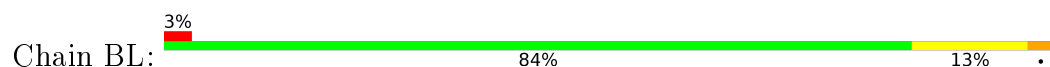
- Molecule 11: 30S ribosomal protein S11



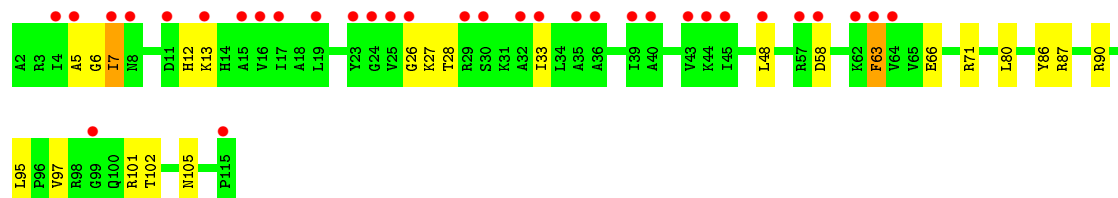
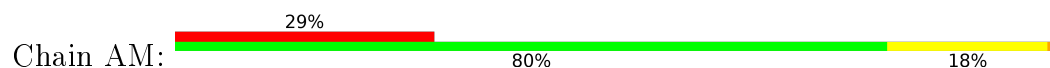
- Molecule 12: 30S ribosomal protein S12



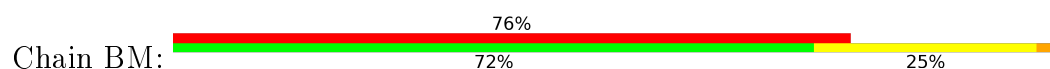
- Molecule 12: 30S ribosomal protein S12

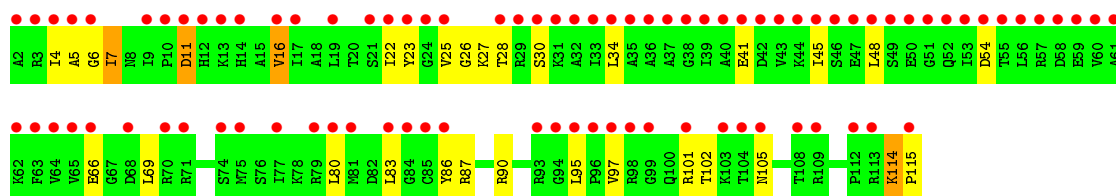


- Molecule 13: 30S ribosomal protein S13

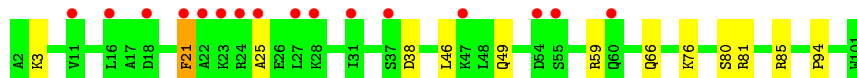
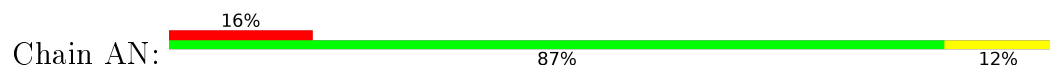


- Molecule 13: 30S ribosomal protein S13

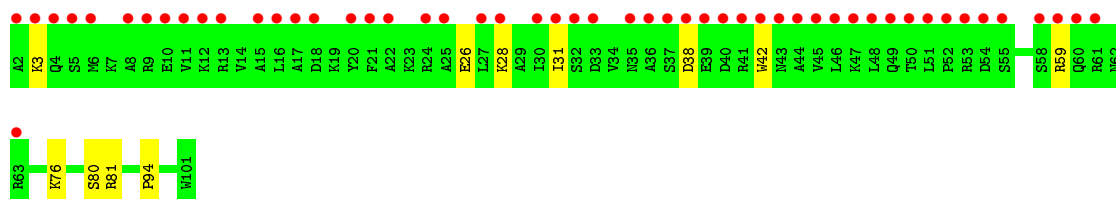
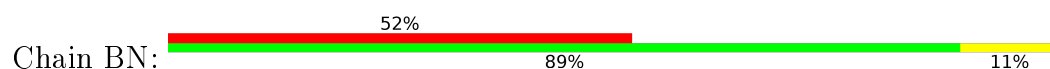




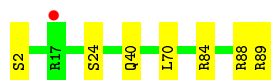
- Molecule 14: 30S ribosomal protein S14



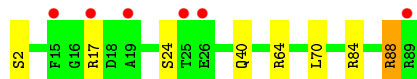
- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15



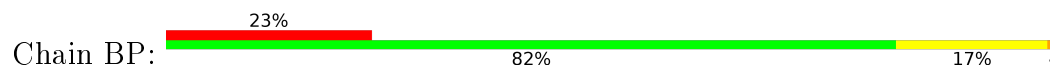
- Molecule 15: 30S ribosomal protein S15

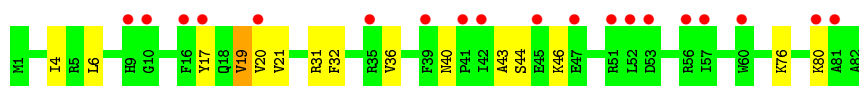


- Molecule 16: 30S ribosomal protein S16

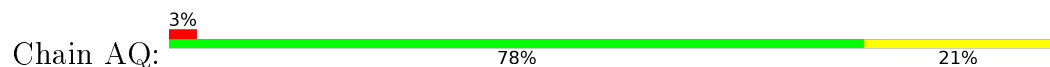


- Molecule 16: 30S ribosomal protein S16

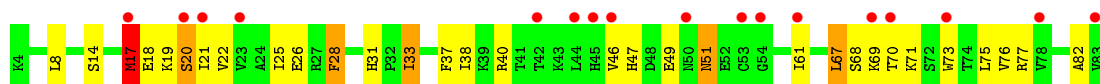




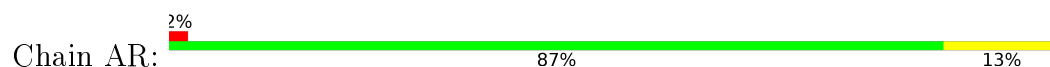
- Molecule 17: 30S ribosomal protein S17



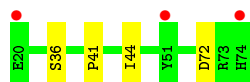
- Molecule 17: 30S ribosomal protein S17



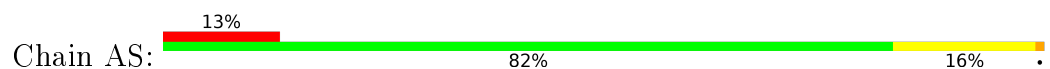
- Molecule 18: 30S ribosomal protein S18



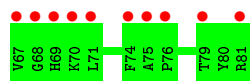
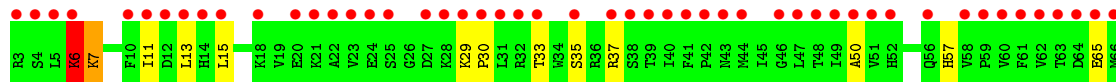
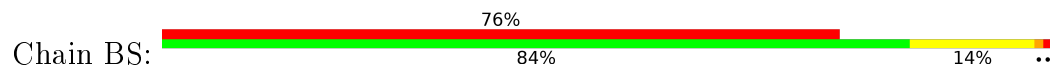
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

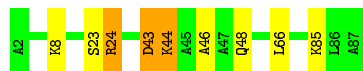


- Molecule 19: 30S ribosomal protein S19




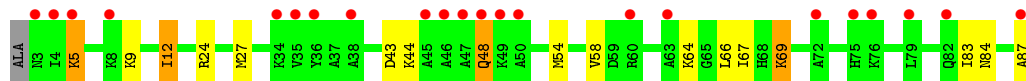
- Molecule 20: 30S ribosomal protein S20

Chain AT:  90% 7% .




- Molecule 20: 30S ribosomal protein S20

Chain BT:  26% 79% 15% 5% .




- Molecule 21: 30S ribosomal protein S21

Chain AU:  4% 88% 13%




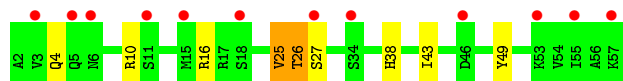
- Molecule 21: 30S ribosomal protein S21

Chain BU:  2% 88% 13%




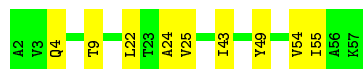
- Molecule 22: 50S ribosomal protein L32

Chain C1:  21% 84% 13% .



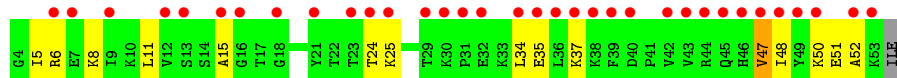
- Molecule 22: 50S ribosomal protein L32

Chain D1:  84% 16%




- Molecule 23: 50S ribosomal protein L33

Chain C2:  67% 69% 27% . .




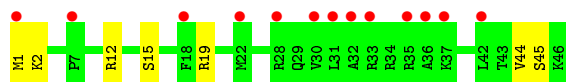
- Molecule 23: 50S ribosomal protein L33

Chain D2:  73% 25% .



- Molecule 24: 50S ribosomal protein L34

Chain C3:  28% 85% 15%




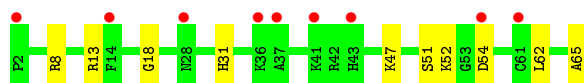
- Molecule 24: 50S ribosomal protein L34

Chain D3:  89% 11%



- Molecule 25: 50S ribosomal protein L35

Chain C4:  14% 84% 16%




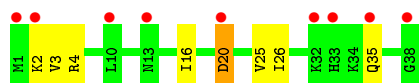
- Molecule 25: 50S ribosomal protein L35

Chain D4:  91% 9%




- Molecule 26: 50S ribosomal protein L36

Chain C5:  24% 79% 18% .




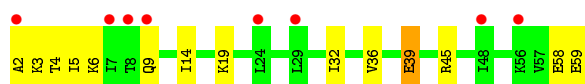
- Molecule 26: 50S ribosomal protein L36

Chain D5:  87% 13%



- Molecule 27: 50S ribosomal protein L30

Chain C0:  14% 76% 22% .



- Molecule 27: 50S ribosomal protein L30

Chain D0: 83% 16%



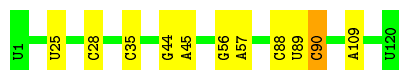
- Molecule 28: 50S ribosomal protein L1

Chain CB: 8% 85% 11%



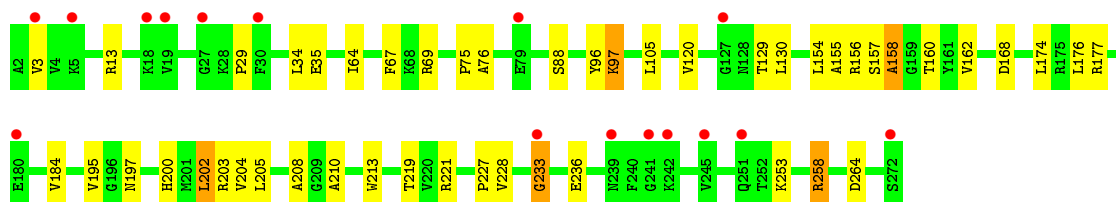
- Molecule 28: 50S ribosomal protein L1

Chain DB: 91% 8%



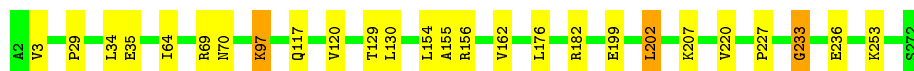
- Molecule 29: 50S ribosomal protein L2

Chain CC: 6% 82% 16%



- Molecule 29: 50S ribosomal protein L2

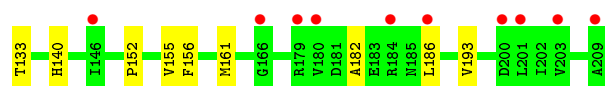
Chain DC: 90% 8%



- Molecule 30: 50S ribosomal protein L3

Chain CD: 15% 88% 11%

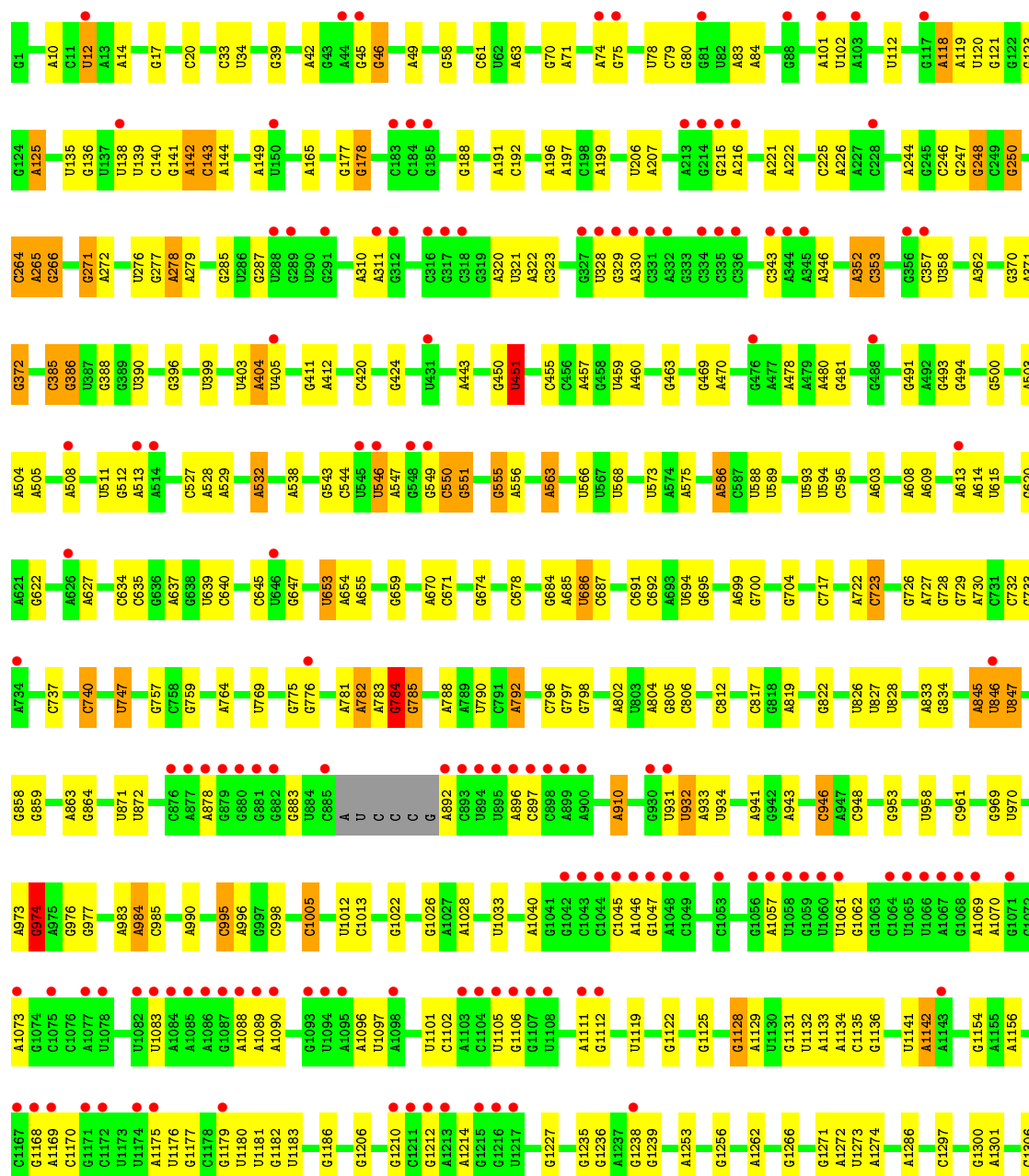
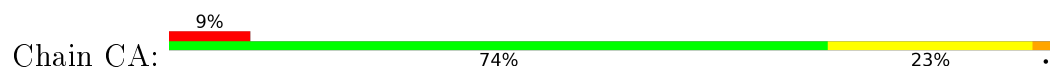


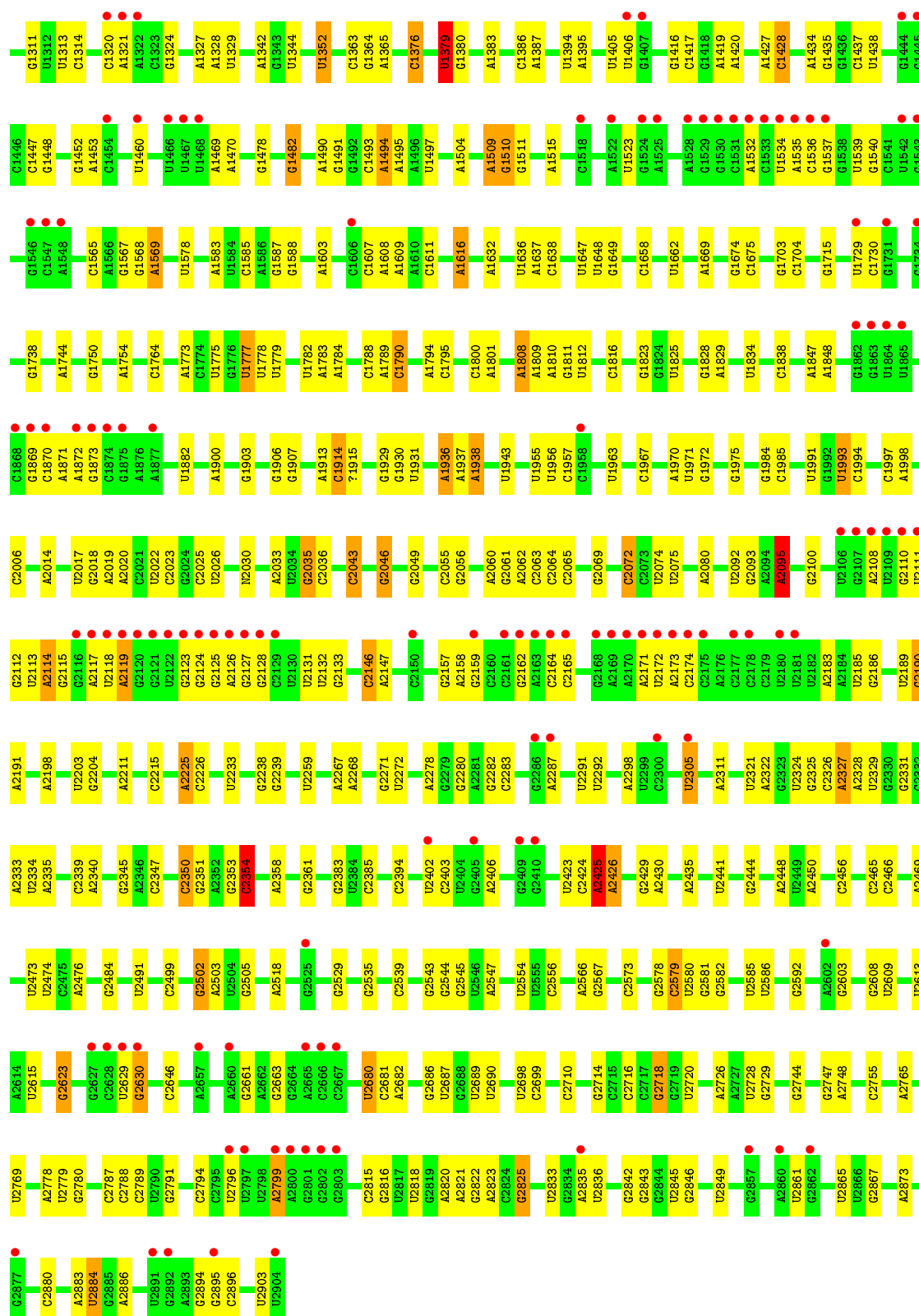


- Molecule 30: 50S ribosomal protein L3

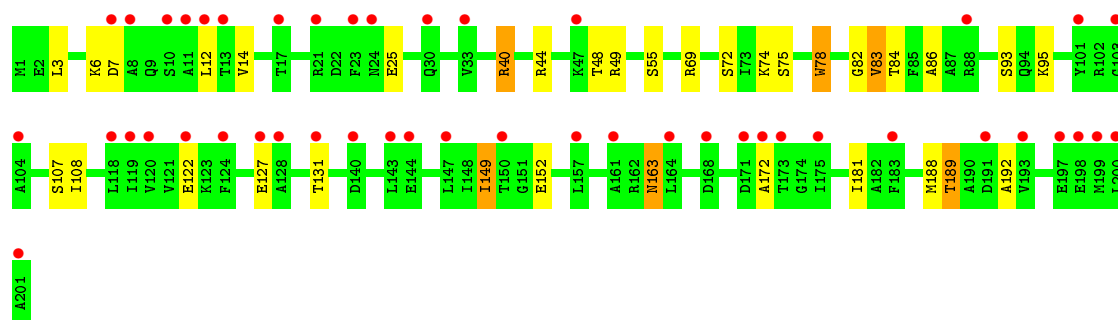


- Molecule 31: 23S rRNA





- Molecule 32: 50S ribosomal protein L4



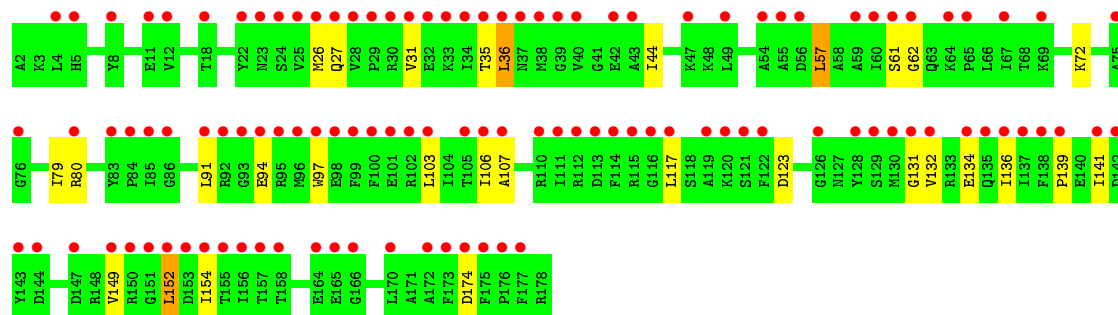
- Molecule 32: 50S ribosomal protein L4

Chain DE: 91% 8% .



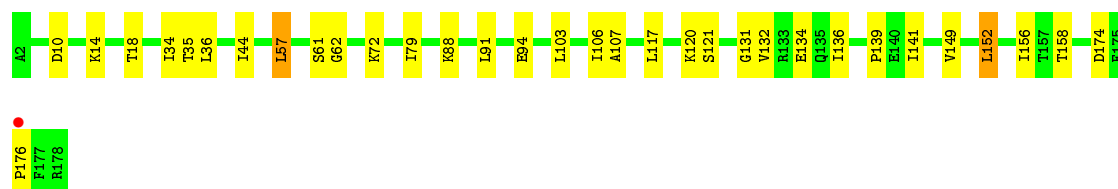
- Molecule 33: 50S ribosomal protein L5

Chain CF: 63% 83% 15% .



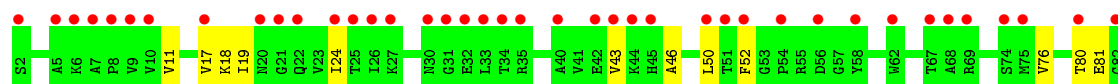
- Molecule 33: 50S ribosomal protein L5

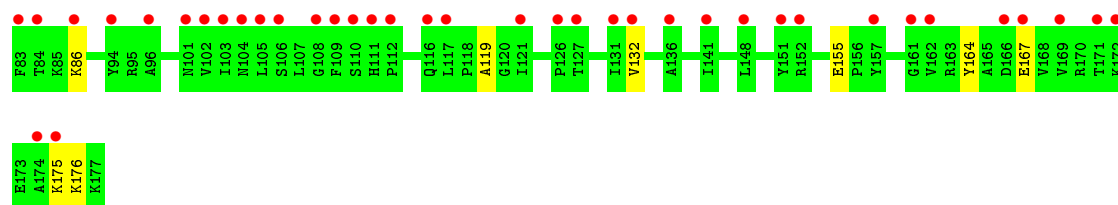
Chain DF: 81% 18% .



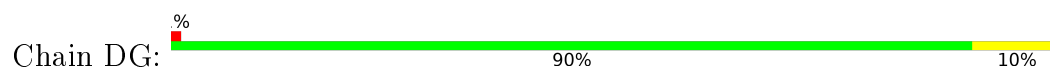
- Molecule 34: 50S ribosomal protein L6

Chain CG: 44% 89% 11% .

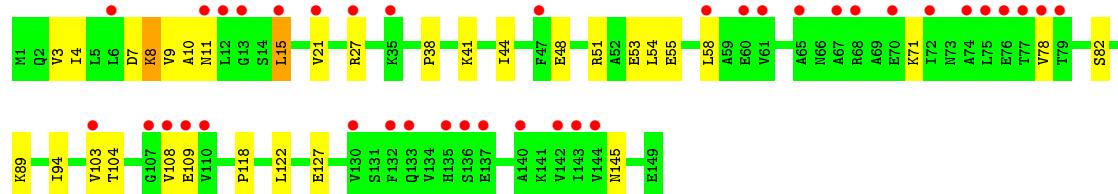
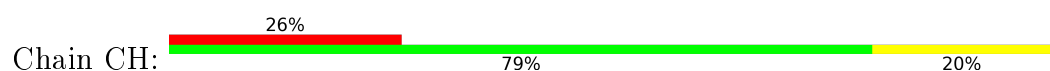




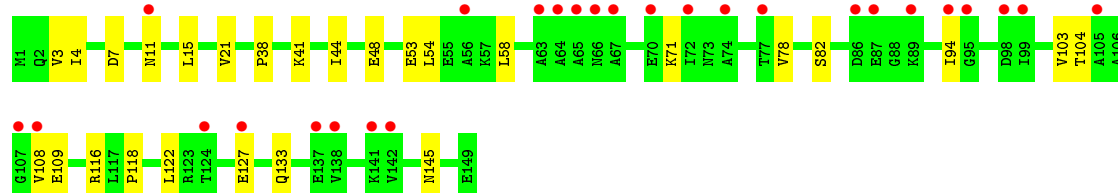
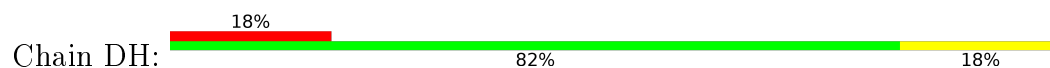
- Molecule 34: 50S ribosomal protein L6



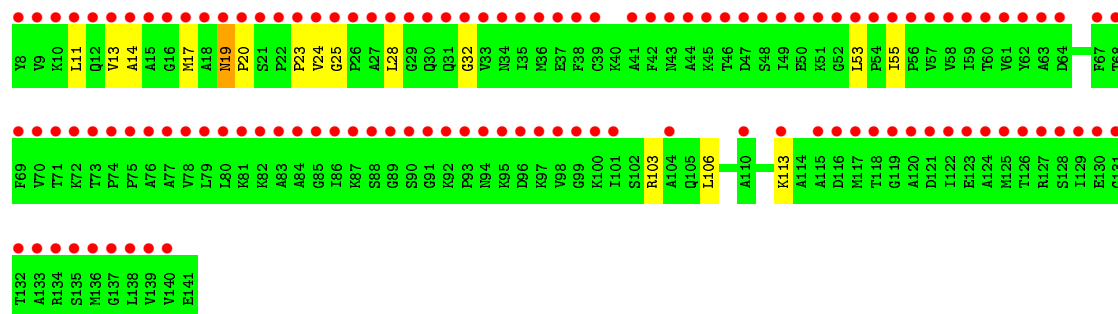
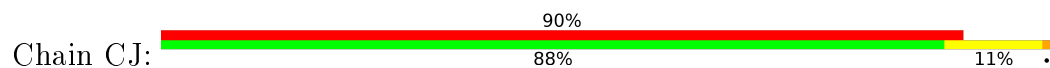
- Molecule 35: 50S ribosomal protein L9



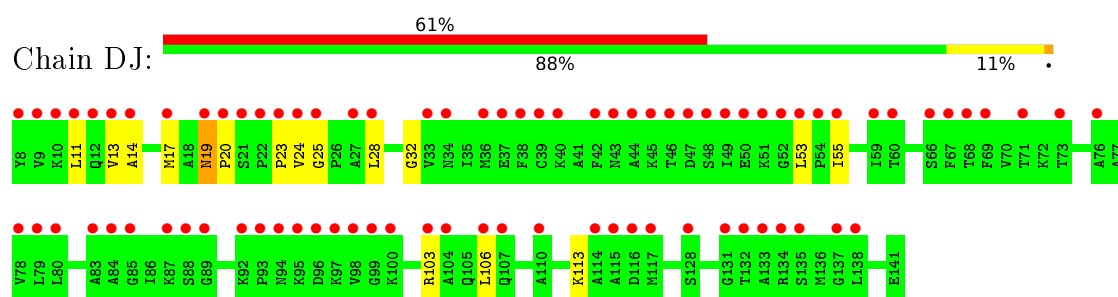
- Molecule 35: 50S ribosomal protein L9



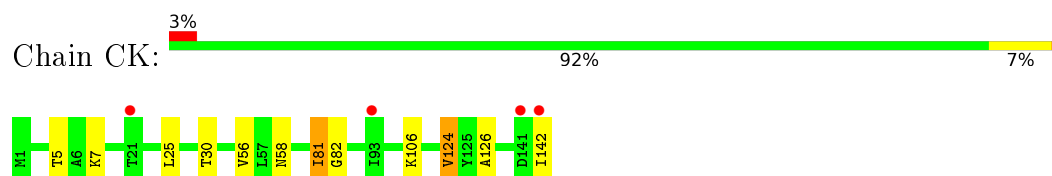
- Molecule 36: 50S ribosomal protein L11



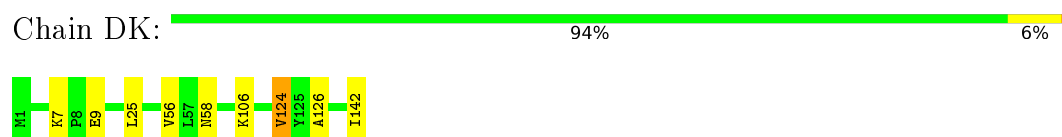
- Molecule 36: 50S ribosomal protein L11



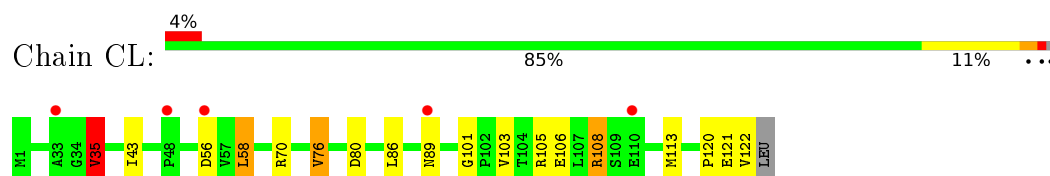
- Molecule 37: 50S ribosomal protein L13



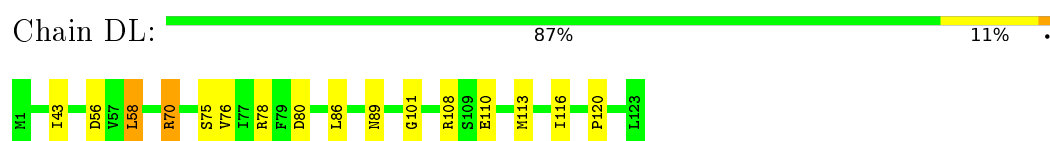
- Molecule 37: 50S ribosomal protein L13



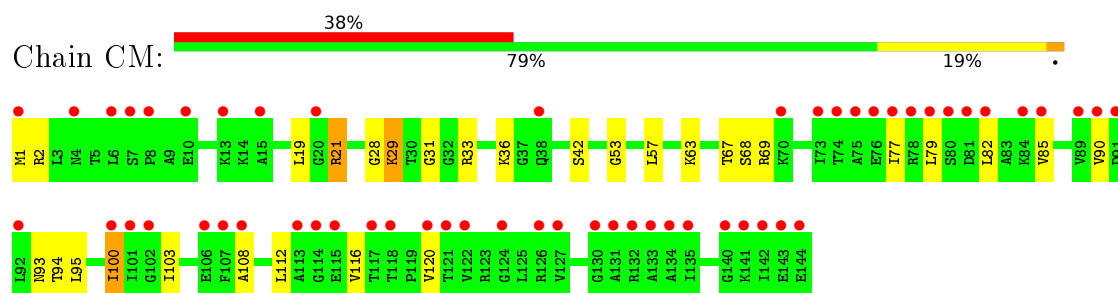
- Molecule 38: 50S ribosomal protein L14



- Molecule 38: 50S ribosomal protein L14

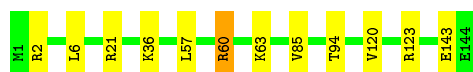


- Molecule 39: 50S ribosomal protein L15

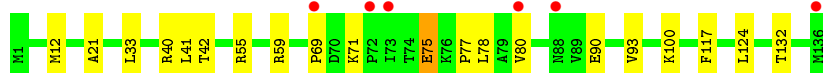
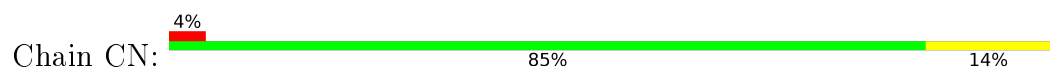


- Molecule 39: 50S ribosomal protein L15

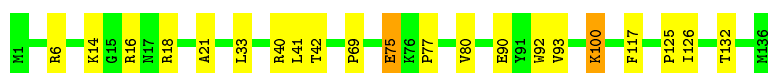
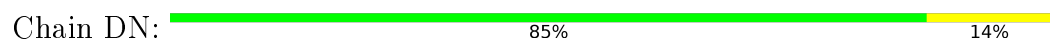




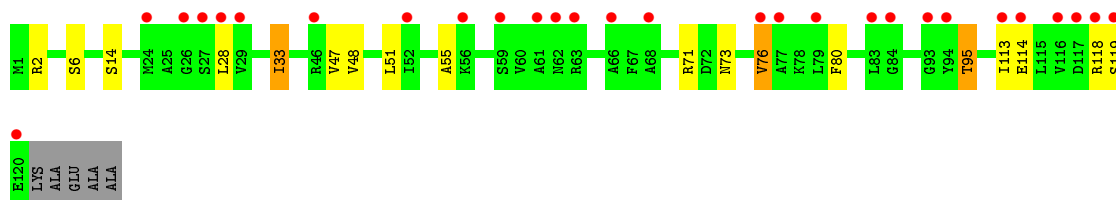
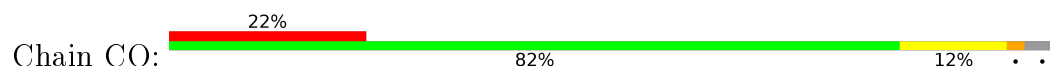
- Molecule 40: 50S ribosomal protein L16



- Molecule 40: 50S ribosomal protein L16



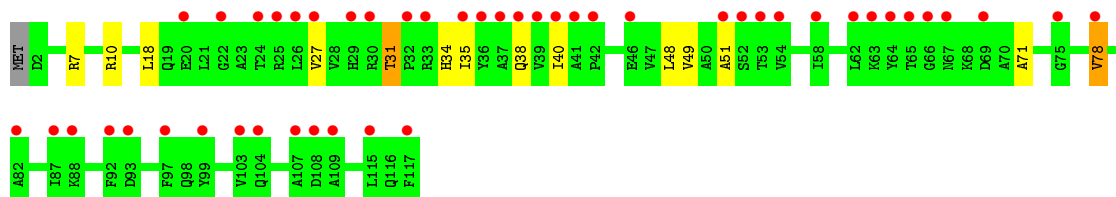
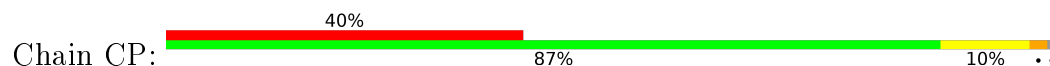
- Molecule 41: 50S ribosomal protein L17



- Molecule 41: 50S ribosomal protein L17

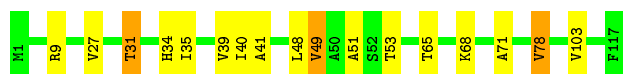


- Molecule 42: 50S ribosomal protein L18

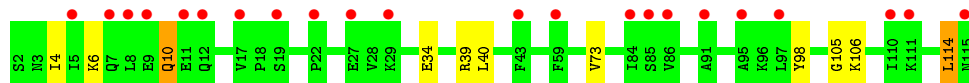
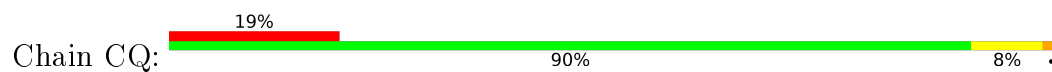


- Molecule 42: 50S ribosomal protein L18

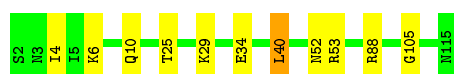




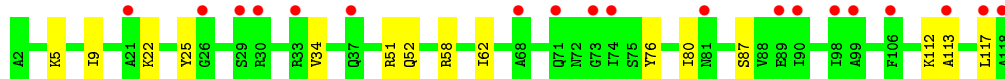
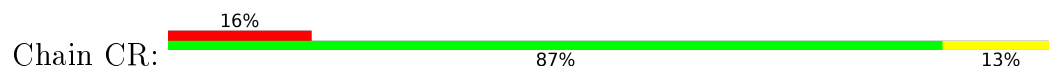
- Molecule 43: 50S ribosomal protein L19



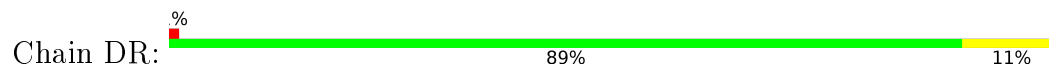
- Molecule 43: 50S ribosomal protein L19



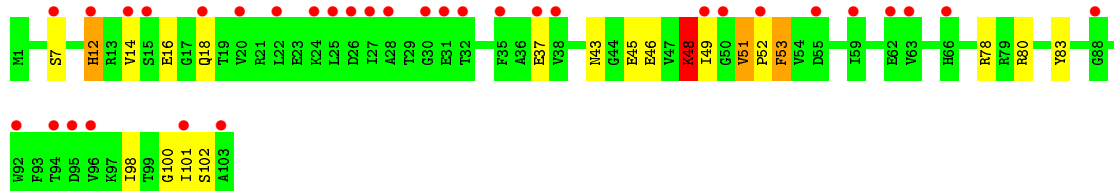
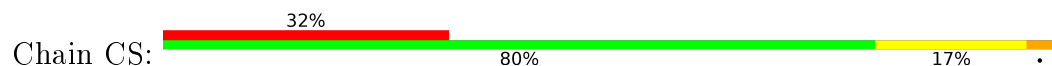
- Molecule 44: 50S ribosomal protein L20



- Molecule 44: 50S ribosomal protein L20



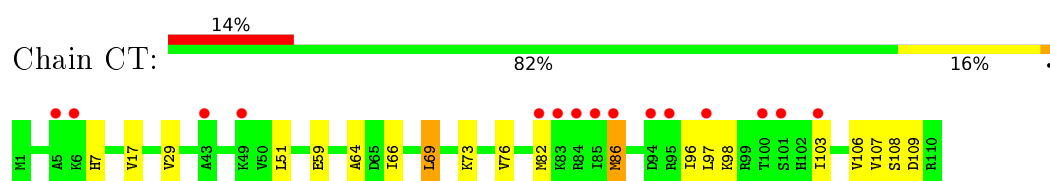
- Molecule 45: 50S ribosomal protein L21



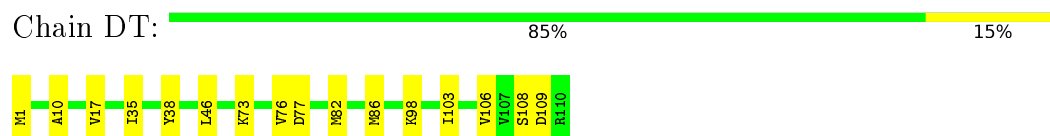
- Molecule 45: 50S ribosomal protein L21



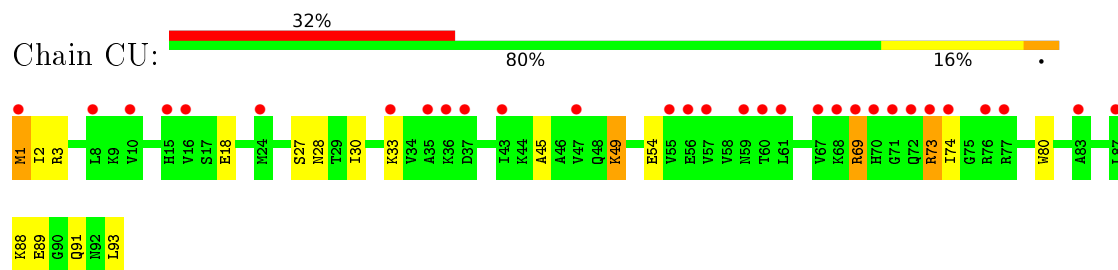
- Molecule 46: 50S ribosomal protein L22



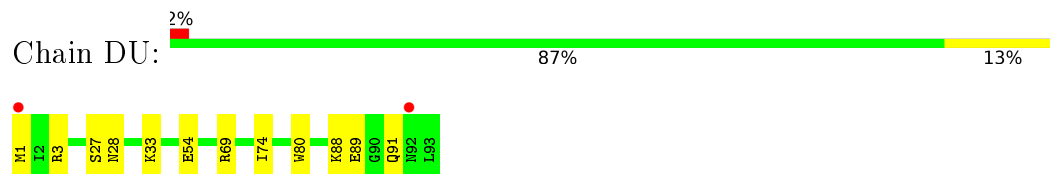
- Molecule 46: 50S ribosomal protein L22



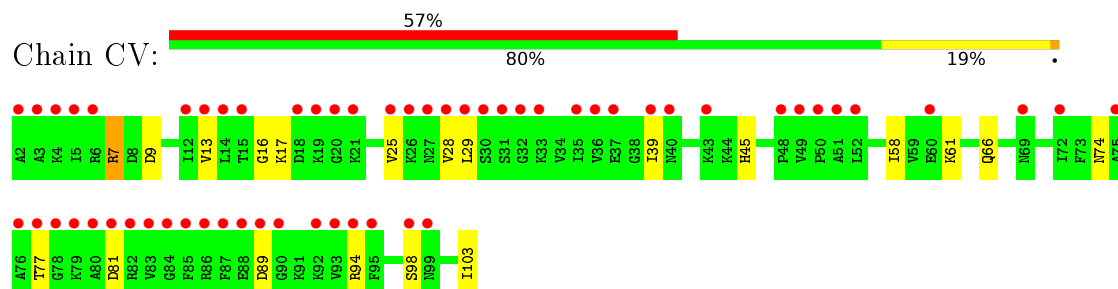
- Molecule 47: 50S ribosomal protein L23



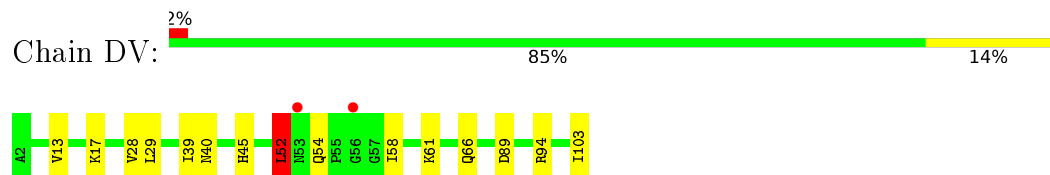
- Molecule 47: 50S ribosomal protein L23



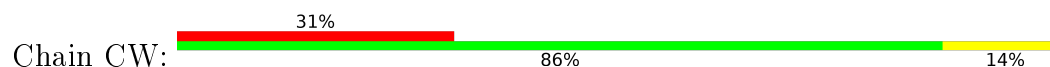
- Molecule 48: 50S ribosomal protein L24

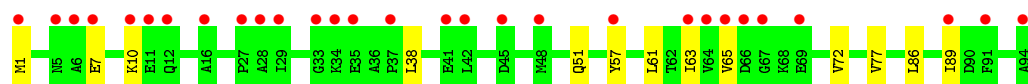


- Molecule 48: 50S ribosomal protein L24



- Molecule 49: 50S ribosomal protein L25





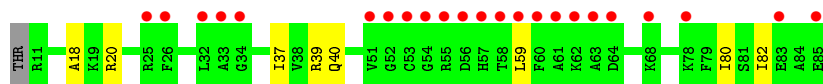
- Molecule 49: 50S ribosomal protein L25

Chain DW: 89% 11%



- Molecule 50: 50S ribosomal protein L27

Chain CX: 30% 88% 11%



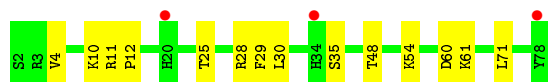
- Molecule 50: 50S ribosomal protein L27

Chain DX: % 87% 9%



- Molecule 51: 50S ribosomal protein L28

Chain CY: 4% 82% 18%



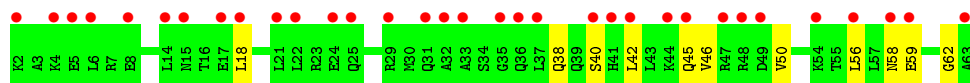
- Molecule 51: 50S ribosomal protein L28

Chain DY: 91% 9%



- Molecule 52: 50S ribosomal protein L29

Chain CZ: 53% 82% 18%



- Molecule 52: 50S ribosomal protein L29

Chain DZ: 2% 92% 8%

G2747	G2570	G2255	C2146	C2043	A1853	G1653
A2748	C2573	G2256	A2157	A2051	G1869	U1871
C2755	G2578	U2262	G2148	C2055	C1870	G1674
A2765	G2585	A2267	A2158	C2056	A1871	A1679
A2778	U2586	A2268	G2159	A2060	G1872	U1680
U2779	G2595	A2273	C2160	G2061	G1881	G1681
C2788	G2603	A2274	G2161	A2062	G1715	G1715
C2789	G2609	A2277	A2162	C2063	U1720	G1721
U2790	U2613	A2278	G2163	C2064	A1913	G1730
G2791	U2614	C2279	C2164	C2065	C1914	G1731
U2796	U2615	G2280	U2166	G2069	G1920	U1729
U2797	A2616	C2283	U2167	A2070	G1929	C1730
U2798	U2617	G2286	A2168	A2071	G1930	G1738
A2799	C2618	A2287	A2169	G2087	U1931	A1739
A2810	U2628	U2291	A2170	G2093	A1936	A1744
A2813	G2629	U2292	U2171	A2097	A1937	A1745
U2818	G2630	C2295	A2172	G2100	A1938	A1746
G2819	G2645	G2304	U2173	U2105	G1954	U1747
A2820	G2661	U2305	C2174	U2106	U1955	G1753
A2821	A2662	G2308	C2175	G2107	C1965	A1754
G2825	G2663	G2484	A2176	A2108	A1966	C1760
U2833	C2678	U2491	C2177	U2109	C1967	C1761
G2834	A2679	U2498	A2182	U2110	A1970	C1764
A2835	U2680	C2498	U2183	U2111	U1971	A1773
U2836	C2681	G2502	U2184	U2112	G1972	U1778
U2845	U2684	A2322	G2186	U2113	G1975	U1782
G2848	U2689	U2324	G2190	A2114	C1985	A1783
C2867	U2690	G2325	A2198	G2115	U1991	A1784
A2868	U2698	C2327	U2203	U2116	G1992	A1794
C2873	C2699	A2328	G2204	U2117	U1993	C1795
C2880	G2714	U2519	A2211	A2118	G1997	C1800
A2883	C2716	C2520	A2225	A2119	G2004	A1801
A2886	G2719	G2529	G2226	G2120	A2014	A1808
A2887	U2720	G2535	A2227	G2121	A2019	U1812
G2895	A2721	U2545	U2233	U2122	A2020	C1816
C2896	G2722	A2546	G2234	G2123	G2021	A1829
U2903	C2723	U2548	G2238	G2124	U2022	A1847
U	A2726	U2556	G2239	A2126	C2023	A1848
	A2727	G2567	U2243	G2127	U2030	
	U2728		U2244	G2128	A2031	
	G2744		G2250	U2131	G2032	
			G2251	U2132	A2033	
				G2133		
				A2134		
				A2135		
				G2141		
				C2145		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.41Å 435.70Å 625.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 3.00 48.61 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.61-3.00) 99.2 (48.61-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.01Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.172 , 0.193 0.184 , 0.207	Depositor DCC
R_{free} test set	4504 reflections (0.40%)	DCC
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 84.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	295261	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.97	8/36597 (0.0%)	0.86	4/57088 (0.0%)
1	BA	0.99	13/36572 (0.0%)	0.86	7/57049 (0.0%)
2	AB	0.45	0/1784	0.64	0/2403
2	BB	0.44	0/1784	0.64	0/2403
3	AC	0.46	0/1652	0.66	0/2225
3	BC	0.45	0/1652	0.68	0/2225
4	AD	0.43	0/1665	0.66	0/2227
4	BD	0.44	0/1665	0.67	0/2227
5	AE	0.47	0/1157	0.75	0/1557
5	BE	0.50	0/1118	0.80	0/1504
6	AF	0.45	0/881	0.70	1/1189 (0.1%)
6	BF	0.46	0/835	0.79	1/1128 (0.1%)
7	AG	0.45	0/1196	0.62	0/1602
7	BG	0.45	0/1196	0.62	0/1602
8	AH	0.43	0/989	0.70	0/1326
8	BH	0.42	0/989	0.69	0/1326
9	AI	0.44	0/1034	0.65	0/1375
9	BI	0.44	0/1034	0.65	0/1375
10	AJ	0.42	0/806	0.66	0/1089
10	BJ	0.48	0/797	0.70	0/1077
11	AK	0.43	0/893	0.63	0/1205
11	BK	0.42	0/893	0.67	0/1205
12	AL	0.44	0/960	0.72	0/1286
12	BL	0.44	0/960	0.73	0/1286
13	AM	0.50	0/893	0.73	0/1193
13	BM	0.49	0/893	0.72	0/1193
14	AN	0.45	0/817	0.64	0/1088
14	BN	0.43	0/817	0.63	0/1088
15	AO	0.45	0/722	0.61	0/964
15	BO	0.43	0/722	0.61	0/964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	AP	0.45	0/659	0.69	0/884
16	BP	0.48	0/659	0.76	0/884
17	AQ	0.46	0/658	0.72	0/881
17	BQ	0.50	0/658	0.76	0/881
18	AR	0.47	0/463	0.65	0/621
18	BR	0.48	0/463	0.65	0/621
19	AS	0.46	0/653	0.60	0/877
19	BS	0.46	0/653	0.61	0/877
20	AT	0.48	0/676	0.67	0/895
20	BT	0.53	0/671	0.69	0/888
21	AU	0.40	0/472	0.61	0/627
21	BU	0.38	0/472	0.62	0/627
22	C1	0.48	0/450	0.67	0/599
22	D1	0.58	0/450	0.72	0/599
23	C2	0.48	0/416	0.70	0/554
23	D2	0.47	0/421	0.69	0/561
24	C3	0.45	0/380	0.68	0/498
24	D3	0.56	0/380	0.76	0/498
25	C4	0.43	0/513	0.65	0/676
25	D4	0.50	0/513	0.68	0/676
26	C5	0.41	0/303	0.79	0/397
26	D5	0.50	0/303	0.78	0/397
27	C0	0.48	0/453	0.77	0/605
27	D0	0.62	0/467	0.79	1/623 (0.2%)
28	CB	0.91	0/2828	0.88	1/4410 (0.0%)
28	DB	1.01	0/2872	0.88	0/4478
29	CC	0.43	0/2122	0.73	0/2852
29	DC	0.48	0/2122	0.74	1/2852 (0.0%)
30	CD	0.42	0/1576	0.67	0/2119
30	DD	0.51	0/1576	0.68	0/2119
31	CA	1.02	39/69143 (0.1%)	0.87	11/107862 (0.0%)
32	CE	0.43	0/1571	0.70	0/2113
32	DE	0.49	0/1571	0.68	0/2113
33	CF	0.41	0/1435	0.67	0/1926
33	DF	0.46	0/1435	0.70	0/1926
34	CG	0.39	0/1343	0.66	0/1816
34	DG	0.43	0/1343	0.64	0/1816
35	CH	0.46	0/1121	0.68	1/1515 (0.1%)
35	DH	0.46	0/1121	0.67	0/1515
36	CJ	0.49	0/993	0.62	0/1341
36	DJ	0.49	0/993	0.62	0/1341
37	CK	0.41	0/1152	0.68	0/1551
37	DK	0.53	0/1152	0.71	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	CL	0.45	0/947	0.71	0/1268
38	DL	0.51	0/955	0.72	0/1279
39	CM	0.45	0/1062	0.73	1/1413 (0.1%)
39	DM	0.47	0/1062	0.70	0/1413
40	CN	0.45	0/1081	0.72	0/1443
40	DN	0.54	0/1092	0.76	0/1457
41	CO	0.44	0/973	0.68	0/1301
41	DO	0.54	0/1006	0.74	0/1345
42	CP	0.42	0/902	0.71	0/1209
42	DP	0.49	0/910	0.71	0/1219
43	CQ	0.40	0/929	0.69	1/1242 (0.1%)
43	DQ	0.45	0/929	0.69	0/1242
44	CR	0.43	0/960	0.65	0/1278
44	DR	0.54	0/960	0.68	0/1278
45	CS	0.42	0/829	0.73	0/1107
45	DS	0.51	0/829	0.74	0/1107
46	CT	0.41	0/864	0.70	0/1156
46	DT	0.53	0/864	0.69	0/1156
47	CU	0.44	0/745	0.71	0/994
47	DU	0.48	0/745	0.72	0/994
48	CV	0.44	0/788	0.75	0/1051
48	DV	0.47	0/788	0.75	0/1051
49	CW	0.40	0/766	0.65	0/1025
49	DW	0.49	0/766	0.68	0/1025
50	CX	0.40	0/576	0.65	0/762
50	DX	0.55	0/598	0.74	0/790
51	CY	0.41	0/635	0.70	0/848
51	DY	0.46	0/635	0.70	0/848
52	CZ	0.42	0/502	0.59	0/667
52	DZ	0.45	0/502	0.59	0/667
53	DI	0.50	0/1037	0.76	1/1402 (0.1%)
54	DA	1.14	49/69364 (0.1%)	0.91	15/108207 (0.0%)
All	All	0.91	109/309249 (0.0%)	0.84	46/462175 (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	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
31	CA	0	8
40	CN	0	1
40	DN	0	1
54	DA	0	41
All	All	0	56

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2095	A	O5'-C5'	-9.26	1.28	1.42
54	DA	12	U	C1'-N1	8.76	1.61	1.48
31	CA	1936	A	N9-C4	-8.51	1.32	1.37
54	DA	2097	A	O5'-C5'	-8.36	1.29	1.42
31	CA	2425	A	C3'-O3'	8.30	1.53	1.42
54	DA	1237	A	C3'-O3'	-7.96	1.31	1.42
31	CA	769	U	C1'-N1	7.92	1.60	1.48
31	CA	12	U	C1'-N1	7.83	1.60	1.48
31	CA	2225	A	C3'-O3'	7.82	1.53	1.42
54	DA	2585	U	C3'-O3'	7.54	1.52	1.42
31	CA	1777	U	C1'-N1	7.22	1.59	1.48
1	BA	5	U	C1'-N1	6.74	1.58	1.48
31	CA	2233	U	C1'-N1	6.72	1.58	1.48
54	DA	788	A	N7-C5	-6.68	1.35	1.39
31	CA	1379	U	C3'-O3'	6.61	1.51	1.42
1	AA	5	U	C1'-N1	6.58	1.58	1.48
31	CA	1658	C	C1'-N1	6.40	1.58	1.48
31	CA	692	C	C1'-N1	6.35	1.58	1.48
1	BA	1493	A	C3'-O3'	6.34	1.51	1.42
54	DA	1607	C	N1-C6	6.22	1.40	1.37
54	DA	12	U	P-O5'	6.16	1.66	1.59
31	CA	946	C	C1'-N1	6.15	1.57	1.48
1	AA	1354	U	C1'-N1	6.12	1.57	1.48
54	DA	1607	C	P-O5'	-6.10	1.53	1.59
54	DA	2585	U	C1'-N1	6.10	1.57	1.48
54	DA	2585	U	N1-C2	6.07	1.44	1.38
31	CA	1825	U	C1'-N1	6.07	1.57	1.48
54	DA	21	A	N3-C4	6.05	1.38	1.34
54	DA	1965	C	C3'-O3'	-6.05	1.33	1.42
31	CA	451	U	C1'-N1	5.96	1.57	1.48
54	DA	12	U	N1-C2	5.95	1.44	1.38
31	CA	404	A	C3'-O3'	5.91	1.50	1.42
1	AA	956	U	C1'-N1	5.89	1.57	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2017	U	C1'-N1	5.89	1.57	1.48
31	CA	546	U	C1'-N1	5.88	1.57	1.48
54	DA	2547	A	O5'-C5'	-5.83	1.33	1.42
1	BA	1008	U	O5'-C5'	-5.82	1.33	1.42
54	DA	613	A	N9-C4	5.80	1.41	1.37
1	BA	1397	C	N1-C2	5.76	1.46	1.40
31	CA	1790	C	C1'-N1	5.75	1.57	1.48
54	DA	1188	U	C3'-O3'	-5.74	1.34	1.42
54	DA	1679	A	N7-C5	-5.72	1.35	1.39
54	DA	653	U	C1'-N1	5.72	1.57	1.48
54	DA	578	G	N7-C5	-5.70	1.35	1.39
31	CA	20	C	C1'-N1	5.70	1.57	1.48
1	BA	306	A	C5-C6	5.67	1.46	1.41
1	BA	306	A	N3-C4	5.66	1.38	1.34
54	DA	2127	G	C3'-O3'	5.65	1.50	1.42
54	DA	2867	G	C3'-O3'	5.64	1.50	1.42
31	CA	1314	C	C1'-N1	5.63	1.57	1.48
54	DA	1313	U	C1'-N1	5.61	1.57	1.48
1	AA	632	U	C1'-N1	5.59	1.57	1.48
54	DA	2051	A	N7-C5	-5.59	1.35	1.39
31	CA	653	U	C1'-N1	5.58	1.57	1.48
31	CA	2146	C	C3'-O3'	5.58	1.50	1.42
1	AA	1397	C	N1-C6	5.54	1.40	1.37
1	AA	955	U	C1'-N1	5.51	1.57	1.48
31	CA	691	C	C1'-N1	5.50	1.57	1.48
1	BA	209	U	C1'-N1	5.50	1.57	1.48
54	DA	2402	U	P-O5'	5.50	1.65	1.59
1	BA	842	U	C3'-O3'	5.50	1.49	1.42
31	CA	817	C	C1'-N1	5.49	1.56	1.48
31	CA	2456	C	C1'-N1	5.47	1.56	1.48
54	DA	2402	U	N1-C2	5.46	1.43	1.38
54	DA	271	G	C3'-O3'	5.45	1.49	1.42
54	DA	784	G	C3'-O3'	5.43	1.49	1.42
54	DA	736	C	C3'-O3'	-5.42	1.34	1.42
31	CA	1376	C	C1'-N1	5.41	1.56	1.48
54	DA	1441	G	O5'-C5'	-5.41	1.34	1.42
31	CA	995	C	O5'-C5'	-5.41	1.34	1.42
1	BA	956	U	C1'-N1	5.38	1.56	1.48
1	BA	1354	U	C1'-N1	5.38	1.56	1.48
1	BA	955	U	C1'-N1	5.37	1.56	1.48
54	DA	2004	G	N3-C4	5.37	1.39	1.35
31	CA	2354	C	C1'-N1	5.36	1.56	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	221	C	C1'-N1	5.30	1.56	1.48
54	DA	1571	A	N7-C5	-5.30	1.36	1.39
54	DA	538	A	N7-C5	-5.30	1.36	1.39
54	DA	2402	U	C1'-N1	5.29	1.56	1.48
31	CA	1788	C	C1'-N1	5.28	1.56	1.48
31	CA	790	U	C1'-N1	5.26	1.56	1.48
31	CA	1352	U	C1'-N1	5.23	1.56	1.48
31	CA	1994	C	C1'-N1	5.23	1.56	1.48
1	AA	221	C	C1'-N1	5.20	1.56	1.48
1	AA	532	A	N9-C4	5.19	1.41	1.37
54	DA	2211	A	C3'-O3'	5.19	1.49	1.42
31	CA	1838	C	N1-C2	5.18	1.45	1.40
31	CA	2680	U	C3'-O3'	5.18	1.49	1.42
54	DA	817	C	C3'-O3'	-5.18	1.34	1.42
54	DA	1920	C	C1'-N1	5.15	1.56	1.48
31	CA	1306	C	C1'-N1	5.14	1.56	1.48
54	DA	1534	U	C1'-N1	5.13	1.56	1.48
54	DA	2810	A	N7-C5	-5.11	1.36	1.39
54	DA	532	A	N7-C5	-5.11	1.36	1.39
31	CA	1938	A	N9-C4	5.09	1.41	1.37
54	DA	2617	U	O5'-C5'	-5.09	1.34	1.42
54	DA	275	C	C1'-N1	5.09	1.56	1.48
31	CA	1971	U	C1'-N1	5.07	1.56	1.48
54	DA	1412	U	C1'-N1	5.07	1.56	1.48
54	DA	1584	U	C1'-N1	5.06	1.56	1.48
1	BA	1067	A	C3'-O3'	5.06	1.49	1.42
31	CA	678	C	C1'-N1	5.06	1.56	1.48
54	DA	2868	A	N7-C5	-5.04	1.36	1.39
54	DA	207	A	C3'-O3'	-5.04	1.35	1.42
54	DA	2227	A	N7-C5	-5.04	1.36	1.39
31	CA	2215	C	C1'-N1	5.02	1.56	1.48
54	DA	353	C	C1'-N1	5.02	1.56	1.48
54	DA	2570	G	C6-N1	-5.00	1.36	1.39
54	DA	34	U	O3'-P	-5.00	1.55	1.61

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	CB	15	A	O4'-C1'-N9	10.03	116.22	108.20
54	DA	1936	A	O4'-C1'-N9	8.20	114.76	108.20
1	BA	1362	A	C1'-O4'-C4'	-7.38	104.00	109.90
1	AA	1	A	OP1-P-OP2	-7.19	108.81	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	271	G	P-O3'-C3'	7.11	128.24	119.70
54	DA	892	A	OP1-P-OP2	-7.08	108.98	119.60
53	DI	132	TYR	C-N-CA	7.07	139.38	121.70
31	CA	892	A	OP1-P-OP2	-6.99	109.12	119.60
54	DA	1	G	OP1-P-OP2	-6.95	109.18	119.60
1	AA	413	G	C1'-O4'-C4'	-6.88	104.40	109.90
1	BA	2	A	OP1-P-OP2	-6.85	109.33	119.60
54	DA	2825	G	O4'-C1'-N9	6.82	113.66	108.20
54	DA	271	G	P-O3'-C3'	6.63	127.66	119.70
54	DA	784	G	P-O3'-C3'	6.62	127.65	119.70
31	CA	2035	G	C1'-O4'-C4'	-6.60	104.62	109.90
29	DC	156	ARG	CB-CG-CD	-6.40	94.96	111.60
31	CA	974	G	N9-C1'-C2'	6.39	122.31	114.00
54	DA	2406	A	C5'-C4'-O4'	-5.91	102.01	109.10
31	CA	2225	A	P-O3'-C3'	5.84	126.70	119.70
31	CA	512	G	O4'-C1'-N9	5.80	112.84	108.20
31	CA	784	G	P-O3'-C3'	5.80	126.66	119.70
31	CA	451	U	C1'-O4'-C4'	-5.70	105.34	109.90
54	DA	1985	C	O4'-C1'-N1	5.69	112.75	108.20
31	CA	1128	G	C1'-O4'-C4'	-5.59	105.42	109.90
54	DA	199	A	C1'-O4'-C4'	-5.52	105.48	109.90
27	D0	10	THR	N-CA-CB	-5.52	99.81	110.30
54	DA	1266	G	C3'-C2'-C1'	-5.46	97.13	101.50
1	BA	328	C	C1'-O4'-C4'	-5.41	105.57	109.90
54	DA	2848	G	O4'-C1'-N9	5.40	112.52	108.20
1	BA	485	U	O4'-C1'-N1	5.38	112.51	108.20
39	CM	68	SER	C-N-CA	5.37	135.13	121.70
54	DA	807	U	C4'-C3'-C2'	-5.35	97.25	102.60
6	AF	55	HIS	N-CA-C	-5.19	97.00	111.00
54	DA	512	G	O4'-C1'-N9	5.18	112.35	108.20
1	AA	841	C	P-O3'-C3'	5.15	125.88	119.70
54	DA	679	C	O4'-C1'-N1	5.15	112.32	108.20
31	CA	2680	U	P-O3'-C3'	5.11	125.83	119.70
1	AA	686	U	C1'-O4'-C4'	-5.10	105.82	109.90
54	DA	729	G	C1'-O4'-C4'	-5.10	105.82	109.90
6	BF	55	HIS	N-CA-C	-5.09	97.25	111.00
31	CA	404	A	P-O3'-C3'	5.06	125.77	119.70
43	CQ	114	LEU	CA-CB-CG	5.05	126.92	115.30
1	BA	686	U	C1'-O4'-C4'	-5.05	105.86	109.90
35	CH	8	LYS	C-N-CA	5.03	134.28	121.70
1	BA	842	U	P-O3'-C3'	5.02	125.73	119.70
1	BA	1362	A	O4'-C1'-N9	5.01	112.21	108.20

There are no chirality outliers.

All (56) 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
1	BA	1432	G	Sidechain
1	BA	898	G	Sidechain
31	CA	2267	A	Sidechain
31	CA	2444	G	Sidechain
31	CA	250	G	Sidechain
31	CA	463	G	Sidechain
31	CA	555	G	Sidechain
31	CA	704	G	Sidechain
31	CA	726	G	Sidechain
31	CA	757	G	Sidechain
40	CN	69	PRO	Mainchain
54	DA	1142	A	Sidechain
54	DA	1212	G	Sidechain
54	DA	1283	G	Sidechain
54	DA	1324	G	Sidechain
54	DA	15	G	Sidechain
54	DA	1631	G	Sidechain
54	DA	1681	G	Sidechain
54	DA	1753	G	Sidechain
54	DA	1761	C	Sidechain
54	DA	177	G	Sidechain
54	DA	1937	A	Sidechain
54	DA	1938	A	Sidechain
54	DA	1954	G	Sidechain
54	DA	221	A	Sidechain
54	DA	2250	G	Sidechain
54	DA	2267	A	Sidechain
54	DA	2323	G	Sidechain
54	DA	2375	G	Sidechain
54	DA	2481	G	Sidechain
54	DA	249	C	Sidechain
54	DA	250	G	Sidechain
54	DA	2529	G	Sidechain
54	DA	2578	G	Sidechain
54	DA	2595	G	Sidechain
54	DA	2645	G	Sidechain
54	DA	2719	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
54	DA	2727	A	Sidechain
54	DA	2728	U	Sidechain
54	DA	2835	A	Sidechain
54	DA	2848	G	Sidechain
54	DA	463	G	Sidechain
54	DA	512	G	Sidechain
54	DA	515	A	Sidechain
54	DA	555	G	Sidechain
54	DA	670	A	Sidechain
54	DA	704	G	Sidechain
54	DA	726	G	Sidechain
54	DA	858	G	Sidechain
54	DA	956	G	Sidechain
54	DA	983	A	Sidechain
54	DA	984	A	Sidechain
40	DN	69	PRO	Mainchain

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	32933	0	16592	113	0
1	BA	32911	0	16581	115	0
2	AB	1753	0	1780	7	0
2	BB	1753	0	1780	9	0
3	AC	1625	0	1696	13	0
3	BC	1625	0	1696	17	0
4	AD	1643	0	1707	11	0
4	BD	1643	0	1707	17	0
5	AE	1144	0	1185	14	0
5	BE	1105	0	1148	25	0
6	AF	862	0	864	7	0
6	BF	817	0	808	7	0
7	AG	1182	0	1238	7	0
7	BG	1182	0	1238	4	0
8	AH	979	0	1031	6	0
8	BH	979	0	1031	3	0
9	AI	1022	0	1070	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	BI	1022	0	1070	7	0
10	AJ	796	0	836	11	0
10	BJ	787	0	828	8	0
11	AK	877	0	887	13	0
11	BK	877	0	887	15	0
12	AL	957	0	1017	5	0
12	BL	957	0	1017	8	0
13	AM	884	0	941	13	0
13	BM	884	0	941	18	0
14	AN	805	0	844	8	0
14	BN	805	0	844	7	0
15	AO	714	0	734	0	0
15	BO	714	0	734	0	0
16	AP	649	0	666	2	0
16	BP	649	0	666	7	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	13	0
18	AR	456	0	478	3	0
18	BR	456	0	478	2	0
19	AS	638	0	665	4	0
19	BS	638	0	665	6	0
20	AT	670	0	719	3	0
20	BT	665	0	714	4	0
21	AU	465	0	491	3	0
21	BU	465	0	491	3	0
22	C1	444	0	458	5	0
22	D1	444	0	458	9	0
23	C2	409	0	440	6	0
23	D2	414	0	442	6	0
24	C3	377	0	418	3	0
24	D3	377	0	418	3	0
25	C4	504	0	572	2	0
25	D4	504	0	572	2	0
26	C5	302	0	340	6	0
26	D5	302	0	340	2	0
27	C0	449	0	488	3	0
27	D0	463	0	504	2	0
28	CB	2529	0	1281	6	0
28	DB	2569	0	1301	3	0
29	CC	2083	0	2154	24	0
29	DC	2083	0	2154	12	0
30	CD	1565	0	1614	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	DD	1576	0	1627	15	0
31	CA	62229	0	31317	224	0
32	CE	1552	0	1619	18	0
32	DE	1552	0	1619	9	0
33	CF	1411	0	1444	14	0
33	DF	1411	0	1444	11	0
34	CG	1323	0	1371	8	0
34	DG	1323	0	1371	8	0
35	CH	1110	0	1148	10	0
35	DH	1110	0	1148	9	0
36	CJ	979	0	1028	5	0
36	DJ	979	0	1028	5	0
37	CK	1129	0	1162	8	0
37	DK	1129	0	1162	4	0
38	CL	938	0	1012	8	0
38	DL	946	0	1023	7	0
39	CM	1053	0	1129	19	0
39	DM	1053	0	1129	6	0
40	CN	1075	0	1154	9	0
40	DN	1092	0	1177	13	0
41	CO	960	0	1000	6	0
41	DO	993	0	1034	5	0
42	CP	892	0	923	6	0
42	DP	900	0	935	11	0
43	CQ	917	0	962	6	0
43	DQ	917	0	962	7	0
44	CR	947	0	1019	11	0
44	DR	947	0	1019	13	0
45	CS	816	0	839	12	0
45	DS	816	0	839	7	0
46	CT	857	0	922	9	0
46	DT	857	0	922	9	0
47	CU	739	0	807	8	0
47	DU	739	0	807	7	0
48	CV	780	0	831	7	0
48	DV	780	0	831	6	0
49	CW	753	0	780	5	0
49	DW	753	0	780	4	0
50	CX	569	0	581	3	0
50	DX	591	0	606	10	0
51	CY	625	0	652	8	0
51	DY	625	0	652	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	CZ	501	0	531	3	0
52	DZ	501	0	531	2	0
53	DI	1023	0	1052	15	0
54	DA	62423	0	31411	176	0
55	AA	72	0	0	0	0
55	BA	45	0	0	0	0
55	CA	156	0	0	0	0
55	CB	3	0	0	0	0
55	DA	183	0	0	0	0
55	DB	9	0	0	0	0
55	DD	1	0	0	0	0
55	DM	1	0	0	0	0
55	DR	2	0	0	0	0
56	AA	13	0	18	1	0
56	BA	13	0	18	1	0
56	DA	26	0	36	3	0
56	DQ	13	0	18	0	0
56	DR	13	0	18	5	0
56	DS	13	0	18	3	0
57	AA	16	0	28	3	0
57	DA	40	0	70	3	0
57	DE	16	0	28	0	0
57	DK	8	0	14	0	0
57	DN	8	0	14	1	0
57	DS	8	0	14	0	0
57	DT	16	0	28	0	0
58	AA	24	0	48	0	0
58	DA	66	0	132	7	0
58	DM	6	0	12	0	0
59	AA	64	1	42	2	0
59	BA	64	1	42	0	0
60	AB	1	0	0	0	0
60	C5	1	0	0	0	0
60	D5	1	0	0	0	0
61	AL	7	0	10	0	0
61	D1	7	0	10	1	0
61	D3	7	0	10	0	0
61	DA	35	0	50	0	0
61	DL	7	0	10	0	0
61	DP	7	0	10	1	0
61	DQ	7	0	10	0	0
62	D1	4	0	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	DA	32	0	48	1	0
62	DB	12	0	18	0	0
63	D1	10	0	14	2	0
63	DA	60	0	84	4	0
63	DS	10	0	14	1	0
63	DU	10	0	14	3	0
64	DA	40	0	76	2	0
65	DA	32	0	44	1	0
66	DA	12	0	9	0	0
67	DA	11	0	5	0	0
68	DA	8	0	12	1	0
69	AA	501	0	0	0	0
69	AC	4	0	0	0	0
69	AD	2	0	0	0	0
69	AE	5	0	0	0	0
69	AG	1	0	0	0	0
69	AH	1	0	0	0	0
69	AJ	2	0	0	0	0
69	AK	6	0	0	0	0
69	AL	10	0	0	0	0
69	AM	5	0	0	2	0
69	AN	6	0	0	1	0
69	AO	2	0	0	0	0
69	AP	2	0	0	0	0
69	AR	1	0	0	0	0
69	AT	3	0	0	0	0
69	AU	3	0	0	0	0
69	BA	287	0	0	1	0
69	BD	13	0	0	0	0
69	BE	1	0	0	0	0
69	BF	2	0	0	0	0
69	BK	2	0	0	0	0
69	BL	4	0	0	0	0
69	BN	2	0	0	0	0
69	BO	1	0	0	0	0
69	BP	3	0	0	0	0
69	BT	2	0	0	0	0
69	BU	2	0	0	0	0
69	C3	4	0	0	0	0
69	C4	1	0	0	0	0
69	CA	691	0	0	3	0
69	CB	13	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	CC	10	0	0	0	0
69	CD	6	0	0	0	0
69	CE	5	0	0	0	0
69	CL	1	0	0	0	0
69	CM	4	0	0	0	0
69	CO	2	0	0	0	0
69	CU	3	0	0	0	0
69	CV	1	0	0	0	0
69	CW	1	0	0	0	0
69	CY	1	0	0	0	0
69	D0	24	0	0	0	0
69	D1	43	0	0	0	0
69	D2	6	0	0	0	0
69	D3	22	0	0	0	0
69	D4	39	0	0	0	0
69	D5	8	0	0	0	0
69	DA	4840	0	0	15	0
69	DB	209	0	0	1	0
69	DC	100	0	0	1	0
69	DD	98	0	0	2	0
69	DE	61	0	0	0	0
69	DF	15	0	0	0	0
69	DG	6	0	0	0	0
69	DH	2	0	0	0	0
69	DK	65	0	0	1	0
69	DL	52	0	0	1	0
69	DM	63	0	0	0	0
69	DN	72	0	0	0	0
69	DO	44	0	0	0	0
69	DP	38	0	0	0	0
69	DQ	33	0	0	0	0
69	DR	62	0	0	1	0
69	DS	46	0	0	2	0
69	DT	69	0	0	1	0
69	DU	18	0	0	0	0
69	DV	20	0	0	0	0
69	DW	31	0	0	0	0
69	DX	25	0	0	1	0
69	DY	9	0	0	0	0
69	DZ	8	0	0	0	0
All	All	295259	2	194493	1263	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 (1263) 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)
45:CS:14:VAL:HG21	45:CS:98:ILE:HG13	1.27	1.10
31:CA:1005:C:O2'	37:CK:30:THR:HG21	1.61	1.00
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.46	0.97
31:CA:1847:A:HO2'	31:CA:1848:A:H8	0.98	0.95
31:CA:528:A:C2	31:CA:2043:C:H4'	2.00	0.95
54:DA:2796:U:H3	54:DA:2799:A:H61	1.11	0.95
54:DA:1847:A:HO2'	54:DA:1848:A:H8	0.98	0.94
2:BB:20:THR:HA	2:BB:39:HIS:CE1	2.02	0.94
26:C5:3:VAL:HG11	31:CA:2539:C:H5'	1.50	0.94
11:BK:88:GLY:H	11:BK:114:THR:HG22	1.34	0.93
31:CA:2796:U:H3	31:CA:2799:A:H61	1.14	0.93
39:CM:77:ILE:HD11	39:CM:108:ALA:HB1	1.50	0.92
31:CA:1936:A:H2	31:CA:1943:U:H3	0.96	0.91
14:AN:66:GLN:HB2	69:AN:206:HOH:O	1.70	0.90
45:CS:14:VAL:CG2	45:CS:98:ILE:HG13	2.00	0.90
1:AA:1492:A:H5''	12:AL:44:LYS:HG2	1.53	0.89
1:AA:307:C:N4	57:AA:1676:MPD:H12	1.88	0.88
12:BL:80:ILE:HD12	12:BL:97:THR:HG22	1.54	0.88
54:DA:1913:A:H4'	54:DA:1913:A:OP1	1.72	0.87
31:CA:135:U:H3	31:CA:144:A:H61	1.20	0.87
54:DA:135:U:H3	54:DA:144:A:H61	1.20	0.87
46:CT:86:MET:HB2	46:CT:96:ILE:HD11	1.54	0.86
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.59	0.85
54:DA:2255:G:H21	68:DA:3220:TRS:H12	1.42	0.85
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.58	0.84
44:DR:20:GLN:HG3	56:DR:202:PG4:H42	1.58	0.84
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.59	0.83
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.61	0.82
31:CA:740:C:H5'	31:CA:1784:A:H3'	1.61	0.82
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.59	0.81
45:CS:14:VAL:HG21	45:CS:98:ILE:CG1	2.10	0.81
1:BA:841:C:H3'	1:BA:842:U:H5''	1.62	0.80
1:BA:664:G:H22	1:BA:741:G:H1	1.29	0.80
2:BB:20:THR:HA	2:BB:39:HIS:HE1	1.46	0.80
31:CA:1779:U:H5	31:CA:1784:A:N7	1.80	0.79
13:BM:6:GLY:HA3	13:BM:66:GLU:HG3	1.63	0.79
1:BA:1052:G:H22	1:BA:1206:G:H1	1.30	0.79
3:BC:123:GLN:HB3	3:BC:128:VAL:HG21	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1305:G:H21	1:AA:1332:A:H2	1.32	0.78
13:AM:33:ILE:HD11	13:AM:63:PHE:HE1	1.48	0.78
44:DR:28:ARG:HD3	69:DR:302:HOH:O	1.85	0.77
1:AA:664:G:H22	1:AA:741:G:H1	1.31	0.77
31:CA:1936:A:H2	31:CA:1943:U:N3	1.80	0.77
8:BH:87:LYS:HB2	8:BH:125:ILE:HD11	1.67	0.77
13:BM:114:LYS:HB3	13:BM:115:PRO:HD3	1.67	0.76
32:DE:33:VAL:HG22	57:DA:3192:MPD:H12	1.66	0.76
17:BQ:14:SER:HB3	17:BQ:22:VAL:HG12	1.68	0.76
1:BA:1305:G:H21	1:BA:1332:A:H2	1.32	0.76
10:AJ:7:ARG:HB3	10:AJ:101:SER:HB2	1.67	0.75
1:AA:202:G:HO2'	1:AA:468:A:H8	1.33	0.75
1:BA:522:C:H5	12:BL:50:ARG:HH12	1.33	0.75
31:CA:846:U:H1'	31:CA:847:U:H5	1.52	0.74
8:AH:87:LYS:HB2	8:AH:125:ILE:HD11	1.69	0.74
30:CD:133:THR:HG22	31:CA:1993:U:H4'	1.68	0.73
54:DA:2127:G:H4'	54:DA:2128:G:OP1	1.89	0.72
1:BA:841:C:H3'	1:BA:842:U:C5'	2.19	0.72
54:DA:568:U:H1'	54:DA:2030:6MZ:H9C1	1.72	0.71
24:C3:12:ARG:HD2	24:C3:44:VAL:HG11	1.71	0.71
34:CG:24:ILE:HD11	34:CG:43:VAL:HG11	1.71	0.71
69:DD:443:HOH:O	54:DA:1671:U:H4'	1.90	0.71
31:CA:1105:U:H2'	31:CA:1106:G:H8	1.56	0.71
34:DG:24:ILE:HD11	34:DG:43:VAL:HG11	1.74	0.70
54:DA:1105:U:H2'	54:DA:1106:G:H8	1.56	0.70
4:AD:107:PHE:HB3	4:AD:145:ILE:HD11	1.74	0.70
5:AE:77:ASN:HB2	5:AE:82:GLN:NE2	2.07	0.69
22:C1:16:ARG:HA	31:CA:2046:G:H5'	1.73	0.69
1:BA:1060:U:C5	3:BC:2:GLY:HA3	2.28	0.69
34:CG:76:VAL:O	34:CG:80:THR:HG22	1.92	0.69
11:BK:89:PRO:HG3	21:BU:32:VAL:HG11	1.74	0.69
29:CC:29:PRO:HG2	29:CC:34:LEU:HD11	1.74	0.69
46:CT:59:GLU:HA	46:CT:64:ALA:HA	1.73	0.69
1:BA:502:A:OP1	12:BL:115:SER:HB2	1.93	0.68
5:BE:72:ILE:HG12	5:BE:145:GLU:HG3	1.75	0.68
65:DA:3202:1PE:H231	69:DA:3678:HOH:O	1.92	0.68
35:DH:41:LYS:HA	35:DH:44:ILE:HG12	1.76	0.68
38:DL:70:ARG:HD3	38:DL:76:VAL:HG22	1.76	0.68
6:BF:38:ARG:HH12	6:BF:99:ALA:HB3	1.59	0.68
29:DC:29:PRO:HG2	29:DC:34:LEU:HD11	1.75	0.68
4:BD:107:PHE:HB3	4:BD:145:ILE:HD11	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:502:A:OP1	12:AL:115:SER:HB2	1.94	0.67
31:CA:2291:U:H2'	31:CA:2292:U:C6	2.28	0.67
47:CU:54:GLU:HB3	47:CU:88:LYS:HD2	1.77	0.67
35:CH:41:LYS:HA	35:CH:44:ILE:HG12	1.75	0.67
29:CC:105:LEU:H	29:CC:105:LEU:HD12	1.59	0.67
12:BL:65:SER:HB2	12:BL:82:ILE:HD11	1.75	0.67
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.77	0.67
5:BE:77:ASN:HB2	5:BE:82:GLN:NE2	2.09	0.67
31:CA:1105:U:H2'	31:CA:1106:G:C8	2.30	0.67
54:DA:2033:A:H5'	69:DA:3362:HOH:O	1.96	0.66
13:AM:33:ILE:HD11	13:AM:63:PHE:CE1	2.29	0.66
69:DK:315:HOH:O	44:DR:93:LYS:HD2	1.93	0.66
31:CA:1394:U:H4'	31:CA:1603:A:H4'	1.78	0.66
35:CH:15:LEU:HD22	35:CH:15:LEU:H	1.60	0.66
5:AE:90:THR:HG22	5:AE:91:GLY:H	1.60	0.66
47:DU:54:GLU:HB3	47:DU:88:LYS:HD2	1.77	0.66
46:CT:73:LYS:HB2	46:CT:106:VAL:HB	1.78	0.66
5:BE:90:THR:HG22	5:BE:91:GLY:H	1.60	0.66
20:BT:9:LYS:O	20:BT:12:ILE:HG13	1.95	0.66
48:CV:7:ARG:O	48:CV:25:VAL:HB	1.95	0.66
25:D4:8:ARG:HD3	54:DA:245:G:O6	1.96	0.66
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.32	0.65
5:AE:157:ARG:HD2	8:AH:43:GLU:O	1.95	0.65
42:DP:39:VAL:HB	42:DP:49:VAL:HG23	1.77	0.65
31:CA:528:A:H2	31:CA:2043:C:H4'	1.57	0.65
1:BA:1323:G:H2'	1:BA:1324:A:C8	2.32	0.65
40:CN:41:LEU:HD21	40:CN:124:LEU:HD22	1.78	0.65
54:DA:1105:U:H2'	54:DA:1106:G:C8	2.30	0.65
39:CM:21:ARG:HH21	39:CM:21:ARG:CG	2.09	0.65
31:CA:528:A:H2'	31:CA:529:A:H5''	1.77	0.65
39:CM:82:LEU:HD11	39:CM:116:VAL:HG23	1.78	0.65
31:CA:2728:U:HO2'	31:CA:2729:G:H8	1.45	0.65
1:AA:1226:C:H2'	13:AM:102:THR:HB	1.80	0.64
31:CA:1311:G:H21	31:CA:1603:A:H62	1.44	0.64
31:CA:674:G:H1'	32:CE:69:ARG:HH11	1.62	0.64
58:DA:3195:PUT:H21	69:DA:5832:HOH:O	1.96	0.64
44:DR:20:GLN:CG	56:DR:202:PG4:H42	2.26	0.64
1:BA:1226:C:H2'	13:BM:102:THR:HB	1.79	0.64
46:DT:73:LYS:HB2	46:DT:106:VAL:HB	1.79	0.64
54:DA:2128:G:H1	54:DA:2160:C:H42	1.44	0.64
26:C5:3:VAL:HG11	31:CA:2539:C:C5'	2.25	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:DN:18[B]:ARG:HG3	28:DB:90:C:H5''	1.79	0.63
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.80	0.63
34:CG:80:THR:HG23	34:CG:81:GLU:H	1.62	0.63
54:DA:1853:A:N1	54:DA:2087:G:H1'	2.14	0.63
1:BA:451:A:H2'	69:BA:1701:HOH:O	1.98	0.63
16:BP:20:VAL:HG13	16:BP:32:PHE:HB2	1.81	0.62
7:AG:22:LEU:HD12	7:AG:62:PHE:HE2	1.64	0.62
54:DA:45:G:H5''	54:DA:46:G:H5'	1.82	0.62
16:BP:4:ILE:HG12	16:BP:21:VAL:HG22	1.82	0.62
1:BA:1012:A:H61	1:BA:1017:U:H3	1.48	0.62
31:CA:1131:G:OP1	37:CK:82:GLY:HA2	1.99	0.61
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.81	0.61
33:CF:36:LEU:HD21	33:CF:91:LEU:HD11	1.82	0.61
1:AA:1012:A:H61	1:AA:1017:U:H3	1.49	0.61
48:DV:52:LEU:HB3	48:DV:54:GLN:HB2	1.81	0.61
11:BK:88:GLY:N	11:BK:114:THR:HG22	2.10	0.61
38:CL:43:ILE:HD12	38:CL:56:ASP:HB2	1.82	0.61
41:CO:33:ILE:HD12	41:CO:114:GLU:HB3	1.82	0.61
40:DN:16:ARG:HG3	40:DN:18[B]:ARG:HH11	1.64	0.61
31:CA:45:G:H5''	31:CA:46:G:H5'	1.82	0.61
31:CA:118:A:N3	31:CA:178:G:H1'	2.16	0.60
46:CT:17:VAL:HG11	46:CT:103:ILE:HG12	1.83	0.60
45:DS:83:TYR:CE1	54:DA:1187:G:H5''	2.36	0.60
31:CA:784:G:H5'	31:CA:785:G:OP1	2.01	0.60
40:DN:77:PRO:HG2	40:DN:80:VAL:HG21	1.84	0.60
46:DT:17:VAL:HG11	46:DT:103:ILE:HG12	1.83	0.60
54:DA:2256:G:H21	56:DA:3193:PG4:H31	1.67	0.60
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.37	0.60
3:BC:40:ARG:HH11	3:BC:55:ILE:HG23	1.67	0.60
1:BA:1151:A:HO2'	1:BA:1152:A:H8	1.48	0.60
30:DD:114:LYS:HE2	54:DA:2681:C:OP2	2.02	0.60
17:BQ:68:SER:OG	17:BQ:71:LYS:HB3	2.02	0.60
53:DI:69:PHE:HB3	53:DI:72:LEU:HD12	1.83	0.60
19:AS:15:LEU:HD13	19:AS:33:THR:HG21	1.84	0.60
38:DL:113:MET:CE	38:DL:116:ILE:HD11	2.32	0.60
1:AA:1396:A:H3'	59:AA:1681:TAC:H433	1.84	0.59
31:CA:674:G:H1'	32:CE:69:ARG:HD2	1.85	0.59
42:DP:31:THR:HG21	28:DB:28:C:OP1	2.02	0.59
1:BA:1218:C:H2'	1:BA:1219:A:C8	2.37	0.59
1:BA:619:U:H3	4:BD:131:ASN:HB3	1.67	0.59
48:CV:13:VAL:HG21	48:CV:39:ILE:HG21	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:DL:43:ILE:HD12	38:DL:56:ASP:HB2	1.84	0.59
3:AC:40:ARG:HG2	3:AC:55:ILE:HG21	1.83	0.59
1:BA:108:G:N3	1:BA:108:G:H5''	2.18	0.59
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	1.85	0.59
53:DI:23:LEU:HD13	53:DI:89:PRO:HD3	1.84	0.59
31:CA:457:A:N1	31:CA:470:A:H5''	2.17	0.59
43:DQ:53:ARG:NH2	54:DA:2720:U:OP1	2.36	0.59
41:DO:33:ILE:HD12	41:DO:114:GLU:HB3	1.83	0.59
39:CM:79:LEU:HD11	39:CM:112:LEU:HD12	1.84	0.59
44:CR:112:LYS:HD3	45:CS:48:LYS:HG3	1.84	0.59
48:CV:45:HIS:HD2	48:CV:58:ILE:HG12	1.68	0.59
54:DA:2796:U:H3	54:DA:2799:A:N6	1.92	0.59
48:DV:13:VAL:HG21	48:DV:39:ILE:HG21	1.84	0.59
31:CA:1638:C:H5''	31:CA:2710:C:O2'	2.03	0.59
31:CA:910:A:H62	40:CN:12:MET:HA	1.67	0.59
1:AA:108:G:H5''	1:AA:108:G:N3	2.17	0.59
4:BD:201:VAL:HG11	5:BE:103:THR:HB	1.85	0.59
13:BM:83:LEU:HD21	19:BS:65:GLU:HB2	1.85	0.59
37:CK:81:ILE:HG23	37:CK:82:GLY:H	1.67	0.59
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.85	0.58
11:BK:23:ILE:HG22	11:BK:32:VAL:HG13	1.86	0.58
50:DX:21:LEU:HD11	50:DX:41[A]:ARG:HE	1.68	0.58
31:CA:974:G:H8	31:CA:990:A:H62	1.52	0.58
31:CA:206:U:H2'	31:CA:207:A:H8	1.69	0.58
30:DD:186:LEU:HD21	43:DQ:4:ILE:HG21	1.85	0.58
11:AK:23:ILE:HG22	11:AK:32:VAL:HG13	1.86	0.58
31:CA:2796:U:H3	31:CA:2799:A:N6	1.94	0.58
54:DA:62:U:O4'	57:DA:3204:MPD:H31	2.03	0.58
50:CX:37:ILE:HG21	50:CX:80:ILE:HG21	1.85	0.58
24:C3:2:LYS:HE2	31:CA:687:C:H5''	1.85	0.58
39:CM:77:ILE:CD1	39:CM:108:ALA:HB1	2.29	0.58
30:DD:99:GLU:HG2	30:DD:182:ALA:HB2	1.86	0.58
50:DX:41[A]:ARG:HG2	50:DX:41[A]:ARG:HH11	1.69	0.58
46:CT:82:MET:HB2	46:CT:98:LYS:HB2	1.85	0.57
48:CV:74:ASN:HD22	48:CV:77:THR:H	1.51	0.57
43:DQ:29:LYS:HB3	43:DQ:40:LEU:HD13	1.85	0.57
46:DT:82:MET:HB2	46:DT:98:LYS:HB2	1.86	0.57
47:DU:80:TRP:HB3	63:DU:101:PGE:H32	1.85	0.57
7:BG:113:ASP:HB2	7:BG:119:ARG:HG3	1.85	0.57
30:DD:140:HIS:HB3	69:DD:487:HOH:O	2.02	0.57
30:CD:4:LEU:HD22	30:CD:101:PHE:CE2	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:129:LEU:HD13	2:AB:134:ALA:HB2	1.87	0.57
29:CC:227:PRO:HA	29:CC:233:GLY:HA2	1.86	0.57
35:CH:4:ILE:HD11	35:CH:44:ILE:HG22	1.86	0.57
38:CL:58:LEU:HD11	38:CL:86:LEU:HD13	1.86	0.57
1:BA:1106:G:H5''	3:BC:172:ARG:HG3	1.87	0.57
54:DA:1975:G:H21	63:DA:3225:PGE:C2	2.18	0.57
31:CA:1936:A:H62	31:CA:1963:U:H3	1.50	0.57
54:DA:1417:C:H5'	54:DA:1588:G:H1'	1.87	0.57
50:DX:59:LEU:HD12	50:DX:80:ILE:HD12	1.87	0.57
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.85	0.57
24:D3:19:ARG:HD3	54:DA:125:A:OP2	2.04	0.57
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.51	0.57
5:AE:38:VAL:HG11	5:AE:114:VAL:HG22	1.87	0.57
1:AA:86:G:H21	1:AA:87:C:H41	1.53	0.57
2:AB:20:THR:HG22	2:AB:39:HIS:CE1	2.40	0.57
11:AK:31:ILE:HG12	11:AK:46:THR:HG22	1.86	0.57
1:BA:1277:C:HO2'	1:BA:1279:G:H8	1.53	0.57
17:BQ:17:MET:HB3	17:BQ:20:SER:HB3	1.86	0.57
42:DP:31:THR:HG22	42:DP:34:HIS:H	1.69	0.57
1:AA:774:G:H21	56:AA:1670:PG4:H51	1.70	0.56
11:AK:67:ALA:HB2	11:AK:96:THR:HG23	1.87	0.56
42:CP:31:THR:HG22	42:CP:34:HIS:H	1.69	0.56
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.87	0.56
1:BA:202:G:H1	1:BA:215:C:H42	1.51	0.56
1:BA:686:U:HO2'	1:BA:687:A:H8	1.52	0.56
33:CF:31:VAL:CG1	33:CF:97:TRP:CH2	2.88	0.56
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.88	0.56
2:BB:129:LEU:HD13	2:BB:134:ALA:HB2	1.87	0.56
31:CA:1156:A:H5''	69:CA:3399:HOH:O	2.05	0.56
30:CD:99:GLU:HG2	30:CD:182:ALA:HB2	1.86	0.56
50:DX:37:ILE:HG21	50:DX:80:ILE:HG21	1.87	0.56
1:BA:9:G:H5'	5:BE:108:GLY:HA3	1.86	0.56
3:BC:77:ILE:HA	3:BC:84:VAL:HG23	1.87	0.56
5:BE:88:VAL:HG12	5:BE:93:ARG:HG2	1.86	0.56
31:CA:244:A:H5''	39:CM:67:THR:HG21	1.87	0.56
54:DA:1746:A:H2'	54:DA:1747:U:C6	2.41	0.56
1:AA:81:A:H61	1:AA:86:G:H1	1.54	0.56
6:BF:38:ARG:NH1	6:BF:99:ALA:HB3	2.20	0.56
11:BK:67:ALA:HB2	11:BK:96:THR:HG23	1.87	0.56
29:CC:210:ALA:HA	29:CC:213:TRP:CE2	2.40	0.56
54:DA:1975:G:H21	63:DA:3225:PGE:H22	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DA:526:A:H2'	69:DA:3716:HOH:O	2.05	0.56
25:C4:54:ASP:HB3	39:CM:57:LEU:HD22	1.86	0.56
11:BK:16:VAL:HG13	11:BK:79:ILE:HG13	1.88	0.56
12:BL:110:ARG:HB2	12:BL:119:VAL:HG21	1.88	0.56
26:C5:3:VAL:CG1	31:CA:2539:C:H5'	2.31	0.56
36:CJ:19:ASN:H	36:CJ:20:PRO:HD2	1.71	0.56
47:CU:18:GLU:H	47:CU:18:GLU:CD	2.08	0.56
22:D1:4:GLN:HA	54:DA:2615:U:C2	2.41	0.56
23:C2:25:LYS:HD2	23:C2:52:ALA:HB1	1.87	0.56
38:DL:58:LEU:HD11	38:DL:86:LEU:HD13	1.88	0.56
1:AA:209:U:H4'	1:AA:210:C:OP2	2.06	0.56
1:AA:137:U:H3	1:AA:226:G:H1	1.53	0.56
17:BQ:19:LYS:HG2	17:BQ:49:GLU:HA	1.87	0.56
31:CA:2019:A:H4'	44:CR:34:VAL:HG21	1.88	0.56
40:CN:77:PRO:HG2	40:CN:80:VAL:HG21	1.87	0.56
5:BE:40:GLY:HA2	5:BE:45:ARG:O	2.06	0.55
30:CD:129:THR:HG23	30:CD:140:HIS:O	2.06	0.55
22:D1:9:THR:CG2	54:DA:2020:A:H5'	2.36	0.55
32:DE:189:THR:HG22	32:DE:192:ALA:H	1.71	0.55
1:AA:202:G:H1	1:AA:215:C:H42	1.54	0.55
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.88	0.55
48:DV:45:HIS:HD2	48:DV:58:ILE:HG12	1.71	0.55
1:BA:240:G:OP1	1:BA:240:G:H4'	2.06	0.55
31:CA:396:G:H1'	51:CY:29:PHE:HB3	1.87	0.55
31:CA:2502:G:H5''	31:CA:2503:2MA:H5''	1.89	0.55
32:DE:48:THR:HG22	32:DE:86:ALA:HB3	1.88	0.55
44:DR:6:ARG:NH1	54:DA:585:G:N7	2.53	0.55
6:BF:45:ARG:O	6:BF:56:LYS:HA	2.07	0.55
8:BH:87:LYS:HB2	8:BH:125:ILE:CD1	2.36	0.55
38:CL:35:VAL:HG12	38:CL:106:GLU:HG2	1.87	0.55
50:CX:59:LEU:HD12	50:CX:80:ILE:HD12	1.87	0.55
9:AI:116:VAL:HG21	10:AJ:62:ARG:HB2	1.89	0.55
1:BA:137:U:H3	1:BA:226:G:H1	1.54	0.55
31:CA:460:A:H5'	47:CU:73:ARG:HH22	1.72	0.55
29:CC:88:SER:HB2	29:CC:158:ALA:HB2	1.88	0.55
29:DC:227:PRO:HA	29:DC:233:GLY:HA2	1.87	0.55
36:DJ:19:ASN:H	36:DJ:20:PRO:HD2	1.71	0.55
2:BB:23:TRP:HB3	2:BB:39:HIS:CE1	2.41	0.55
40:DN:16:ARG:HG3	40:DN:18[B]:ARG:NH1	2.22	0.55
10:AJ:35:GLN:HB2	10:AJ:77:VAL:HB	1.89	0.55
1:AA:1329:A:H5''	13:AM:26:GLY:H	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:374:A:H5''	1:BA:452:A:C2	2.41	0.55
12:BL:80:ILE:HD12	12:BL:97:THR:CG2	2.30	0.55
31:CA:1028:A:N6	31:CA:1125:G:H2'	2.22	0.55
32:CE:3:LEU:HD12	32:CE:14:VAL:HG11	1.89	0.55
23:D2:35:GLU:HG2	23:D2:50:LYS:HG2	1.89	0.55
31:CA:699:A:H2'	31:CA:700:G:O4'	2.07	0.54
22:D1:54:VAL:HG23	22:D1:55:ILE:HG12	1.89	0.54
46:CT:66:ILE:HA	46:CT:69:LEU:HD22	1.89	0.54
1:AA:1144:G:H21	1:AA:1146:A:H62	1.54	0.54
31:CA:2043:C:C6	31:CA:2043:C:H5''	2.42	0.54
31:CA:247:G:H4'	31:CA:386:G:C5	2.41	0.54
45:CS:78:ARG:HB2	45:CS:83:TYR:HD1	1.71	0.54
54:DA:789:A:OP1	58:DA:3222:PUT:H11	2.07	0.54
31:CA:863:A:H2'	31:CA:864:G:C8	2.42	0.54
31:CA:822:G:O6	31:CA:943:A:H2	1.89	0.54
54:DA:2065:C:H4'	54:DA:2251:OMG:HM22	1.89	0.54
54:DA:1482:G:H1'	54:DA:1509:A:H61	1.73	0.54
6:AF:45:ARG:O	6:AF:56:LYS:HA	2.07	0.54
1:BA:1329:A:H5''	13:BM:26:GLY:H	1.73	0.54
1:BA:769:G:H4'	1:BA:1513:A:H4'	1.88	0.54
5:BE:106:ILE:HD11	5:BE:124:LEU:HD23	1.88	0.54
28:CB:55:U:H1'	33:CF:26:MET:HG3	1.88	0.54
1:AA:1343:G:H2'	1:AA:1344:C:C6	2.42	0.54
1:BA:1144:G:H21	1:BA:1146:A:H62	1.54	0.54
17:BQ:76:VAL:HG12	17:BQ:77:ARG:HG3	1.89	0.54
32:CE:149:ILE:HG12	32:CE:188:MET:HG2	1.90	0.54
52:CZ:56:LEU:HA	52:CZ:59:GLU:HG2	1.89	0.54
63:D1:102:PGE:H4	69:DT:311:HOH:O	2.08	0.54
54:DA:1180:U:H5''	54:DA:1180:U:H6	1.73	0.54
22:C1:43:ILE:HG22	22:C1:49:TYR:HB2	1.89	0.54
41:DO:2:ARG:HG3	54:DA:1653:G:H3'	1.90	0.54
32:DE:3:LEU:HD12	32:DE:14:VAL:HG11	1.90	0.54
1:AA:412:A:H3'	1:AA:413:G:H5'	1.90	0.54
1:AA:307:C:N4	57:AA:1676:MPD:C1	2.68	0.53
31:CA:550:C:H2'	31:CA:551:G:H5''	1.90	0.53
10:BJ:5:ARG:HG2	10:BJ:79:PRO:HG3	1.90	0.53
30:CD:133:THR:CG2	31:CA:1993:U:H4'	2.38	0.53
31:CA:2425:A:H4'	31:CA:2426:A:O5'	2.08	0.53
31:CA:2815:C:H2'	31:CA:2816:G:O4'	2.08	0.53
33:CF:61:SER:HB2	33:CF:91:LEU:HD21	1.90	0.53
54:DA:1847:A:O2'	54:DA:1848:A:H8	1.78	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:73:C:HO2'	1:AA:74:A:H8	1.56	0.53
12:AL:110:ARG:HB2	12:AL:119:VAL:HG21	1.90	0.53
17:AQ:76:VAL:HG12	17:AQ:77:ARG:HG3	1.89	0.53
47:CU:69:ARG:HB2	47:CU:74:ILE:HG22	1.90	0.53
47:CU:28:ASN:HD21	47:CU:91:GLN:HB3	1.74	0.53
11:AK:84:VAL:HG11	11:AK:97:ILE:HG12	1.90	0.53
5:BE:72:ILE:HG13	5:BE:73:ASN:N	2.23	0.53
31:CA:2190:G:H2'	31:CA:2191:A:H8	1.73	0.53
22:C1:4:GLN:HA	31:CA:2615:U:C2	2.43	0.53
31:CA:782:A:H5'	31:CA:783:A:C2	2.44	0.53
33:DF:61:SER:HB2	33:DF:91:LEU:HD21	1.90	0.53
52:DZ:56:LEU:HA	52:DZ:59:GLU:HG2	1.89	0.53
1:BA:374:A:H5''	1:BA:452:A:N1	2.23	0.53
46:CT:69:LEU:HG	46:CT:107:VAL:HG22	1.91	0.53
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	1.90	0.53
22:C1:38:HIS:HE1	31:CA:2884:U:O4	1.91	0.53
24:D3:2:LYS:HE2	54:DA:687:C:H5''	1.90	0.53
1:AA:404:G:N7	4:AD:2:ALA:HB3	2.23	0.53
7:AG:22:LEU:HD12	7:AG:62:PHE:CE2	2.42	0.53
46:CT:29:VAL:HG22	46:CT:51:LEU:HD11	1.89	0.53
33:DF:132:VAL:HG22	33:DF:152:LEU:HG	1.91	0.53
1:BA:73:C:HO2'	1:BA:74:A:H8	1.55	0.53
5:BE:90:THR:HG22	5:BE:91:GLY:N	2.23	0.53
31:CA:1363:C:H2'	31:CA:1364:G:C8	2.44	0.53
32:CE:189:THR:HG22	32:CE:192:ALA:H	1.73	0.53
33:CF:44:ILE:HG21	33:CF:79:ILE:HG22	1.91	0.53
37:DK:9:GLU:HG2	69:DA:5751:HOH:O	2.09	0.53
4:BD:85:ASN:HA	5:BE:102:GLY:CA	2.34	0.52
34:DG:17:VAL:HG11	34:DG:50:LEU:HD21	1.90	0.52
1:BA:209:U:H4'	1:BA:210:C:OP2	2.08	0.52
11:BK:84:VAL:HG11	11:BK:97:ILE:HG12	1.91	0.52
30:DD:152:PRO:HG3	30:DD:156:PHE:CZ	2.45	0.52
54:DA:550:C:H2'	54:DA:551:G:H5''	1.91	0.52
56:DS:202:PG4:H21	69:DS:315:HOH:O	2.09	0.52
10:AJ:52:LEU:HB2	14:AN:81:ARG:HD2	1.91	0.52
1:BA:12:U:H4'	1:BA:526:C:H4'	1.91	0.52
1:BA:404:G:N7	4:BD:2:ALA:HB3	2.24	0.52
9:BI:19:VAL:HG22	9:BI:65:ILE:HG22	1.91	0.52
34:CG:17:VAL:HG11	34:CG:50:LEU:HD21	1.90	0.52
5:AE:90:THR:HG22	5:AE:91:GLY:N	2.22	0.52
17:BQ:8:LEU:HD23	17:BQ:25:ILE:HG21	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DH:4:ILE:HD11	35:DH:44:ILE:HG22	1.91	0.52
53:DI:8:LYS:O	53:DI:12:VAL:HG23	2.09	0.52
1:AA:1126:U:O2	1:AA:1280:A:H5'	2.09	0.52
41:CO:73:ASN:HA	41:CO:76:VAL:HG13	1.92	0.52
33:DF:44:ILE:HG21	33:DF:79:ILE:HG22	1.91	0.52
28:CB:28:C:OP1	42:CP:31:THR:HG21	2.10	0.52
32:CE:48:THR:HG22	32:CE:86:ALA:HB3	1.91	0.52
31:CA:2718:G:OP1	43:CQ:98:TYR:HD2	1.93	0.52
50:DX:18:ALA:HB3	50:DX:20:ARG:NH1	2.24	0.52
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.44	0.52
17:BQ:8:LEU:HD13	17:BQ:73:TRP:CH2	2.45	0.52
54:DA:2291:U:H2'	54:DA:2292:U:C6	2.45	0.52
18:AR:36:SER:HA	18:AR:72:ASP:HB3	1.91	0.52
19:BS:15:LEU:HD13	19:BS:33:THR:HG21	1.91	0.52
31:CA:1274:A:N3	31:CA:1297:C:H1'	2.24	0.52
31:CA:1482:G:H1'	31:CA:1509:A:H61	1.75	0.52
54:DA:551:G:H8	54:DA:551:G:H5''	1.75	0.52
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	1.91	0.52
1:BA:1126:U:O2	1:BA:1280:A:H5'	2.09	0.52
1:BA:1343:G:H2'	1:BA:1344:C:C6	2.44	0.52
31:CA:1636:U:H2'	31:CA:1637:A:C8	2.45	0.52
31:CA:846:U:H1'	31:CA:847:U:C5	2.40	0.52
38:CL:121:GLU:HG2	38:CL:122:VAL:HG23	1.92	0.52
45:DS:16:GLU:HG2	45:DS:100:GLY:HA2	1.92	0.52
9:AI:19:VAL:HG22	9:AI:65:ILE:HG22	1.91	0.51
23:C2:35:GLU:HG2	23:C2:50:LYS:HG2	1.91	0.51
31:CA:566:U:O4	45:CS:80:ARG:HD3	2.10	0.51
54:DA:837:C:H5	69:DA:6614:HOH:O	1.93	0.51
1:AA:673:A:H2'	1:AA:674:G:C8	2.45	0.51
53:DI:132:TYR:H	53:DI:133:GLU:HB2	1.75	0.51
31:CA:1363:C:H2'	31:CA:1364:G:H8	1.76	0.51
31:CA:784:G:H3'	69:CA:3435:HOH:O	2.10	0.51
51:CY:4:VAL:HG22	51:CY:11:ARG:HG3	1.91	0.51
1:AA:1151:A:O2'	1:AA:1152:A:H8	1.94	0.51
1:AA:686:U:HO2'	1:AA:687:A:H8	1.58	0.51
1:BA:1068:G:N7	1:BA:1094:G:H2'	2.25	0.51
33:CF:36:LEU:HB2	33:CF:57:LEU:HD21	1.92	0.51
54:DA:793:A:OP1	64:DA:3224:SPD:H81	2.10	0.51
33:DF:36:LEU:HB2	33:DF:57:LEU:HD21	1.92	0.51
1:AA:528:C:H5''	1:AA:528:C:H6	1.76	0.51
5:AE:107:ALA:HB2	5:AE:125:ALA:HB3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AH:2:SER:HB2	8:AH:4:GLN:HE21	1.76	0.51
10:BJ:52:LEU:HB2	14:BN:81:ARG:HD2	1.92	0.51
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.40	0.51
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.41	0.51
8:AH:87:LYS:HB2	8:AH:125:ILE:CD1	2.39	0.51
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.76	0.51
29:CC:208:ALA:HB2	31:CA:1790:C:O2'	2.11	0.51
39:CM:21:ARG:HH21	39:CM:21:ARG:HG2	1.75	0.51
43:DQ:52:ASN:O	54:DA:2845:U:H5''	2.10	0.51
56:DA:3216:PG4:H31	69:DA:4497:HOH:O	2.11	0.51
37:DK:56:VAL:HB	37:DK:124:VAL:HB	1.93	0.51
13:AM:12:HIS:HB3	69:AM:305:HOH:O	2.10	0.51
31:CA:1810:A:H2'	31:CA:1811:G:O4'	2.08	0.51
40:CN:40:ARG:HD3	40:CN:93:VAL:HG21	1.93	0.51
54:DA:2273:A:H2'	54:DA:2274:A:C8	2.45	0.51
44:DR:6:ARG:HD3	54:DA:1250:G:C5'	2.41	0.51
9:BI:116:VAL:HG21	10:BJ:62:ARG:HB2	1.93	0.51
31:CA:1447:C:H2'	31:CA:1448:G:C8	2.46	0.51
42:DP:68:LYS:HB3	61:DP:201:PEG:H22	1.92	0.51
4:BD:177:LYS:HB3	4:BD:179:GLU:HG2	1.92	0.51
26:C5:2:LYS:HE3	26:C5:4:ARG:HH11	1.76	0.51
64:DA:3224:SPD:H82	69:DA:5291:HOH:O	2.10	0.51
53:DI:50:VAL:HG13	53:DI:85:VAL:HG22	1.93	0.51
13:AM:86:TYR:CZ	13:AM:90:ARG:HD2	2.46	0.50
13:BM:90:ARG:HH21	13:BM:95:LEU:HB3	1.76	0.50
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.47	0.50
32:CE:149:ILE:HD12	32:CE:172:ALA:HA	1.93	0.50
34:DG:164:TYR:HB2	34:DG:167:GLU:HB2	1.93	0.50
4:AD:177:LYS:HB3	4:AD:179:GLU:HG2	1.93	0.50
1:AA:1328:C:H5''	13:AM:28:THR:HG21	1.93	0.50
13:BM:22:ILE:HB	13:BM:25:VAL:HG12	1.93	0.50
41:DO:73:ASN:HA	41:DO:76:VAL:HG13	1.93	0.50
1:BA:1151:A:O2'	1:BA:1152:A:H8	1.94	0.50
1:BA:1518:MA6:H103	1:BA:1519:MA6:C10	2.39	0.50
54:DA:12:U:H6	69:DA:4057:HOH:O	1.93	0.50
1:AA:845:A:O4'	1:AA:845:A:P	2.69	0.50
6:AF:47:LEU:HD13	6:AF:51:ILE:HG12	1.94	0.50
13:AM:90:ARG:HD3	13:AM:97:VAL:HA	1.92	0.50
31:CA:792:A:H1'	31:CA:2072:C:O2'	2.11	0.50
30:CD:152:PRO:HG3	30:CD:156:PHE:CZ	2.46	0.50
33:CF:132:VAL:HG22	33:CF:152:LEU:HG	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:781:A:H2'	31:CA:1777:U:O2'	2.11	0.50
37:CK:81:ILE:CG2	37:CK:82:GLY:H	2.24	0.50
30:DD:150[A]:MEQ:HE3	54:DA:2032:G:C8	2.47	0.50
54:DA:287:G:H1	54:DA:353:C:H42	1.60	0.50
34:DG:86:LYS:HG2	34:DG:132:VAL:HG22	1.93	0.50
46:DT:10:ALA:HB1	46:DT:46:LEU:HD13	1.94	0.50
31:CA:1405:U:H2'	31:CA:1406:U:C6	2.47	0.50
31:CA:1809:A:H2'	31:CA:1810:A:C8	2.45	0.50
54:DA:1738:G:HO2'	54:DA:1739:A:H8	1.58	0.50
1:BA:374:A:OP1	1:BA:452:A:N1	2.44	0.50
13:BM:86:TYR:CZ	13:BM:90:ARG:HD2	2.46	0.50
1:BA:1493:A:H1'	31:CA:1913:A:H61	1.77	0.50
31:CA:328:U:O3'	48:CV:66:GLN:HG3	2.11	0.50
35:CH:27:ARG:HH11	51:CY:60:ASP:HA	1.77	0.50
54:DA:2886[A]:A:C2	54:DA:2887[A]:A:H1'	2.46	0.50
36:DJ:14:ALA:HB3	36:DJ:17:MET:HB2	1.94	0.50
1:AA:412:A:H3'	1:AA:413:G:C5'	2.42	0.50
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	1.94	0.50
31:CA:1469:A:H2'	31:CA:1470:A:C8	2.47	0.50
38:CL:76:VAL:HG12	43:CQ:73:VAL:HB	1.93	0.50
13:BM:90:ARG:HD3	13:BM:97:VAL:HA	1.93	0.49
1:BA:202:G:O2'	1:BA:468:A:H8	1.94	0.49
5:BE:81:LEU:HB3	5:BE:147:MET:SD	2.52	0.49
35:CH:94:ILE:HB	35:CH:122:LEU:HB2	1.95	0.49
37:CK:81:ILE:HG23	37:CK:82:GLY:N	2.27	0.49
33:DF:88:LYS:HD3	54:DA:2313:C:H5''	1.93	0.49
1:BA:1328:C:H5''	13:BM:28:THR:HG21	1.95	0.49
1:BA:518:C:H2'	1:BA:530:G:C8	2.48	0.49
31:CA:593:U:H2'	31:CA:594:U:C6	2.47	0.49
54:DA:1172:C:C5	54:DA:1173:U:H1'	2.47	0.49
54:DA:1515:A:H2'	54:DA:1516:G:O4'	2.12	0.49
54:DA:118:A:N3	54:DA:178:G:H1'	2.26	0.49
31:CA:2189:U:H2'	31:CA:2190:G:H8	1.78	0.49
53:DI:64:VAL:HG22	53:DI:69:PHE:HB2	1.95	0.49
1:AA:131:A:H2'	1:AA:132:C:C6	2.48	0.49
1:BA:845:A:H8	1:BA:845:A:O5'	1.96	0.49
5:BE:72:ILE:HG13	5:BE:73:ASN:H	1.77	0.49
31:CA:1847:A:O2'	31:CA:1848:A:H8	1.78	0.49
36:CJ:14:ALA:HB3	36:CJ:17:MET:HB2	1.93	0.49
30:DD:161:MET:HG2	69:DA:6194:HOH:O	2.12	0.49
21:AU:51:SER:HA	21:AU:54:LYS:HE3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:8:A:C6	4:BD:206:LYS:HB3	2.48	0.49
31:CA:1775:U:O4	31:CA:1789:A:H2	1.95	0.49
26:D5:25:VAL:HB	26:D5:35:GLN:HB2	1.94	0.49
20:AT:43:ASP:HB3	20:AT:46:ALA:HB3	1.95	0.49
41:CO:95:THR:HG21	41:CO:113:ILE:HD11	1.94	0.49
54:DA:136:G:H1	54:DA:143:C:H42	1.61	0.49
54:DA:593:U:H2'	54:DA:594:U:C6	2.48	0.49
30:DD:150[A]:MEQ:HG2	69:DA:3634:HOH:O	2.13	0.49
53:DI:126:LEU:HA	53:DI:129:LEU:HD12	1.94	0.49
31:CA:551:G:H8	31:CA:551:G:H5''	1.76	0.49
34:CG:86:LYS:HG2	34:CG:132:VAL:HG22	1.95	0.49
38:CL:103:VAL:O	38:CL:122:VAL:HB	2.13	0.49
6:AF:3:HIS:CE1	6:AF:65:GLU:HG3	2.48	0.49
10:BJ:26:VAL:HG21	10:BJ:39:PRO:HD3	1.95	0.49
11:BK:52:PHE:HE2	11:BK:65:VAL:HG21	1.78	0.49
13:BM:16:VAL:HG13	13:BM:34:LEU:HD12	1.94	0.49
54:DA:2327:A:H2'	54:DA:2328:A:C8	2.48	0.49
54:DA:2813:A:C2	54:DA:2887[B]:A:N6	2.80	0.49
41:DO:55:ALA:HA	41:DO:80:PHE:CE2	2.48	0.49
44:DR:31:VAL:HG13	54:DA:580:U:O3'	2.13	0.49
48:DV:94:ARG:HB3	48:DV:103:ILE:HD12	1.95	0.49
1:AA:1518:MA6:H103	1:AA:1519:MA6:C10	2.37	0.48
2:AB:111:ILE:HD12	2:AB:152:LYS:HA	1.95	0.48
1:AA:439:U:H5''	4:AD:121:LYS:HD2	1.95	0.48
10:AJ:5:ARG:HE	10:AJ:77:VAL:HG22	1.78	0.48
11:AK:16:VAL:HG23	11:AK:79:ILE:HG13	1.94	0.48
1:BA:1190:G:H5'	3:BC:176:HIS:NE2	2.28	0.48
45:CS:49:ILE:HB	45:CS:51:VAL:O	2.13	0.48
22:D1:24:ALA:HB3	63:D1:102:PGE:H5	1.95	0.48
54:DA:12:U:O2	54:DA:12:U:H2'	2.13	0.48
54:DA:1536:C:H4'	54:DA:1537:G:H5''	1.94	0.48
54:DA:572:A:H5''	54:DA:573:U:OP2	2.13	0.48
54:DA:784:G:H5'	54:DA:785:G:OP1	2.13	0.48
1:AA:1277:C:HO2'	1:AA:1279:G:H8	1.61	0.48
54:DA:1773:A:H5''	69:DA:4750:HOH:O	2.12	0.48
11:AK:52:PHE:HE2	11:AK:65:VAL:HG21	1.78	0.48
1:BA:1001:C:H2'	1:BA:1002:G:H8	1.78	0.48
6:AF:16:GLU:HB3	4:BD:189:SER:HA	1.95	0.48
8:BH:2:SER:HB2	8:BH:4:GLN:HE21	1.78	0.48
31:CA:1379:U:H6	31:CA:1379:U:H5'	1.78	0.48
31:CA:1956:U:O2	31:CA:1985:C:H4'	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:67:PHE:CD1	29:CC:105:LEU:HD11	2.48	0.48
40:DN:21:ALA:HB1	40:DN:100:LYS:HG2	1.95	0.48
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.79	0.48
3:AC:20:SER:HB3	14:AN:94:PRO:HG3	1.95	0.48
31:CA:12:U:H2'	31:CA:12:U:O2	2.14	0.48
29:CC:3:VAL:HG21	29:CC:202:LEU:HD23	1.96	0.48
33:CF:106:ILE:HD12	33:CF:139:PRO:HG2	1.95	0.48
37:CK:56:VAL:HB	37:CK:124:VAL:HB	1.93	0.48
29:DC:233:GLY:HA3	69:DC:309:HOH:O	2.12	0.48
33:DF:131:GLY:HA3	54:DA:2305:U:H5''	1.95	0.48
35:DH:94:ILE:HB	35:DH:122:LEU:HB2	1.95	0.48
40:DN:18[B]:ARG:HG3	28:DB:90:C:C5'	2.43	0.48
1:AA:413:G:H5''	1:AA:414:A:H5'	1.96	0.48
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	1.96	0.48
36:CJ:103:ARG:HA	36:CJ:106:LEU:HD12	1.95	0.48
32:CE:108:ILE:HG22	39:CM:1:MET:SD	2.54	0.48
54:DA:1794:A:H2'	54:DA:1795:C:C6	2.47	0.48
54:DA:2628:C:H5'	58:DA:3195:PUT:H11	1.95	0.48
42:DP:35:ILE:HG21	42:DP:71:ALA:HA	1.94	0.48
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.48	0.48
1:AA:1250:A:O3'	9:AI:69:GLY:HA2	2.14	0.48
21:AU:4:ILE:HG13	21:AU:19:PHE:HA	1.96	0.48
19:BS:6:LYS:HD2	19:BS:7:LYS:H	1.78	0.48
31:CA:287:G:H1	31:CA:353:C:H42	1.61	0.48
33:DF:106:ILE:HD12	33:DF:139:PRO:HG2	1.94	0.48
1:AA:1346:A:H61	1:AA:1374:A:H3'	1.77	0.48
13:AM:26:GLY:HA2	69:AM:303:HOH:O	2.13	0.48
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	1.95	0.48
31:CA:747:5MU:O2	31:CA:2014:A:H1'	2.14	0.48
36:DJ:103:ARG:HA	36:DJ:106:LEU:HD12	1.95	0.48
1:BA:131:A:H2'	1:BA:132:C:C6	2.49	0.48
26:C5:25:VAL:HB	26:C5:35:GLN:HB2	1.95	0.48
31:CA:136:G:H1	31:CA:143:C:H42	1.62	0.48
31:CA:450:G:H2'	31:CA:451:U:H5''	1.96	0.48
45:CS:16:GLU:HG2	45:CS:100:GLY:HA2	1.95	0.48
54:DA:2628:C:H5'	58:DA:3195:PUT:C1	2.44	0.48
54:DA:588:U:H2'	54:DA:589:U:C6	2.49	0.48
53:DI:50:VAL:HG11	53:DI:92:ALA:HB2	1.94	0.48
1:BA:1493:A:H8	1:BA:1493:A:OP2	1.97	0.48
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.79	0.48
31:CA:323:C:H5'	32:CE:163:ASN:HD21	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:DS:92:TRP:CZ2	63:DS:201:PGE:H2	2.49	0.48
1:AA:451:A:H61	1:AA:481:G:H5'	1.79	0.48
13:BM:22:ILE:HB	13:BM:25:VAL:CG1	2.44	0.48
13:BM:11:ASP:HA	13:BM:45:ILE:HD13	1.94	0.48
31:CA:538:A:H4'	37:CK:7:LYS:HG2	1.96	0.48
31:CA:674:G:H2'	31:CA:804:A:H61	1.79	0.48
31:CA:796:C:H2'	31:CA:797:G:C8	2.49	0.48
54:DA:2262:U:H4'	54:DA:2328:A:C2	2.49	0.48
54:DA:2262:U:H4'	54:DA:2328:A:H2	1.79	0.48
54:DA:2031:A:C6	54:DA:2498:OMC:H1'	2.48	0.48
31:CA:2271:G:H2'	31:CA:2272:U:C6	2.49	0.47
31:CA:1783:A:H5'	31:CA:2608:G:H4'	1.95	0.47
29:CC:228:VAL:HG21	69:CA:3410:HOH:O	2.13	0.47
35:CH:82:SER:HB2	35:CH:94:ILE:HD11	1.96	0.47
48:DV:17:LYS:HE3	48:DV:40:ASN:HA	1.96	0.47
1:BA:1346:A:H61	1:BA:1374:A:H3'	1.78	0.47
21:BU:4:ILE:HG13	21:BU:19:PHE:HA	1.95	0.47
41:CO:55:ALA:HA	41:CO:80:PHE:CE2	2.49	0.47
42:CP:35:ILE:HG21	42:CP:71:ALA:HA	1.96	0.47
54:DA:1433:A:O2'	54:DA:1434:A:H5'	2.14	0.47
20:AT:24:ARG:HD3	20:AT:24:ARG:N	2.30	0.47
6:BF:47:LEU:HD13	6:BF:51:ILE:HG12	1.96	0.47
34:CG:164:TYR:HB2	34:CG:167:GLU:HB2	1.95	0.47
44:CR:58:ARG:HH11	44:CR:62:ILE:HD11	1.79	0.47
52:CZ:42:LEU:HD23	52:CZ:45:GLN:HE21	1.79	0.47
54:DA:1509:A:HO2'	54:DA:1510:G:H8	1.62	0.47
40:DN:33:LEU:HD13	40:DN:117:PHE:HB3	1.95	0.47
1:AA:1190:G:H5'	3:AC:176:HIS:NE2	2.30	0.47
11:AK:30:THR:HG21	11:AK:92:GLY:HA3	1.97	0.47
31:CA:804:A:H2'	31:CA:806:C:C4	2.49	0.47
53:DI:44:ALA:HB1	53:DI:95:LEU:HD11	1.96	0.47
1:AA:518:C:H2'	1:AA:530:G:C8	2.48	0.47
17:BQ:31:HIS:HE1	17:BQ:33:ILE:HD12	1.79	0.47
31:CA:2822:G:H2'	31:CA:2823:A:H5''	1.97	0.47
31:CA:588:U:H2'	31:CA:589:U:C6	2.49	0.47
31:CA:634:C:H2'	31:CA:635:C:C6	2.50	0.47
39:CM:85:VAL:HG11	39:CM:90:VAL:HG22	1.96	0.47
42:DP:9:ARG:HH22	54:DA:2295:C:P	2.38	0.47
54:DA:2520:C:C6	54:DA:2567:G:H1'	2.50	0.47
29:DC:3:VAL:HG21	29:DC:202:LEU:HD23	1.96	0.47
44:DR:19:LYS:HD3	56:DR:202:PG4:H22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AQ:15:ASP:HA	17:AQ:21:ILE:HG22	1.96	0.47
2:BB:41:ILE:HD13	2:BB:202:GLY:HA2	1.96	0.47
31:CA:2686:G:H2'	31:CA:2687:U:C6	2.50	0.47
31:CA:70:G:H5''	31:CA:112:U:O2	2.14	0.47
39:CM:28:GLY:O	39:CM:29:LYS:O	2.33	0.47
39:CM:19:LEU:HD23	39:CM:31:GLY:O	2.15	0.47
44:CR:87:SER:HB3	45:CS:52:PRO:HD3	1.96	0.47
22:D1:43:ILE:HG22	22:D1:49:TYR:HB2	1.95	0.47
24:D3:7:PRO:HB2	54:DA:1309:G:H4'	1.95	0.47
1:AA:1305:G:HO2'	1:AA:1306:A:H8	1.63	0.47
3:BC:26:THR:HG23	14:BN:76:LYS:HD2	1.96	0.47
31:CA:2350:C:H2'	31:CA:2351:G:O4'	2.15	0.47
31:CA:737:C:H42	31:CA:759:G:H1	1.63	0.47
49:CW:51:GLN:HG2	49:CW:86:LEU:HD11	1.97	0.47
54:DA:2324:U:H3'	54:DA:2325:G:H5''	1.97	0.47
1:AA:946:A:H2'	1:AA:947:G:C8	2.50	0.47
2:AB:41:ILE:HD13	2:AB:202:GLY:HA2	1.95	0.47
1:BA:1391:U:H2'	1:BA:1392:G:C8	2.49	0.47
1:BA:10:A:OP2	5:BE:131:THR:HG21	2.15	0.47
29:CC:155:ALA:HB2	29:CC:162:VAL:HG23	1.96	0.47
1:BA:214:C:H2'	1:BA:215:C:H6	1.80	0.47
1:BA:946:A:H2'	1:BA:947:G:C8	2.50	0.47
1:BA:957:U:O2	1:BA:959:A:H8	1.98	0.47
31:CA:248:G:H5'	31:CA:250:G:N7	2.29	0.47
31:CA:2623:G:H4'	31:CA:2825:G:H8	1.80	0.47
40:CN:21:ALA:HB1	40:CN:100:LYS:HG2	1.97	0.47
48:CV:94:ARG:HB3	48:CV:103:ILE:HD12	1.97	0.47
54:DA:5:A:H2'	54:DA:6:A:C8	2.50	0.47
31:CA:1182:G:H2'	31:CA:1183:U:O4'	2.15	0.47
31:CA:1914:C:H2'	31:CA:1915:3TD:H6	1.96	0.47
31:CA:2025:C:H2'	31:CA:2026:U:C6	2.50	0.47
31:CA:2328:A:H2'	31:CA:2329:U:C6	2.51	0.47
29:CC:75:PRO:HG2	29:CC:97:LYS:HD3	1.97	0.47
41:CO:47:VAL:O	41:CO:51:LEU:HD23	2.15	0.47
22:D1:22:LEU:HD23	61:D1:103:PEG:H31	1.96	0.47
39:DM:21:ARG:HA	54:DA:811:U:H2'	1.96	0.47
1:AA:620:C:H2'	1:AA:621:A:O4'	2.14	0.46
10:AJ:26:VAL:HG21	10:AJ:39:PRO:HD3	1.97	0.46
11:AK:84:VAL:HG21	11:AK:97:ILE:HG23	1.97	0.46
1:BA:1356:G:H2'	1:BA:1357:A:C8	2.50	0.46
1:BA:1250:A:O3'	9:BI:69:GLY:HA2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1494:A:H2'	31:CA:1495:A:C8	2.50	0.46
31:CA:2327:A:H2'	31:CA:2328:A:C8	2.50	0.46
31:CA:976:G:H2'	31:CA:977:G:H8	1.80	0.46
54:DA:933:A:H5'	54:DA:934:U:OP2	2.14	0.46
35:DH:82:SER:HB2	35:DH:94:ILE:HD11	1.95	0.46
2:AB:129:LEU:H	2:AB:129:LEU:HG	1.54	0.46
1:BA:1069:C:H4'	1:BA:1192:C:O2	2.16	0.46
31:CA:443:A:H2'	32:CE:40:ARG:NH1	2.29	0.46
39:CM:21:ARG:NH2	39:CM:21:ARG:CG	2.76	0.46
54:DA:2128:G:H1	54:DA:2160:C:N4	2.12	0.46
1:AA:429:U:H1'	1:AA:430:A:H5''	1.97	0.46
7:BG:69:VAL:HG23	7:BG:100:ALA:HB1	1.98	0.46
42:CP:7:ARG:HA	42:CP:10:ARG:HE	1.79	0.46
19:AS:32:ARG:HE	19:AS:57:HIS:CE1	2.34	0.46
1:BA:1152:A:H2'	1:BA:1153:G:C8	2.51	0.46
1:BA:411:A:P	4:BD:26:ARG:HH12	2.38	0.46
1:BA:429:U:H1'	1:BA:430:A:H5''	1.98	0.46
31:CA:727:A:H2'	31:CA:728:G:C8	2.50	0.46
31:CA:833:A:H2'	31:CA:834:G:C8	2.50	0.46
29:DC:207:LYS:HB2	54:DA:729:G:C6	2.50	0.46
7:AG:132:GLY:H	7:AG:135:VAL:HG22	1.80	0.46
31:CA:1386:C:H2'	31:CA:1387:A:C8	2.51	0.46
31:CA:933:A:H5'	31:CA:934:U:OP2	2.16	0.46
54:DA:265:A:H4'	54:DA:266:G:OP1	2.16	0.46
54:DA:2895:G:H2'	54:DA:2896:C:C6	2.51	0.46
34:DG:52:PHE:N	34:DG:52:PHE:CD1	2.84	0.46
38:DL:101:GLY:O	38:DL:120:PRO:HD2	2.16	0.46
1:AA:1053:G:H4'	1:AA:1054:C:H5'	1.97	0.46
12:BL:110:ARG:NH2	12:BL:117:TYR:CE2	2.84	0.46
18:BR:36:SER:HA	18:BR:72:ASP:HB3	1.96	0.46
20:BT:44:LYS:HB3	20:BT:87:ALA:HB2	1.98	0.46
42:CP:51:ALA:HB3	42:CP:78:VAL:HG13	1.98	0.46
51:DY:10:LYS:HE3	51:DY:54:LYS:HG2	1.97	0.46
18:BR:41:PRO:HG2	18:BR:44:ILE:HD12	1.97	0.46
29:CC:35:GLU:HG3	29:CC:64:ILE:HD11	1.98	0.46
40:CN:33:LEU:HD13	40:CN:117:PHE:HB3	1.97	0.46
44:CR:22:LYS:HE2	44:CR:22:LYS:HA	1.97	0.46
54:DA:2243:U:H2'	54:DA:2244:U:C6	2.51	0.46
29:DC:35:GLU:HG3	29:DC:64:ILE:HD11	1.96	0.46
30:DD:121:THR:HB	30:DD:127:PHE:CD2	2.51	0.46
49:DW:51:GLN:HG2	49:DW:86:LEU:HD11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:76:G:H22	1:AA:93:U:H3	1.64	0.46
3:BC:5:VAL:HG21	3:BC:10:ILE:HD13	1.98	0.46
31:CA:2728:U:O2'	31:CA:2729:G:H8	1.98	0.46
31:CA:2788:C:H2'	31:CA:2789:C:C6	2.51	0.46
31:CA:686:U:H2'	31:CA:788:A:N1	2.31	0.46
45:CS:7:SER:HB3	45:CS:12:HIS:HE1	1.79	0.46
54:DA:1168:G:H2'	54:DA:1169:A:O4'	2.15	0.46
1:AA:1239:A:H62	1:AA:1299:A:N6	2.14	0.46
1:AA:619:U:C2	4:AD:132:ILE:HD11	2.51	0.46
14:BN:31:ILE:HG23	14:BN:42:TRP:HZ2	1.81	0.46
31:CA:2353:G:H2'	31:CA:2354:C:O4'	2.15	0.46
31:CA:2030:6MZ:C2	31:CA:2499:C:H5"	2.46	0.46
31:CA:493:G:H2'	31:CA:494:G:O4'	2.16	0.46
23:D2:10:LYS:HE3	23:D2:53:LYS:O	2.16	0.46
54:DA:1738:G:O2'	54:DA:1739:A:H8	1.99	0.46
54:DA:493:G:H2'	54:DA:494:G:O4'	2.16	0.46
38:DL:76:VAL:CG2	54:DA:2684:U:H4'	2.46	0.46
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.51	0.46
31:CA:1510:G:H2'	31:CA:1511:G:O4'	2.16	0.46
31:CA:1638:C:H4'	31:CA:2710:C:O2	2.16	0.46
31:CA:2630:G:O4'	31:CA:2894:G:H1'	2.15	0.46
31:CA:2845:U:H2'	31:CA:2846:G:O4'	2.16	0.46
33:CF:31:VAL:HG11	33:CF:97:TRP:CH2	2.51	0.46
50:DX:11:ARG:HH11	54:DA:2256:G:H4'	1.81	0.46
1:AA:1289:A:H3'	1:AA:1290:G:H8	1.82	0.45
1:AA:957:U:O2	1:AA:959:A:H8	1.98	0.45
8:AH:66:PHE:CD2	8:AH:67:GLN:HG2	2.51	0.45
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.80	0.45
1:BA:439:U:H5"	4:BD:121:LYS:HD2	1.97	0.45
3:BC:20:SER:HB3	14:BN:94:PRO:HG3	1.97	0.45
54:DA:1510:G:H2'	54:DA:1511:G:O4'	2.16	0.45
54:DA:2133:G:H21	54:DA:2158:A:N6	2.14	0.45
54:DA:68:G:H2'	54:DA:69:C:O4'	2.16	0.45
40:DN:75:GLU:HB2	40:DN:90:GLU:HG3	1.97	0.45
3:AC:26:THR:HG23	14:AN:76:LYS:HD2	1.97	0.45
5:AE:15:LEU:HA	5:AE:37:THR:HG22	1.98	0.45
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.97	0.45
13:BM:6:GLY:O	13:BM:7:ILE:HG13	2.15	0.45
30:CD:25:THR:HG21	30:CD:193:VAL:HG22	1.98	0.45
51:CY:10:LYS:HE3	51:CY:54:LYS:HG2	1.96	0.45
54:DA:722:A:H2'	54:DA:723:C:O4'	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:DX:39:ARG:HD3	69:DX:118:HOH:O	2.16	0.45
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	1.98	0.45
5:BE:15:LEU:HA	5:BE:37:THR:HG22	1.98	0.45
31:CA:2095:A:H8	31:CA:2095:A:H5''	1.81	0.45
31:CA:2895:G:H2'	31:CA:2896:C:C6	2.51	0.45
31:CA:998:C:OP2	44:CR:58:ARG:NH2	2.49	0.45
54:DA:2547:A:H2'	54:DA:2548:U:C6	2.52	0.45
1:BA:76:G:H22	1:BA:93:U:H3	1.64	0.45
6:BF:99:ALA:O	6:BF:100:SER:HB3	2.16	0.45
31:CA:722:A:H2'	31:CA:723:C:O4'	2.17	0.45
31:CA:969:G:H2'	31:CA:970:U:C6	2.52	0.45
54:DA:1386:C:H2'	54:DA:1387:A:C8	2.51	0.45
54:DA:2328:A:H2'	54:DA:2329:U:C6	2.51	0.45
10:AJ:5:ARG:HG3	10:AJ:77:VAL:HA	1.99	0.45
31:CA:1936:A:N6	31:CA:1963:U:H3	2.14	0.45
27:D0:45:ARG:HH12	27:D0:59:GLU:CD	2.20	0.45
30:DD:150[B]:MEQ:HE2	54:DA:2033:A:O5'	2.16	0.45
54:DA:788:A:H5''	58:DA:3222:PUT:H12	1.99	0.45
54:DA:686:U:H2'	54:DA:788:A:N1	2.31	0.45
12:AL:110:ARG:NH2	12:AL:117:TYR:CE2	2.85	0.45
18:AR:41:PRO:HG2	18:AR:44:ILE:HD12	1.98	0.45
1:BA:1239:A:H62	1:BA:1299:A:N6	2.14	0.45
1:BA:451:A:H61	1:BA:481:G:H5'	1.81	0.45
1:BA:545:C:H5'	4:BD:69:GLU:HB2	1.98	0.45
11:BK:45:ALA:HB3	11:BK:70:CYS:HB2	1.97	0.45
20:BT:48:GLN:HE21	20:BT:83:ILE:HD13	1.81	0.45
31:CA:278:A:N3	31:CA:278:A:H2'	2.32	0.45
38:CL:101:GLY:O	38:CL:120:PRO:HD2	2.15	0.45
1:AA:604:G:H2'	1:AA:605:U:O4'	2.17	0.45
3:AC:7:PRO:HD2	3:AC:184:TYR:CD1	2.51	0.45
1:BA:328:C:H2'	1:BA:328:C:O2	2.17	0.45
4:BD:48:LEU:HD21	4:BD:56:ARG:HG3	1.97	0.45
31:CA:1936:A:C2	31:CA:1943:U:N3	2.61	0.45
30:CD:129:THR:CG2	30:CD:140:HIS:O	2.65	0.45
54:DA:1494:A:H2'	54:DA:1495:A:C8	2.51	0.45
54:DA:747:5MU:O2	54:DA:2014:A:H1'	2.17	0.45
44:DR:34:VAL:HG21	54:DA:2019:A:H4'	1.98	0.45
54:DA:788:A:H3'	58:DA:3222:PUT:H41	1.98	0.45
1:AA:1239:A:H62	1:AA:1299:A:H62	1.64	0.45
1:AA:411:A:P	4:AD:26:ARG:HH12	2.40	0.45
1:BA:1003:G:H21	1:BA:1005:A:H5'	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:972:C:H4'	10:BJ:59:LYS:HG2	1.99	0.45
5:BE:76:LEU:HD21	5:BE:120:VAL:HG22	1.99	0.45
11:BK:30:THR:HG21	11:BK:92:GLY:HA3	1.98	0.45
31:CA:1324:G:H1'	31:CA:1616:A:N6	2.32	0.45
48:CV:45:HIS:CD2	48:CV:58:ILE:HG12	2.50	0.45
54:DA:136:G:H1	54:DA:143:C:N4	2.15	0.45
33:DF:121:SER:HB2	54:DA:2304:G:H5'	1.98	0.45
42:DP:51:ALA:HB3	42:DP:78:VAL:HG13	1.99	0.45
1:AA:528:C:C6	1:AA:528:C:H5''	2.52	0.45
1:BA:49:U:O2	1:BA:362:G:H1'	2.17	0.45
7:BG:132:GLY:H	7:BG:135:VAL:HG22	1.81	0.45
31:CA:639:U:H2'	31:CA:640:C:C6	2.51	0.45
40:DN:14:LYS:HE2	69:DA:3581:HOH:O	2.16	0.45
1:AA:1068:G:N7	1:AA:1094:G:H2'	2.32	0.45
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.82	0.45
1:BA:1289:A:H3'	1:BA:1290:G:H8	1.81	0.45
1:BA:604:G:H2'	1:BA:605:U:O4'	2.17	0.45
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	1.98	0.45
31:CA:2842:G:H2'	31:CA:2843:G:O4'	2.17	0.45
54:DA:2788:C:H2'	54:DA:2789:C:C6	2.52	0.45
54:DA:278:A:H2'	54:DA:278:A:N3	2.32	0.45
54:DA:825:A:H2'	54:DA:826:U:O4'	2.17	0.45
1:BA:1081:A:H5'	5:BE:23:LYS:HG3	1.98	0.44
3:BC:47:LEU:HD22	3:BC:76:VAL:HG22	1.99	0.44
9:BI:57:MET:HG3	9:BI:61:LEU:HG	1.99	0.44
9:BI:7:TYR:HE1	9:BI:18:ARG:HB2	1.81	0.44
17:BQ:51:ASN:N	17:BQ:51:ASN:HD22	2.15	0.44
23:C2:15:ALA:HB2	23:C2:47:VAL:HG21	1.99	0.44
31:CA:1327:A:H2'	31:CA:1328:A:O4'	2.17	0.44
29:CC:105:LEU:HD12	29:CC:105:LEU:N	2.30	0.44
22:D1:25:VAL:HG11	46:DT:38:TYR:HB2	1.99	0.44
54:DA:639:U:H2'	54:DA:640:C:C6	2.52	0.44
1:AA:545:C:H5'	4:AD:69:GLU:HB2	1.98	0.44
20:BT:69:LYS:HG3	20:BT:69:LYS:H	1.54	0.44
31:CA:1214:A:H4'	31:CA:1239:G:H4'	2.00	0.44
54:DA:1101:U:H2'	54:DA:1102:C:C6	2.52	0.44
1:AA:79:G:H22	1:AA:90:C:H42	1.66	0.44
3:AC:5:VAL:HG21	3:AC:10:ILE:HD13	1.98	0.44
4:AD:48:LEU:HD21	4:AD:56:ARG:HG3	2.00	0.44
17:AQ:31:HIS:HE1	17:AQ:33:ILE:HD12	1.81	0.44
44:CR:58:ARG:NH1	44:CR:62:ILE:HD11	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D2:15:ALA:HB2	23:D2:47:VAL:HG21	1.99	0.44
54:DA:455:C:N3	54:DA:472:A:H2'	2.31	0.44
7:AG:69:VAL:HG21	7:AG:104:ILE:HD11	1.98	0.44
1:BA:1069:C:O4'	1:BA:1191:A:H2	2.00	0.44
1:BA:134:G:H2'	1:BA:135:C:O4'	2.18	0.44
14:BN:31:ILE:HG23	14:BN:42:TRP:CZ2	2.52	0.44
31:CA:1509:A:HO2'	31:CA:1510:G:H8	1.66	0.44
31:CA:2339:C:H2'	31:CA:2340:A:C8	2.53	0.44
31:CA:2030:6MZ:N3	31:CA:2499:C:H5''	2.33	0.44
31:CA:320:A:H4'	31:CA:322:A:N7	2.31	0.44
23:D2:11:LEU:HD21	23:D2:34:LEU:HD23	1.99	0.44
54:DA:2722:G:H2'	54:DA:2723:C:C6	2.53	0.44
54:DA:2747:G:O6	54:DA:2755:C:H5''	2.17	0.44
40:DN:41:LEU:CD2	40:DN:125:PRO:HD2	2.47	0.44
1:AA:345:C:H5''	43:DQ:34:GLU:O	2.17	0.44
9:AI:57:MET:HG3	9:AI:61:LEU:HG	1.99	0.44
1:AA:1329:A:H5''	13:AM:26:GLY:N	2.33	0.44
2:BB:129:LEU:H	2:BB:129:LEU:HG	1.54	0.44
6:BF:3:HIS:H	6:BF:92:THR:HG23	1.82	0.44
31:CA:136:G:H1	31:CA:143:C:N4	2.16	0.44
34:CG:52:PHE:N	34:CG:52:PHE:CD2	2.86	0.44
40:CN:75:GLU:HB2	40:CN:90:GLU:HG3	2.00	0.44
54:DA:2339:C:H2'	54:DA:2340:A:C8	2.53	0.44
53:DI:132:TYR:N	53:DI:133:GLU:HB2	2.32	0.44
50:DX:11:ARG:H	50:DX:11:ARG:HE	1.65	0.44
11:BK:84:VAL:HG21	11:BK:97:ILE:HG23	1.99	0.44
31:CA:1587:G:H2'	31:CA:1588:G:H8	1.83	0.44
31:CA:694:U:OP1	31:CA:1569:A:H1'	2.17	0.44
29:CC:219:THR:O	31:CA:1789:A:H5''	2.17	0.44
41:CO:28:LEU:HD23	41:CO:48:VAL:HG21	1.99	0.44
54:DA:1637:A:H5'	54:DA:1760:C:O2'	2.17	0.44
54:DA:2723:C:O5'	54:DA:2723:C:H6	2.01	0.44
39:DM:85:VAL:HB	39:DM:94:THR:HG22	1.99	0.44
45:DS:21:ARG:HH21	56:DS:202:PG4:H71	1.81	0.44
1:AA:1003:G:H21	1:AA:1005:A:H5'	1.82	0.44
3:BC:47:LEU:HB3	3:BC:50:ALA:HB3	1.99	0.44
7:BG:69:VAL:HG21	7:BG:104:ILE:HD11	1.99	0.44
31:CA:1434:A:H2'	31:CA:1435:G:C8	2.52	0.44
31:CA:17:G:H4'	44:CR:25:TYR:HE2	1.81	0.44
31:CA:2298:A:C2	31:CA:2321:U:N3	2.85	0.44
30:CD:121:THR:HB	30:CD:127:PHE:CD2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:CH:104:THR:HG22	35:CH:109:GLU:HA	2.00	0.44
31:CA:2394:C:H5''	39:CM:63:LYS:HE2	2.00	0.44
54:DA:2117:A:H61	54:DA:2171:A:H61	1.66	0.44
30:DD:55:LYS:HD3	30:DD:60:VAL:HG22	2.00	0.44
53:DI:50:VAL:HG22	53:DI:85:VAL:HG13	1.99	0.44
21:BU:51:SER:HA	21:BU:54:LYS:HE3	2.00	0.44
31:CA:1101:U:H2'	31:CA:1102:C:C6	2.52	0.44
31:CA:2074:U:H2'	31:CA:2075:U:C6	2.52	0.44
31:CA:671:C:C5	39:CM:33:ARG:NH2	2.86	0.44
40:CN:42:THR:HA	40:CN:93:VAL:HG12	2.00	0.44
31:CA:142:A:H1'	47:CU:1:MET:HB3	1.99	0.44
54:DA:2473:U:O2	54:DA:2473:U:H2'	2.18	0.44
35:DH:104:THR:HG22	35:DH:109:GLU:HA	1.99	0.44
1:AA:240:G:OP1	1:AA:240:G:H4'	2.17	0.44
1:AA:328:C:H2'	1:AA:328:C:O2	2.17	0.44
2:AB:188:ASP:HB2	2:AB:204:ASP:OD2	2.17	0.44
1:BA:677:U:H3	1:BA:713:G:H22	1.66	0.44
31:CA:2747:G:O6	31:CA:2755:C:H5''	2.17	0.44
28:CB:89:U:C6	31:CA:958:U:H2'	2.52	0.44
1:BA:1432:G:H3'	43:CQ:106:LYS:HE2	1.99	0.44
54:DA:352:A:H5''	54:DA:352:A:H8	1.82	0.44
47:DU:33:LYS:HG3	47:DU:80:TRP:CE3	2.52	0.44
1:AA:1152:A:H2'	1:AA:1153:G:C8	2.53	0.43
3:AC:47:LEU:HD22	3:AC:76:VAL:HG22	2.00	0.43
5:AE:133:PRO:O	5:AE:137:VAL:HG13	2.18	0.43
1:BA:1239:A:H62	1:BA:1299:A:H62	1.64	0.43
3:BC:22:TRP:HB3	3:BC:59:ARG:H	1.83	0.43
17:BQ:28:PHE:HD2	17:BQ:37:PHE:HB3	1.83	0.43
54:DA:1180:U:H5''	54:DA:1180:U:C6	2.52	0.43
54:DA:142:A:H2'	54:DA:143:C:C6	2.52	0.43
54:DA:207:A:H2'	54:DA:208:C:O4'	2.17	0.43
48:DV:66:GLN:HG3	54:DA:328:U:O3'	2.17	0.43
1:BA:774:G:H21	56:BA:1642:PG4:H62	1.84	0.43
22:C1:25:VAL:HG13	22:C1:26:THR:H	1.83	0.43
38:CL:105:ARG:HH21	43:CQ:34:GLU:HG2	1.84	0.43
47:CU:33:LYS:HG3	47:CU:80:TRP:CE3	2.53	0.43
54:DA:31:C:O3'	54:DA:1238:G:H5''	2.17	0.43
30:DD:25:THR:HG21	30:DD:193:VAL:HG22	2.00	0.43
40:DN:42:THR:HG22	40:DN:93:VAL:HG12	1.99	0.43
42:DP:27:VAL:HG21	42:DP:40:ILE:HD12	2.00	0.43
44:DR:19:LYS:HB3	56:DR:202:PG4:H41	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:844:G:H2'	1:BA:844:G:N3	2.32	0.43
29:CC:154:LEU:HD13	29:CC:176:LEU:HD21	1.99	0.43
30:CD:35:THR:HG22	30:CD:73:VAL:HG21	1.99	0.43
35:CH:78:VAL:HG21	35:CH:103:VAL:HG22	2.00	0.43
54:DA:553:G:H2'	54:DA:554:U:O4'	2.18	0.43
49:DW:51:GLN:HB2	49:DW:57:TYR:OH	2.18	0.43
1:AA:1358:U:H3	1:AA:1363:A:H62	1.66	0.43
1:BA:1329:A:H5''	13:BM:26:GLY:N	2.33	0.43
31:CA:2473:U:O2	31:CA:2473:U:H2'	2.18	0.43
1:AA:202:G:H21	1:AA:466:A:H61	1.65	0.43
1:BA:1152:A:H2'	1:BA:1153:G:H8	1.82	0.43
2:BB:188:ASP:HB2	2:BB:204:ASP:OD2	2.18	0.43
27:C0:2:ALA:CB	27:C0:39:GLU:HB3	2.49	0.43
31:CA:142:A:H2'	31:CA:143:C:C6	2.53	0.43
31:CA:2114:A:N6	31:CA:2119:A:H62	2.16	0.43
31:CA:265:A:H4'	31:CA:266:G:OP1	2.19	0.43
28:CB:57:A:C4'	33:CF:27:GLN:HG3	2.49	0.43
28:CB:57:A:O4'	33:CF:27:GLN:HG3	2.17	0.43
32:DE:45:ALA:HB3	54:DA:38:A:H5'	2.01	0.43
53:DI:94:ARG:HG2	53:DI:127:ALA:HA	2.01	0.43
40:DN:40:ARG:HD3	40:DN:93:VAL:HG21	2.00	0.43
1:AA:923:A:OP1	5:AE:26:LYS:HG2	2.18	0.43
1:BA:322:C:H5	1:BA:328:C:C5	2.36	0.43
1:BA:8:A:H5'	5:BE:125:ALA:O	2.18	0.43
13:BM:23:TYR:HD1	13:BM:69:LEU:HD23	1.84	0.43
16:BP:20:VAL:CG1	16:BP:32:PHE:HB2	2.48	0.43
23:C2:11:LEU:HD21	23:C2:34:LEU:HD23	2.00	0.43
23:C2:37:LYS:HG2	23:C2:48:ILE:HG13	2.01	0.43
31:CA:459:U:C5	31:CA:469:G:N2	2.87	0.43
31:CA:871:U:H2'	31:CA:872:U:C6	2.53	0.43
33:CF:103:LEU:HA	33:CF:107:ALA:HB3	2.01	0.43
30:DD:150[B]:MEQ:HG3	54:DA:2032:G:N3	2.33	0.43
54:DA:26:G:H1'	54:DA:514:A:N6	2.33	0.43
1:AA:1338:G:H2'	1:AA:1339:A:C8	2.54	0.43
4:AD:27:ALA:HB3	4:AD:30:THR:HG23	2.00	0.43
5:BE:126:LYS:HG2	5:BE:128:TYR:CZ	2.54	0.43
31:CA:1794:A:H2'	31:CA:1795:C:C6	2.54	0.43
31:CA:2064:C:H2'	31:CA:2065:C:C6	2.53	0.43
31:CA:532:A:N1	31:CA:2020:A:H1'	2.34	0.43
54:DA:1778:U:H2'	54:DA:1784:A:N6	2.34	0.43
54:DA:984:A:N3	54:DA:984:A:H2'	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:216:U:H2'	1:AA:217:C:C6	2.53	0.43
11:AK:34:ILE:HG12	11:AK:70:CYS:SG	2.59	0.43
5:BE:88:VAL:CG1	5:BE:93:ARG:HG2	2.48	0.43
19:BS:29:LYS:HB3	19:BS:30:PRO:HD2	2.01	0.43
31:CA:321:U:H5''	32:CE:131:THR:HG23	2.01	0.43
54:DA:1469:A:H2'	54:DA:1470:A:C8	2.54	0.43
54:DA:1587:G:H2'	54:DA:1588:G:H8	1.84	0.43
54:DA:2233:U:H2'	54:DA:2234:G:C8	2.54	0.43
29:DC:155:ALA:HB2	29:DC:162:VAL:HG23	2.00	0.43
32:DE:23:PHE:HE2	32:DE:25:GLU:HG3	1.84	0.43
33:DF:103:LEU:HA	33:DF:107:ALA:HB3	2.00	0.43
1:AA:567:G:H2'	1:AA:568:G:O4'	2.19	0.43
4:BD:27:ALA:HB3	4:BD:30:THR:HG23	2.00	0.43
31:CA:1028:A:H61	31:CA:1125:G:H2'	1.84	0.43
32:CE:75:SER:O	32:CE:78:TRP:HB2	2.18	0.43
49:CW:77:VAL:HG23	49:CW:89:ILE:HG12	2.00	0.43
54:DA:2097:A:H5''	54:DA:2097:A:H8	1.84	0.43
54:DA:644:A:H2'	54:DA:645:C:O4'	2.19	0.43
36:DJ:19:ASN:N	36:DJ:20:PRO:HD2	2.33	0.43
17:AQ:68:SER:OG	17:AQ:71:LYS:HB2	2.19	0.43
1:BA:663:A:H5'	1:BA:836:G:OP1	2.19	0.43
1:BA:8:A:H1'	5:BE:108:GLY:HA2	2.00	0.43
25:C4:62:LEU:HB3	25:C4:65:ALA:HB2	2.01	0.43
31:CA:1101:U:H2'	31:CA:1102:C:H6	1.84	0.43
31:CA:1427:A:H4'	31:CA:1428:C:O4'	2.18	0.43
31:CA:1662:U:H3	31:CA:1998:A:H61	1.66	0.43
29:CC:258:ARG:NH1	29:CC:264:ASP:OD1	2.52	0.43
33:CF:36:LEU:HD12	33:CF:154:ILE:HG12	2.01	0.43
43:DQ:6:LYS:O	43:DQ:10:GLN:HG2	2.19	0.43
47:DU:28:ASN:OD1	47:DU:91:GLN:HB3	2.19	0.43
1:BA:1171:A:H2'	1:BA:1172:C:C6	2.53	0.42
4:BD:28:ILE:HG12	4:BD:34:ILE:HD13	2.01	0.42
29:CC:69:ARG:HB2	29:CC:129:THR:HG21	2.00	0.42
29:CC:160:THR:HG22	29:CC:177:ARG:HG2	1.99	0.42
29:CC:174:LEU:HD21	29:CC:184:VAL:HB	2.00	0.42
34:CG:19:ILE:HG12	34:CG:24:ILE:HG12	2.01	0.42
52:CZ:46:VAL:O	52:CZ:50:VAL:HG23	2.19	0.42
51:DY:57:ARG:NH1	54:DA:400:G:N7	2.55	0.42
50:DX:41[B]:ARG:HA	50:DX:41[B]:ARG:HD3	1.77	0.42
1:AA:1366:C:H2'	1:AA:1367:C:C6	2.54	0.42
1:AA:268:U:H2'	1:AA:269:C:C6	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1081:A:H5'	5:AE:23:LYS:HG3	2.00	0.42
5:AE:81:LEU:HB3	5:AE:147:MET:SD	2.59	0.42
13:AM:80:LEU:HD22	13:AM:87:ARG:HB3	2.02	0.42
1:BA:1411:C:H2'	1:BA:1412:C:C6	2.54	0.42
31:CA:2543:G:H2'	31:CA:2544:G:C8	2.55	0.42
31:CA:352:A:H8	31:CA:352:A:H5''	1.84	0.42
28:CB:14:U:H2'	28:CB:15:A:C2	2.53	0.42
39:CM:77:ILE:HD11	39:CM:108:ALA:CB	2.35	0.42
45:CS:16:GLU:HG3	45:CS:101:ILE:HG12	1.99	0.42
54:DA:1026:G:H2'	54:DA:1027:A:C8	2.54	0.42
54:DA:476:G:H4'	54:DA:502:A:N1	2.34	0.42
25:D4:13:ARG:HG3	39:DM:63:LYS:HA	2.01	0.42
51:DY:7:VAL:HG23	51:DY:51:VAL:HG12	2.00	0.42
4:AD:28:ILE:HG12	4:AD:34:ILE:HD13	2.01	0.42
8:AH:94:LYS:HB3	8:AH:117:ARG:HH22	1.85	0.42
10:BJ:10:LEU:HB2	10:BJ:72:ARG:HB2	2.01	0.42
35:CH:3:VAL:HG12	35:CH:38:PRO:HA	2.00	0.42
45:CS:37:GLU:HB3	45:CS:53:PHE:CD1	2.54	0.42
54:DA:2051:A:OP2	54:DA:2051:A:H8	2.02	0.42
32:DE:94:GLN:HG2	54:DA:660:C:H5''	2.02	0.42
30:DD:35:THR:HG22	30:DD:73:VAL:HG21	2.01	0.42
41:DO:28:LEU:HD23	41:DO:48:VAL:HG21	2.00	0.42
1:AA:134:G:H2'	1:AA:135:C:O4'	2.19	0.42
1:AA:663:A:H5'	1:AA:836:G:OP1	2.19	0.42
9:BI:98:LEU:HB3	9:BI:104:VAL:HG13	2.01	0.42
9:BI:19:VAL:HG11	9:BI:83:ILE:HA	2.02	0.42
31:CA:123:G:H4'	31:CA:1376:C:O5'	2.20	0.42
31:CA:948:C:H1'	31:CA:984:A:C8	2.54	0.42
36:CJ:19:ASN:N	36:CJ:20:PRO:HD2	2.33	0.42
37:CK:58:ASN:HA	37:CK:126:ALA:O	2.19	0.42
54:DA:2813:A:H2	54:DA:2887[B]:A:N6	2.17	0.42
1:AA:967:5MC:O3'	9:AI:127:PHE:HE1	2.03	0.42
16:BP:6:LEU:HB3	16:BP:17:TYR:HB3	2.01	0.42
31:CA:2579:C:H2'	31:CA:2580:PSU:O4'	2.19	0.42
31:CA:478:A:H61	31:CA:500:G:H4'	1.84	0.42
29:CC:208:ALA:CB	31:CA:1790:C:H4'	2.50	0.42
47:CU:45:ALA:O	47:CU:49:LYS:HG2	2.19	0.42
49:CW:38:LEU:HD21	49:CW:65:VAL:HG11	2.01	0.42
50:CX:18:ALA:HB3	50:CX:20:ARG:NH1	2.33	0.42
53:DI:130:PRO:HG2	53:DI:134:GLU:HG2	2.01	0.42
6:AF:38:ARG:HE	6:AF:63:ASN:ND2	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:34:ILE:HB	11:AK:74:VAL:HG11	2.02	0.42
11:BK:34:ILE:HB	11:BK:74:VAL:HG11	2.01	0.42
31:CA:121:G:H4'	31:CA:149:A:H5'	2.02	0.42
31:CA:608:A:H2'	31:CA:609:A:C8	2.55	0.42
30:CD:101:PHE:O	30:CD:104:VAL:HG22	2.19	0.42
30:CD:186:LEU:HD21	43:CQ:4:ILE:HG21	2.01	0.42
30:CD:55:LYS:HD3	30:CD:60:VAL:HG22	2.02	0.42
43:CQ:6:LYS:O	43:CQ:10:GLN:HG2	2.20	0.42
54:DA:191:A:H2'	54:DA:192:C:C6	2.55	0.42
34:DG:19:ILE:HG12	34:DG:24:ILE:HG12	2.00	0.42
19:AS:29:LYS:HB3	19:AS:30:PRO:HD2	2.02	0.42
1:BA:1338:G:H2'	1:BA:1339:A:C8	2.54	0.42
16:BP:6:LEU:HD23	16:BP:19:VAL:HB	2.00	0.42
31:CA:1539:U:H2'	31:CA:1540:G:C8	2.55	0.42
31:CA:785:G:H4'	31:CA:1779:U:H4'	2.00	0.42
31:CA:1957:C:H5'	31:CA:1984:G:O2'	2.20	0.42
31:CA:659:G:H4'	32:CE:95:LYS:HD3	2.02	0.42
31:CA:732:C:H2'	31:CA:733:G:O4'	2.20	0.42
54:DA:1168:G:H5''	54:DA:1168:G:H8	1.84	0.42
29:DC:69:ARG:HB2	29:DC:129:THR:HG21	2.01	0.42
35:DH:116:ARG:HH21	35:DH:133:GLN:HB2	1.85	0.42
53:DI:26:VAL:HB	53:DI:83:ALA:HB3	2.00	0.42
1:AA:1171:A:H2'	1:AA:1172:C:C6	2.54	0.42
1:BA:216:U:H2'	1:BA:217:C:C6	2.54	0.42
1:BA:923:A:OP1	5:BE:26:LYS:HG2	2.19	0.42
27:C0:6:LYS:HB2	27:C0:58:GLU:HG3	2.02	0.42
31:CA:1703:G:H2'	31:CA:1704:C:C6	2.55	0.42
31:CA:191:A:H2'	31:CA:192:C:C6	2.55	0.42
31:CA:528:A:H3'	31:CA:528:A:H8	1.84	0.42
42:CP:27:VAL:HG21	42:CP:40:ILE:HD12	2.00	0.42
23:D2:6:ARG:HG2	23:D2:24:THR:HB	2.02	0.42
54:DA:1236:G:N7	58:DA:3189:PUT:H41	2.35	0.42
1:AA:202:G:O2'	1:AA:468:A:H8	1.95	0.42
6:AF:9:MET:HG2	6:AF:86:ARG:HB3	2.01	0.42
9:AI:98:LEU:HB3	9:AI:104:VAL:HG13	2.01	0.42
10:AJ:10:LEU:HB2	10:AJ:72:ARG:HB2	2.01	0.42
1:BA:216:U:H4'	1:BA:464:U:H4'	2.02	0.42
1:BA:73:C:O2'	1:BA:74:A:H8	2.03	0.42
11:BK:25:ALA:HA	11:BK:30:THR:HG22	2.02	0.42
13:BM:23:TYR:CD1	13:BM:69:LEU:HD23	2.55	0.42
31:CA:246:C:O2'	31:CA:385:C:H4'	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DA:1424:G:H21	63:DA:3214:PGE:H32	1.84	0.42
35:DH:78:VAL:HG21	35:DH:103:VAL:HG22	2.02	0.42
45:DS:16:GLU:HG3	45:DS:101:ILE:HG12	2.02	0.42
49:DW:38:LEU:HD21	49:DW:65:VAL:HG11	2.01	0.42
1:AA:932:C:H5'	7:AG:4:ARG:HE	1.84	0.42
1:AA:1048:G:H4'	14:AN:3:LYS:HE2	2.01	0.42
1:BA:1308:U:H2'	1:BA:1309:G:H8	1.85	0.42
31:CA:1141:U:H4'	31:CA:1142:A:O4'	2.20	0.42
31:CA:834:G:H1'	31:CA:2358:A:N3	2.35	0.42
54:DA:2479:U:OP1	54:DA:2537:U:H1'	2.20	0.42
54:DA:357:C:H2'	54:DA:358:U:C6	2.55	0.42
39:DM:57:LEU:HA	39:DM:60:ARG:HG3	2.02	0.42
44:DR:6:ARG:HD3	54:DA:1250:G:H5''	2.02	0.42
1:AA:1396:A:H3'	59:AA:1681:TAC:C43	2.48	0.41
1:AA:49:U:O2	1:AA:362:G:H1'	2.20	0.41
1:AA:73:C:O2'	1:AA:74:A:H8	2.02	0.41
1:BA:1366:C:H2'	1:BA:1367:C:C6	2.55	0.41
1:BA:1347:G:N2	1:BA:1373:G:H2'	2.35	0.41
1:BA:567:G:H2'	1:BA:568:G:O4'	2.18	0.41
23:C2:6:ARG:HG2	23:C2:24:THR:HB	2.01	0.41
24:C3:19:ARG:HD3	31:CA:125:A:OP2	2.20	0.41
26:C5:4:ARG:HB2	31:CA:2466:C:OP1	2.19	0.41
31:CA:2623:G:H4'	31:CA:2825:G:C8	2.55	0.41
30:CD:155:VAL:HG11	30:CD:161:MET:CE	2.50	0.41
32:CE:149:ILE:HG23	32:CE:188:MET:HG2	2.02	0.41
32:CE:49:ARG:O	32:CE:74:LYS:HD2	2.20	0.41
36:CJ:11:LEU:HD22	36:CJ:24:VAL:HG23	2.02	0.41
44:CR:113:ALA:O	44:CR:117:LEU:HD12	2.20	0.41
54:DA:527:C:H4'	54:DA:528:A:O5'	2.19	0.41
37:DK:58:ASN:HA	37:DK:126:ALA:O	2.20	0.41
40:DN:92:TRP:HE1	57:DN:201:MPD:HM1	1.83	0.41
42:DP:41:ALA:HB2	42:DP:48:LEU:HD21	2.01	0.41
44:DR:20:GLN:HG3	56:DR:202:PG4:C4	2.40	0.41
5:AE:76:LEU:HD11	5:AE:120:VAL:HG22	2.01	0.41
1:BA:716:A:N3	11:BK:119:ASN:O	2.53	0.41
1:BA:1048:G:H4'	14:BN:3:LYS:HE2	2.02	0.41
17:BQ:46:VAL:HG11	17:BQ:61:ILE:CG2	2.50	0.41
17:BQ:47:HIS:HB2	17:BQ:67:LEU:HD13	2.01	0.41
27:C0:9:GLN:HB3	27:C0:32:ILE:HA	2.03	0.41
31:CA:2544:G:H2'	31:CA:2545:G:O4'	2.20	0.41
29:CC:76:ALA:HB2	29:CC:96:TYR:CD1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DA:264:C:O2'	54:DA:265:A:H2'	2.20	0.41
29:DC:220:VAL:HG21	54:DA:782:A:N7	2.36	0.41
54:DA:871:U:H2'	54:DA:872:U:C6	2.55	0.41
36:DJ:11:LEU:HD22	36:DJ:24:VAL:HG23	2.03	0.41
45:DS:86:GLN:HG2	69:DS:318:HOH:O	2.20	0.41
1:BA:268:U:H2'	1:BA:269:C:C6	2.55	0.41
19:BS:33:THR:HG22	19:BS:35:SER:H	1.86	0.41
31:CA:826:U:O2'	39:CM:53:GLY:HA3	2.19	0.41
44:CR:76:TYR:CZ	44:CR:80:ILE:HG13	2.55	0.41
51:CY:12:PRO:HB3	51:CY:30:LEU:HD23	2.02	0.41
34:DG:26:ILE:O	34:DG:79:VAL:HG11	2.20	0.41
1:AA:1347:G:N2	1:AA:1373:G:H2'	2.35	0.41
1:AA:307:C:C4	57:AA:1676:MPD:H12	2.52	0.41
1:AA:77:A:H2'	1:AA:78:A:C8	2.56	0.41
1:AA:438:U:H5'	4:AD:120:HIS:HB3	2.03	0.41
1:AA:716:A:N3	11:AK:119:ASN:O	2.53	0.41
1:BA:1402:4OC:H2'	1:BA:1403:C:O4'	2.21	0.41
1:BA:79:G:H22	1:BA:90:C:H42	1.67	0.41
3:BC:113:ALA:O	3:BC:200:VAL:HG11	2.19	0.41
5:BE:149:SER:HB2	5:BE:151:GLU:HG2	2.02	0.41
39:CM:95:LEU:HD22	39:CM:100:ILE:HG12	2.02	0.41
54:DA:2063:C:O2	54:DA:2450:A:N1	2.53	0.41
29:DC:97:LYS:HD3	29:DC:97:LYS:HA	1.72	0.41
35:DH:71:LYS:HB3	35:DH:108:VAL:HG22	2.02	0.41
52:DZ:46:VAL:O	52:DZ:50:VAL:HG23	2.19	0.41
12:AL:36:ARG:HH11	12:AL:54:ARG:NH1	2.18	0.41
31:CA:511:U:H5''	31:CA:1235:G:H4'	2.03	0.41
49:CW:51:GLN:HB2	49:CW:57:TYR:OH	2.21	0.41
29:DC:154:LEU:HD13	29:DC:176:LEU:HD21	2.01	0.41
33:DF:34:ILE:HG12	33:DF:156:ILE:HG12	2.02	0.41
34:DG:24:ILE:HG21	34:DG:72:LEU:HD21	2.02	0.41
53:DI:65:GLU:HA	53:DI:70:GLU:HG3	2.01	0.41
1:AA:649:A:H2'	1:AA:650:G:O4'	2.20	0.41
5:AE:126:LYS:HG2	5:AE:128:TYR:CZ	2.56	0.41
17:AQ:21:ILE:HD12	17:AQ:23:VAL:CG2	2.50	0.41
1:BA:1530:G:H2'	1:BA:1531:A:C8	2.56	0.41
1:BA:269:C:H2'	1:BA:270:A:C8	2.56	0.41
5:BE:57:PRO:O	5:BE:60:ILE:HG13	2.21	0.41
11:BK:43:GLY:HA3	11:BK:74:VAL:HG12	2.03	0.41
31:CA:729:G:H2'	31:CA:1775:U:H1'	2.02	0.41
31:CA:783:A:H2	31:CA:1778:U:H4'	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:264:C:O2'	31:CA:265:A:H2'	2.20	0.41
31:CA:594:U:H2'	31:CA:595:C:C6	2.55	0.41
29:CC:174:LEU:CD2	29:CC:184:VAL:HB	2.50	0.41
39:CM:79:LEU:O	39:CM:82:LEU:HG	2.21	0.41
31:CA:1154:G:OP1	44:CR:58:ARG:HD3	2.20	0.41
54:DA:1539:U:H2'	54:DA:1540:G:C8	2.55	0.41
54:DA:2698:U:H2'	54:DA:2699:C:C6	2.56	0.41
35:DH:3:VAL:HG12	35:DH:38:PRO:HA	2.03	0.41
42:DP:53:THR:HB	42:DP:65:THR:HG22	2.02	0.41
22:D1:25:VAL:HG11	46:DT:38:TYR:CB	2.51	0.41
1:AA:1152:A:H2'	1:AA:1153:G:H8	1.85	0.41
1:AA:1308:U:H2'	1:AA:1309:G:H8	1.85	0.41
10:AJ:80:THR:HG22	10:AJ:82:LYS:H	1.85	0.41
1:BA:591:U:H2'	1:BA:592:G:C8	2.55	0.41
1:BA:1108:G:H5''	3:BC:176:HIS:CE1	2.56	0.41
10:BJ:80:THR:HG22	10:BJ:82:LYS:H	1.86	0.41
1:BA:310:G:H5''	16:BP:31:ARG:HB2	2.02	0.41
27:D0:8:THR:O	27:D0:55:VAL:HA	2.21	0.41
54:DA:121:G:H4'	54:DA:149:A:H5'	2.02	0.41
1:BA:629:A:H2'	1:BA:630:A:O4'	2.21	0.41
2:BB:12:ALA:HB2	2:BB:212:LEU:HD13	2.02	0.41
13:BM:80:LEU:HD22	13:BM:87:ARG:HB3	2.03	0.41
31:CA:1779:U:C5	31:CA:1784:A:N7	2.73	0.41
31:CA:563:A:H1'	31:CA:2018:G:N2	2.36	0.41
31:CA:845:A:H61	31:CA:932:U:H3	1.68	0.41
23:D2:39:PHE:HB2	23:D2:46:HIS:CE1	2.56	0.41
54:DA:1720:U:H2'	54:DA:1721:G:O4'	2.20	0.41
54:DA:2070:A:H2'	54:DA:2071:A:O4'	2.21	0.41
43:DQ:25:THR:HB	43:DQ:88:ARG:HB3	2.03	0.41
1:AA:591:U:H2'	1:AA:592:G:C8	2.55	0.41
2:AB:163:VAL:HG11	2:AB:173:ILE:HD11	2.03	0.41
31:CA:2063:C:O2	31:CA:2450:A:N1	2.54	0.41
31:CA:388:G:N7	31:CA:390:U:H2'	2.35	0.41
29:CC:200:HIS:O	29:CC:203:ARG:HG2	2.21	0.41
54:DA:2123:G:H2'	54:DA:2124:G:H8	1.85	0.41
54:DA:2813:A:H2	54:DA:2887[B]:A:H61	1.66	0.41
57:DA:3207:MPD:H11	57:DA:3207:MPD:H4	1.99	0.41
32:DE:49:ARG:O	32:DE:74:LYS:HD2	2.21	0.41
32:DE:32:VAL:HG21	39:DM:6:LEU:HD13	2.03	0.41
49:DW:77:VAL:HG23	49:DW:89:ILE:HG12	2.03	0.41
1:AA:1402:4OC:H2'	1:AA:1403:C:O4'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AK:25:ALA:HA	11:AK:30:THR:HG22	2.03	0.41
1:BA:202:G:H21	1:BA:466:A:H61	1.67	0.41
1:BA:438:U:H5'	4:BD:120:HIS:HB3	2.02	0.41
31:CA:357:C:H2'	31:CA:358:U:C6	2.55	0.41
31:CA:797:G:H5''	32:CE:55:SER:HB2	2.02	0.41
40:CN:71:LYS:HB3	40:CN:93:VAL:O	2.20	0.41
31:CA:396:G:C1'	51:CY:29:PHE:HB3	2.49	0.41
1:AA:269:C:H2'	1:AA:270:A:C8	2.55	0.41
1:AA:677:U:H3	1:AA:713:G:H22	1.69	0.41
1:AA:9:G:H5'	5:AE:108:GLY:HA3	2.03	0.41
9:AI:19:VAL:HG11	9:AI:83:ILE:HA	2.02	0.41
20:AT:44:LYS:HG3	20:AT:44:LYS:H	1.54	0.41
4:BD:197:GLU:HA	4:BD:200:ILE:HD12	2.03	0.41
16:BP:40:ASN:O	16:BP:43:ALA:HB2	2.21	0.41
49:CW:63:ILE:CD1	49:CW:72:VAL:HG21	2.50	0.41
54:DA:2336:A:N3	54:DA:2385:C:H1'	2.36	0.41
45:DS:21:ARG:HH21	56:DS:202:PG4:C7	2.34	0.41
46:DT:17:VAL:HB	46:DT:76:VAL:HG11	2.03	0.41
46:DT:77:ASP:HB3	54:DA:24:G:O2'	2.20	0.41
1:AA:629:A:H2'	1:AA:630:A:O4'	2.21	0.40
31:CA:1181:U:H2'	31:CA:1182:G:C8	2.56	0.40
31:CA:1662:U:O2'	31:CA:2687:U:H5''	2.21	0.40
31:CA:225:C:H2'	31:CA:226:A:O4'	2.21	0.40
31:CA:372:G:H5''	51:CY:61:LYS:HD3	2.03	0.40
30:DD:167:ASN:HD21	62:DA:3198:EDO:H11	1.86	0.40
42:DP:103:VAL:HG23	69:DB:307:HOH:O	2.21	0.40
1:AA:1463:U:H2'	1:AA:1464:U:C6	2.56	0.40
1:AA:322:C:H5	1:AA:328:C:C5	2.38	0.40
1:BA:1463:U:H2'	1:BA:1464:U:C6	2.56	0.40
31:CA:2698:U:H2'	31:CA:2699:C:C6	2.56	0.40
30:CD:63:PRO:HG3	31:CA:2787:C:H1'	2.02	0.40
32:CE:108:ILE:HG21	32:CE:181:ILE:HD11	2.04	0.40
26:D5:2:LYS:HE2	26:D5:4:ARG:HH11	1.86	0.40
54:DA:1093:G:H1'	54:DA:1099:G:N2	2.37	0.40
54:DA:1354:A:H2'	54:DA:1355:G:O4'	2.21	0.40
54:DA:2678:C:H2'	54:DA:2679:A:O4'	2.20	0.40
54:DA:78:U:H2'	54:DA:79:C:C6	2.57	0.40
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.56	0.40
1:AA:244:U:O4	1:AA:906:A:H1'	2.22	0.40
1:AA:920:U:H2'	1:AA:921:U:C6	2.57	0.40
1:BA:1411:C:H2'	1:BA:1412:C:H6	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BL:33:VAL:HG22	12:BL:79:VAL:HG22	2.04	0.40
29:CC:13:ARG:HD3	31:CA:728:G:H4'	2.03	0.40
35:CH:71:LYS:HB3	35:CH:108:VAL:HG22	2.04	0.40
31:CA:1808:A:N1	51:CY:28:ARG:HD2	2.36	0.40
22:D1:24:ALA:HB1	46:DT:35:ILE:HG12	2.03	0.40
54:DA:2022:U:H1'	69:DA:3881:HOH:O	2.21	0.40
54:DA:2545:G:N3	54:DA:2565:A:H2	2.20	0.40
54:DA:909:A:O2'	54:DA:910:A:H5'	2.21	0.40
29:DC:199:GLU:O	29:DC:202:LEU:HB2	2.22	0.40
44:DR:76:TYR:CZ	44:DR:80:ILE:HG13	2.56	0.40
47:DU:33:LYS:HE2	63:DU:101:PGE:C2	2.52	0.40
47:DU:33:LYS:NZ	63:DU:101:PGE:H62	2.36	0.40
47:DU:69:ARG:HG3	47:DU:74:ILE:HG22	2.03	0.40
50:DX:11:ARG:HG2	56:DA:3193:PG4:H12	2.04	0.40
3:AC:151:VAL:HG12	3:AC:200:VAL:HG22	2.02	0.40
10:AJ:53:ILE:HG13	14:AN:85:ARG:HD2	2.04	0.40
14:AN:21:PHE:HA	14:AN:25:ALA:HB3	2.02	0.40
14:AN:46:LEU:HA	14:AN:49:GLN:HE21	1.86	0.40
16:AP:6:LEU:HB3	16:AP:17:TYR:HB3	2.02	0.40
1:BA:649:A:H2'	1:BA:650:G:O4'	2.21	0.40
1:BA:1108:G:H5''	3:BC:176:HIS:ND1	2.37	0.40
31:CA:2185:U:H2'	31:CA:2186:G:C8	2.57	0.40
31:CA:78:U:H2'	31:CA:79:C:C6	2.57	0.40
31:CA:586:A:H5'	32:CE:84:THR:HG21	2.02	0.40
31:CA:2305:U:H5''	33:CF:131:GLY:HA3	2.04	0.40
46:CT:17:VAL:HB	46:CT:76:VAL:HG11	2.03	0.40
63:DA:3001:PGE:H52	69:DA:5960:HOH:O	2.22	0.40
54:DA:340:A:H2'	54:DA:341:C:O4'	2.22	0.40
38:DL:78:ARG:HD3	69:DL:308:HOH:O	2.21	0.40
1:AA:1108:G:H5''	3:AC:176:HIS:ND1	2.37	0.40
54:DA:2324:U:H3'	54:DA:2325:G:C5'	2.52	0.40
54:DA:364:C:H2'	54:DA:365:U:C6	2.57	0.40
33:DF:14:LYS:O	33:DF:18:THR:HG22	2.21	0.40
37:DK:7:LYS:HG2	54:DA:538:A:H4'	2.03	0.40
39:DM:123:ARG:HG3	39:DM:143:GLU:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	207 (93%)	11 (5%)	4 (2%)	11	45
2	BB	222/224 (99%)	208 (94%)	10 (4%)	4 (2%)	11	45
3	AC	204/206 (99%)	193 (95%)	10 (5%)	1 (0%)	34	76
3	BC	204/206 (99%)	194 (95%)	7 (3%)	3 (2%)	13	50
4	AD	203/205 (99%)	196 (97%)	6 (3%)	1 (0%)	34	76
4	BD	203/205 (99%)	196 (97%)	6 (3%)	1 (0%)	34	76
5	AE	153/155 (99%)	145 (95%)	7 (5%)	1 (1%)	26	70
5	BE	148/155 (96%)	134 (90%)	8 (5%)	6 (4%)	3	20
6	AF	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
6	BF	98/106 (92%)	93 (95%)	1 (1%)	4 (4%)	3	20
7	AG	149/151 (99%)	134 (90%)	14 (9%)	1 (1%)	26	70
7	BG	149/151 (99%)	137 (92%)	11 (7%)	1 (1%)	26	70
8	AH	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	24	66
8	BH	127/129 (98%)	121 (95%)	4 (3%)	2 (2%)	12	48
9	AI	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
9	BI	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
10	AJ	97/99 (98%)	89 (92%)	6 (6%)	2 (2%)	9	40
10	BJ	96/99 (97%)	76 (79%)	14 (15%)	6 (6%)	2	9
11	AK	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	21	64
11	BK	115/117 (98%)	102 (89%)	12 (10%)	1 (1%)	21	64
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
12	BL	120/123 (98%)	116 (97%)	3 (2%)	1 (1%)	24	66
13	AM	112/114 (98%)	100 (89%)	9 (8%)	3 (3%)	6	32
13	BM	112/114 (98%)	99 (88%)	8 (7%)	5 (4%)	3	18
14	AN	98/100 (98%)	86 (88%)	10 (10%)	2 (2%)	9	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	BN	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	19	61
15	AO	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
15	BO	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	16	56
16	AP	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	15	53
16	BP	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	7	34
17	AQ	78/80 (98%)	71 (91%)	6 (8%)	1 (1%)	15	53
17	BQ	78/80 (98%)	67 (86%)	7 (9%)	4 (5%)	2	15
18	AR	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/79 (98%)	68 (88%)	9 (12%)	0	100	100
19	BS	77/79 (98%)	66 (86%)	10 (13%)	1 (1%)	15	53
20	AT	84/86 (98%)	81 (96%)	2 (2%)	1 (1%)	16	56
20	BT	83/86 (96%)	79 (95%)	2 (2%)	2 (2%)	7	35
21	AU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
21	BU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
22	C1	54/56 (96%)	47 (87%)	4 (7%)	3 (6%)	2	13
22	D1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	3	20
23	D2	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
24	C3	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	8	36
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	C4	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	12	48
25	D4	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	12	48
26	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	6	30
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	4	24
27	D0	57/58 (98%)	53 (93%)	4 (7%)	0	100	100
29	CC	269/271 (99%)	250 (93%)	15 (6%)	4 (2%)	13	50
29	DC	269/271 (99%)	250 (93%)	17 (6%)	2 (1%)	26	70
30	CD	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
30	DD	206/209 (99%)	197 (96%)	9 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	CE	199/201 (99%)	187 (94%)	9 (4%)	3 (2%)	13	50
32	DE	199/201 (99%)	192 (96%)	6 (3%)	1 (0%)	34	76
33	CF	175/177 (99%)	164 (94%)	10 (6%)	1 (1%)	30	72
33	DF	175/177 (99%)	166 (95%)	7 (4%)	2 (1%)	17	58
34	CG	174/176 (99%)	160 (92%)	10 (6%)	4 (2%)	8	36
34	DG	174/176 (99%)	162 (93%)	11 (6%)	1 (1%)	30	72
35	CH	147/149 (99%)	128 (87%)	14 (10%)	5 (3%)	5	25
35	DH	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	14	51
36	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	5	29
36	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	5	29
37	CK	140/142 (99%)	134 (96%)	4 (3%)	2 (1%)	14	51
37	DK	140/142 (99%)	136 (97%)	3 (2%)	1 (1%)	26	70
38	CL	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	11	46
38	DL	121/123 (98%)	115 (95%)	4 (3%)	2 (2%)	11	46
39	CM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	9	40
39	DM	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	26	70
40	CN	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
40	DN	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
41	CO	118/125 (94%)	111 (94%)	5 (4%)	2 (2%)	11	46
41	DO	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
42	CP	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
42	DP	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
43	CQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	21	64
43	DQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	21	64
44	CR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
44	DR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
45	CS	101/103 (98%)	90 (89%)	8 (8%)	3 (3%)	5	29
45	DS	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	19	61
46	CT	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
46	DT	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
47	CU	91/93 (98%)	85 (93%)	5 (6%)	1 (1%)	17	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	DU	91/93 (98%)	84 (92%)	6 (7%)	1 (1%)	17	58
48	CV	100/102 (98%)	89 (89%)	7 (7%)	4 (4%)	4	21
48	DV	100/102 (98%)	94 (94%)	4 (4%)	2 (2%)	9	41
49	CW	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
49	DW	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
50	CX	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
50	DX	75/76 (99%)	73 (97%)	2 (3%)	0	100	100
51	CY	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
51	DY	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
52	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11	46
52	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
53	DI	133/135 (98%)	115 (86%)	12 (9%)	6 (4%)	3	18
All	All	11406/11629 (98%)	10673 (94%)	590 (5%)	143 (1%)	15	53

All (143) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE
3	AC	156	ARG
10	AJ	57	VAL
13	AM	5	ALA
17	AQ	82	ALA
23	C2	5	ILE
27	C0	4	THR
2	BB	126	PHE
3	BC	156	ARG
6	BF	98	GLU
10	BJ	38	GLY
10	BJ	57	VAL
10	BJ	91	ASP
13	BM	7	ILE
16	BP	80	LYS
17	BQ	82	ALA
29	CC	158	ALA
32	CE	82	GLY
32	CE	83	VAL
34	CG	119	ALA
34	CG	175	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	CG	176	LYS
35	CH	10	ALA
36	CJ	19	ASN
37	CK	81	ILE
38	CL	35	VAL
39	CM	29	LYS
39	CM	69	ARG
48	CV	7	ARG
48	CV	16	GLY
35	DH	11	ASN
36	DJ	19	ASN
48	DV	52	LEU
53	DI	91	ALA
7	AG	56	LYS
13	AM	7	ILE
13	AM	105	ASN
14	AN	38	ASP
22	C1	25	VAL
22	C1	27	SER
27	C0	14	ILE
2	BB	95	ARG
3	BC	61	ALA
5	BE	51	GLY
5	BE	103	THR
6	BF	92	THR
12	BL	44	LYS
13	BM	5	ALA
13	BM	105	ASN
13	BM	114	LYS
14	BN	38	ASP
15	BO	88	ARG
19	BS	6	LYS
20	BT	5	LYS
29	CC	233	GLY
29	CC	253	LYS
29	DC	233	GLY
29	DC	253	LYS
34	CG	46	ALA
36	CJ	25	GLY
38	CL	108	ARG
47	CU	89	GLU
48	CV	17	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	CV	89	ASP
34	DG	46	ALA
36	DJ	25	GLY
38	DL	108	ARG
43	DQ	105	GLY
48	DV	89	ASP
2	AB	95	ARG
4	AD	197	GLU
5	AE	162	GLU
8	AH	66	PHE
11	AK	89	PRO
23	C2	51	GLU
24	C3	45	SER
26	C5	20	ASP
2	BB	127	ASP
5	BE	110	ALA
5	BE	157	ARG
8	BH	66	PHE
10	BJ	36	VAL
10	BJ	95	GLY
11	BK	89	PRO
13	BM	4	ILE
17	BQ	17	MET
17	BQ	70	THR
20	BT	43	ASP
29	CC	197	ASN
32	CE	6	LYS
35	CH	11	ASN
39	CM	36	LYS
41	CO	118	ARG
41	CO	119	SER
32	DE	6	LYS
53	DI	70	GLU
53	DI	109	LYS
53	DI	130	PRO
2	AB	125	THR
2	AB	127	ASP
16	AP	45	GLU
22	C1	26	THR
2	BB	125	THR
4	BD	197	GLU
5	BE	24	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	BF	99	ALA
16	BP	44	SER
35	CH	9	VAL
36	CJ	23	PRO
37	CK	25	LEU
43	CQ	105	GLY
45	CS	43	ASN
45	CS	48	LYS
36	DJ	23	PRO
38	DL	75	SER
45	DS	44	GLY
53	DI	88	HIS
14	AN	21	PHE
20	AT	43	ASP
8	BH	67	GLN
17	BQ	18	GLU
35	CH	8	LYS
52	CZ	62	GLY
37	DK	25	LEU
39	DM	36	LYS
47	DU	89	GLU
53	DI	108	VAL
3	BC	127	ARG
6	BF	94	HIS
7	BG	56	LYS
10	BJ	93	ALA
45	CS	53	PHE
5	BE	105	ILE
35	CH	118	PRO
36	CJ	32	GLY
35	DH	118	PRO
36	DJ	32	GLY
10	AJ	33	GLY
33	CF	62	GLY
33	DF	62	GLY
25	D4	18	GLY
33	DF	176	PRO
25	C4	18	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%)	172 (92%)	14 (8%)	17	51
2	BB	186/186 (100%)	172 (92%)	14 (8%)	17	51
3	AC	170/170 (100%)	156 (92%)	14 (8%)	14	46
3	BC	170/170 (100%)	156 (92%)	14 (8%)	14	46
4	AD	172/172 (100%)	165 (96%)	7 (4%)	37	76
4	BD	172/172 (100%)	163 (95%)	9 (5%)	29	68
5	AE	118/118 (100%)	103 (87%)	15 (13%)	5	23
5	BE	113/118 (96%)	91 (80%)	22 (20%)	2	9
6	AF	92/92 (100%)	84 (91%)	8 (9%)	13	43
6	BF	87/92 (95%)	73 (84%)	14 (16%)	3	14
7	AG	124/124 (100%)	109 (88%)	15 (12%)	6	25
7	BG	124/124 (100%)	106 (86%)	18 (14%)	4	18
8	AH	104/104 (100%)	90 (86%)	14 (14%)	5	20
8	BH	104/104 (100%)	88 (85%)	16 (15%)	3	16
9	AI	105/105 (100%)	99 (94%)	6 (6%)	25	64
9	BI	105/105 (100%)	99 (94%)	6 (6%)	25	64
10	AJ	87/87 (100%)	80 (92%)	7 (8%)	15	47
10	BJ	86/87 (99%)	76 (88%)	10 (12%)	7	27
11	AK	90/90 (100%)	90 (100%)	0	100	100
11	BK	90/90 (100%)	84 (93%)	6 (7%)	20	57
12	AL	102/102 (100%)	93 (91%)	9 (9%)	12	42
12	BL	102/102 (100%)	90 (88%)	12 (12%)	6	26
13	AM	92/92 (100%)	84 (91%)	8 (9%)	13	43
13	BM	92/92 (100%)	84 (91%)	8 (9%)	13	43
14	AN	83/83 (100%)	81 (98%)	2 (2%)	57	87
14	BN	83/83 (100%)	80 (96%)	3 (4%)	42	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	76/76 (100%)	69 (91%)	7 (9%)	11	40
15	BO	76/76 (100%)	68 (90%)	8 (10%)	8	32
16	AP	65/65 (100%)	62 (95%)	3 (5%)	33	73
16	BP	65/65 (100%)	61 (94%)	4 (6%)	23	60
17	AQ	74/74 (100%)	66 (89%)	8 (11%)	8	30
17	BQ	74/74 (100%)	63 (85%)	11 (15%)	4	17
18	AR	48/48 (100%)	47 (98%)	1 (2%)	61	89
18	BR	48/48 (100%)	48 (100%)	0	100	100
19	AS	70/70 (100%)	62 (89%)	8 (11%)	7	28
19	BS	70/70 (100%)	65 (93%)	5 (7%)	18	54
20	AT	65/65 (100%)	58 (89%)	7 (11%)	8	30
20	BT	65/65 (100%)	53 (82%)	12 (18%)	2	10
21	AU	48/48 (100%)	46 (96%)	2 (4%)	36	76
21	BU	48/48 (100%)	46 (96%)	2 (4%)	36	76
22	C1	47/47 (100%)	46 (98%)	1 (2%)	61	89
22	D1	47/47 (100%)	47 (100%)	0	100	100
23	C2	45/46 (98%)	43 (96%)	2 (4%)	35	74
23	D2	45/46 (98%)	42 (93%)	3 (7%)	20	57
24	C3	38/38 (100%)	36 (95%)	2 (5%)	28	67
24	D3	38/38 (100%)	36 (95%)	2 (5%)	28	67
25	C4	51/51 (100%)	45 (88%)	6 (12%)	6	26
25	D4	51/51 (100%)	48 (94%)	3 (6%)	24	63
26	C5	34/34 (100%)	31 (91%)	3 (9%)	12	42
26	D5	34/34 (100%)	33 (97%)	1 (3%)	50	84
27	C0	48/48 (100%)	41 (85%)	7 (15%)	4	18
27	D0	49/48 (102%)	43 (88%)	6 (12%)	6	25
29	CC	216/216 (100%)	203 (94%)	13 (6%)	24	62
29	DC	216/216 (100%)	208 (96%)	8 (4%)	41	79
30	CD	163/163 (100%)	159 (98%)	4 (2%)	55	86
30	DD	163/163 (100%)	160 (98%)	3 (2%)	66	91
32	CE	165/165 (100%)	149 (90%)	16 (10%)	10	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	DE	165/165 (100%)	159 (96%)	6 (4%)	42	79
33	CF	148/148 (100%)	134 (90%)	14 (10%)	11	38
33	DF	148/148 (100%)	134 (90%)	14 (10%)	11	38
34	CG	137/137 (100%)	134 (98%)	3 (2%)	60	88
34	DG	137/137 (100%)	133 (97%)	4 (3%)	50	84
35	CH	114/114 (100%)	102 (90%)	12 (10%)	8	32
35	DH	114/114 (100%)	105 (92%)	9 (8%)	15	48
36	CJ	104/104 (100%)	99 (95%)	5 (5%)	31	71
36	DJ	104/104 (100%)	99 (95%)	5 (5%)	31	71
37	CK	116/116 (100%)	112 (97%)	4 (3%)	44	81
37	DK	116/116 (100%)	113 (97%)	3 (3%)	54	85
38	CL	103/104 (99%)	95 (92%)	8 (8%)	16	49
38	DL	104/104 (100%)	99 (95%)	5 (5%)	31	71
39	CM	103/103 (100%)	95 (92%)	8 (8%)	16	49
39	DM	103/103 (100%)	100 (97%)	3 (3%)	50	84
40	CN	108/108 (100%)	103 (95%)	5 (5%)	33	73
40	DN	109/108 (101%)	104 (95%)	5 (5%)	33	73
41	CO	100/102 (98%)	93 (93%)	7 (7%)	19	55
41	DO	102/102 (100%)	97 (95%)	5 (5%)	31	71
42	CP	86/87 (99%)	80 (93%)	6 (7%)	19	55
42	DP	87/87 (100%)	84 (97%)	3 (3%)	44	81
43	CQ	99/99 (100%)	95 (96%)	4 (4%)	38	77
43	DQ	99/99 (100%)	98 (99%)	1 (1%)	82	95
44	CR	89/89 (100%)	85 (96%)	4 (4%)	34	74
44	DR	89/89 (100%)	85 (96%)	4 (4%)	34	74
45	CS	84/84 (100%)	77 (92%)	7 (8%)	14	46
45	DS	84/84 (100%)	82 (98%)	2 (2%)	57	87
46	CT	93/93 (100%)	87 (94%)	6 (6%)	21	58
46	DT	93/93 (100%)	89 (96%)	4 (4%)	35	75
47	CU	80/80 (100%)	71 (89%)	9 (11%)	7	28
47	DU	80/80 (100%)	77 (96%)	3 (4%)	40	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	CV	83/83 (100%)	77 (93%)	6 (7%)	18	53
48	DV	83/83 (100%)	79 (95%)	4 (5%)	31	71
49	CW	78/78 (100%)	74 (95%)	4 (5%)	29	69
49	DW	78/78 (100%)	75 (96%)	3 (4%)	40	78
50	CX	56/58 (97%)	53 (95%)	3 (5%)	27	66
50	DX	58/58 (100%)	53 (91%)	5 (9%)	13	44
51	CY	67/67 (100%)	63 (94%)	4 (6%)	24	62
51	DY	67/67 (100%)	65 (97%)	2 (3%)	48	83
52	CZ	54/54 (100%)	50 (93%)	4 (7%)	17	52
52	DZ	54/54 (100%)	53 (98%)	1 (2%)	65	90
53	DI	103/103 (100%)	96 (93%)	7 (7%)	20	56
All	All	9460/9477 (100%)	8810 (93%)	650 (7%)	19	56

All (650) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	23	TRP
2	AB	73	LYS
2	AB	93	ASN
2	AB	105	LYS
2	AB	108	ARG
2	AB	125	THR
2	AB	129	LEU
2	AB	130	THR
2	AB	135	LEU
2	AB	137	ARG
2	AB	147	SER
2	AB	161	LEU
2	AB	205	ASP
2	AB	212	LEU
3	AC	14	ILE
3	AC	21	THR
3	AC	33	LEU
3	AC	46	GLU
3	AC	55	ILE
3	AC	60	PRO
3	AC	75	ILE
3	AC	107	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	AC	110	GLU
3	AC	168	TYR
3	AC	175	LEU
3	AC	178	LEU
3	AC	185	ASN
3	AC	207	ILE
4	AD	10	LYS
4	AD	17	THR
4	AD	22	LYS
4	AD	26	ARG
4	AD	28	ILE
4	AD	143	VAL
4	AD	194	ASP
5	AE	11	LEU
5	AE	14	LYS
5	AE	43	ASN
5	AE	46	VAL
5	AE	76	LEU
5	AE	78	ASN
5	AE	82	GLN
5	AE	94	VAL
5	AE	101	GLU
5	AE	106	ILE
5	AE	123	VAL
5	AE	126	LYS
5	AE	137	VAL
5	AE	148	ASN
5	AE	149	SER
6	AF	36	ILE
6	AF	39	LEU
6	AF	62	MET
6	AF	69	GLU
6	AF	71	ILE
6	AF	74	LEU
6	AF	89	VAL
6	AF	93	LYS
7	AG	18	PHE
7	AG	22	LEU
7	AG	23	LEU
7	AG	30	LEU
7	AG	36	LYS
7	AG	59	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	AG	63	GLU
7	AG	76	LYS
7	AG	83	SER
7	AG	92	ARG
7	AG	95	ARG
7	AG	120	LEU
7	AG	131	LYS
7	AG	133	THR
7	AG	142	HIS
8	AH	3	MET
8	AH	13	ARG
8	AH	38	ASN
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	96	MET
8	AH	107	SER
8	AH	117	ARG
8	AH	129	VAL
9	AI	11	ARG
9	AI	61	LEU
9	AI	63	LEU
9	AI	66	THR
9	AI	96	SER
9	AI	99	ARG
10	AJ	6	ILE
10	AJ	19	ASP
10	AJ	62	ARG
10	AJ	63	ASP
10	AJ	69	THR
10	AJ	89	ARG
10	AJ	90	LEU
12	AL	24	LEU
12	AL	55	VAL
12	AL	74	LEU
12	AL	82	ILE
12	AL	86	ARG
12	AL	88	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	AL	110	ARG
12	AL	115	SER
12	AL	121	ARG
13	AM	7	ILE
13	AM	13	LYS
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	59	ARG
14	AN	80	SER
15	AO	2	SER
15	AO	24	SER
15	AO	40	GLN
15	AO	70	LEU
15	AO	84	ARG
15	AO	88	ARG
15	AO	89	ARG
16	AP	36	VAL
16	AP	48	GLU
16	AP	54	LEU
17	AQ	5	ILE
17	AQ	16	LYS
17	AQ	26	GLU
17	AQ	33	ILE
17	AQ	38	ILE
17	AQ	51	ASN
17	AQ	75	LEU
17	AQ	83	VAL
18	AR	66	SER
19	AS	5	LEU
19	AS	7	LYS
19	AS	11	ILE
19	AS	13	LEU
19	AS	27	ASP
19	AS	33	THR
19	AS	37	ARG
19	AS	56	GLN
20	AT	8	LYS
20	AT	23	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	AT	24	ARG
20	AT	44	LYS
20	AT	48	GLN
20	AT	66	LEU
20	AT	85	LYS
21	AU	13	ASP
21	AU	56	HIS
22	C1	10	ARG
23	C2	8	LYS
23	C2	47	VAL
24	C3	1	MET
24	C3	15	SER
25	C4	8	ARG
25	C4	13	ARG
25	C4	31	HIS
25	C4	47	LYS
25	C4	51	SER
25	C4	52	LYS
26	C5	16	ILE
26	C5	20	ASP
26	C5	26	ILE
27	C0	3	LYS
27	C0	5	ILE
27	C0	19	LYS
27	C0	36	VAL
27	C0	39	GLU
27	C0	45	ARG
27	C0	59	GLU
2	BB	23	TRP
2	BB	73	LYS
2	BB	93	ASN
2	BB	105	LYS
2	BB	108	ARG
2	BB	125	THR
2	BB	129	LEU
2	BB	130	THR
2	BB	135	LEU
2	BB	137	ARG
2	BB	147	SER
2	BB	161	LEU
2	BB	205	ASP
2	BB	212	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	BC	3	GLN
3	BC	14	ILE
3	BC	21	THR
3	BC	33	LEU
3	BC	37	PHE
3	BC	38	LYS
3	BC	46	GLU
3	BC	75	ILE
3	BC	107	ARG
3	BC	110	GLU
3	BC	152	GLU
3	BC	168	TYR
3	BC	185	ASN
3	BC	207	ILE
4	BD	10	LYS
4	BD	17	THR
4	BD	22	LYS
4	BD	26	ARG
4	BD	28	ILE
4	BD	143	VAL
4	BD	173	VAL
4	BD	194	ASP
4	BD	206	LYS
5	BE	11	LEU
5	BE	14	LYS
5	BE	19	ASN
5	BE	24	THR
5	BE	43	ASN
5	BE	46	VAL
5	BE	76	LEU
5	BE	81	LEU
5	BE	82	GLN
5	BE	88	VAL
5	BE	94	VAL
5	BE	101	GLU
5	BE	103	THR
5	BE	114	VAL
5	BE	115	LEU
5	BE	123	VAL
5	BE	126	LYS
5	BE	137	VAL
5	BE	148	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	BE	149	SER
5	BE	151	GLU
5	BE	159	LYS
6	BF	14	GLN
6	BF	16	GLU
6	BF	36	ILE
6	BF	39	LEU
6	BF	53	LYS
6	BF	62	MET
6	BF	68	GLN
6	BF	69	GLU
6	BF	71	ILE
6	BF	74	LEU
6	BF	79	ARG
6	BF	84	VAL
6	BF	89	VAL
6	BF	93	LYS
7	BG	4	ARG
7	BG	5	ARG
7	BG	10	ARG
7	BG	18	PHE
7	BG	23	LEU
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	92	ARG
7	BG	95	ARG
7	BG	109	ARG
7	BG	120	LEU
7	BG	131	LYS
7	BG	133	THR
7	BG	142	HIS
8	BH	3	MET
8	BH	13	ARG
8	BH	38	ASN
8	BH	47	GLU
8	BH	51	VAL
8	BH	52	GLU
8	BH	60	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	BH	76	GLN
8	BH	77	ARG
8	BH	80	ARG
8	BH	83	LEU
8	BH	90	ASP
8	BH	96	MET
8	BH	107	SER
8	BH	117	ARG
8	BH	129	VAL
9	BI	11	ARG
9	BI	61	LEU
9	BI	63	LEU
9	BI	66	THR
9	BI	96	SER
9	BI	99	ARG
10	BJ	5	ARG
10	BJ	6	ILE
10	BJ	19	ASP
10	BJ	59	LYS
10	BJ	62	ARG
10	BJ	63	ASP
10	BJ	69	THR
10	BJ	78	GLU
10	BJ	89	ARG
10	BJ	90	LEU
11	BK	18	ASP
11	BK	22	HIS
11	BK	31	ILE
11	BK	38	GLN
11	BK	72	ASP
11	BK	118	HIS
12	BL	4	VAL
12	BL	24	LEU
12	BL	44	LYS
12	BL	55	VAL
12	BL	58	THR
12	BL	74	LEU
12	BL	82	ILE
12	BL	86	ARG
12	BL	88	LYS
12	BL	110	ARG
12	BL	115	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	BL	121	ARG
13	BM	11	ASP
13	BM	16	VAL
13	BM	27	LYS
13	BM	30	SER
13	BM	41	GLU
13	BM	48	LEU
13	BM	54	ASP
13	BM	101	ARG
14	BN	26	GLU
14	BN	59	ARG
14	BN	80	SER
15	BO	2	SER
15	BO	17	ARG
15	BO	24	SER
15	BO	40	GLN
15	BO	64	ARG
15	BO	70	LEU
15	BO	84	ARG
15	BO	88	ARG
16	BP	19	VAL
16	BP	36	VAL
16	BP	46	LYS
16	BP	76	LYS
17	BQ	17	MET
17	BQ	20	SER
17	BQ	21	ILE
17	BQ	26	GLU
17	BQ	28	PHE
17	BQ	33	ILE
17	BQ	38	ILE
17	BQ	40	ARG
17	BQ	51	ASN
17	BQ	67	LEU
17	BQ	75	LEU
19	BS	6	LYS
19	BS	7	LYS
19	BS	11	ILE
19	BS	13	LEU
19	BS	37	ARG
20	BT	5	LYS
20	BT	12	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	BT	24	ARG
20	BT	27	MET
20	BT	48	GLN
20	BT	54	MET
20	BT	58	VAL
20	BT	64	LYS
20	BT	66	LEU
20	BT	67	ILE
20	BT	69	LYS
20	BT	84	ASN
21	BU	13	ASP
21	BU	56	HIS
23	D2	5	ILE
23	D2	8	LYS
23	D2	47	VAL
24	D3	1	MET
24	D3	15	SER
25	D4	31	HIS
25	D4	47	LYS
25	D4	52	LYS
26	D5	16	ILE
27	D0	10	THR
27	D0	19	LYS
27	D0	25	LEU
27	D0	36	VAL
27	D0	39	GLU
27	D0	58	GLU
29	CC	97	LYS
29	CC	120	VAL
29	CC	130	LEU
29	CC	156	ARG
29	CC	157	SER
29	CC	168	ASP
29	CC	195	VAL
29	CC	202	LEU
29	CC	204	VAL
29	CC	205	LEU
29	CC	221	ARG
29	CC	236	GLU
29	CC	258	ARG
30	CD	4	LEU
30	CD	18	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	CD	32	ASN
30	CD	95	SER
29	DC	70	ASN
29	DC	97	LYS
29	DC	117	GLN
29	DC	120	VAL
29	DC	130	LEU
29	DC	182	ARG
29	DC	202	LEU
29	DC	236	GLU
30	DD	18	ASP
30	DD	32	ASN
30	DD	95	SER
32	CE	7	ASP
32	CE	12	LEU
32	CE	25	GLU
32	CE	40	ARG
32	CE	44	ARG
32	CE	72	SER
32	CE	78	TRP
32	CE	83	VAL
32	CE	93	SER
32	CE	107	SER
32	CE	122	GLU
32	CE	127	GLU
32	CE	149	ILE
32	CE	152	GLU
32	CE	163	ASN
32	CE	189	THR
33	CF	35	THR
33	CF	36	LEU
33	CF	57	LEU
33	CF	72	LYS
33	CF	80	ARG
33	CF	94	GLU
33	CF	117	LEU
33	CF	123	ASP
33	CF	134	GLU
33	CF	136	ILE
33	CF	141	ILE
33	CF	149	VAL
33	CF	152	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	CF	174	ASP
34	CG	11	VAL
34	CG	18	LYS
34	CG	155	GLU
35	CH	7	ASP
35	CH	15	LEU
35	CH	21	VAL
35	CH	48	GLU
35	CH	51	ARG
35	CH	53	GLU
35	CH	54	LEU
35	CH	55	GLU
35	CH	58	LEU
35	CH	89	LYS
35	CH	127	GLU
35	CH	145	ASN
36	CJ	13	VAL
36	CJ	28	LEU
36	CJ	53	LEU
36	CJ	55	ILE
36	CJ	113	LYS
37	CK	5	THR
37	CK	106	LYS
37	CK	124	VAL
37	CK	142	ILE
38	CL	35	VAL
38	CL	58	LEU
38	CL	70	ARG
38	CL	76	VAL
38	CL	80	ASP
38	CL	89	ASN
38	CL	108	ARG
38	CL	113	MET
39	CM	2	ARG
39	CM	21	ARG
39	CM	42	SER
39	CM	93	ASN
39	CM	94	THR
39	CM	100	ILE
39	CM	103	ILE
39	CM	120	VAL
40	CN	55	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	CN	59	ARG
40	CN	75	GLU
40	CN	78	LEU
40	CN	132	THR
41	CO	2	ARG
41	CO	6	SER
41	CO	14	SER
41	CO	33	ILE
41	CO	71	ARG
41	CO	76	VAL
41	CO	95	THR
42	CP	18	LEU
42	CP	31	THR
42	CP	38	GLN
42	CP	48	LEU
42	CP	49	VAL
42	CP	78	VAL
43	CQ	10	GLN
43	CQ	39	ARG
43	CQ	40	LEU
43	CQ	114	LEU
44	CR	5	LYS
44	CR	9	ILE
44	CR	51	ARG
44	CR	52	GLN
45	CS	12	HIS
45	CS	18	GLN
45	CS	45	GLU
45	CS	46	GLU
45	CS	48	LYS
45	CS	51	VAL
45	CS	102	SER
46	CT	7	HIS
46	CT	69	LEU
46	CT	86	MET
46	CT	97	LEU
46	CT	108	SER
46	CT	109	ASP
47	CU	1	MET
47	CU	2	ILE
47	CU	3	ARG
47	CU	27	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	CU	30	ILE
47	CU	49	LYS
47	CU	69	ARG
47	CU	73	ARG
47	CU	93	LEU
48	CV	9	ASP
48	CV	28	VAL
48	CV	29	LEU
48	CV	61	LYS
48	CV	81	ASP
48	CV	98	SER
49	CW	1	MET
49	CW	7	GLU
49	CW	10	LYS
49	CW	61	LEU
50	CX	39	ARG
50	CX	40	GLN
50	CX	82	ILE
51	CY	25	THR
51	CY	35	SER
51	CY	48	THR
51	CY	71	LEU
52	CZ	18	LEU
52	CZ	38	GLN
52	CZ	40	SER
52	CZ	58	ASN
32	DE	12	LEU
32	DE	25	GLU
32	DE	107	SER
32	DE	127	GLU
32	DE	163	ASN
32	DE	189	THR
33	DF	10	ASP
33	DF	35	THR
33	DF	57	LEU
33	DF	72	LYS
33	DF	94	GLU
33	DF	117	LEU
33	DF	120	LYS
33	DF	134	GLU
33	DF	136	ILE
33	DF	141	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	DF	149	VAL
33	DF	152	LEU
33	DF	158	THR
33	DF	174	ASP
34	DG	11	VAL
34	DG	18	LYS
34	DG	155	GLU
34	DG	168	VAL
35	DH	7	ASP
35	DH	15	LEU
35	DH	21	VAL
35	DH	48	GLU
35	DH	53	GLU
35	DH	54	LEU
35	DH	58	LEU
35	DH	127	GLU
35	DH	145	ASN
36	DJ	13	VAL
36	DJ	28	LEU
36	DJ	53	LEU
36	DJ	55	ILE
36	DJ	113	LYS
37	DK	106	LYS
37	DK	124	VAL
37	DK	142	ILE
38	DL	58	LEU
38	DL	70	ARG
38	DL	80	ASP
38	DL	89	ASN
38	DL	110	GLU
39	DM	2	ARG
39	DM	60	ARG
39	DM	120	VAL
40	DN	6	ARG
40	DN	75	GLU
40	DN	100	LYS
40	DN	126	ILE
40	DN	132	THR
41	DO	2	ARG
41	DO	6	SER
41	DO	14	SER
41	DO	33	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	DO	76	VAL
42	DP	31	THR
42	DP	49	VAL
42	DP	78	VAL
43	DQ	40	LEU
44	DR	5	LYS
44	DR	9	ILE
44	DR	13	ARG
44	DR	51	ARG
45	DS	38	VAL
45	DS	102	SER
46	DT	1	MET
46	DT	86	MET
46	DT	108	SER
46	DT	109	ASP
47	DU	1	MET
47	DU	3	ARG
47	DU	27	SER
48	DV	28	VAL
48	DV	29	LEU
48	DV	52	LEU
48	DV	61	LYS
49	DW	7	GLU
49	DW	53	LYS
49	DW	61	LEU
50	DX	11	ARG
50	DX	39	ARG
50	DX	41[A]	ARG
50	DX	41[B]	ARG
50	DX	82	ILE
51	DY	25	THR
51	DY	71	LEU
52	DZ	38	GLN
53	DI	7	ASP
53	DI	16	SER
53	DI	31	ARG
53	DI	53	ARG
53	DI	60	LEU
53	DI	64	VAL
53	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	93	ASN
2	AB	120	GLN
2	AB	146	ASN
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
16	AP	9	HIS
17	AQ	51	ASN
19	AS	57	HIS
20	AT	52	ASN
22	C1	38	HIS
2	BB	39	HIS
2	BB	93	ASN
2	BB	120	GLN
2	BB	146	ASN
3	BC	3	GLN
5	BE	70	ASN
5	BE	89	HIS
6	BF	3	HIS
7	BG	97	ASN
8	BH	4	GLN
16	BP	9	HIS
17	BQ	45	HIS
17	BQ	51	ASN
20	BT	48	GLN
20	BT	52	ASN
32	CE	115	GLN
32	CE	163	ASN
34	CG	38	ASN
36	CJ	43	ASN
45	CS	12	HIS
48	CV	74	ASN
50	CX	57	HIS
52	CZ	45	GLN
34	DG	116	GLN
36	DJ	43	ASN
41	DO	31	HIS
48	DV	54	GLN
53	DI	122	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	255 (16%)	32 (2%)
1	BA	1529/1534 (99%)	255 (16%)	36 (2%)
28	CB	117/120 (97%)	12 (10%)	1 (0%)
28	DB	119/120 (99%)	10 (8%)	0
31	CA	2892/2904 (99%)	468 (16%)	79 (2%)
54	DA	2880/2904 (99%)	397 (13%)	60 (2%)
All	All	9067/9116 (99%)	1397 (15%)	208 (2%)

All (1397) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	28	A
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	69	G
1	AA	70	U
1	AA	71	A
1	AA	72	A
1	AA	74	A
1	AA	80	A
1	AA	81	A
1	AA	82	G
1	AA	83	C
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	88	U
1	AA	89	U
1	AA	90	C
1	AA	94	G
1	AA	95	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	108	G
1	AA	120	A
1	AA	128	G
1	AA	130	A
1	AA	131	A
1	AA	137	U
1	AA	141	G
1	AA	142	G
1	AA	144	G
1	AA	149	A
1	AA	159	G
1	AA	163	C
1	AA	168	G
1	AA	197	A
1	AA	200	G
1	AA	205	A
1	AA	210	C
1	AA	211	G
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	298	A
1	AA	306	A
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	346	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	382	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	384	G
1	AA	398	U
1	AA	406	G
1	AA	411	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	466	A
1	AA	467	U
1	AA	468	A
1	AA	474	G
1	AA	479	U
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	495	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	579	A
1	AA	615	G
1	AA	632	U
1	AA	633	G
1	AA	650	G
1	AA	653	U
1	AA	661	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	665	A
1	AA	682	G
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	818	G
1	AA	821	G
1	AA	828	U
1	AA	836	G
1	AA	839	C
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	873	A
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	932	C
1	AA	934	C
1	AA	935	A
1	AA	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	971	G
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	987	G
1	AA	992	U
1	AA	993	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	996	A
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	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	1052	G
1	AA	1053	G
1	AA	1054	C
1	AA	1055	A
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
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	1146	A
1	AA	1152	A
1	AA	1159	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1160	G
1	AA	1168	U
1	AA	1184	G
1	AA	1196	A
1	AA	1197	A
1	AA	1200	C
1	AA	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	1323	G
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1379	G
1	AA	1381	U
1	AA	1397	C
1	AA	1398	A
1	AA	1429	A
1	AA	1441	A
1	AA	1446	A
1	AA	1447	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	1448	C
1	AA	1451	U
1	AA	1452	C
1	AA	1453	G
1	AA	1475	G
1	AA	1487	G
1	AA	1492	A
1	AA	1497	G
1	AA	1503	A
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1534	A
1	BA	4	U
1	BA	5	U
1	BA	6	G
1	BA	9	G
1	BA	22	G
1	BA	28	A
1	BA	32	A
1	BA	39	G
1	BA	47	C
1	BA	48	C
1	BA	50	A
1	BA	51	A
1	BA	52	C
1	BA	69	G
1	BA	70	U
1	BA	71	A
1	BA	72	A
1	BA	74	A
1	BA	80	A
1	BA	82	G
1	BA	83	C
1	BA	84	U
1	BA	85	U
1	BA	87	C
1	BA	88	U
1	BA	89	U
1	BA	90	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	144	G
1	BA	149	A
1	BA	159	G
1	BA	163	C
1	BA	168	G
1	BA	197	A
1	BA	200	G
1	BA	205	A
1	BA	210	C
1	BA	211	G
1	BA	212	G
1	BA	226	G
1	BA	240	G
1	BA	245	U
1	BA	247	G
1	BA	250	A
1	BA	251	G
1	BA	266	G
1	BA	267	C
1	BA	289	G
1	BA	298	A
1	BA	306	A
1	BA	321	A
1	BA	328	C
1	BA	329	A
1	BA	330	C
1	BA	332	G
1	BA	346	G
1	BA	352	C
1	BA	354	G
1	BA	367	U
1	BA	372	C
1	BA	373	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BA	382	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	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	511	C
1	BA	527	G7M
1	BA	528	C
1	BA	531	U
1	BA	532	A
1	BA	533	A
1	BA	547	A
1	BA	559	A
1	BA	562	U
1	BA	564	C
1	BA	568	G
1	BA	572	A
1	BA	573	A
1	BA	576	C
1	BA	577	G
1	BA	579	A
1	BA	615	G
1	BA	632	U
1	BA	633	G
1	BA	650	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BA	653	U
1	BA	661	G
1	BA	665	A
1	BA	682	G
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	812	G
1	BA	814	A
1	BA	815	A
1	BA	817	C
1	BA	818	G
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	873	A
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
1	BA	975	A
1	BA	976	G
1	BA	977	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BA	987	G
1	BA	992	U
1	BA	993	G
1	BA	996	A
1	BA	1004	A
1	BA	1008	U
1	BA	1009	U
1	BA	1015	G
1	BA	1019	A
1	BA	1024	G
1	BA	1026	G
1	BA	1027	C
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	1053	G
1	BA	1054	C
1	BA	1055	A
1	BA	1065	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
1	BA	1141	C
1	BA	1142	G
1	BA	1143	G
1	BA	1145	A
1	BA	1146	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BA	1152	A
1	BA	1159	U
1	BA	1160	G
1	BA	1168	U
1	BA	1196	A
1	BA	1197	A
1	BA	1200	C
1	BA	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	1323	G
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	1397	C
1	BA	1398	A
1	BA	1419	G
1	BA	1429	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	BA	1441	A
1	BA	1446	A
1	BA	1447	A
1	BA	1448	C
1	BA	1451	U
1	BA	1452	C
1	BA	1453	G
1	BA	1475	G
1	BA	1487	G
1	BA	1493	A
1	BA	1497	G
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	44	G
28	CB	45	A
28	CB	56	G
28	CB	57	A
28	CB	88	C
28	CB	89	U
28	CB	90	C
28	CB	99	A
28	CB	109	A
31	CA	10	A
31	CA	14	A
31	CA	34	U
31	CA	39	G
31	CA	42	A
31	CA	46	G
31	CA	49	A
31	CA	58	G
31	CA	61	C
31	CA	63	A
31	CA	71	A
31	CA	74	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	75	G
31	CA	80	G
31	CA	83	A
31	CA	84	A
31	CA	101	A
31	CA	102	U
31	CA	118	A
31	CA	119	A
31	CA	120	U
31	CA	125	A
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	165	A
31	CA	177	G
31	CA	178	G
31	CA	188	G
31	CA	196	A
31	CA	197	A
31	CA	199	A
31	CA	215	G
31	CA	216	A
31	CA	221	A
31	CA	222	A
31	CA	248	G
31	CA	264	C
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	352	A
31	CA	353	C
31	CA	362	A
31	CA	370	G
31	CA	371	A
31	CA	372	G
31	CA	385	C
31	CA	386	G
31	CA	399	U
31	CA	404	A
31	CA	405	U
31	CA	411	G
31	CA	412	A
31	CA	420	C
31	CA	424	G
31	CA	451	U
31	CA	455	C
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	513	A
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	573	U
31	CA	575	A
31	CA	586	A
31	CA	603	A
31	CA	613	A
31	CA	614	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	615	U
31	CA	622	G
31	CA	627	A
31	CA	637	A
31	CA	645	C
31	CA	647	G
31	CA	653	U
31	CA	654	A
31	CA	655	A
31	CA	670	A
31	CA	684	G
31	CA	685	A
31	CA	686	U
31	CA	695	G
31	CA	717	C
31	CA	723	C
31	CA	730	A
31	CA	740	C
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	798	G
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
31	CA	984	A
31	CA	985	C
31	CA	995	C
31	CA	996	A
31	CA	1005	C
31	CA	1012	U
31	CA	1013	C
31	CA	1022	G
31	CA	1026	G
31	CA	1033	U
31	CA	1040	A
31	CA	1046	A
31	CA	1047	G
31	CA	1057	A
31	CA	1061	U
31	CA	1062	G
31	CA	1070	A
31	CA	1073	A
31	CA	1083	U
31	CA	1088	A
31	CA	1089	A
31	CA	1090	A
31	CA	1096	A
31	CA	1097	U
31	CA	1111	A
31	CA	1112	G
31	CA	1119	U
31	CA	1122	G
31	CA	1128	G
31	CA	1129	A
31	CA	1132	U
31	CA	1133	A
31	CA	1134	A
31	CA	1135	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	1136	G
31	CA	1142	A
31	CA	1168	G
31	CA	1169	A
31	CA	1170	C
31	CA	1175	A
31	CA	1176	U
31	CA	1177	G
31	CA	1179	G
31	CA	1180	U
31	CA	1186	G
31	CA	1206	G
31	CA	1210	G
31	CA	1212	G
31	CA	1227	G
31	CA	1236	G
31	CA	1238	G
31	CA	1253	A
31	CA	1256	G
31	CA	1262	A
31	CA	1266	G
31	CA	1271	G
31	CA	1272	A
31	CA	1273	U
31	CA	1300	G
31	CA	1301	A
31	CA	1313	U
31	CA	1321	A
31	CA	1329	U
31	CA	1342	A
31	CA	1344	U
31	CA	1352	U
31	CA	1365	A
31	CA	1379	U
31	CA	1380	G
31	CA	1383	A
31	CA	1395	A
31	CA	1416	G
31	CA	1417	C
31	CA	1419	A
31	CA	1420	A
31	CA	1428	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	1437	C
31	CA	1438	U
31	CA	1452	G
31	CA	1453	A
31	CA	1460	U
31	CA	1478	G
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	1504	A
31	CA	1509	A
31	CA	1510	G
31	CA	1515	A
31	CA	1523	U
31	CA	1532	A
31	CA	1534	U
31	CA	1535	A
31	CA	1536	C
31	CA	1537	G
31	CA	1565	C
31	CA	1567	G
31	CA	1568	G
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	1609	A
31	CA	1611	C
31	CA	1616	A
31	CA	1632	A
31	CA	1647	U
31	CA	1648	U
31	CA	1649	G
31	CA	1669	A
31	CA	1674	G
31	CA	1675	C
31	CA	1715	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	1729	U
31	CA	1730	C
31	CA	1738	G
31	CA	1744	A
31	CA	1750	G
31	CA	1754	A
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	1812	U
31	CA	1816	C
31	CA	1823	G
31	CA	1828	G
31	CA	1829	A
31	CA	1834	U
31	CA	1869	G
31	CA	1870	C
31	CA	1871	A
31	CA	1872	A
31	CA	1873	G
31	CA	1882	U
31	CA	1900	A
31	CA	1903	G
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	1975	G
31	CA	1991	U
31	CA	1993	U
31	CA	1997	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	2006	C
31	CA	2022	U
31	CA	2023	C
31	CA	2033	A
31	CA	2035	G
31	CA	2036	C
31	CA	2043	C
31	CA	2046	G
31	CA	2049	G
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	2092	U
31	CA	2093	G
31	CA	2095	A
31	CA	2100	G
31	CA	2108	A
31	CA	2110	G
31	CA	2111	U
31	CA	2112	G
31	CA	2113	U
31	CA	2114	A
31	CA	2115	G
31	CA	2117	A
31	CA	2118	U
31	CA	2119	A
31	CA	2123	G
31	CA	2124	G
31	CA	2125	G
31	CA	2126	A
31	CA	2127	G
31	CA	2128	G
31	CA	2131	U
31	CA	2132	U
31	CA	2133	G
31	CA	2146	C
31	CA	2147	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	2157	G
31	CA	2158	A
31	CA	2159	G
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	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	2278	A
31	CA	2280	G
31	CA	2283	C
31	CA	2287	A
31	CA	2305	U
31	CA	2311	A
31	CA	2322	A
31	CA	2325	G
31	CA	2326	C
31	CA	2327	A
31	CA	2331	G
31	CA	2333	A
31	CA	2334	U
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	2385	C
31	CA	2402	U
31	CA	2403	C
31	CA	2406	A
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	2469	A
31	CA	2474	U
31	CA	2476	A
31	CA	2484	G
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	2579	C
31	CA	2582	G
31	CA	2585	U
31	CA	2586	U
31	CA	2592	G
31	CA	2603	G
31	CA	2609	U
31	CA	2613	U
31	CA	2623	G
31	CA	2629	U
31	CA	2630	G
31	CA	2646	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2716	C
31	CA	2718	G
31	CA	2720	U
31	CA	2726	A
31	CA	2744	G
31	CA	2748	A
31	CA	2765	A
31	CA	2769	U
31	CA	2778	A
31	CA	2779	U
31	CA	2780	G
31	CA	2791	G
31	CA	2794	C
31	CA	2799	A
31	CA	2818	U
31	CA	2820	A
31	CA	2821	A
31	CA	2825	G
31	CA	2833	U
31	CA	2835	A
31	CA	2836	U
31	CA	2861	U
31	CA	2865	U
31	CA	2867	G
31	CA	2880	C
31	CA	2883	A
31	CA	2884	U
31	CA	2886	A
31	CA	2903	U
28	DB	25	U
28	DB	35	C
28	DB	44	G
28	DB	45	A
28	DB	56	G
28	DB	57	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	DB	88	C
28	DB	89	U
28	DB	90	C
28	DB	109	A
54	DA	10	A
54	DA	12	U
54	DA	14	A
54	DA	15	G
54	DA	34	U
54	DA	39	G
54	DA	42	A
54	DA	46	G
54	DA	58	G
54	DA	61	C
54	DA	63	A
54	DA	71	A
54	DA	74	A
54	DA	75	G
54	DA	84	A
54	DA	101	A
54	DA	102	U
54	DA	118	A
54	DA	119	A
54	DA	120	U
54	DA	125	A
54	DA	138	U
54	DA	139	U
54	DA	140	C
54	DA	141	G
54	DA	142	A
54	DA	143	C
54	DA	165	A
54	DA	196	A
54	DA	197	A
54	DA	199	A
54	DA	200	U
54	DA	215	G
54	DA	216	A
54	DA	221	A
54	DA	222	A
54	DA	248	G
54	DA	264	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	265	A
54	DA	266	G
54	DA	272	A
54	DA	276	U
54	DA	277	G
54	DA	278	A
54	DA	279	A
54	DA	285	G
54	DA	302	C
54	DA	311	A
54	DA	329	G
54	DA	330	A
54	DA	343	C
54	DA	352	A
54	DA	353	C
54	DA	362	A
54	DA	370	G
54	DA	372	G
54	DA	385	C
54	DA	386	G
54	DA	399	U
54	DA	411	G
54	DA	412	A
54	DA	420	C
54	DA	424	G
54	DA	451	U
54	DA	480	A
54	DA	481	G
54	DA	491	G
54	DA	504	A
54	DA	505	A
54	DA	508	A
54	DA	513	A
54	DA	528	A
54	DA	532	A
54	DA	533	G
54	DA	543	G
54	DA	544	C
54	DA	546	U
54	DA	547	A
54	DA	548	G
54	DA	549	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	550	C
54	DA	551	G
54	DA	563	A
54	DA	573	U
54	DA	575	A
54	DA	586	A
54	DA	603	A
54	DA	613	A
54	DA	614	A
54	DA	615	U
54	DA	627	A
54	DA	637	A
54	DA	645	C
54	DA	647	G
54	DA	653	U
54	DA	654	A
54	DA	655	A
54	DA	686	U
54	DA	717	C
54	DA	723	C
54	DA	730	A
54	DA	747	5MU
54	DA	764	A
54	DA	765	C
54	DA	775	G
54	DA	776	G
54	DA	782	A
54	DA	784	G
54	DA	785	G
54	DA	790	U
54	DA	805	G
54	DA	812	C
54	DA	827	U
54	DA	828	U
54	DA	858	G
54	DA	859	G
54	DA	878	A
54	DA	883	G
54	DA	885	C
54	DA	896	A
54	DA	897	C
54	DA	910	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	931	U
54	DA	932	U
54	DA	933	A
54	DA	946	C
54	DA	953	G
54	DA	961	C
54	DA	974	G
54	DA	983	A
54	DA	985	C
54	DA	996	A
54	DA	1012	U
54	DA	1013	C
54	DA	1022	G
54	DA	1026	G
54	DA	1033	U
54	DA	1040	A
54	DA	1047	G
54	DA	1057	A
54	DA	1061	U
54	DA	1062	G
54	DA	1068	G
54	DA	1070	A
54	DA	1073	A
54	DA	1083	U
54	DA	1088	A
54	DA	1089	A
54	DA	1090	A
54	DA	1096	A
54	DA	1097	U
54	DA	1112	G
54	DA	1119	U
54	DA	1128	G
54	DA	1129	A
54	DA	1132	U
54	DA	1133	A
54	DA	1134	A
54	DA	1135	C
54	DA	1136	G
54	DA	1142	A
54	DA	1155	A
54	DA	1168	G
54	DA	1171	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	1172	C
54	DA	1176	U
54	DA	1177	G
54	DA	1180	U
54	DA	1206	G
54	DA	1212	G
54	DA	1238	G
54	DA	1253	A
54	DA	1256	G
54	DA	1271	G
54	DA	1272	A
54	DA	1273	U
54	DA	1300	G
54	DA	1301	A
54	DA	1321	A
54	DA	1329	U
54	DA	1342	A
54	DA	1352	U
54	DA	1365	A
54	DA	1379	U
54	DA	1383	A
54	DA	1416	G
54	DA	1417	C
54	DA	1427	A
54	DA	1428	C
54	DA	1435	G
54	DA	1452	G
54	DA	1453	A
54	DA	1460	U
54	DA	1478	G
54	DA	1482	G
54	DA	1490	A
54	DA	1491	G
54	DA	1493	C
54	DA	1494	A
54	DA	1497	U
54	DA	1504	A
54	DA	1508	A
54	DA	1509	A
54	DA	1510	G
54	DA	1515	A
54	DA	1523	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	1532	A
54	DA	1534	U
54	DA	1535	A
54	DA	1536	C
54	DA	1537	G
54	DA	1569	A
54	DA	1578	U
54	DA	1583	A
54	DA	1585	C
54	DA	1607	C
54	DA	1608	A
54	DA	1609	A
54	DA	1616	A
54	DA	1647	U
54	DA	1648	U
54	DA	1649	G
54	DA	1674	G
54	DA	1715	G
54	DA	1729	U
54	DA	1730	C
54	DA	1738	G
54	DA	1744	A
54	DA	1754	A
54	DA	1764	C
54	DA	1773	A
54	DA	1782	U
54	DA	1800	C
54	DA	1801	A
54	DA	1808	A
54	DA	1812	U
54	DA	1816	C
54	DA	1829	A
54	DA	1869	G
54	DA	1870	C
54	DA	1871	A
54	DA	1872	A
54	DA	1873	G
54	DA	1906	G
54	DA	1907	G
54	DA	1913	A
54	DA	1914	C
54	DA	1929	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	1930	G
54	DA	1931	U
54	DA	1937	A
54	DA	1938	A
54	DA	1955	U
54	DA	1965	C
54	DA	1967	C
54	DA	1970	A
54	DA	1972	G
54	DA	1991	U
54	DA	1993	U
54	DA	1997	C
54	DA	2023	C
54	DA	2031	A
54	DA	2033	A
54	DA	2043	C
54	DA	2055	C
54	DA	2056	G
54	DA	2060	A
54	DA	2061	G
54	DA	2062	A
54	DA	2069	G7M
54	DA	2093	G
54	DA	2097	A
54	DA	2100	G
54	DA	2105	U
54	DA	2111	U
54	DA	2112	G
54	DA	2113	U
54	DA	2116	G
54	DA	2117	A
54	DA	2118	U
54	DA	2119	A
54	DA	2120	G
54	DA	2123	G
54	DA	2125	G
54	DA	2126	A
54	DA	2128	G
54	DA	2131	U
54	DA	2132	U
54	DA	2133	G
54	DA	2134	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	2135	A
54	DA	2145	C
54	DA	2146	C
54	DA	2148	G
54	DA	2158	A
54	DA	2159	G
54	DA	2160	C
54	DA	2161	C
54	DA	2162	G
54	DA	2163	A
54	DA	2164	C
54	DA	2165	C
54	DA	2167	U
54	DA	2168	G
54	DA	2169	A
54	DA	2170	A
54	DA	2171	A
54	DA	2172	U
54	DA	2173	A
54	DA	2178	C
54	DA	2179	C
54	DA	2181	U
54	DA	2183	A
54	DA	2185	U
54	DA	2186	G
54	DA	2190	G
54	DA	2198	A
54	DA	2203	U
54	DA	2204	G
54	DA	2211	A
54	DA	2225	A
54	DA	2238	G
54	DA	2239	G
54	DA	2268	A
54	DA	2278	A
54	DA	2280	G
54	DA	2283	C
54	DA	2286	G
54	DA	2287	A
54	DA	2305	U
54	DA	2308	G
54	DA	2312	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	2322	A
54	DA	2324	U
54	DA	2325	G
54	DA	2327	A
54	DA	2331	G
54	DA	2335	A
54	DA	2345	G
54	DA	2347	C
54	DA	2383	G
54	DA	2385	C
54	DA	2402	U
54	DA	2406	A
54	DA	2407	A
54	DA	2424	C
54	DA	2425	A
54	DA	2435	A
54	DA	2441	U
54	DA	2448	A
54	DA	2465	C
54	DA	2474	U
54	DA	2476	A
54	DA	2484	G
54	DA	2491	U
54	DA	2502	G
54	DA	2505	G
54	DA	2518	A
54	DA	2529	G
54	DA	2535	G
54	DA	2547	A
54	DA	2556	C
54	DA	2566	A
54	DA	2567	G
54	DA	2573	C
54	DA	2585	U
54	DA	2586	U
54	DA	2603	G
54	DA	2609	U
54	DA	2613	U
54	DA	2629	U
54	DA	2630	G
54	DA	2661	G
54	DA	2663	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	2689	U
54	DA	2690	U
54	DA	2714	G
54	DA	2716	C
54	DA	2726	A
54	DA	2744	G
54	DA	2748	A
54	DA	2765	A
54	DA	2778	A
54	DA	2791	G
54	DA	2798	U
54	DA	2799	A
54	DA	2818	U
54	DA	2820	A
54	DA	2821	A
54	DA	2825	G
54	DA	2833	U
54	DA	2835	A
54	DA	2836	U
54	DA	2867	G
54	DA	2880	C
54	DA	2883	A
54	DA	2903	U

All (208) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	30	U
1	AA	70	U
1	AA	88	U
1	AA	89	U
1	AA	209	U
1	AA	305	G
1	AA	367	U
1	AA	413	G
1	AA	422	C
1	AA	429	U
1	AA	576	C
1	AA	653	U
1	AA	702	A
1	AA	733	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	793	U
1	AA	841	C
1	AA	884	U
1	AA	992	U
1	AA	1086	U
1	AA	1094	G
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1225	A
1	AA	1281	C
1	AA	1299	A
1	AA	1301	U
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	305	G
1	BA	367	U
1	BA	422	C
1	BA	429	U
1	BA	559	A
1	BA	560	A
1	BA	561	U
1	BA	576	C
1	BA	653	U
1	BA	702	A
1	BA	733	G
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

Continued on next page...

Continued from previous page...

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	1301	U
1	BA	1362	A
1	BA	1363	A
1	BA	1397	C
1	BA	1447	A
1	BA	1452	C
28	CB	89	U
31	CA	33	C
31	CA	83	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	371	A
31	CA	403	U
31	CA	404	A
31	CA	411	G
31	CA	503	A
31	CA	527	C
31	CA	555	G
31	CA	620	G
31	CA	764	A
31	CA	775	G
31	CA	784	G
31	CA	827	U
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	1070	A
31	CA	1088	A
31	CA	1089	A
31	CA	1128	G
31	CA	1132	U
31	CA	1133	A
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	1567	G
31	CA	1607	C
31	CA	1609	A
31	CA	1647	U
31	CA	1870	C
31	CA	1871	A
31	CA	1900	A
31	CA	1929	G
31	CA	1970	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	2172	U
31	CA	2225	A
31	CA	2282	G
31	CA	2324	U
31	CA	2326	C
31	CA	2423	U
31	CA	2425	A
31	CA	2581	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	CA	2680	U
31	CA	2681	C
31	CA	2778	A
31	CA	2779	U
31	CA	2820	A
31	CA	2849	U
31	CA	2873	A
54	DA	138	U
54	DA	141	G
54	DA	196	A
54	DA	199	A
54	DA	271	G
54	DA	278	A
54	DA	310	A
54	DA	370	G
54	DA	371	A
54	DA	403	U
54	DA	503	A
54	DA	620	G
54	DA	764	A
54	DA	784	G
54	DA	984	A
54	DA	1061	U
54	DA	1069	A
54	DA	1070	A
54	DA	1087	G
54	DA	1089	A
54	DA	1128	G
54	DA	1133	A
54	DA	1141	U
54	DA	1142	A
54	DA	1171	G
54	DA	1175	A
54	DA	1253	A
54	DA	1286	A
54	DA	1300	G
54	DA	1301	A
54	DA	1320	C
54	DA	1490	A
54	DA	1497	U
54	DA	1508	A
54	DA	1509	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	DA	1535	A
54	DA	1607	C
54	DA	1609	A
54	DA	1647	U
54	DA	1870	C
54	DA	1871	A
54	DA	2062	A
54	DA	2097	A
54	DA	2119	A
54	DA	2127	G
54	DA	2146	C
54	DA	2157	G
54	DA	2158	A
54	DA	2164	C
54	DA	2172	U
54	DA	2286	G
54	DA	2311	A
54	DA	2324	U
54	DA	2406	A
54	DA	2423	U
54	DA	2585	U
54	DA	2779	U
54	DA	2798	U
54	DA	2820	A
54	DA	2873	A

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

77 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	1.02	1 (5%)	21,38,41	2.53	4 (19%)
1	4OC	AA	1402	1	15,23,24	0.79	0	21,32,35	1.22	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	AA	1407	1	14,22,23	0.93	1 (7%)	17,32,35	0.74	1 (5%)
1	UR3	AA	1498	1	13,22,23	1.12	2 (15%)	18,32,35	0.69	0
1	2MG	AA	1516	1	18,26,27	1.28	2 (11%)	21,38,41	2.44	4 (19%)
1	MA6	AA	1518	1	18,26,27	0.67	0	15,38,41	0.59	0
1	MA6	AA	1519	1	18,26,27	0.75	0	15,38,41	0.60	0
1	PSU	AA	516	1,55	15,21,22	1.19	2 (13%)	16,30,33	3.49	2 (12%)
1	G7M	AA	527	1	18,26,27	1.12	2 (11%)	21,39,42	3.53	6 (28%)
1	2MG	AA	966	1	18,26,27	1.14	2 (11%)	21,38,41	2.50	3 (14%)
1	5MC	AA	967	1	14,22,23	0.81	1 (7%)	17,32,35	0.66	1 (5%)
12	D2T	AL	89	12	4,9,10	0.58	0	4,11,13	1.66	2 (50%)
1	2MG	BA	1207	1	18,26,27	1.12	2 (11%)	21,38,41	2.54	4 (19%)
1	4OC	BA	1402	1	15,23,24	0.79	0	21,32,35	1.23	2 (9%)
1	5MC	BA	1407	1	14,22,23	0.95	1 (7%)	17,32,35	0.72	1 (5%)
1	UR3	BA	1498	1	13,22,23	0.96	1 (7%)	18,32,35	0.53	0
1	2MG	BA	1516	1	18,26,27	1.19	2 (11%)	21,38,41	2.42	3 (14%)
1	MA6	BA	1518	1	18,26,27	0.61	0	15,38,41	0.58	0
1	MA6	BA	1519	1	18,26,27	0.69	0	15,38,41	0.60	0
1	PSU	BA	516	1	15,21,22	1.20	2 (13%)	16,30,33	3.48	2 (12%)
1	G7M	BA	527	1	18,26,27	0.94	1 (5%)	21,39,42	3.53	5 (23%)
1	2MG	BA	966	1	18,26,27	1.08	1 (5%)	21,38,41	2.55	4 (19%)
1	5MC	BA	967	1	14,22,23	0.79	1 (7%)	17,32,35	0.68	1 (5%)
12	D2T	BL	89	12	4,9,10	0.49	0	4,11,13	1.71	1 (25%)
31	6MZ	CA	1618	31	17,25,26	0.83	0	15,36,39	0.87	1 (6%)
31	2MG	CA	1835	31	18,26,27	1.14	1 (5%)	21,38,41	2.36	3 (14%)
31	PSU	CA	1911	31	15,21,22	1.12	2 (13%)	16,30,33	3.46	1 (6%)
31	3TD	CA	1915	31	15,22,23	1.01	2 (13%)	17,32,35	0.99	1 (5%)
31	PSU	CA	1917	31	15,21,22	1.16	2 (13%)	16,30,33	3.54	1 (6%)
31	5MU	CA	1939	31	13,22,23	1.19	1 (7%)	16,32,35	4.77	3 (18%)
31	5MC	CA	1962	31	14,22,23	0.82	1 (7%)	17,32,35	0.65	1 (5%)
31	6MZ	CA	2030	31	17,25,26	0.89	0	15,36,39	0.88	1 (6%)
31	G7M	CA	2069	31	18,26,27	0.93	1 (5%)	21,39,42	3.68	6 (28%)
31	OMG	CA	2251	31	18,26,27	1.14	2 (11%)	21,38,41	2.77	4 (19%)
31	2MG	CA	2445	31	18,26,27	1.30	2 (11%)	21,38,41	2.62	4 (19%)
31	PSU	CA	2457	31	15,21,22	1.21	2 (13%)	16,30,33	3.50	1 (6%)
31	OMC	CA	2498	55,31	15,22,23	0.87	1 (6%)	20,31,34	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	2MA	CA	2503	31	17,25,26	0.89	0	18,37,40	1.04	1 (5%)
31	PSU	CA	2504	31	15,21,22	1.15	2 (13%)	16,30,33	3.47	1 (6%)
31	OMU	CA	2552	31	14,22,23	1.22	2 (14%)	19,31,34	2.93	2 (10%)
31	PSU	CA	2580	31	15,21,22	1.26	2 (13%)	16,30,33	3.57	3 (18%)
31	PSU	CA	2604	31	15,21,22	17.92	2 (13%)	16,30,33	9.22	2 (12%)
31	PSU	CA	2605	31	15,21,22	1.21	2 (13%)	16,30,33	3.51	1 (6%)
31	1MG	CA	745	31	17,26,27	1.20	1 (5%)	19,39,42	1.18	2 (10%)
31	PSU	CA	746	55,31	15,21,22	1.35	3 (20%)	16,30,33	3.47	2 (12%)
31	5MU	CA	747	31	13,22,23	1.09	1 (7%)	16,32,35	4.77	3 (18%)
31	PSU	CA	955	31	15,21,22	1.14	2 (13%)	16,30,33	3.44	1 (6%)
30	MEQ	CD	150	30	6,8,10	0.43	0	7,9,12	0.98	1 (14%)
40	4D4	CN	81	40	7,11,12	0.59	0	5,13,15	0.93	0
54	6MZ	DA	1618	54	17,25,26	0.91	0	15,36,39	0.61	0
54	2MG	DA	1835	54	18,26,27	1.08	1 (5%)	21,38,41	2.38	3 (14%)
54	PSU	DA	1911	54	15,21,22	1.15	2 (13%)	16,30,33	3.43	1 (6%)
54	3TD	DA	1915	54	15,22,23	0.93	1 (6%)	17,32,35	1.04	1 (5%)
54	PSU	DA	1917	54	15,21,22	1.27	2 (13%)	16,30,33	3.53	1 (6%)
54	5MU	DA	1939	54	13,22,23	1.48	3 (23%)	16,32,35	4.72	3 (18%)
54	5MC	DA	1962	54	14,22,23	0.88	1 (7%)	17,32,35	0.76	1 (5%)
54	6MZ	DA	2030	54	17,25,26	1.24	2 (11%)	15,36,39	0.98	1 (6%)
54	G7M	DA	2069	54	18,26,27	1.00	1 (5%)	21,39,42	3.16	5 (23%)
54	OMG	DA	2251	54	18,26,27	0.92	1 (5%)	21,38,41	2.59	4 (19%)
54	2MG	DA	2445	54	18,26,27	1.42	4 (22%)	21,38,41	2.74	4 (19%)
54	H2U	DA	2449	54	17,21,22	0.50	0	23,30,33	0.52	0
54	PSU	DA	2457	54	15,21,22	1.37	2 (13%)	16,30,33	3.48	2 (12%)
54	OMC	DA	2498	55,54	15,22,23	1.00	0	20,31,34	0.57	0
54	2MA	DA	2503	55,54	17,25,26	0.80	0	18,37,40	1.09	2 (11%)
54	PSU	DA	2504	54	15,21,22	1.19	2 (13%)	16,30,33	3.47	1 (6%)
54	OMU	DA	2552	54	14,22,23	1.13	1 (7%)	19,31,34	2.91	2 (10%)
54	PSU	DA	2580	54	15,21,22	1.61	5 (33%)	16,30,33	3.53	2 (12%)
54	PSU	DA	2604	54	15,21,22	1.63	5 (33%)	16,30,33	3.53	1 (6%)
54	PSU	DA	2605	54	15,21,22	1.33	3 (20%)	16,30,33	3.54	2 (12%)
54	1MG	DA	745	54	17,26,27	1.24	2 (11%)	19,39,42	1.21	2 (10%)
54	PSU	DA	746	55,54	15,21,22	1.72	5 (33%)	16,30,33	3.57	2 (12%)
54	5MU	DA	747	54	13,22,23	1.15	2 (15%)	16,32,35	4.72	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	DA	955	54	15,21,22	1.37	3 (20%)	16,30,33	3.47	1 (6%)
30	MEQ	DD	150[A]	30	7,9,10	0.40	0	8,10,12	1.36	2 (25%)
30	MEQ	DD	150[B]	30	7,9,10	1.55	1 (14%)	8,10,12	1.67	2 (25%)
40	4D4	DN	81[A]	-	7,11,12	0.56	0	5,13,15	0.99	0
40	4D4	DN	81[B]	-	7,11,12	0.91	1 (14%)	5,13,15	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	AA	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	AA	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	AA	516	1,55	-	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	55,31	-	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	2604	31	-	0/7/25/26	1/2/2/2
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	55,31	-	0/7/25/26	0/2/2/2
31	5MU	CA	747	31	-	0/3/25/26	0/2/2/2
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
30	MEQ	CD	150	30	-	0/5/7/11	0/0/0/0
40	4D4	CN	81	40	-	0/8/12/14	0/0/0/0
54	6MZ	DA	1618	54	-	0/5/27/28	0/3/3/3
54	2MG	DA	1835	54	-	0/5/27/28	0/3/3/3
54	PSU	DA	1911	54	-	0/7/25/26	0/2/2/2
54	3TD	DA	1915	54	-	0/7/25/26	0/2/2/2
54	PSU	DA	1917	54	-	0/7/25/26	0/2/2/2
54	5MU	DA	1939	54	-	0/3/25/26	0/2/2/2
54	5MC	DA	1962	54	-	0/3/25/26	0/2/2/2
54	6MZ	DA	2030	54	-	0/5/27/28	0/3/3/3
54	G7M	DA	2069	54	-	0/3/25/26	0/3/3/3
54	OMG	DA	2251	54	-	0/5/27/28	0/3/3/3
54	2MG	DA	2445	54	-	0/5/27/28	0/3/3/3
54	H2U	DA	2449	54	-	0/7/38/39	0/2/2/2
54	PSU	DA	2457	54	-	0/7/25/26	0/2/2/2
54	OMC	DA	2498	55,54	-	0/5/27/28	0/2/2/2
54	2MA	DA	2503	55,54	-	0/3/25/26	0/3/3/3
54	PSU	DA	2504	54	-	0/7/25/26	0/2/2/2
54	OMU	DA	2552	54	-	0/5/27/28	0/2/2/2
54	PSU	DA	2580	54	-	0/7/25/26	0/2/2/2
54	PSU	DA	2604	54	-	0/7/25/26	0/2/2/2
54	PSU	DA	2605	54	-	0/7/25/26	0/2/2/2
54	1MG	DA	745	54	-	0/3/25/26	0/3/3/3
54	PSU	DA	746	55,54	-	0/7/25/26	0/2/2/2
54	5MU	DA	747	54	-	0/3/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	DA	955	54	-	0/7/25/26	0/2/2/2
30	MEQ	DD	150[A]	30	-	0/7/9/11	0/0/0/0
30	MEQ	DD	150[B]	30	-	0/7/9/11	0/0/0/0
40	4D4	DN	81[A]	-	-	0/8/12/14	0/0/0/0
40	4D4	DN	81[B]	-	-	0/8/12/14	0/0/0/0

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	DA	746	PSU	C2'-C1'	-3.45	1.50	1.53
54	DA	1939	5MU	C2'-C1'	-3.29	1.48	1.53
54	DA	746	PSU	O4'-C1'	-3.13	1.39	1.44
54	DA	2030	6MZ	C2'-C1'	-2.98	1.48	1.53
54	DA	2580	PSU	C5-C1'	-2.94	1.49	1.52
54	DA	2030	6MZ	O4'-C1'	-2.72	1.37	1.41
54	DA	745	1MG	O3'-C3'	-2.70	1.36	1.43
54	DA	2604	PSU	C5-C1'	-2.64	1.49	1.52
54	DA	2604	PSU	O3'-C3'	-2.51	1.37	1.43
54	DA	2457	PSU	C5-C1'	-2.48	1.50	1.52
54	DA	746	PSU	C5-C1'	-2.46	1.50	1.52
54	DA	2604	PSU	C6-C5	-2.39	1.35	1.38
54	DA	2580	PSU	O4'-C1'	-2.35	1.40	1.44
54	DA	955	PSU	C2'-C1'	-2.30	1.51	1.53
54	DA	2580	PSU	C6-C5	-2.29	1.35	1.38
54	DA	2605	PSU	C6-C5	-2.26	1.35	1.38
54	DA	2445	2MG	O3'-C3'	-2.24	1.37	1.43
54	DA	2604	PSU	C2'-C1'	-2.19	1.51	1.53
31	CA	746	PSU	O4'-C1'	-2.19	1.41	1.44
31	CA	1915	3TD	C6-C5	-2.18	1.35	1.38
54	DA	1917	PSU	C6-C5	-2.13	1.35	1.38
54	DA	2445	2MG	C2'-C1'	-2.13	1.50	1.53
31	CA	2605	PSU	C6-C5	-2.12	1.35	1.38
31	CA	955	PSU	C6-C5	-2.12	1.35	1.38
54	DA	2504	PSU	C6-C5	-2.11	1.35	1.38
1	AA	516	PSU	C6-C5	-2.11	1.35	1.38
54	DA	955	PSU	C6-C5	-2.11	1.35	1.38
54	DA	746	PSU	C6-C5	-2.10	1.35	1.38
54	DA	2580	PSU	C2'-C1'	-2.10	1.51	1.53
1	AA	1407	5MC	C6-C5	-2.10	1.34	1.40
54	DA	1911	PSU	C6-C5	-2.10	1.35	1.38
1	BA	516	PSU	C6-C5	-2.10	1.35	1.38
54	DA	1915	3TD	C6-C5	-2.09	1.35	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	1962	5MC	C6-C5	-2.09	1.34	1.40
54	DA	1962	5MC	C6-C5	-2.09	1.34	1.40
31	CA	1917	PSU	C6-C5	-2.08	1.35	1.38
31	CA	2580	PSU	C6-C5	-2.08	1.35	1.38
1	BA	1407	5MC	C6-C5	-2.07	1.34	1.40
31	CA	2457	PSU	C6-C5	-2.06	1.35	1.38
31	CA	1911	PSU	C6-C5	-2.05	1.35	1.38
54	DA	747	5MU	C6-C5	-2.05	1.34	1.40
31	CA	746	PSU	C6-C5	-2.03	1.35	1.38
54	DA	2605	PSU	C5-C1'	-2.03	1.50	1.52
1	AA	967	5MC	C6-C5	-2.03	1.34	1.40
1	BA	967	5MC	C6-C5	-2.03	1.34	1.40
31	CA	2504	PSU	C6-C5	-2.01	1.35	1.38
54	DA	1939	5MU	C6-C5	-2.01	1.34	1.40
1	AA	1498	UR3	O3'-C3'	2.04	1.47	1.43
31	CA	2498	OMC	C6-N1	2.06	1.38	1.35
40	DN	81[B]	4D4	CB-CA	2.08	1.57	1.54
1	AA	527	G7M	C6-C5	2.10	1.45	1.41
31	CA	2251	OMG	C6-C5	2.11	1.45	1.41
1	AA	1498	UR3	C6-N1	2.15	1.38	1.35
1	AA	966	2MG	C6-C5	2.23	1.45	1.41
31	CA	1915	3TD	C4-N3	2.24	1.41	1.38
1	BA	1498	UR3	C4-N3	2.27	1.41	1.38
1	BA	1207	2MG	C6-C5	2.30	1.45	1.41
1	BA	1516	2MG	C6-C5	2.46	1.46	1.41
31	CA	2552	OMU	C6-N1	2.51	1.39	1.35
31	CA	2604	PSU	C4-N3	2.70	1.37	1.33
54	DA	745	1MG	C6-C5	2.72	1.46	1.40
1	BA	527	G7M	C6-N1	2.78	1.38	1.33
54	DA	1835	2MG	C6-N1	2.86	1.38	1.33
54	DA	2445	2MG	C6-C5	2.87	1.47	1.41
54	DA	2552	OMU	C4-N3	2.91	1.38	1.33
54	DA	2604	PSU	C4-N3	2.92	1.38	1.33
54	DA	2605	PSU	C4-N3	2.95	1.38	1.33
31	CA	2069	G7M	C6-N1	3.01	1.38	1.33
54	DA	746	PSU	C4-N3	3.03	1.38	1.33
54	DA	2251	OMG	C6-N1	3.04	1.38	1.33
1	AA	1516	2MG	C6-C5	3.10	1.47	1.41
31	CA	2445	2MG	C6-C5	3.11	1.47	1.41
1	AA	1207	2MG	C6-N1	3.15	1.38	1.33
1	AA	527	G7M	C6-N1	3.15	1.38	1.33
31	CA	2457	PSU	C4-N3	3.16	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	DA	1917	PSU	C4-N3	3.19	1.38	1.33
54	DA	747	5MU	C4-N3	3.20	1.38	1.33
31	CA	1911	PSU	C4-N3	3.22	1.38	1.33
54	DA	1939	5MU	C4-N3	3.23	1.38	1.33
54	DA	2445	2MG	C6-N1	3.23	1.38	1.33
1	BA	516	PSU	C4-N3	3.24	1.38	1.33
1	BA	966	2MG	C6-N1	3.24	1.38	1.33
54	DA	2504	PSU	C4-N3	3.25	1.38	1.33
31	CA	2580	PSU	C4-N3	3.25	1.38	1.33
54	DA	2580	PSU	C4-N3	3.26	1.38	1.33
31	CA	955	PSU	C4-N3	3.28	1.38	1.33
31	CA	2552	OMU	C4-N3	3.29	1.39	1.33
31	CA	747	5MU	C4-N3	3.29	1.39	1.33
31	CA	1917	PSU	C4-N3	3.29	1.39	1.33
54	DA	1911	PSU	C4-N3	3.30	1.39	1.33
31	CA	2251	OMG	C6-N1	3.31	1.39	1.33
54	DA	2069	G7M	C6-N1	3.32	1.39	1.33
31	CA	1835	2MG	C6-N1	3.33	1.39	1.33
54	DA	955	PSU	C4-N3	3.34	1.39	1.33
1	BA	1207	2MG	C6-N1	3.35	1.39	1.33
54	DA	2457	PSU	C4-N3	3.35	1.39	1.33
31	CA	2605	PSU	C4-N3	3.36	1.39	1.33
31	CA	2445	2MG	C6-N1	3.36	1.39	1.33
31	CA	2504	PSU	C4-N3	3.38	1.39	1.33
31	CA	1939	5MU	C4-N3	3.39	1.39	1.33
1	AA	516	PSU	C4-N3	3.40	1.39	1.33
1	AA	1516	2MG	C6-N1	3.43	1.39	1.33
31	CA	746	PSU	C4-N3	3.47	1.39	1.33
1	BA	1516	2MG	C6-N1	3.51	1.39	1.33
1	AA	966	2MG	C6-N1	3.51	1.39	1.33
31	CA	745	1MG	C6-C5	3.79	1.48	1.40
30	DD	150[B]	MEQ	CB-CA	3.95	1.59	1.53
31	CA	2604	PSU	C2-N1	69.29	2.82	1.38

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DA	747	5MU	C5-C4-N3	-12.16	115.14	125.35
31	CA	747	5MU	C5-C4-N3	-12.15	115.15	125.35
31	CA	1939	5MU	C5-C4-N3	-12.04	115.25	125.35
54	DA	1939	5MU	C5-C4-N3	-12.00	115.27	125.35
1	BA	527	G7M	C5-C6-N1	-10.03	110.41	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2069	G7M	C5-C6-N1	-9.93	110.55	123.52
54	DA	2069	G7M	C5-C6-N1	-9.92	110.56	123.52
1	AA	527	G7M	C5-C6-N1	-9.86	110.63	123.52
31	CA	2069	G7M	C6-C5-C4	-9.85	109.61	120.86
54	DA	2445	2MG	C5-C6-N1	-9.28	111.39	123.52
31	CA	2445	2MG	C5-C6-N1	-8.83	111.97	123.52
31	CA	2251	OMG	C5-C6-N1	-8.63	112.23	123.52
1	AA	1207	2MG	C5-C6-N1	-8.61	112.27	123.52
1	BA	966	2MG	C5-C6-N1	-8.56	112.34	123.52
1	AA	966	2MG	C5-C6-N1	-8.48	112.43	123.52
1	BA	527	G7M	C6-C5-C4	-8.46	111.19	120.86
1	BA	1207	2MG	C5-C6-N1	-8.26	112.72	123.52
54	DA	1835	2MG	C5-C6-N1	-8.21	112.79	123.52
1	BA	1516	2MG	C5-C6-N1	-8.15	112.86	123.52
31	CA	1835	2MG	C5-C6-N1	-8.11	112.92	123.52
1	AA	1516	2MG	C5-C6-N1	-8.10	112.93	123.52
54	DA	2251	OMG	C5-C6-N1	-7.93	113.15	123.52
1	AA	527	G7M	C6-C5-C4	-6.97	112.89	120.86
54	DA	2069	G7M	C6-C5-C4	-4.38	115.85	120.86
1	BA	527	G7M	N3-C2-N1	-4.20	121.85	127.56
54	DA	745	1MG	C6-C5-C4	-4.00	117.08	119.93
31	CA	2069	G7M	N3-C2-N1	-3.86	122.30	127.56
1	AA	527	G7M	N3-C2-N1	-3.83	122.34	127.56
54	DA	746	PSU	C4-C5-C1'	-3.71	114.97	121.22
31	CA	745	1MG	C6-C5-C4	-3.70	117.29	119.93
54	DA	2069	G7M	N3-C2-N1	-3.64	122.61	127.56
31	CA	2552	OMU	C5-C4-N3	-3.48	114.75	123.28
54	DA	2552	OMU	C5-C4-N3	-3.43	114.85	123.28
1	AA	527	G7M	C1'-N9-C4	-3.38	123.04	126.81
54	DA	2251	OMG	N3-C2-N1	-3.25	123.13	127.56
1	AA	1516	2MG	C6-C5-C4	-3.15	117.26	120.86
54	DA	1915	3TD	C5-C4-N3	-3.15	116.08	118.65
31	CA	1915	3TD	C5-C4-N3	-3.04	116.17	118.65
31	CA	2251	OMG	N3-C2-N1	-2.96	123.53	127.56
30	DD	150[A]	MEQ	CG-CB-CA	-2.93	107.37	114.03
1	BA	1207	2MG	C6-C5-C4	-2.91	117.54	120.86
1	AA	966	2MG	C6-C5-C4	-2.90	117.54	120.86
1	BA	1516	2MG	C6-C5-C4	-2.88	117.56	120.86
31	CA	2445	2MG	C6-C5-C4	-2.78	117.68	120.86
31	CA	2251	OMG	C6-C5-C4	-2.63	117.85	120.86
54	DA	2445	2MG	C6-C5-C4	-2.60	117.89	120.86
1	BA	966	2MG	C6-C5-C4	-2.52	117.98	120.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2069	G7M	C1'-N9-C4	-2.45	124.08	126.81
31	CA	1835	2MG	C6-C5-C4	-2.44	118.07	120.86
31	CA	745	1MG	C5-C6-N1	-2.40	115.21	118.35
30	DD	150[B]	MEQ	O-C-CA	-2.36	119.38	125.72
54	DA	2605	PSU	C4-C5-C1'	-2.33	117.29	121.22
30	CD	150	MEQ	O-C-CA	-2.31	119.54	125.72
31	CA	746	PSU	C4-C5-C1'	-2.30	117.34	121.22
1	AA	1207	2MG	C6-C5-C4	-2.27	118.26	120.86
54	DA	1835	2MG	C6-C5-C4	-2.25	118.29	120.86
31	CA	2580	PSU	C4-C5-C1'	-2.25	117.44	121.22
30	DD	150[A]	MEQ	O-C-CA	-2.23	119.75	125.72
54	DA	745	1MG	C5-C6-N1	-2.19	115.48	118.35
12	AL	89	D2T	O-C-CA	-2.10	119.96	125.69
54	DA	2251	OMG	C6-C5-C4	-2.02	118.55	120.86
54	DA	2503	2MA	CM2-C2-N3	2.00	120.62	117.22
1	BA	516	PSU	O4'-C1'-C2'	2.00	106.86	104.69
1	AA	516	PSU	O4'-C1'-C2'	2.01	106.86	104.69
54	DA	747	5MU	C5M-C5-C6	2.03	122.74	118.63
1	AA	1516	2MG	N2-C2-N3	2.07	119.35	116.94
54	DA	1939	5MU	C5M-C5-C6	2.14	122.97	118.63
31	CA	747	5MU	C5M-C5-C6	2.16	123.00	118.63
31	CA	1962	5MC	CM5-C5-C6	2.18	123.05	118.63
1	AA	967	5MC	CM5-C5-C6	2.18	123.05	118.63
1	BA	1407	5MC	CM5-C5-C6	2.19	123.07	118.63
31	CA	1939	5MU	C5M-C5-C6	2.22	123.13	118.63
1	AA	1207	2MG	N2-C2-N3	2.24	119.54	116.94
1	AA	1407	5MC	CM5-C5-C6	2.24	123.17	118.63
54	DA	2445	2MG	N2-C2-N3	2.25	119.55	116.94
1	BA	967	5MC	CM5-C5-C6	2.26	123.20	118.63
54	DA	2457	PSU	O4'-C1'-C2'	2.29	107.16	104.69
31	CA	2503	2MA	C2-N3-C4	2.31	116.40	115.29
31	CA	2445	2MG	N2-C2-N3	2.34	119.66	116.94
54	DA	2503	2MA	C2-N3-C4	2.34	116.42	115.29
12	AL	89	D2T	C-CA-N	2.35	115.15	109.95
54	DA	1962	5MC	CM5-C5-C6	2.43	123.56	118.63
31	CA	2030	6MZ	C2-N1-C6	2.46	118.24	116.47
1	BA	966	2MG	N2-C2-N3	2.50	119.84	116.94
12	BL	89	D2T	C-CA-N	2.57	115.62	109.95
1	BA	1207	2MG	N2-C2-N3	2.59	119.94	116.94
31	CA	2580	PSU	O4'-C1'-C2'	2.78	107.69	104.69
31	CA	1618	6MZ	C2-N1-C6	2.87	118.53	116.47
1	BA	1402	4OC	CM4-N4-C4	2.93	125.34	122.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1402	4OC	CM4-N4-C4	2.99	125.39	122.87
54	DA	2580	PSU	O4'-C1'-C2'	3.11	108.05	104.69
54	DA	2030	6MZ	C2-N1-C6	3.16	118.74	116.47
30	DD	150[B]	MEQ	CB-CA-N	3.19	119.52	110.54
1	AA	1402	4OC	C2-N3-C4	3.99	120.51	115.43
31	CA	2069	G7M	O4'-C1'-N9	4.01	115.69	108.11
54	DA	2069	G7M	O4'-C1'-N9	4.02	115.70	108.11
1	BA	1402	4OC	C2-N3-C4	4.07	120.60	115.43
1	BA	527	G7M	O4'-C1'-N9	5.41	118.33	108.11
1	AA	527	G7M	O4'-C1'-N9	5.44	118.38	108.11
1	BA	527	G7M	C6-N1-C2	5.95	122.86	115.88
31	CA	1835	2MG	C6-N1-C2	5.95	123.77	115.24
1	BA	1516	2MG	C6-N1-C2	6.00	123.84	115.24
54	DA	1835	2MG	C6-N1-C2	6.01	123.85	115.24
1	AA	1516	2MG	C6-N1-C2	6.02	123.86	115.24
1	AA	966	2MG	C6-N1-C2	6.42	124.44	115.24
1	AA	1207	2MG	C6-N1-C2	6.52	124.58	115.24
1	BA	966	2MG	C6-N1-C2	6.58	124.67	115.24
1	BA	1207	2MG	C6-N1-C2	6.61	124.71	115.24
31	CA	2069	G7M	C6-N1-C2	6.62	123.64	115.88
31	CA	2445	2MG	C6-N1-C2	6.74	124.89	115.24
54	DA	2445	2MG	C6-N1-C2	7.12	125.43	115.24
1	AA	527	G7M	C6-N1-C2	7.12	124.23	115.88
54	DA	2069	G7M	C6-N1-C2	7.38	124.53	115.88
54	DA	2251	OMG	C6-N1-C2	7.54	124.72	115.88
31	CA	2251	OMG	C6-N1-C2	8.02	125.28	115.88
54	DA	2552	OMU	C4-N3-C2	12.04	126.89	114.21
31	CA	2552	OMU	C4-N3-C2	12.13	126.99	114.21
54	DA	2605	PSU	C4-N3-C2	13.41	126.35	115.16
31	CA	955	PSU	C4-N3-C2	13.43	126.36	115.16
54	DA	2580	PSU	C4-N3-C2	13.43	126.37	115.16
54	DA	2457	PSU	C4-N3-C2	13.44	126.37	115.16
54	DA	955	PSU	C4-N3-C2	13.46	126.39	115.16
54	DA	1911	PSU	C4-N3-C2	13.47	126.40	115.16
31	CA	746	PSU	C4-N3-C2	13.48	126.41	115.16
54	DA	2604	PSU	C4-N3-C2	13.51	126.43	115.16
31	CA	2504	PSU	C4-N3-C2	13.53	126.45	115.16
31	CA	1911	PSU	C4-N3-C2	13.54	126.46	115.16
31	CA	2605	PSU	C4-N3-C2	13.56	126.48	115.16
54	DA	1917	PSU	C4-N3-C2	13.59	126.50	115.16
1	BA	516	PSU	C4-N3-C2	13.60	126.50	115.16
31	CA	2580	PSU	C4-N3-C2	13.60	126.51	115.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	AA	516	PSU	C4-N3-C2	13.61	126.51	115.16
31	CA	2457	PSU	C4-N3-C2	13.64	126.53	115.16
54	DA	746	PSU	C4-N3-C2	13.64	126.54	115.16
54	DA	2504	PSU	C4-N3-C2	13.64	126.54	115.16
31	CA	1917	PSU	C4-N3-C2	13.73	126.61	115.16
54	DA	747	5MU	C4-N3-C2	14.17	126.98	115.16
54	DA	1939	5MU	C4-N3-C2	14.26	127.05	115.16
31	CA	2604	PSU	C4-N3-C2	14.30	127.09	115.16
31	CA	747	5MU	C4-N3-C2	14.43	127.20	115.16
31	CA	1939	5MU	C4-N3-C2	14.52	127.27	115.16
31	CA	2604	PSU	C4-C5-C1'	33.81	178.16	121.22

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	CA	2604	PSU	C2-C4-C5-C6-N1-N3

18 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1402	4OC	1	0
1	AA	1518	MA6	2	0
1	AA	1519	MA6	2	0
1	AA	967	5MC	1	0
1	BA	1402	4OC	1	0
1	BA	1518	MA6	2	0
1	BA	1519	MA6	2	0
31	CA	1915	3TD	1	0
31	CA	2030	6MZ	3	0
31	CA	2503	2MA	1	0
31	CA	2580	PSU	1	0
31	CA	747	5MU	1	0
54	DA	2030	6MZ	1	0
54	DA	2251	OMG	1	0
54	DA	2498	OMC	1	0
54	DA	747	5MU	1	0
30	DD	150[A]	MEQ	2	0
30	DD	150[B]	MEQ	2	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 559 ligands modelled in this entry, 475 are monoatomic - leaving 84 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	$\# Z > 2$
56	PG4	AA	1670	-	12,12,12	0.35	0	11,11,11	0.41	0
57	MPD	AA	1671	-	6,7,7	0.38	0	6,10,10	0.40	0
58	PUT	AA	1672	-	5,5,5	0.29	0	4,4,4	0.30	0
58	PUT	AA	1673	-	5,5,5	0.18	0	4,4,4	0.18	0
58	PUT	AA	1674	-	5,5,5	0.21	0	4,4,4	0.17	0
58	PUT	AA	1675	-	5,5,5	0.23	0	4,4,4	0.12	0
57	MPD	AA	1676	-	6,7,7	0.52	0	6,10,10	0.39	0
59	TAC	AA	1680	55	33,35,35	0.52	0	42,58,58	0.64	0
59	TAC	AA	1681	55	33,35,35	0.55	0	42,58,58	0.71	1 (2%)
61	PEG	AL	201	-	6,6,6	0.33	0	5,5,5	0.13	0
56	PG4	BA	1642	-	12,12,12	0.25	0	11,11,11	0.16	0
59	TAC	BA	1643	55	33,35,35	0.46	0	42,58,58	0.82	0
59	TAC	BA	1644	55	33,35,35	0.58	0	42,58,58	0.68	0
62	EDO	D1	101	-	3,3,3	0.70	0	2,2,2	0.10	0
63	PGE	D1	102	-	9,9,9	0.26	0	8,8,8	0.21	0
61	PEG	D1	103	-	6,6,6	0.39	0	5,5,5	0.17	0
61	PEG	D3	101	-	6,6,6	0.30	0	5,5,5	0.28	0
63	PGE	DA	3001	-	9,9,9	0.33	0	8,8,8	0.32	0
62	EDO	DA	3002	-	3,3,3	0.59	0	2,2,2	0.41	0
62	EDO	DA	3003	-	3,3,3	0.59	0	2,2,2	0.27	0
64	SPD	DA	3183	-	9,9,9	0.13	0	8,8,8	0.17	0
58	PUT	DA	3184	-	5,5,5	0.46	0	4,4,4	0.25	0
65	1PE	DA	3185	-	15,15,15	0.21	0	14,14,14	0.37	0
63	PGE	DA	3186	-	9,9,9	0.39	0	8,8,8	0.44	0
64	SPD	DA	3187	-	9,9,9	0.22	0	8,8,8	0.35	0
58	PUT	DA	3188	-	5,5,5	0.28	0	4,4,4	0.15	0
58	PUT	DA	3189	-	5,5,5	0.30	0	4,4,4	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	MPD	DA	3190	-	6,7,7	0.32	0	6,10,10	0.36	0
66	ACY	DA	3191	-	0,3,3	0.00	-	0,3,3	0.00	-
57	MPD	DA	3192	-	6,7,7	0.35	0	6,10,10	0.39	0
56	PG4	DA	3193	-	12,12,12	0.42	0	11,11,11	0.33	0
62	EDO	DA	3194	-	3,3,3	0.92	0	2,2,2	0.15	0
58	PUT	DA	3195	-	5,5,5	0.42	0	4,4,4	0.56	0
66	ACY	DA	3196	-	0,3,3	0.00	-	0,3,3	0.00	-
62	EDO	DA	3197	-	3,3,3	0.74	0	2,2,2	0.12	0
62	EDO	DA	3198	-	3,3,3	0.58	0	2,2,2	0.44	0
61	PEG	DA	3199	-	6,6,6	0.24	0	5,5,5	0.15	0
61	PEG	DA	3200	-	6,6,6	0.40	0	5,5,5	0.21	0
66	ACY	DA	3201	-	0,3,3	0.00	-	0,3,3	0.00	-
65	1PE	DA	3202	-	15,15,15	0.37	0	14,14,14	0.36	0
63	PGE	DA	3203	-	9,9,9	0.33	0	8,8,8	0.25	0
57	MPD	DA	3204	-	6,7,7	0.58	0	6,10,10	0.62	0
58	PUT	DA	3205	-	5,5,5	0.25	0	4,4,4	0.22	0
64	SPD	DA	3206	-	9,9,9	0.27	0	8,8,8	0.23	0
57	MPD	DA	3207	-	6,7,7	0.55	0	6,10,10	0.47	0
62	EDO	DA	3208	-	3,3,3	0.62	0	2,2,2	0.30	0
62	EDO	DA	3209	-	3,3,3	0.63	0	2,2,2	0.33	0
57	MPD	DA	3210	-	6,7,7	0.48	0	6,10,10	0.31	0
67	GUN	DA	3211	-	9,12,12	1.71	2 (22%)	7,17,17	4.69	5 (71%)
58	PUT	DA	3212	-	5,5,5	0.30	0	4,4,4	0.03	0
58	PUT	DA	3213	-	5,5,5	0.25	0	4,4,4	0.24	0
63	PGE	DA	3214	-	9,9,9	0.31	0	8,8,8	0.41	0
62	EDO	DA	3215	-	3,3,3	0.75	0	2,2,2	0.18	0
56	PG4	DA	3216	-	12,12,12	0.19	0	11,11,11	0.23	0
63	PGE	DA	3217	-	9,9,9	0.20	0	8,8,8	0.24	0
61	PEG	DA	3218	-	6,6,6	0.27	0	5,5,5	0.06	0
58	PUT	DA	3219	-	5,5,5	0.24	0	4,4,4	0.15	0
68	TRS	DA	3220	-	7,7,7	0.51	0	9,9,9	0.42	0
58	PUT	DA	3221	-	5,5,5	0.26	0	4,4,4	0.15	0
58	PUT	DA	3222	-	5,5,5	0.54	0	4,4,4	0.66	0
58	PUT	DA	3223	-	5,5,5	0.27	0	4,4,4	0.21	0
64	SPD	DA	3224	-	9,9,9	0.26	0	8,8,8	0.44	0
63	PGE	DA	3225	-	9,9,9	0.18	0	8,8,8	0.15	0
61	PEG	DA	3226	-	6,6,6	0.47	0	5,5,5	0.16	0
61	PEG	DA	3227	-	6,6,6	0.28	0	5,5,5	0.14	0
62	EDO	DB	201	-	3,3,3	0.66	0	2,2,2	0.20	0
62	EDO	DB	211	-	3,3,3	0.63	0	2,2,2	0.23	0
62	EDO	DB	212	-	3,3,3	0.75	0	2,2,2	0.15	0
57	MPD	DE	301	-	6,7,7	0.46	0	6,10,10	0.50	0
57	MPD	DE	302	-	6,7,7	0.53	0	6,10,10	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	MPD	DK	201	-	6,7,7	0.39	0	6,10,10	0.20	0
61	PEG	DL	201	-	6,6,6	0.11	0	5,5,5	0.16	0
58	PUT	DM	201	-	5,5,5	0.17	0	4,4,4	0.14	0
57	MPD	DN	201	-	6,7,7	0.67	0	6,10,10	0.38	0
61	PEG	DP	201	-	6,6,6	0.31	0	5,5,5	0.13	0
61	PEG	DQ	201	-	6,6,6	0.21	0	5,5,5	0.17	0
56	PG4	DQ	202	-	12,12,12	0.23	0	11,11,11	0.15	0
56	PG4	DR	202	-	12,12,12	0.30	0	11,11,11	0.38	0
63	PGE	DS	201	-	9,9,9	0.42	0	8,8,8	0.31	0
56	PG4	DS	202	-	12,12,12	0.41	0	11,11,11	0.33	0
57	MPD	DS	203	-	6,7,7	0.23	0	6,10,10	0.27	0
57	MPD	DT	201	-	6,7,7	0.43	0	6,10,10	0.21	0
57	MPD	DT	202	-	6,7,7	0.47	0	6,10,10	0.40	0
63	PGE	DU	101	-	9,9,9	0.23	0	8,8,8	0.11	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
56	PG4	AA	1670	-	-	0/10/10/10	0/0/0/0
57	MPD	AA	1671	-	-	0/5/5/5	0/0/0/0
58	PUT	AA	1672	-	-	0/3/3/3	0/0/0/0
58	PUT	AA	1673	-	-	0/3/3/3	0/0/0/0
58	PUT	AA	1674	-	-	0/3/3/3	0/0/0/0
58	PUT	AA	1675	-	-	0/3/3/3	0/0/0/0
57	MPD	AA	1676	-	-	0/5/5/5	0/0/0/0
59	TAC	AA	1680	55	-	0/8/74/74	0/4/4/4
59	TAC	AA	1681	55	-	0/8/74/74	0/4/4/4
61	PEG	AL	201	-	-	0/4/4/4	0/0/0/0
56	PG4	BA	1642	-	-	0/10/10/10	0/0/0/0
59	TAC	BA	1643	55	-	0/8/74/74	0/4/4/4
59	TAC	BA	1644	55	-	0/8/74/74	0/4/4/4
62	EDO	D1	101	-	-	0/1/1/1	0/0/0/0
63	PGE	D1	102	-	-	0/7/7/7	0/0/0/0
61	PEG	D1	103	-	-	0/4/4/4	0/0/0/0
61	PEG	D3	101	-	-	0/4/4/4	0/0/0/0
63	PGE	DA	3001	-	-	0/7/7/7	0/0/0/0
62	EDO	DA	3002	-	-	0/1/1/1	0/0/0/0
62	EDO	DA	3003	-	-	0/1/1/1	0/0/0/0
64	SPD	DA	3183	-	-	0/7/7/7	0/0/0/0
58	PUT	DA	3184	-	-	0/3/3/3	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
65	1PE	DA	3185	-	-	0/13/13/13	0/0/0/0
63	PGE	DA	3186	-	-	0/7/7/7	0/0/0/0
64	SPD	DA	3187	-	-	0/7/7/7	0/0/0/0
58	PUT	DA	3188	-	-	0/3/3/3	0/0/0/0
58	PUT	DA	3189	-	-	0/3/3/3	0/0/0/0
57	MPD	DA	3190	-	-	0/5/5/5	0/0/0/0
66	ACY	DA	3191	-	-	0/0/0/0	0/0/0/0
57	MPD	DA	3192	-	-	0/5/5/5	0/0/0/0
56	PG4	DA	3193	-	-	0/10/10/10	0/0/0/0
62	EDO	DA	3194	-	-	0/1/1/1	0/0/0/0
58	PUT	DA	3195	-	-	0/3/3/3	0/0/0/0
66	ACY	DA	3196	-	-	0/0/0/0	0/0/0/0
62	EDO	DA	3197	-	-	0/1/1/1	0/0/0/0
62	EDO	DA	3198	-	-	0/1/1/1	0/0/0/0
61	PEG	DA	3199	-	-	0/4/4/4	0/0/0/0
61	PEG	DA	3200	-	-	0/4/4/4	0/0/0/0
66	ACY	DA	3201	-	-	0/0/0/0	0/0/0/0
65	1PE	DA	3202	-	-	0/13/13/13	0/0/0/0
63	PGE	DA	3203	-	-	0/7/7/7	0/0/0/0
57	MPD	DA	3204	-	-	0/5/5/5	0/0/0/0
58	PUT	DA	3205	-	-	0/3/3/3	0/0/0/0
64	SPD	DA	3206	-	-	0/7/7/7	0/0/0/0
57	MPD	DA	3207	-	-	0/5/5/5	0/0/0/0
62	EDO	DA	3208	-	-	0/1/1/1	0/0/0/0
62	EDO	DA	3209	-	-	0/1/1/1	0/0/0/0
57	MPD	DA	3210	-	-	0/5/5/5	0/0/0/0
67	GUN	DA	3211	-	-	0/0/0/0	0/2/2/2
58	PUT	DA	3212	-	-	0/3/3/3	0/0/0/0
58	PUT	DA	3213	-	-	0/3/3/3	0/0/0/0
63	PGE	DA	3214	-	-	0/7/7/7	0/0/0/0
62	EDO	DA	3215	-	-	0/1/1/1	0/0/0/0
56	PG4	DA	3216	-	-	0/10/10/10	0/0/0/0
63	PGE	DA	3217	-	-	0/7/7/7	0/0/0/0
61	PEG	DA	3218	-	-	0/4/4/4	0/0/0/0
58	PUT	DA	3219	-	-	0/3/3/3	0/0/0/0
68	TRS	DA	3220	-	-	0/9/9/9	0/0/0/0
58	PUT	DA	3221	-	-	0/3/3/3	0/0/0/0
58	PUT	DA	3222	-	-	0/3/3/3	0/0/0/0
58	PUT	DA	3223	-	-	0/3/3/3	0/0/0/0
64	SPD	DA	3224	-	-	0/7/7/7	0/0/0/0
63	PGE	DA	3225	-	-	0/7/7/7	0/0/0/0
61	PEG	DA	3226	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	PEG	DA	3227	-	-	0/4/4/4	0/0/0/0
62	EDO	DB	201	-	-	0/1/1/1	0/0/0/0
62	EDO	DB	211	-	-	0/1/1/1	0/0/0/0
62	EDO	DB	212	-	-	0/1/1/1	0/0/0/0
57	MPD	DE	301	-	-	0/5/5/5	0/0/0/0
57	MPD	DE	302	-	-	0/5/5/5	0/0/0/0
57	MPD	DK	201	-	-	0/5/5/5	0/0/0/0
61	PEG	DL	201	-	-	0/4/4/4	0/0/0/0
58	PUT	DM	201	-	-	0/3/3/3	0/0/0/0
57	MPD	DN	201	-	-	0/5/5/5	0/0/0/0
61	PEG	DP	201	-	-	0/4/4/4	0/0/0/0
61	PEG	DQ	201	-	-	0/4/4/4	0/0/0/0
56	PG4	DQ	202	-	-	0/10/10/10	0/0/0/0
56	PG4	DR	202	-	-	0/10/10/10	0/0/0/0
63	PGE	DS	201	-	-	0/7/7/7	0/0/0/0
56	PG4	DS	202	-	-	0/10/10/10	0/0/0/0
57	MPD	DS	203	-	-	0/5/5/5	0/0/0/0
57	MPD	DT	201	-	-	0/5/5/5	0/0/0/0
57	MPD	DT	202	-	-	0/5/5/5	0/0/0/0
63	PGE	DU	101	-	-	0/7/7/7	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	DA	3211	GUN	C6-C5	3.17	1.47	1.41
67	DA	3211	GUN	C6-N1	3.29	1.39	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	DA	3211	GUN	C5-C6-N1	-8.21	112.79	123.52
67	DA	3211	GUN	C5-C4-N9	-3.15	105.53	111.12
67	DA	3211	GUN	C6-C5-C4	-3.08	117.34	120.86
67	DA	3211	GUN	N3-C2-N1	-2.94	123.56	127.56
59	AA	1681	TAC	C42-N4-C4	2.12	119.17	114.11
67	DA	3211	GUN	C6-N1-C2	7.56	124.74	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

27 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	AA	1670	PG4	1	0
57	AA	1676	MPD	3	0
59	AA	1681	TAC	2	0
56	BA	1642	PG4	1	0
63	D1	102	PGE	2	0
61	D1	103	PEG	1	0
63	DA	3001	PGE	1	0
58	DA	3189	PUT	1	0
57	DA	3192	MPD	1	0
56	DA	3193	PG4	2	0
58	DA	3195	PUT	3	0
62	DA	3198	EDO	1	0
65	DA	3202	1PE	1	0
57	DA	3204	MPD	1	0
57	DA	3207	MPD	1	0
63	DA	3214	PGE	1	0
56	DA	3216	PG4	1	0
68	DA	3220	TRS	1	0
58	DA	3222	PUT	3	0
64	DA	3224	SPD	2	0
63	DA	3225	PGE	2	0
57	DN	201	MPD	1	0
61	DP	201	PEG	1	0
56	DR	202	PG4	5	0
63	DS	201	PGE	1	0
56	DS	202	PG4	3	0
63	DU	101	PGE	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1523/1534 (99%)	-0.06	30 (1%) 68 39	37, 86, 227, 287	0
1	BA	1522/1534 (99%)	0.47	167 (10%) 7 3	58, 109, 255, 271	0
2	AB	224/224 (100%)	0.64	28 (12%) 5 2	65, 117, 185, 228	0
2	BB	224/224 (100%)	0.89	36 (16%) 3 1	89, 139, 197, 228	0
3	AC	206/206 (100%)	-0.11	2 (0%) 84 60	67, 98, 127, 149	0
3	BC	206/206 (100%)	0.97	40 (19%) 1 1	90, 138, 170, 184	0
4	AD	205/205 (100%)	-0.31	0 100 100	63, 92, 129, 160	0
4	BD	205/205 (100%)	-0.45	0 100 100	53, 77, 106, 132	0
5	AE	155/155 (100%)	-0.10	0 100 100	54, 75, 108, 159	0
5	BE	150/155 (96%)	0.07	2 (1%) 79 53	61, 92, 129, 201	0
6	AF	106/106 (100%)	0.01	2 (1%) 70 41	63, 93, 120, 134	0
6	BF	100/106 (94%)	0.44	2 (2%) 68 39	77, 117, 140, 153	0
7	AG	151/151 (100%)	0.87	30 (19%) 1 1	95, 136, 160, 174	0
7	BG	151/151 (100%)	2.32	75 (49%) 0 0	136, 196, 213, 220	0
8	AH	129/129 (100%)	-0.08	1 (0%) 87 67	59, 82, 107, 122	0
8	BH	129/129 (100%)	0.03	4 (3%) 52 24	85, 110, 137, 152	0
9	AI	127/127 (100%)	1.12	27 (21%) 1 1	75, 135, 164, 171	0
9	BI	127/127 (100%)	1.90	49 (38%) 0 0	133, 164, 201, 210	0
10	AJ	99/99 (100%)	0.62	11 (11%) 7 3	83, 118, 141, 147	0
10	BJ	98/99 (98%)	3.09	59 (60%) 0 0	134, 168, 189, 195	0
11	AK	117/117 (100%)	0.24	5 (4%) 39 16	44, 100, 129, 139	0
11	BK	117/117 (100%)	0.24	3 (2%) 59 29	59, 104, 132, 163	0
12	AL	122/123 (99%)	-0.28	1 (0%) 87 67	43, 60, 92, 130	0
12	BL	122/123 (99%)	0.33	4 (3%) 50 22	65, 86, 114, 137	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	1.42	33 (28%) 1 0	108, 130, 165, 171	0
13	BM	114/114 (100%)	3.34	87 (76%) 0 0	195, 230, 238, 247	0
14	AN	100/100 (100%)	1.01	16 (16%) 3 1	77, 117, 178, 184	0
14	BN	100/100 (100%)	2.55	52 (52%) 0 0	124, 178, 216, 222	0
15	AO	88/88 (100%)	-0.07	1 (1%) 82 58	54, 84, 107, 129	0
15	BO	88/88 (100%)	0.45	6 (6%) 20 7	75, 109, 133, 153	0
16	AP	82/82 (100%)	0.40	3 (3%) 45 19	55, 75, 121, 140	0
16	BP	82/82 (100%)	1.16	19 (23%) 1 1	81, 98, 148, 155	0
17	AQ	80/80 (100%)	0.01	2 (2%) 61 30	58, 78, 113, 129	0
17	BQ	80/80 (100%)	1.10	17 (21%) 1 1	83, 120, 145, 157	0
18	AR	55/55 (100%)	0.15	1 (1%) 71 43	63, 89, 130, 153	0
18	BR	55/55 (100%)	0.26	3 (5%) 29 11	65, 86, 129, 168	0
19	AS	79/79 (100%)	0.82	10 (12%) 5 2	114, 135, 155, 163	0
19	BS	79/79 (100%)	3.80	60 (75%) 0 0	210, 226, 239, 245	0
20	AT	86/86 (100%)	0.01	0 100 100	54, 77, 108, 129	0
20	BT	85/86 (98%)	1.28	22 (25%) 1 1	93, 119, 147, 159	0
21	AU	56/56 (100%)	0.26	2 (3%) 46 20	66, 107, 153, 165	0
21	BU	56/56 (100%)	0.29	1 (1%) 71 43	63, 95, 134, 143	0
22	C1	56/56 (100%)	1.10	12 (21%) 1 1	78, 133, 163, 173	0
22	D1	56/56 (100%)	-0.56	0 100 100	18, 37, 65, 104	0
23	C2	50/51 (98%)	2.98	34 (68%) 0 0	131, 157, 168, 196	0
23	D2	51/51 (100%)	-0.01	0 100 100	46, 60, 87, 104	0
24	C3	46/46 (100%)	1.49	13 (28%) 1 0	90, 117, 130, 138	0
24	D3	46/46 (100%)	-0.38	0 100 100	23, 31, 48, 112	0
25	C4	64/64 (100%)	0.89	9 (14%) 4 1	96, 120, 140, 154	0
25	D4	64/64 (100%)	-0.46	0 100 100	23, 35, 48, 61	0
26	C5	38/38 (100%)	1.23	9 (23%) 1 1	91, 114, 127, 138	0
26	D5	38/38 (100%)	-0.33	0 100 100	30, 44, 62, 80	0
27	C0	58/58 (100%)	0.79	8 (13%) 4 1	90, 111, 135, 139	0
27	D0	58/58 (100%)	-0.53	0 100 100	21, 30, 53, 80	0
28	CB	118/120 (98%)	0.64	9 (7%) 17 6	102, 170, 229, 238	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	120/120 (100%)	-0.35	0 100 100	29, 53, 95, 122	0
29	CC	271/271 (100%)	0.36	16 (5%) 26 10	71, 94, 116, 128	0
29	DC	271/271 (100%)	-0.47	0 100 100	22, 49, 76, 92	0
30	CD	208/209 (99%)	0.91	31 (14%) 3 1	73, 111, 141, 155	0
30	DD	208/209 (99%)	-0.51	0 100 100	13, 34, 66, 93	0
31	CA	2875/2904 (99%)	0.61	264 (9%) 11 4	61, 127, 244, 289	0
32	CE	201/201 (100%)	1.29	46 (22%) 1 1	85, 153, 183, 194	0
32	DE	201/201 (100%)	-0.40	1 (0%) 91 76	19, 50, 97, 132	0
33	CF	177/177 (100%)	3.03	112 (63%) 0 0	193, 211, 219, 227	0
33	DF	177/177 (100%)	-0.17	1 (0%) 90 73	44, 75, 117, 142	0
34	CG	176/176 (100%)	1.95	78 (44%) 0 0	130, 159, 185, 198	0
34	DG	176/176 (100%)	-0.16	1 (0%) 90 73	38, 66, 97, 123	0
35	CH	149/149 (100%)	1.38	38 (25%) 1 1	79, 144, 170, 184	0
35	DH	149/149 (100%)	0.85	27 (18%) 2 1	55, 142, 179, 198	0
36	CJ	134/134 (100%)	6.11	120 (89%) 0 0	235, 251, 263, 270	0
36	DJ	134/134 (100%)	3.48	82 (61%) 0 0	200, 227, 240, 245	0
37	CK	142/142 (100%)	0.34	4 (2%) 56 27	84, 101, 127, 139	0
37	DK	142/142 (100%)	-0.57	0 100 100	18, 30, 57, 82	0
38	CL	122/123 (99%)	0.28	5 (4%) 41 16	73, 101, 135, 154	0
38	DL	123/123 (100%)	-0.52	0 100 100	20, 38, 66, 94	0
39	CM	144/144 (100%)	2.01	55 (38%) 0 0	88, 144, 181, 214	0
39	DM	144/144 (100%)	-0.53	0 100 100	10, 45, 79, 102	0
40	CN	135/136 (99%)	0.34	6 (4%) 38 16	71, 104, 130, 165	0
40	DN	135/136 (99%)	-0.65	0 100 100	21, 34, 63, 95	0
41	CO	120/125 (96%)	1.29	28 (23%) 1 1	94, 117, 139, 181	0
41	DO	125/125 (100%)	-0.48	0 100 100	16, 32, 66, 128	0
42	CP	116/117 (99%)	1.93	47 (40%) 0 0	133, 156, 174, 184	0
42	DP	117/117 (100%)	-0.36	0 100 100	34, 52, 82, 94	0
43	CQ	114/114 (100%)	1.18	22 (19%) 2 1	98, 114, 134, 148	0
43	DQ	114/114 (100%)	-0.49	0 100 100	26, 43, 75, 116	0
44	CR	117/117 (100%)	0.95	19 (16%) 3 1	81, 103, 125, 141	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DR	117/117 (100%)	-0.46	1 (0%) 85 64	14, 25, 43, 75	0
45	CS	103/103 (100%)	1.66	33 (32%) 1 0	101, 121, 157, 167	0
45	DS	103/103 (100%)	-0.53	0 100 100	15, 39, 68, 94	0
46	CT	110/110 (100%)	0.84	15 (13%) 4 1	98, 120, 152, 162	0
46	DT	110/110 (100%)	-0.59	0 100 100	15, 28, 56, 111	0
47	CU	93/93 (100%)	1.59	30 (32%) 1 0	124, 146, 173, 182	0
47	DU	93/93 (100%)	-0.00	2 (2%) 65 35	27, 52, 110, 129	0
48	CV	102/102 (100%)	2.59	58 (56%) 0 0	124, 156, 188, 199	0
48	DV	102/102 (100%)	-0.26	2 (1%) 68 39	36, 56, 101, 131	0
49	CW	94/94 (100%)	1.46	29 (30%) 1 0	111, 134, 151, 161	0
49	DW	94/94 (100%)	-0.52	0 100 100	32, 48, 80, 91	0
50	CX	75/76 (98%)	1.41	23 (30%) 1 0	86, 118, 132, 172	0
50	DX	76/76 (100%)	-0.52	1 (1%) 79 53	25, 36, 62, 104	0
51	CY	77/77 (100%)	0.43	3 (3%) 43 18	78, 113, 143, 161	0
51	DY	77/77 (100%)	-0.43	0 100 100	24, 50, 85, 112	0
52	CZ	62/62 (100%)	2.35	33 (53%) 0 0	123, 162, 179, 190	0
52	DZ	62/62 (100%)	-0.03	1 (1%) 74 47	41, 67, 104, 131	0
53	DI	135/135 (100%)	1.22	29 (21%) 1 1	75, 153, 204, 213	1 (0%)
54	DA	2873/2904 (98%)	-0.09	88 (3%) 52 24	16, 39, 206, 298	0
All	All	20632/20745 (99%)	0.49	2358 (11%) 7 2	10, 100, 227, 298	1 (0%)

All (2358) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	CJ	13	VAL	23.0
36	DJ	54	PRO	22.7
36	CJ	54	PRO	20.7
36	CJ	14	ALA	17.1
36	CJ	87	LYS	16.7
36	CJ	76	ALA	16.3
36	CJ	69	PHE	16.0
36	CJ	23	PRO	15.4
36	CJ	12	GLN	13.2
9	BI	128	SER	12.9
36	CJ	55	ILE	12.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	CA	2172	U	12.6
36	CJ	17	MET	12.5
36	DJ	135	SER	12.2
36	CJ	53	LEU	12.1
36	DJ	53	LEU	11.8
36	CJ	21	SER	11.6
10	BJ	74	VAL	11.4
10	BJ	75	ASP	11.3
31	CA	1067	A	11.1
54	DA	2120	G	11.0
36	CJ	20	PRO	11.0
36	CJ	56	PRO	11.0
36	DJ	67	PHE	10.7
36	DJ	79	LEU	10.6
31	CA	1068	G	10.4
36	CJ	57	VAL	10.3
36	CJ	59	ILE	10.3
36	CJ	51	LYS	10.1
45	CS	50	GLY	10.1
36	CJ	11	LEU	10.1
36	DJ	94	ASN	10.0
19	BS	48	THR	10.0
36	DJ	96	ASP	9.9
54	DA	2111	U	9.9
1	AA	1030	U	9.8
36	CJ	75	PRO	9.8
36	CJ	42	PHE	9.7
36	DJ	80	LEU	9.5
36	CJ	82	LYS	9.5
36	DJ	24	VAL	9.4
54	DA	2110	G	9.4
53	DI	131	THR	9.3
14	AN	23	LYS	9.2
19	BS	66	MET	9.2
23	C2	52	ALA	9.1
36	CJ	22	PRO	9.1
14	AN	21	PHE	9.1
9	BI	31	ASN	9.0
39	CM	81	ASP	9.0
36	CJ	47	ASP	9.0
31	CA	2174	C	9.0
10	BJ	76	ILE	9.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	CJ	46	THR	8.8
10	BJ	8	ILE	8.8
31	CA	2402	U	8.7
1	BA	1302	C	8.7
36	CJ	89	GLY	8.7
33	CF	128	TYR	8.7
9	BI	67	VAL	8.7
36	CJ	80	LEU	8.6
20	BT	4	ILE	8.6
36	CJ	86	ILE	8.6
9	BI	126	GLN	8.5
36	DJ	23	PRO	8.5
19	BS	39	THR	8.4
19	BS	38	SER	8.4
36	CJ	60	THR	8.4
33	CF	154	ILE	8.3
36	CJ	68	THR	8.3
36	CJ	132	THR	8.3
1	BA	983	A	8.3
7	BG	62	PHE	8.3
54	DA	2163	A	8.3
36	CJ	126	THR	8.3
36	CJ	120	ALA	8.2
39	CM	82	LEU	8.2
36	CJ	52	GLY	8.2
36	CJ	88	SER	8.1
36	CJ	138	LEU	8.1
33	CF	106	ILE	8.1
10	BJ	73	LEU	8.1
36	CJ	78	VAL	8.1
1	BA	1242	G	8.0
19	BS	12	ASP	8.0
14	BN	60	GLN	8.0
31	CA	2110	G	8.0
13	BM	23	TYR	8.0
36	DJ	20	PRO	7.9
52	CZ	45	GLN	7.9
31	CA	1087	G	7.9
36	CJ	83	ALA	7.9
10	BJ	41	PRO	7.9
54	DA	2124	G	7.9
33	CF	153	ASP	7.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	BN	54	ASP	7.9
36	CJ	121	ASP	7.9
33	CF	85	ILE	7.8
54	DA	2125	G	7.8
31	CA	2126	A	7.7
36	DJ	55	ILE	7.7
36	CJ	38	PHE	7.7
36	CJ	61	VAL	7.7
13	BM	45	ILE	7.7
36	CJ	71	THR	7.7
33	CF	156	ILE	7.7
13	BM	10	PRO	7.7
34	CG	32	GLU	7.7
36	CJ	77	ALA	7.7
36	CJ	9	VAL	7.6
48	CV	87	PHE	7.6
19	BS	14	HIS	7.6
9	BI	16	ALA	7.6
33	CF	117	LEU	7.6
54	DA	2127	G	7.5
19	BS	60	VAL	7.5
48	CV	80	ALA	7.5
36	DJ	13	VAL	7.5
31	CA	2125	G	7.4
36	CJ	24	VAL	7.4
31	CA	2173	A	7.4
19	BS	74	PHE	7.3
39	CM	114	GLY	7.3
7	BG	42	ILE	7.3
36	CJ	129	ILE	7.2
36	CJ	139	VAL	7.2
14	BN	35	ASN	7.2
23	C2	24	THR	7.1
31	CA	1066	U	7.1
19	BS	49	ILE	7.1
10	BJ	90	LEU	7.1
13	BM	39	ILE	7.1
13	BM	105	ASN	7.1
33	CF	132	VAL	7.1
10	BJ	26	VAL	7.0
33	CF	155	THR	7.0
1	BA	211	G	7.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	CJ	99	GLY	7.0
14	BN	21	PHE	7.0
48	CV	20	GLY	6.9
36	CJ	50	GLU	6.9
36	CJ	79	LEU	6.9
33	CF	176	PRO	6.9
45	CS	27	ILE	6.9
48	CV	3	ALA	6.9
31	CA	1084	A	6.9
48	CV	89	ASP	6.9
31	CA	1104	C	6.9
14	BN	36	ALA	6.9
1	BA	82	G	6.9
10	BJ	39	PRO	6.9
13	BM	84	GLY	6.8
33	CF	113	ASP	6.8
54	DA	884	U	6.8
19	BS	29	LYS	6.8
7	BG	151	PHE	6.8
14	BN	49	GLN	6.8
48	CV	36	VAL	6.7
18	BR	20	GLU	6.7
19	BS	63	THR	6.7
1	AA	86	G	6.7
13	BM	40	ALA	6.7
36	CJ	15	ALA	6.7
54	DA	1172	C	6.7
36	DJ	76	ALA	6.7
40	CN	136	MET	6.7
10	BJ	38	GLY	6.7
34	CG	103	ILE	6.7
50	CX	54	GLY	6.6
7	BG	116	MET	6.6
33	CF	95	ARG	6.6
36	CJ	73	THR	6.6
9	BI	130	ARG	6.6
36	CJ	90	SER	6.6
36	CJ	96	ASP	6.6
9	AI	130	ARG	6.6
31	CA	1537	G	6.6
43	CQ	85	SER	6.6
14	BN	17	ALA	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	BS	28	LYS	6.5
13	BM	47	GLU	6.5
31	CA	1085	A	6.5
1	AA	844	G	6.5
1	BA	1241	G	6.5
19	BS	32	ARG	6.5
31	CA	1103	A	6.5
1	BA	1030	U	6.5
13	BM	48	LEU	6.5
34	CG	33	LEU	6.5
19	BS	41	PHE	6.5
33	CF	97	TRP	6.5
33	CF	136	ILE	6.5
1	BA	209	U	6.5
33	CF	144	ASP	6.5
7	BG	52	GLN	6.5
52	CZ	15	ASN	6.4
36	DJ	138	LEU	6.4
36	CJ	119	GLY	6.4
36	CJ	131	GLY	6.4
9	BI	17	ALA	6.4
13	BM	64	VAL	6.4
39	CM	144	GLU	6.4
10	BJ	91	ASP	6.4
36	DJ	114	ALA	6.4
13	BM	96	PRO	6.4
1	AA	87	C	6.4
7	BG	43	VAL	6.4
36	DJ	137	GLY	6.3
14	BN	43	ASN	6.3
53	DI	128	THR	6.3
36	DJ	12	GLN	6.3
10	BJ	7	ARG	6.3
9	AI	20	PHE	6.3
23	C2	47	VAL	6.3
14	BN	40	ASP	6.2
48	CV	31	SER	6.2
36	DJ	38	PHE	6.2
1	BA	1243	C	6.2
31	CA	1057	A	6.2
33	CF	92	ARG	6.2
2	AB	123	ASP	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	BJ	6	ILE	6.1
54	DA	2123	G	6.1
10	BJ	35	GLN	6.1
54	DA	2174	C	6.1
19	BS	37	ARG	6.1
10	BJ	37	ARG	6.1
33	CF	96	MET	6.1
17	BQ	70	THR	6.1
19	BS	61	PHE	6.1
36	CJ	19	ASN	6.1
36	DJ	87	LYS	6.1
36	DJ	36	MET	6.0
39	CM	101	ILE	6.0
36	CJ	45	LYS	6.0
13	BM	22	ILE	6.0
33	CF	23	ASN	6.0
54	DA	2121	G	6.0
36	DJ	88	SER	6.0
7	AG	62	PHE	6.0
10	BJ	102	LEU	6.0
31	CA	331	C	6.0
34	CG	105	LEU	6.0
36	DJ	42	PHE	6.0
54	DA	885	C	6.0
14	BN	52	PRO	6.0
34	CG	2	SER	6.0
52	CZ	40	SER	6.0
36	CJ	18	ALA	6.0
31	CA	1065	U	5.9
23	C2	37	LYS	5.9
36	CJ	74	PRO	5.9
50	CX	52	GLY	5.9
36	CJ	84	ALA	5.9
1	BA	1016	A	5.9
31	CA	1175	A	5.9
36	DJ	21	SER	5.9
7	BG	39	ALA	5.9
39	CM	8	PRO	5.9
52	CZ	17	GLU	5.9
54	DA	892	A	5.9
48	CV	88	GLU	5.9
14	BN	50	THR	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	BJ	40	ILE	5.9
36	DJ	133	ALA	5.9
1	AA	1032	G	5.9
36	CJ	44	ALA	5.9
20	BT	36	TYR	5.9
13	BM	46	SER	5.9
36	CJ	28	LEU	5.9
33	CF	175	PHE	5.8
10	BJ	77	VAL	5.8
31	CA	1105	U	5.8
48	CV	13	VAL	5.8
1	AA	1031	C	5.8
7	BG	41	SER	5.8
45	CS	32	THR	5.8
1	BA	1032	G	5.8
10	BJ	25	ILE	5.8
52	CZ	49	ASP	5.8
33	CF	116	GLY	5.8
48	CV	32	GLY	5.8
1	BA	1017	U	5.8
1	BA	1024	G	5.8
36	CJ	118	THR	5.8
36	DJ	68	THR	5.8
33	CF	112	ARG	5.7
12	AL	124	ALA	5.7
54	DA	1729	U	5.7
7	BG	45	SER	5.7
33	CF	147	ASP	5.7
34	CG	40	ALA	5.7
13	AM	33	ILE	5.7
54	DA	2118	U	5.7
36	DJ	19	ASN	5.7
13	BM	95	LEU	5.7
33	CF	65	PRO	5.6
32	CE	104	ALA	5.6
48	CV	33	LYS	5.6
1	BA	1296	C	5.6
49	CW	94	ALA	5.6
54	DA	2175	C	5.6
31	CA	2127	G	5.6
36	CJ	116	ASP	5.6
36	DJ	132	THR	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	BN	55	SER	5.6
26	C5	38	GLY	5.6
33	CF	40	VAL	5.6
54	DA	1731	G	5.6
1	BA	1240	U	5.6
33	CF	157	THR	5.5
31	CA	877	A	5.5
7	BG	75	VAL	5.5
14	BN	58	SER	5.5
19	BS	13	LEU	5.5
14	BN	45	VAL	5.5
19	BS	76	PRO	5.5
9	AI	21	ILE	5.5
13	BM	83	LEU	5.5
31	CA	2120	G	5.5
36	CJ	43	ASN	5.5
7	BG	91	VAL	5.5
23	C2	31	PRO	5.4
33	CF	93	GLY	5.4
7	BG	65	ALA	5.4
9	BI	38	TYR	5.4
39	CM	92	LEU	5.4
7	BG	148	ASN	5.4
33	CF	135	GLN	5.4
54	DA	1065	U	5.4
31	CA	1086	A	5.4
33	CF	130	MET	5.4
7	BG	8	GLY	5.4
33	CF	131	GLY	5.4
9	AI	90	TYR	5.4
36	DJ	22	PRO	5.4
19	BS	42	PRO	5.4
53	DI	130	PRO	5.4
13	BM	31	LYS	5.4
10	BJ	27	GLU	5.4
54	DA	2116	G	5.3
36	CJ	62	TYR	5.3
13	BM	104	THR	5.3
19	BS	65	GLU	5.3
31	CA	1095	A	5.3
10	BJ	87	LEU	5.3
33	CF	35	THR	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	BS	31	LEU	5.3
36	CJ	33	VAL	5.3
36	CJ	98	VAL	5.3
36	CJ	67	PHE	5.3
54	DA	2172	U	5.3
33	CF	102	ARG	5.3
53	DI	96	PHE	5.3
13	BM	33	ILE	5.3
36	CJ	122	ILE	5.3
13	AM	30	SER	5.3
1	BA	1020	G	5.3
13	BM	56	LEU	5.3
37	CK	142	ILE	5.3
53	DI	134	GLU	5.2
47	CU	43	ILE	5.2
36	CJ	8	TYR	5.2
34	CG	102	VAL	5.2
19	BS	30	PRO	5.2
45	CS	63	VAL	5.2
31	CA	878	A	5.2
48	CV	98	SER	5.2
31	CA	1083	U	5.2
3	BC	192	THR	5.2
39	CM	78	ARG	5.2
19	BS	11	ILE	5.2
9	BI	68	LYS	5.2
35	CH	11	ASN	5.2
36	CJ	94	ASN	5.2
33	CF	31	VAL	5.2
53	DI	121	SER	5.2
39	CM	10	GLU	5.2
33	CF	152	LEU	5.2
9	BI	127	PHE	5.2
33	CF	60	ILE	5.2
13	AM	13	LYS	5.2
14	BN	51	LEU	5.2
7	BG	150	ALA	5.2
39	CM	80	SER	5.2
31	CA	2123	G	5.2
43	CQ	111	LYS	5.2
14	BN	53	ARG	5.2
31	CA	931	U	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	DJ	69	PHE	5.1
13	BM	19	LEU	5.1
33	CF	34	ILE	5.1
31	CA	75	G	5.1
10	BJ	72	ARG	5.1
31	CA	2119	A	5.1
31	CA	2171	A	5.1
42	CP	64	TYR	5.1
12	BL	124	ALA	5.1
15	BO	17	ARG	5.1
45	CS	96	VAL	5.1
31	CA	2161	C	5.1
36	DJ	78	VAL	5.1
23	C2	35	GLU	5.1
10	BJ	21	ALA	5.1
13	BM	85	CYS	5.1
23	C2	21	TYR	5.1
23	C2	36	LEU	5.1
52	CZ	32	ALA	5.1
33	CF	170	LEU	5.0
54	DA	883	G	5.0
14	BN	48	LEU	5.0
1	BA	1218	C	5.0
31	CA	2163	A	5.0
31	CA	1536	C	5.0
49	CW	6	ALA	5.0
14	BN	37	SER	5.0
14	BN	20	TYR	5.0
33	CF	36	LEU	5.0
9	BI	32	GLN	5.0
9	BI	5	GLN	5.0
19	BS	5	LEU	5.0
54	DA	896	A	5.0
54	DA	2167	U	5.0
48	CV	79	LYS	5.0
36	CJ	26	PRO	5.0
31	CA	2128	G	5.0
33	CF	151	GLY	5.0
7	BG	49	THR	4.9
36	CJ	85	GLY	4.9
13	AM	43	VAL	4.9
23	C2	18	GLY	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	BG	71	PRO	4.9
34	CG	52	PHE	4.9
10	BJ	22	THR	4.9
14	BN	31	ILE	4.9
48	CV	29	LEU	4.9
7	BG	4	ARG	4.9
13	BM	30	SER	4.9
7	BG	134	ALA	4.9
14	BN	27	LEU	4.9
32	CE	119	ILE	4.9
13	BM	61	ALA	4.9
31	CA	546	U	4.9
42	CP	29	HIS	4.9
36	CJ	123	GLU	4.9
43	CQ	115	ASN	4.9
32	CE	143	LEU	4.9
48	CV	35	ILE	4.9
1	BA	949	A	4.9
33	CF	86	GLY	4.9
54	DA	138	U	4.8
16	AP	47	GLU	4.8
7	BG	37	SER	4.8
1	BA	1026	G	4.8
13	BM	41	GLU	4.8
31	CA	318	C	4.8
16	BP	57	ILE	4.8
36	CJ	48	SER	4.8
42	CP	40	ILE	4.8
39	CM	77	ILE	4.8
48	CV	5	ILE	4.8
33	CF	107	ALA	4.8
31	CA	846	U	4.8
33	CF	143	TYR	4.8
13	BM	29	ARG	4.8
29	CC	27	GLY	4.8
41	CO	63	ARG	4.8
13	BM	32	ALA	4.8
31	CA	896	A	4.8
9	AI	5	GLN	4.8
39	CM	126	ARG	4.8
13	BM	38	GLY	4.8
9	BI	44	ALA	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	CF	173	PHE	4.7
31	CA	879	G	4.7
2	BB	123	ASP	4.7
36	DJ	110	ALA	4.7
21	AU	2	PRO	4.7
36	CJ	70	VAL	4.7
33	CF	28	VAL	4.7
52	CZ	33	ALA	4.7
52	CZ	63	ALA	4.7
36	CJ	113	LYS	4.7
54	DA	882	G	4.7
13	BM	65	VAL	4.7
19	BS	43	ASN	4.7
44	CR	118	ALA	4.7
31	CA	1535	A	4.7
31	CA	1179	G	4.7
32	CE	164	LEU	4.7
13	BM	55	THR	4.7
13	AM	5	ALA	4.7
42	CP	52	SER	4.7
34	CG	111	HIS	4.7
32	CE	172	ALA	4.7
13	AM	24	GLY	4.7
14	BN	39	GLU	4.7
36	DJ	40	LYS	4.7
33	CF	25	VAL	4.7
9	AI	22	LYS	4.6
10	BJ	86	ALA	4.6
7	BG	48	GLU	4.6
48	CV	81	ASP	4.6
42	CP	63	LYS	4.6
45	CS	49	ILE	4.6
39	CM	89	VAL	4.6
39	CM	120	VAL	4.6
42	CP	41	ALA	4.6
44	CR	73	GLY	4.6
31	CA	2124	G	4.6
54	DA	2126	A	4.6
23	C2	53	LYS	4.6
1	BA	1028	C	4.6
7	AG	4	ARG	4.6
36	CJ	135	SER	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	CO	119	SER	4.6
33	CF	122	PHE	4.6
42	CP	38	GLN	4.6
9	BI	40	GLY	4.6
19	BS	24	GLU	4.6
36	CJ	58	VAL	4.6
17	BQ	78	VAL	4.6
3	BC	196	ILE	4.6
42	CP	117	PHE	4.6
1	BA	954	G	4.6
19	BS	27	ASP	4.6
53	DI	136	ILE	4.5
36	CJ	32	GLY	4.5
48	CV	19	LYS	4.5
3	BC	71	ALA	4.5
13	BM	5	ALA	4.5
35	CH	78	VAL	4.5
36	DJ	134	ARG	4.5
13	BM	34	LEU	4.5
13	BM	11	ASP	4.5
33	CF	32	GLU	4.5
47	CU	83	ALA	4.5
39	CM	100	ILE	4.5
1	BA	1031	C	4.5
19	BS	23	VAL	4.5
26	C5	1	MET	4.5
31	CA	81	G	4.5
31	CA	1090	A	4.5
41	CO	28	LEU	4.5
52	CZ	42	LEU	4.5
1	BA	844	G	4.5
1	BA	1025	U	4.5
33	CF	105	THR	4.5
54	DA	2109	U	4.5
14	BN	47	LYS	4.5
7	BG	35	LYS	4.5
10	BJ	42	LEU	4.5
36	CJ	41	ALA	4.5
42	CP	24	THR	4.4
36	DJ	66	SER	4.4
31	CA	329	G	4.4
33	CF	37	ASN	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	CX	63	ALA	4.4
36	DJ	131	GLY	4.4
13	AM	32	ALA	4.4
36	CJ	27	ALA	4.4
41	CO	120	GLU	4.4
13	BM	12	HIS	4.4
14	BN	13	ARG	4.4
48	CV	78	GLY	4.4
54	DA	1068	G	4.4
36	CJ	133	ALA	4.4
43	CQ	12	GLN	4.4
14	AN	31	ILE	4.4
31	CA	549	G	4.4
7	BG	133	THR	4.4
13	BM	2	ALA	4.4
54	DA	2147	A	4.4
36	CJ	130	GLU	4.4
10	BJ	19	ASP	4.4
9	BI	14	SER	4.4
16	BP	17	TYR	4.4
32	CE	183	PHE	4.4
19	BS	69	HIS	4.4
49	CW	27	PRO	4.4
2	BB	82	ASP	4.3
10	AJ	35	GLN	4.3
52	CZ	22	LEU	4.3
33	CF	129	SER	4.3
3	BC	206	GLU	4.3
36	CJ	95	LYS	4.3
36	CJ	136	MET	4.3
54	DA	2166	U	4.3
14	BN	41	ARG	4.3
7	BG	72	THR	4.3
19	BS	51	VAL	4.3
31	CA	2121	G	4.3
52	CZ	31	GLN	4.3
1	BA	1314	C	4.3
10	BJ	101	SER	4.3
1	BA	1126	U	4.3
49	CW	48	MET	4.3
9	AI	128	SER	4.3
30	CD	10	GLY	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	CE	33	VAL	4.3
14	BN	30	ILE	4.3
14	BN	33	ASP	4.3
19	BS	71	LEU	4.3
36	DJ	49	ILE	4.3
10	AJ	75	ASP	4.3
39	CM	115	GLU	4.3
26	C5	32	LYS	4.3
54	DA	1077	A	4.3
31	CA	2164	C	4.3
31	CA	1047	G	4.3
2	BB	135	LEU	4.3
7	BG	5	ARG	4.3
10	BJ	80	THR	4.3
1	BA	213	G	4.3
1	BA	953	G	4.3
48	CV	30	SER	4.3
52	CZ	41	HIS	4.3
7	AG	58	GLU	4.2
9	AI	32	GLN	4.2
7	AG	8	GLY	4.2
13	BM	24	GLY	4.2
36	CJ	25	GLY	4.2
7	BG	144	MET	4.2
45	CS	20	VAL	4.2
34	CG	104	ASN	4.2
31	CA	1731	G	4.2
33	CF	137	ILE	4.2
10	BJ	10	LEU	4.2
20	BT	3	ASN	4.2
54	DA	881	G	4.2
43	CQ	110	ILE	4.2
19	BS	33	THR	4.2
1	BA	1321	U	4.2
31	CA	2116	G	4.2
39	CM	142	ILE	4.2
36	CJ	125	MET	4.2
1	BA	1247	U	4.2
36	DJ	25	GLY	4.2
32	CE	197	GLU	4.2
36	DJ	28	LEU	4.2
1	BA	1022	A	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	CM	130	GLY	4.2
54	DA	1067	A	4.2
1	AA	1020	G	4.2
39	CM	108	ALA	4.2
13	BM	13	LYS	4.2
34	CG	27	LYS	4.2
9	BI	39	PHE	4.2
13	AM	64	VAL	4.2
13	BM	25	VAL	4.2
31	CA	2170	A	4.1
23	C2	46	HIS	4.1
54	DA	2176	A	4.1
31	CA	1106	G	4.1
34	CG	26	ILE	4.1
3	BC	53	SER	4.1
45	CS	26	ASP	4.1
31	CA	1064	C	4.1
31	CA	1211	C	4.1
36	DJ	52	GLY	4.1
50	CX	53	CYS	4.1
54	DA	893	C	4.1
47	CU	8	LEU	4.1
42	CP	36	TYR	4.1
31	CA	1048	A	4.1
39	CM	79	LEU	4.1
1	BA	1245	C	4.1
33	CF	76	GLY	4.1
13	BM	36	ALA	4.1
34	CG	83	PHE	4.1
36	DJ	97	LYS	4.1
31	CA	344	A	4.1
36	DJ	93	PRO	4.1
1	BA	208	U	4.1
1	BA	1235	U	4.1
14	BN	4	GLN	4.1
31	CA	2797	U	4.1
32	CE	201	ALA	4.1
13	BM	6	GLY	4.1
1	BA	1305	G	4.1
1	BA	985	C	4.1
7	BG	54	SER	4.1
53	DI	124	ASP	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	CA	613	A	4.1
9	AI	6	TYR	4.1
9	AI	129	LYS	4.1
10	BJ	99	GLN	4.1
31	CA	1046	A	4.1
14	BN	16	LEU	4.1
31	CA	138	U	4.1
31	CA	2666	C	4.1
13	BM	4	ILE	4.1
2	BB	34	ALA	4.0
16	BP	52	LEU	4.0
31	CA	2802	G	4.0
42	CP	92	PHE	4.0
13	BM	35	ALA	4.0
1	BA	942	G	4.0
3	BC	159	GLY	4.0
1	BA	1244	G	4.0
35	CH	72	ILE	4.0
36	CJ	31	GLN	4.0
39	CM	90	VAL	4.0
13	BM	70	ARG	4.0
34	CG	17	VAL	4.0
36	DJ	99	GLY	4.0
16	BP	60	TRP	4.0
9	AI	89	GLU	4.0
13	BM	58	ASP	4.0
43	CQ	27	GLU	4.0
54	DA	1062	G	4.0
31	CA	1078	U	4.0
47	CU	55	VAL	4.0
48	CV	28	VAL	4.0
10	BJ	36	VAL	4.0
33	CF	174	ASP	4.0
31	CA	12	U	4.0
31	CA	1107	G	4.0
48	CV	95	PHE	4.0
33	CF	139	PRO	4.0
36	DJ	11	LEU	4.0
42	CP	65	THR	4.0
47	DU	1	MET	4.0
43	CQ	84	ILE	4.0
54	DA	879	G	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	CA	183	C	4.0
36	CJ	117	MET	4.0
53	DI	38	MET	4.0
24	C3	35	ARG	4.0
54	DA	1847	A	3.9
10	BJ	89	ARG	3.9
14	BN	6	MET	3.9
31	CA	1049	C	3.9
52	CZ	24	GLU	3.9
54	DA	2146	C	3.9
54	DA	2178	C	3.9
3	BC	193	TYR	3.9
31	CA	2162	G	3.9
54	DA	2115	G	3.9
19	BS	68	GLY	3.9
1	BA	955	U	3.9
33	CF	111	ILE	3.9
33	CF	94	GLU	3.9
15	BO	89	ARG	3.9
39	CM	70	LYS	3.9
1	BA	1125	U	3.9
13	AM	25	VAL	3.9
13	BM	60	VAL	3.9
47	CU	57	VAL	3.9
36	DJ	85	GLY	3.9
48	DV	56	GLY	3.9
7	AG	54	SER	3.9
36	DJ	48	SER	3.9
7	AG	109	ARG	3.9
10	BJ	94	ALA	3.9
45	CS	31	GLU	3.9
1	BA	85	U	3.9
32	CE	144	GLU	3.9
23	C2	39	PHE	3.9
44	CR	71	GLN	3.9
31	CA	1530	G	3.9
7	BG	66	LEU	3.9
7	BG	137	LYS	3.9
31	CA	2665	A	3.9
23	C2	45	GLN	3.9
44	CR	74	ILE	3.9
49	CW	29	ILE	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	CJ	97	LYS	3.9
49	CW	67	GLY	3.9
10	BJ	24	GLU	3.9
31	CA	2169	A	3.9
31	CA	880	G	3.9
1	AA	1286	U	3.8
35	CH	61	VAL	3.8
15	AO	17	ARG	3.8
7	BG	69	VAL	3.8
24	C3	32	ALA	3.8
42	CP	93	ASP	3.8
2	AB	46	THR	3.8
7	BG	38	THR	3.8
47	CU	60	THR	3.8
36	DJ	59	ILE	3.8
30	CD	4	LEU	3.8
45	CS	24	LYS	3.8
9	BI	92	GLU	3.8
48	CV	50	PRO	3.8
3	BC	76	VAL	3.8
14	AN	25	ALA	3.8
1	BA	4	U	3.8
1	BA	842	U	3.8
41	CO	76	VAL	3.8
9	BI	64	TYR	3.8
7	BG	88	PRO	3.8
31	CA	1094	U	3.8
13	BM	113	ARG	3.8
39	CM	132	ARG	3.8
14	AN	18	ASP	3.8
31	CA	876	C	3.8
1	BA	1034	G	3.8
24	C3	1	MET	3.8
6	BF	39	LEU	3.8
48	CV	4	LYS	3.8
2	AB	4	VAL	3.8
9	AI	19	VAL	3.8
10	BJ	34	ALA	3.8
7	BG	15	ASP	3.8
3	BC	197	GLY	3.8
7	BG	46	ALA	3.8
7	AG	7	ILE	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	CU	15	HIS	3.8
23	C2	23	THR	3.8
31	CA	1547	C	3.8
31	CA	1870	C	3.8
31	CA	2667	C	3.8
35	CH	136	SER	3.8
35	DH	137	GLU	3.8
54	DA	1089	A	3.8
52	CZ	37	LEU	3.8
13	BM	97	VAL	3.8
31	CA	1045	C	3.8
34	CG	43	VAL	3.8
39	CM	85	VAL	3.8
41	CO	116	VAL	3.8
47	CU	1	MET	3.7
7	BG	129	GLU	3.7
13	BM	37	ALA	3.7
36	CJ	81	LYS	3.7
9	BI	117	GLY	3.7
10	BJ	100	ILE	3.7
33	CF	67	ILE	3.7
9	BI	20	PHE	3.7
14	BN	32	SER	3.7
42	CP	30	ARG	3.7
46	CT	84	ARG	3.7
54	DA	1064	C	3.7
16	BP	42	ILE	3.7
9	BI	66	THR	3.7
14	BN	2	ALA	3.7
14	BN	22	ALA	3.7
53	DI	104	ALA	3.7
1	BA	1219	A	3.7
14	BN	28	LYS	3.7
23	C2	48	ILE	3.7
33	CF	141	ILE	3.7
53	DI	135	ALA	3.7
9	BI	15	SER	3.7
10	BJ	20	GLN	3.7
33	CF	138	PHE	3.7
2	AB	225	ARG	3.7
2	BB	67	ILE	3.7
41	CO	26	GLY	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	AG	5	ARG	3.7
10	BJ	9	ARG	3.7
49	CW	42	LEU	3.7
10	BJ	28	THR	3.7
30	CD	26	VAL	3.7
33	CF	99	PHE	3.7
47	CU	72	GLN	3.7
7	BG	16	PRO	3.7
16	BP	56	ARG	3.7
13	BM	52	GLN	3.7
13	BM	63	PHE	3.7
19	AS	56	GLN	3.7
33	CF	62	GLY	3.7
48	CV	18	ASP	3.7
54	DA	2162	G	3.7
17	BQ	45	HIS	3.7
1	BA	984	C	3.7
7	BG	109	ARG	3.7
34	CG	112	PRO	3.7
32	CE	200	LEU	3.7
35	CH	140	ALA	3.7
36	CJ	35	ILE	3.7
9	BI	41	ARG	3.7
7	BG	73	VAL	3.7
53	DI	132	TYR	3.7
42	CP	67	ASN	3.7
39	CM	117	THR	3.6
34	CG	121	ILE	3.6
48	CV	39	ILE	3.6
31	CA	1044	C	3.6
39	CM	133	ALA	3.6
34	CG	108	GLY	3.6
7	BG	106	GLU	3.6
54	DA	1078	U	3.6
19	BS	15	LEU	3.6
54	DA	2168	G	3.6
52	CZ	29	ARG	3.6
16	AP	82	ALA	3.6
10	BJ	81	GLU	3.6
1	AA	121	U	3.6
32	CE	17	THR	3.6
14	AN	24	ARG	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	DJ	60	THR	3.6
49	CW	45	ASP	3.6
52	CZ	6	LEU	3.6
9	BI	125	PRO	3.6
14	BN	9	ARG	3.6
31	CA	1524	G	3.6
32	CE	12	LEU	3.6
19	BS	21	LYS	3.6
31	CA	895	U	3.6
13	AM	7	ILE	3.6
3	BC	179	ARG	3.6
2	BB	33	GLY	3.6
13	AM	44	LYS	3.6
30	CD	186	LEU	3.6
34	CG	56	ASP	3.6
39	CM	91	ASP	3.6
17	BQ	17	MET	3.6
43	CQ	9	GLU	3.6
47	CU	69	ARG	3.6
48	CV	25	VAL	3.6
48	CV	51	ALA	3.6
36	DJ	98	VAL	3.6
31	CA	1167	C	3.6
2	BB	35	ARG	3.6
32	CE	118	LEU	3.6
1	BA	1201	A	3.6
3	BC	80	LYS	3.6
34	CG	106	SER	3.6
34	CG	148	LEU	3.6
36	DJ	89	GLY	3.6
42	CP	66	GLY	3.6
3	BC	79	LYS	3.5
19	BS	75	ALA	3.5
22	C1	46	ASP	3.5
33	CF	56	ASP	3.5
20	BT	48	GLN	3.5
34	CG	62	TRP	3.5
41	CO	62	ASN	3.5
1	BA	1145	A	3.5
20	BT	49	LYS	3.5
35	CH	76	GLU	3.5
48	CV	2	ALA	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	BN	18	ASP	3.5
1	BA	94	G	3.5
31	CA	1171	G	3.5
42	CP	46	GLU	3.5
7	BG	141	VAL	3.5
17	BQ	83	VAL	3.5
34	CG	169	VAL	3.5
1	AA	81	A	3.5
27	C0	56	LYS	3.5
32	CE	23	PHE	3.5
42	CP	20	GLU	3.5
48	CV	40	ASN	3.5
1	BA	1018	G	3.5
7	BG	87	VAL	3.5
7	BG	113	ASP	3.5
23	C2	43	VAL	3.5
47	CU	16	VAL	3.5
7	BG	103	TRP	3.5
36	DJ	51	LYS	3.5
54	DA	546	U	3.5
50	CX	59	LEU	3.5
1	BA	1221	G	3.5
19	BS	22	ALA	3.5
20	BT	46	ALA	3.5
36	DJ	100	LYS	3.5
50	CX	85	GLU	3.5
16	BP	53	ASP	3.5
36	DJ	37	GLU	3.5
7	BG	6	VAL	3.5
31	CA	2178	C	3.5
47	CU	10	VAL	3.5
1	BA	958	A	3.5
35	CH	74	ALA	3.5
43	CQ	91	ALA	3.5
13	BM	42	ASP	3.5
13	BM	54	ASP	3.5
1	BA	121	U	3.5
31	CA	1077	A	3.5
52	DZ	63	ALA	3.5
54	DA	2122	U	3.5
45	CS	35	PHE	3.5
44	DR	118	ALA	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	BM	49	SER	3.4
48	CV	83	VAL	3.4
30	CD	6	GLY	3.4
9	BI	4	ASN	3.4
13	BM	109	ARG	3.4
34	CG	9	VAL	3.4
34	CG	24	ILE	3.4
54	DA	2132	U	3.4
17	BQ	53	CYS	3.4
31	CA	1548	A	3.4
36	DJ	106	LEU	3.4
36	CJ	29	GLY	3.4
31	CA	513	A	3.4
50	CX	57	HIS	3.4
1	BA	1304	G	3.4
52	CZ	36	GLN	3.4
13	AM	19	LEU	3.4
7	BG	111	ARG	3.4
52	CZ	18	LEU	3.4
33	CF	142	ASP	3.4
35	CH	132	PHE	3.4
19	BS	18	LYS	3.4
16	BP	81	ALA	3.4
34	CG	80	THR	3.4
39	CM	131	ALA	3.4
31	CA	2168	G	3.4
42	CP	103	VAL	3.4
34	CG	166	ASP	3.4
1	BA	80	A	3.4
10	BJ	32	THR	3.4
30	CD	25	THR	3.4
10	BJ	82	LYS	3.4
35	CH	142	VAL	3.4
13	BM	74	SER	3.4
1	BA	1275	A	3.4
36	DJ	46	THR	3.4
16	BP	80	LYS	3.4
20	BT	79	LEU	3.4
34	CG	172	LYS	3.4
36	DJ	83	ALA	3.4
1	BA	90	C	3.4
2	BB	89	GLN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	CH	107	GLY	3.4
45	CS	7	SER	3.4
1	BA	81	A	3.4
2	BB	37	LYS	3.4
19	BS	70	LYS	3.4
31	CA	101	A	3.4
13	AM	36	ALA	3.4
13	BM	9	ILE	3.4
1	BA	1001	C	3.4
1	BA	1222	G	3.4
50	CX	83	GLU	3.4
41	CO	56	LYS	3.4
48	CV	26	LYS	3.4
54	DA	277	G	3.4
3	BC	156	ARG	3.4
10	AJ	76	ILE	3.3
50	CX	25	ARG	3.3
50	CX	55	ARG	3.3
31	CA	2175	C	3.3
41	CO	29	VAL	3.3
13	BM	77	ILE	3.3
1	BA	1274	A	3.3
31	CA	345	A	3.3
34	CG	45	HIS	3.3
38	CL	48	PRO	3.3
53	DI	2	ALA	3.3
13	BM	50	GLU	3.3
17	AQ	53	CYS	3.3
36	CJ	16	GLY	3.3
39	CM	102	GLY	3.3
31	CA	2181	U	3.3
1	BA	250	A	3.3
2	AB	14	VAL	3.3
19	AS	39	THR	3.3
33	CF	172	ALA	3.3
1	BA	1307	U	3.3
54	DA	2106	U	3.3
31	CA	1734	G	3.3
54	DA	1087	G	3.3
1	BA	1271	A	3.3
1	BA	1303	C	3.3
2	AB	135	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	AG	59	LEU	3.3
31	CA	431	U	3.3
31	CA	2111	U	3.3
7	BG	152	ALA	3.3
32	CE	10	SER	3.3
46	CT	101	SER	3.3
49	CW	89	ILE	3.3
53	DI	133	GLU	3.3
31	CA	214	G	3.3
7	AG	52	GLN	3.3
46	CT	94	ASP	3.3
36	DJ	43	ASN	3.3
13	AM	115	PRO	3.3
14	BN	42	TRP	3.3
1	BA	79	G	3.3
31	CA	332	A	3.3
31	CA	882	G	3.3
31	CA	1407	G	3.3
54	DA	2141	G	3.3
13	BM	94	GLY	3.3
36	DJ	27	ALA	3.3
50	CX	61	ALA	3.3
1	BA	1015	G	3.3
31	CA	1061	U	3.3
13	BM	28	THR	3.3
32	CE	199	MET	3.3
31	CA	2107	G	3.3
1	BA	948	C	3.3
48	CV	15	THR	3.3
54	DA	1072	C	3.3
7	AG	50	LEU	3.3
11	AK	18	ASP	3.3
23	C2	50	LYS	3.3
1	BA	1019	A	3.2
1	BA	1035	A	3.2
31	CA	1069	A	3.2
31	CA	881	G	3.2
32	DE	7	ASP	3.2
36	CJ	127	ARG	3.2
19	BS	59	PRO	3.2
33	CF	26	MET	3.2
1	AA	88	U	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BA	1021	A	3.2
31	CA	2109	U	3.2
48	CV	52	LEU	3.2
3	BC	195	VAL	3.2
16	BP	39	PHE	3.2
39	CM	124	GLY	3.2
42	CP	87	ILE	3.2
2	BB	12	ALA	3.2
52	CZ	14	LEU	3.2
34	CG	84	THR	3.2
1	BA	1000	A	3.2
1	BA	1236	A	3.2
29	CC	30	PHE	3.2
45	CS	62	GLU	3.2
35	CH	133	GLN	3.2
7	BG	145	ALA	3.2
31	CA	1056	G	3.2
35	CH	15	LEU	3.2
36	CJ	34	ASN	3.2
1	BA	843	U	3.2
54	DA	2171	A	3.2
3	BC	155	GLY	3.2
1	BA	1317	C	3.2
43	CQ	8	LEU	3.2
46	CT	5	ALA	3.2
1	BA	1033	G	3.2
7	BG	58	GLU	3.2
54	DA	880	G	3.2
1	AA	1025	U	3.2
31	CA	2118	U	3.2
33	CF	39	GLY	3.2
33	CF	110	ARG	3.2
36	CJ	49	ILE	3.2
31	CA	1531	C	3.2
48	DV	53	ASN	3.2
54	DA	2165	C	3.2
52	CZ	5	GLU	3.2
19	BS	40	ILE	3.2
31	CA	2180	U	3.2
19	BS	50	ALA	3.2
23	C2	49	TYR	3.2
35	DH	87	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	CG	25	THR	3.2
36	CJ	36	MET	3.2
39	CM	20	GLY	3.2
42	CP	69	ASP	3.2
9	AI	17	ALA	3.2
34	CG	7	ALA	3.2
42	CP	107	ALA	3.2
39	CM	127	VAL	3.2
52	CZ	59	GLU	3.2
1	BA	1534	A	3.2
9	BI	21	ILE	3.2
31	CA	892	A	3.2
42	CP	115	LEU	3.2
1	BA	1217	C	3.2
23	C2	38	LYS	3.2
31	CA	184	C	3.2
27	C0	2	ALA	3.2
36	DJ	14	ALA	3.2
1	BA	632	U	3.2
33	CF	80	ARG	3.2
42	CP	99	TYR	3.2
23	C2	16	GLY	3.2
42	CP	62	LEU	3.2
30	CD	1	MET	3.2
1	BA	1248	A	3.2
13	AM	11	ASP	3.2
42	CP	108	ASP	3.2
1	BA	83	C	3.2
1	BA	1038	C	3.2
2	BB	201	PRO	3.2
31	CA	1468	U	3.2
33	CF	27	GLN	3.2
36	DJ	84	ALA	3.2
1	AA	1019	A	3.2
31	CA	1111	A	3.2
23	C2	25	LYS	3.1
48	CV	12	ILE	3.1
7	AG	57	SER	3.1
7	AG	106	GLU	3.1
11	AK	81	ASN	3.1
33	CF	149	VAL	3.1
31	CA	330	A	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	DA	2180	U	3.1
10	BJ	98	VAL	3.1
13	BM	43	VAL	3.1
14	BN	10	GLU	3.1
47	CU	47	VAL	3.1
2	BB	21	ARG	3.1
19	AS	55	ARG	3.1
34	CG	8	PRO	3.1
34	CG	141	ILE	3.1
48	CV	84	GLY	3.1
41	CO	24	MET	3.1
39	CM	113	ALA	3.1
3	BC	126	ARG	3.1
46	CT	97	LEU	3.1
42	CP	58	ILE	3.1
44	CR	99	ALA	3.1
31	CA	1059	G	3.1
2	BB	14	VAL	3.1
10	AJ	74	VAL	3.1
34	CG	132	VAL	3.1
36	DJ	33	VAL	3.1
7	AG	42	ILE	3.1
31	CA	1082	U	3.1
35	CH	35	LYS	3.1
54	DA	1175	A	3.1
2	AB	136	MET	3.1
32	CE	140	ASP	3.1
54	DA	2164	C	3.1
9	BI	58	VAL	3.1
39	CM	121	THR	3.1
31	CA	1546	G	3.1
44	CR	106	PHE	3.1
1	BA	84	U	3.1
9	BI	124	ARG	3.1
1	BA	1005	A	3.1
13	BM	108	THR	3.1
30	CD	43	ASP	3.1
41	CO	59	SER	3.1
31	CA	228	C	3.1
31	CA	893	C	3.1
22	C1	57	LYS	3.1
34	CG	157	TYR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	CP	26	LEU	3.1
3	BC	170	GLU	3.1
31	CA	1729	U	3.1
49	CW	5	ASN	3.1
29	CC	242	LYS	3.1
45	CS	28	ALA	3.1
24	C3	33	ARG	3.1
1	AA	4	U	3.1
1	BA	950	U	3.1
14	AN	55	SER	3.1
31	CA	1529	G	3.1
34	CG	54	PRO	3.1
39	CM	75	ALA	3.1
42	CP	33	ARG	3.1
36	CJ	140	VAL	3.1
45	CS	25	LEU	3.1
32	CE	24	ASN	3.1
1	BA	89	U	3.1
31	CA	1873	G	3.1
35	DH	63	ALA	3.1
10	AJ	6	ILE	3.0
17	BQ	50	ASN	3.0
19	BS	64	ASP	3.0
50	CX	60	PHE	3.0
39	CM	122	VAL	3.0
45	CS	37	GLU	3.0
54	DA	1066	U	3.0
7	BG	53	ARG	3.0
9	BI	129	LYS	3.0
31	CA	2150	C	3.0
54	DA	2177	C	3.0
30	CD	30	GLU	3.0
54	DA	1061	U	3.0
36	CJ	72	LYS	3.0
31	CA	1093	G	3.0
9	BI	48	VAL	3.0
17	BQ	23	VAL	3.0
26	C5	10	LEU	3.0
9	BI	81	HIS	3.0
12	BL	70	GLU	3.0
2	AB	42	ASN	3.0
25	C4	28	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	CG	20	ASN	3.0
13	AM	57	ARG	3.0
14	BN	61	ARG	3.0
18	BR	74	HIS	3.0
42	CP	54	VAL	3.0
14	AN	47	LYS	3.0
36	DJ	34	ASN	3.0
51	CY	20	HIS	3.0
19	BS	56	GLN	3.0
2	AB	27	MET	3.0
23	C2	40	ASP	3.0
9	BI	69	GLY	3.0
2	BB	213	TYR	3.0
44	CR	113	ALA	3.0
29	CC	5	LYS	3.0
33	CF	69	LYS	3.0
49	CW	57	TYR	3.0
2	AB	210	VAL	3.0
19	BS	47	LEU	3.0
50	CX	32	LEU	3.0
7	BG	60	GLU	3.0
22	C1	27	SER	3.0
44	CR	117	LEU	3.0
48	CV	6	ARG	3.0
31	CA	1089	A	3.0
31	CA	1071	G	3.0
48	CV	69	ASN	3.0
14	BN	46	LEU	3.0
48	CV	86	ARG	3.0
3	BC	50	ALA	3.0
49	CW	63	ILE	3.0
13	BM	16	VAL	3.0
34	CG	162	VAL	3.0
42	CP	39	VAL	3.0
8	AH	121	LEU	3.0
36	DJ	95	LYS	3.0
33	CF	29	PRO	3.0
38	CL	110	GLU	3.0
31	CA	1060	U	3.0
33	CF	75	ALA	3.0
35	DH	86	ASP	3.0
19	BS	52	HIS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	CJ	137	GLY	2.9
39	CM	106	GLU	3.0
1	BA	1002	G	2.9
47	CU	71	GLY	2.9
54	DA	2128	G	2.9
1	BA	1049	U	2.9
23	C2	34	LEU	2.9
31	CA	1217	U	2.9
1	BA	1004	A	2.9
31	CA	213	A	2.9
17	BQ	21	ILE	2.9
49	CW	34	LYS	2.9
1	BA	1048	G	2.9
31	CA	1534	U	2.9
31	CA	311	A	2.9
1	BA	203	G	2.9
13	BM	103	LYS	2.9
39	CM	1	MET	2.9
2	BB	40	ILE	2.9
54	DA	1063	G	2.9
7	BG	89	VAL	2.9
20	BT	38	ALA	2.9
33	CF	91	LEU	2.9
34	CG	126	PRO	2.9
31	CA	2860	A	2.9
1	BA	981	U	2.9
2	AB	9	MET	2.9
34	CG	31	GLY	2.9
46	CT	82	MET	2.9
42	CP	37	ALA	2.9
44	CR	81	ASN	2.9
45	CS	22	LEU	2.9
1	BA	977	A	2.9
1	BA	1014	A	2.9
10	BJ	85	ASP	2.9
22	C1	15	MET	2.9
9	BI	37	GLN	2.9
11	BK	84	VAL	2.9
45	CS	18	GLN	2.9
7	AG	53	ARG	2.9
33	CF	8	TYR	2.9
42	CP	53	THR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	CA	289	G	2.9
24	C3	28	ARG	2.9
33	CF	30	ARG	2.9
35	DH	98	ASP	2.9
1	BA	1023	U	2.9
36	CJ	10	LYS	2.9
49	CW	10	LYS	2.9
10	BJ	95	GLY	2.9
1	BA	1003	G	2.9
31	CA	2801	G	2.9
34	CG	94	TYR	2.9
19	BS	4	SER	2.9
21	AU	9	ASN	2.9
9	AI	63	LEU	2.9
25	C4	36	LYS	2.9
36	DJ	17	MET	2.9
2	BB	32	PHE	2.9
36	CJ	124	ALA	2.9
31	CA	1172	C	2.9
2	AB	49	MET	2.9
42	CP	82	ALA	2.9
19	BS	46	GLY	2.9
1	BA	999	C	2.9
1	BA	219	U	2.9
19	BS	67	VAL	2.9
7	BG	79	ARG	2.9
31	CA	312	G	2.9
32	CE	8	ALA	2.9
13	BM	14	HIS	2.9
17	BQ	44	LEU	2.9
31	CA	1075	C	2.8
20	BT	87	ALA	2.8
42	CP	51	ALA	2.8
50	CX	62	LYS	2.8
16	BP	41	PRO	2.8
23	C2	12	VAL	2.8
1	BA	989	U	2.8
9	BI	90	TYR	2.8
5	BE	91	GLY	2.8
43	CQ	86	VAL	2.8
31	CA	626	A	2.8
54	DA	2119	A	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	CS	92	TRP	2.8
27	C0	8	THR	2.8
5	BE	159	LYS	2.8
34	CG	86	LYS	2.8
41	CO	52	ILE	2.8
35	DH	66	ASN	2.8
35	CH	130	VAL	2.8
48	CV	82	ARG	2.8
52	CZ	47	ARG	2.8
2	AB	6	MET	2.8
13	BM	93	ARG	2.8
19	BS	3	ARG	2.8
22	C1	11	SER	2.8
12	BL	108	LYS	2.8
29	CC	233	GLY	2.8
3	BC	106	VAL	2.8
31	CA	1143	A	2.8
33	CF	126	GLY	2.8
36	DJ	92	LYS	2.8
9	BI	43	THR	2.8
35	CH	108	VAL	2.8
35	DH	142	VAL	2.8
36	CJ	101	ILE	2.8
49	CW	65	VAL	2.8
31	CA	1466	U	2.8
36	CJ	110	ALA	2.8
14	AN	27	LEU	2.8
33	CF	4	LEU	2.8
39	CM	84	LYS	2.8
2	AB	30	PHE	2.8
35	CH	47	PHE	2.8
40	CN	80	VAL	2.8
32	CE	127	GLU	2.8
3	BC	127	ARG	2.8
9	AI	62	ASP	2.8
30	CD	39	ASP	2.8
36	DJ	103	ARG	2.8
45	CS	66	HIS	2.8
6	AF	61	LEU	2.8
15	BO	19	ALA	2.8
23	C2	15	ALA	2.8
41	CO	79	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	C4	61	CYS	2.8
31	CA	317	G	2.8
36	CJ	128	SER	2.8
42	CP	78	VAL	2.8
33	CF	38	MET	2.8
1	BA	1362	A	2.8
13	AM	35	ALA	2.8
32	CE	171	ASP	2.8
54	DA	1088	A	2.8
32	CE	103	GLY	2.8
30	CD	180	VAL	2.8
1	BA	1209	C	2.8
2	AB	131	LYS	2.8
31	CA	1543	G	2.8
39	CM	118	THR	2.8
10	BJ	71	LEU	2.8
1	BA	218	U	2.8
1	BA	1029	U	2.8
22	C1	3	VAL	2.8
54	DA	2117	A	2.8
7	BG	17	LYS	2.8
22	C1	34	SER	2.8
13	AM	48	LEU	2.8
14	AN	22	ALA	2.8
34	CG	51	THR	2.8
31	CA	1238	G	2.8
33	CF	166	GLY	2.8
7	AG	69	VAL	2.8
7	BG	18	PHE	2.8
9	BI	30	ILE	2.8
30	CD	8	LYS	2.8
36	DJ	9	VAL	2.8
48	CV	85	PHE	2.8
1	BA	957	U	2.8
9	AI	59	GLU	2.8
14	BN	15	ALA	2.8
36	DJ	71	THR	2.8
1	BA	1027	C	2.8
47	CU	37	ASP	2.8
36	DJ	50	GLU	2.7
31	CA	1210	G	2.7
9	BI	33	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	CA	2660	A	2.7
33	CF	61	SER	2.7
46	CT	43	ALA	2.7
14	BN	11	VAL	2.7
13	AM	39	ILE	2.7
13	BM	17	ILE	2.7
32	CE	173	THR	2.7
33	CF	18	THR	2.7
41	CO	114	GLU	2.7
31	CA	1606	C	2.7
47	CU	24	MET	2.7
19	BS	6	LYS	2.7
35	CH	58	LEU	2.7
1	AA	1026	G	2.7
1	BA	1276	G	2.7
7	AG	26	PHE	2.7
31	CA	2862	G	2.7
34	CG	30	ASN	2.7
10	BJ	83	THR	2.7
33	CF	158	THR	2.7
36	CJ	64	ASP	2.7
48	CV	77	THR	2.7
36	DJ	39	CYS	2.7
7	BG	112	GLY	2.7
9	BI	10	GLY	2.7
54	DA	897	C	2.7
2	BB	187	VAL	2.7
35	CH	144	VAL	2.7
1	BA	951	G	2.7
27	C0	9	GLN	2.7
12	BL	109	ASP	2.7
20	BT	76	LYS	2.7
31	CA	88	G	2.7
35	DH	67	ALA	2.7
49	CW	91	PHE	2.7
31	CA	1518	C	2.7
33	CF	165	GLU	2.7
35	CH	60	GLU	2.7
7	AG	110	LYS	2.7
54	DA	1094	U	2.7
41	CO	118	ARG	2.7
3	BC	43	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
24	C3	42	LEU	2.7
1	AA	82	G	2.7
1	AA	1024	G	2.7
31	CA	103	A	2.7
35	DH	74	ALA	2.7
9	BI	122	ARG	2.7
1	BA	982	U	2.7
13	BM	51	GLY	2.7
14	BN	38	ASP	2.7
33	CF	100	PHE	2.7
10	BJ	30	LYS	2.7
23	C2	32	GLU	2.7
1	BA	1280	A	2.7
31	CA	1322	A	2.7
1	BA	979	C	2.7
54	DA	2105	U	2.7
2	BB	119	THR	2.7
7	AG	65	ALA	2.7
13	AM	16	VAL	2.7
14	BN	8	ALA	2.7
49	CW	16	ALA	2.7
39	CM	135	ILE	2.7
44	CR	90	ILE	2.7
1	BA	959	A	2.7
9	AI	127	PHE	2.7
13	AM	62	LYS	2.7
36	DJ	128	SER	2.7
45	CS	12	HIS	2.7
1	AA	84	U	2.7
1	BA	1123	U	2.7
31	CA	117	G	2.7
31	CA	1863	G	2.7
54	DA	2133	G	2.7
1	BA	1230	C	2.7
9	AI	7	TYR	2.7
16	AP	45	GLU	2.7
24	C3	30	VAL	2.7
34	CG	110	SER	2.7
33	CF	43	ALA	2.7
49	CW	69	GLU	2.7
31	CA	1108	U	2.7
49	CW	66	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BA	847	G	2.7
53	DI	129	LEU	2.7
2	BB	210	VAL	2.7
13	BM	99	GLY	2.7
14	BN	25	ALA	2.7
1	BA	1287	A	2.7
31	CA	1321	A	2.7
31	CA	1525	A	2.7
31	CA	2287	A	2.7
53	DI	103	ASN	2.7
32	CE	150	THR	2.7
31	CA	1533	C	2.7
31	CA	1444	G	2.7
32	CE	193	VAL	2.7
34	CG	161	GLY	2.7
23	C2	7	GLU	2.7
14	BN	44	ALA	2.7
32	CE	128	ALA	2.7
2	BB	57	LEU	2.6
3	BC	111	LEU	2.6
32	CE	124	PHE	2.6
1	AA	1441	A	2.6
11	AK	19	GLY	2.6
31	CA	1098	A	2.6
31	CA	2108	A	2.6
34	CG	10	VAL	2.6
35	CH	13	GLY	2.6
45	CS	88	GLY	2.6
54	DA	654	A	2.6
49	CW	7	GLU	2.6
1	BA	1273	C	2.6
13	AM	45	ILE	2.6
3	BC	124	LEU	2.6
7	BG	59	LEU	2.6
28	CB	23	G	2.6
30	CD	201	LEU	2.6
31	CA	2803	G	2.6
54	DA	1059	G	2.6
7	BG	130	ASN	2.6
2	BB	80	VAL	2.6
36	CJ	91	GLY	2.6
41	CO	84	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	BB	131	LYS	2.6
20	BT	47	ALA	2.6
24	C3	31	LEU	2.6
39	CM	134	ALA	2.6
48	CV	48	PRO	2.6
8	BH	54	ASP	2.6
17	BQ	54	GLY	2.6
26	C5	20	ASP	2.6
36	DJ	116	ASP	2.6
37	CK	141	ASP	2.6
47	CU	56	GLU	2.6
48	CV	93	VAL	2.6
49	CW	35	GLU	2.6
31	CA	2891	U	2.6
24	C3	18	PHE	2.6
1	BA	1320	C	2.6
31	CA	2165	C	2.6
48	CV	90	GLY	2.6
9	AI	9	THR	2.6
13	AM	17	ILE	2.6
50	CX	58	THR	2.6
1	BA	1039	G	2.6
31	CA	2627	G	2.6
32	CE	11	ALA	2.6
53	DI	84	TYR	2.6
14	BN	3	LYS	2.6
3	BC	172	ARG	2.6
10	BJ	78	GLU	2.6
19	BS	58	VAL	2.6
3	AC	189	ALA	2.6
9	BI	9	THR	2.6
13	BM	44	LYS	2.6
18	BR	51	TYR	2.6
36	CJ	63	ALA	2.6
36	DJ	115	ALA	2.6
33	CF	177	PHE	2.6
34	CG	152	ARG	2.6
1	BA	102	G	2.6
7	BG	77	SER	2.6
3	BC	181	ASP	2.6
10	BJ	29	ALA	2.6
7	AG	49	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	C2	6	ARG	2.6
28	CB	49	C	2.6
35	CH	65	ALA	2.6
47	CU	35	ALA	2.6
30	CD	166	GLY	2.6
35	DH	127	GLU	2.6
31	CA	1169	A	2.6
40	CN	88	ASN	2.6
1	BA	207	C	2.6
1	BA	962	C	2.6
52	CZ	8	GLU	2.6
54	DA	1870	C	2.6
33	CF	33	LYS	2.6
9	BI	61	LEU	2.6
34	CG	50	LEU	2.6
34	CG	131	ILE	2.6
32	CE	191	ASP	2.6
36	DJ	104	ALA	2.6
41	CO	77	ALA	2.6
17	BQ	46	VAL	2.6
23	C2	29	THR	2.6
29	CC	241	GLY	2.6
32	CE	198	GLU	2.6
31	CA	2877	G	2.6
35	DH	95	GLY	2.6
39	CM	74	THR	2.6
28	CB	19	C	2.6
33	CF	103	LEU	2.6
35	CH	67	ALA	2.6
35	DH	11	ASN	2.6
45	CS	14	VAL	2.6
2	BB	130	THR	2.6
10	AJ	73	LEU	2.6
46	CT	103	ILE	2.6
1	BA	1270	G	2.6
19	BS	10	PHE	2.6
31	CA	215	G	2.6
31	CA	1073	A	2.6
31	CA	1532	A	2.6
2	BB	206	ALA	2.6
20	BT	50	ALA	2.6
44	CR	68	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	CZ	25	GLN	2.6
31	CA	1406	U	2.6
31	CA	2122	U	2.6
34	CG	69	ARG	2.6
3	BC	109	PRO	2.6
35	CH	143	ILE	2.6
33	CF	114	PHE	2.5
32	CE	47	LYS	2.5
33	CF	83	TYR	2.5
41	CO	61	ALA	2.5
44	CR	89	GLU	2.5
13	BM	79	ARG	2.5
16	BP	10	GLY	2.5
54	DA	1098	A	2.5
54	DA	2108	A	2.5
13	AM	58	ASP	2.5
14	AN	37	SER	2.5
19	AS	25	SER	2.5
21	BU	9	ASN	2.5
42	CP	35	ILE	2.5
43	CQ	22	PRO	2.5
48	CV	72	ILE	2.5
49	CW	37	PRO	2.5
34	CG	171	THR	2.5
32	CE	88	ARG	2.5
33	CF	101	GLU	2.5
34	CG	151	TYR	2.5
35	CH	70	GLU	2.5
31	CA	898	C	2.5
52	CZ	4	LYS	2.5
31	CA	2410	G	2.5
13	BM	57	ARG	2.5
49	CW	41	GLU	2.5
32	CE	147	LEU	2.5
34	CG	6	LYS	2.5
47	CU	68	LYS	2.5
13	BM	3	ARG	2.5
7	BG	68	ASN	2.5
33	CF	59	ALA	2.5
35	DH	105	ALA	2.5
47	DU	92	ASN	2.5
45	CS	30	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	DA	1093	G	2.5
35	DH	94	ILE	2.5
14	BN	5	SER	2.5
29	CC	272	SER	2.5
13	BM	59	GLU	2.5
31	CA	1542	U	2.5
9	AI	64	TYR	2.5
1	AA	959	A	2.5
1	AA	1492	A	2.5
3	BC	78	GLY	2.5
13	AM	40	ALA	2.5
19	BS	81	ARG	2.5
36	CJ	134	ARG	2.5
1	AA	1015	G	2.5
2	BB	88	ASP	2.5
45	CS	95	ASP	2.5
25	C4	37	ALA	2.5
33	CF	12	VAL	2.5
47	CU	59	ASN	2.5
35	CH	79	THR	2.5
1	AA	1022	A	2.5
1	BA	1036	A	2.5
31	CA	74	A	2.5
34	CG	109	PHE	2.5
2	BB	9	MET	2.5
49	CW	11	GLU	2.5
1	BA	1124	G	2.5
10	AJ	36	VAL	2.5
31	CA	1168	G	2.5
35	DH	107	GLY	2.5
31	CA	405	U	2.5
35	CH	27	ARG	2.5
52	CZ	48	ARG	2.5
48	CV	92	LYS	2.5
14	BN	59	ARG	2.5
33	CF	115	ARG	2.5
33	CF	121	SER	2.5
13	BM	53	ILE	2.5
27	C0	48	ILE	2.5
31	CA	545	U	2.5
39	CM	107	PHE	2.5
50	CX	26	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
24	C3	22	MET	2.5
54	DA	1071	G	2.5
7	BG	70	ARG	2.5
10	AJ	5	ARG	2.5
1	BA	1132	C	2.5
7	AG	66	LEU	2.5
10	BJ	23	ALA	2.5
34	CG	136	ALA	2.5
50	CX	51	VAL	2.5
31	CA	316	C	2.5
23	C2	9	ILE	2.5
29	CC	79	GLU	2.5
1	AA	1127	G	2.5
7	AG	6	VAL	2.5
48	CV	49	VAL	2.5
36	CJ	30	GLN	2.5
43	CQ	59	PHE	2.5
1	BA	1322	C	2.5
7	BG	90	GLU	2.5
41	CO	113	ILE	2.5
54	DA	613	A	2.5
13	BM	101	ARG	2.5
7	BG	132	GLY	2.5
3	BC	108	LYS	2.5
36	DJ	10	LYS	2.5
28	CB	51	G	2.5
34	CG	35	ARG	2.5
44	CR	30	ARG	2.5
10	BJ	88	MET	2.4
2	AB	221	VAL	2.4
6	BF	97	THR	2.4
31	CA	646	U	2.4
9	AI	18	ARG	2.4
13	AM	4	ILE	2.4
32	CE	175	ILE	2.4
39	CM	73	ILE	2.4
47	CU	76	ARG	2.4
33	CF	120	LYS	2.4
44	CR	29	SER	2.4
10	BJ	33	GLY	2.4
31	CA	45	G	2.4
31	CA	343	C	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	CA	548	G	2.4
48	CV	14	LEU	2.4
29	CC	239	ASN	2.4
30	CD	41	ALA	2.4
15	BO	25	THR	2.4
19	BS	79	THR	2.4
9	AI	55	VAL	2.4
13	BM	21	SER	2.4
1	BA	202	G	2.4
32	CE	131	THR	2.4
1	BA	1364	U	2.4
31	CA	1058	U	2.4
31	CA	2904	U	2.4
34	CG	175	LYS	2.4
9	BI	91	ASP	2.4
41	CO	83	LEU	2.4
7	BG	83	SER	2.4
8	BH	2	SER	2.4
36	CJ	92	LYS	2.4
39	CM	76	GLU	2.4
34	CG	67	THR	2.4
34	CG	116	GLN	2.4
36	DJ	107	GLN	2.4
19	AS	67	VAL	2.4
31	CA	1864	U	2.4
31	CA	2177	C	2.4
47	CU	87	LEU	2.4
1	BA	978	A	2.4
31	CA	1528	A	2.4
50	CX	34	GLY	2.4
17	BQ	20	SER	2.4
34	CG	68	ALA	2.4
44	CR	37	GLN	2.4
7	BG	120	LEU	2.4
24	C3	7	PRO	2.4
35	CH	77	THR	2.4
36	DJ	117	MET	2.4
1	BA	980	C	2.4
23	C2	30	LYS	2.4
7	BG	74	GLU	2.4
31	CA	2117	A	2.4
10	AJ	37	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	AK	82	LEU	2.4
36	CJ	115	ALA	2.4
1	BA	210	C	2.4
31	CA	897	C	2.4
54	DA	2114	A	2.4
3	BC	2	GLY	2.4
31	CA	1215	G	2.4
52	CZ	35	GLY	2.4
2	AB	12	ALA	2.4
10	BJ	31	ARG	2.4
19	AS	27	ASP	2.4
50	CX	33	ALA	2.4
45	CS	101	ILE	2.4
46	CT	85	ILE	2.4
35	CH	110	VAL	2.4
41	CO	27	SER	2.4
53	DI	72	LEU	2.4
11	BK	64	GLN	2.4
33	CF	84	PRO	2.4
9	BI	11	ARG	2.4
48	CV	27	ASN	2.4
48	CV	37	GLU	2.4
31	CA	1112	G	2.4
19	BS	35	SER	2.4
35	DH	108	VAL	2.4
1	AA	1027	C	2.4
1	BA	532	A	2.4
38	CL	89	ASN	2.4
33	CF	64	LYS	2.4
13	BM	68	ASP	2.4
41	CO	117	ASP	2.4
3	BC	198	VAL	2.4
13	BM	98	ARG	2.4
19	AS	74	PHE	2.4
28	CB	24	G	2.4
31	CA	894	U	2.4
31	CA	2892	G	2.4
33	CF	42	GLU	2.4
33	CF	119	ALA	2.4
38	CL	33	ALA	2.4
41	CO	68	ALA	2.4
47	CU	74	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	BT	75	HIS	2.4
19	BS	62	VAL	2.3
31	CA	900	A	2.3
30	CD	97	SER	2.3
9	BI	7	TYR	2.3
13	BM	115	PRO	2.3
31	CA	2630	G	2.3
48	CV	43	LYS	2.3
50	CX	56	ASP	2.3
32	CE	101	TYR	2.3
39	CM	6	LEU	2.3
1	BA	1297	G	2.3
1	BA	1312	G	2.3
17	BQ	73	TRP	2.3
34	CG	21	GLY	2.3
14	AN	54	ASP	2.3
31	CA	1868	C	2.3
7	AG	79	ARG	2.3
16	BP	51	ARG	2.3
40	CN	72	PRO	2.3
2	BB	16	PHE	2.3
20	BT	34	LYS	2.3
50	CX	78	LYS	2.3
2	BB	36	ASN	2.3
34	CG	75	MET	2.3
42	CP	104	GLN	2.3
53	DI	29	ASP	2.3
1	BA	1006	G	2.3
9	BI	119	ARG	2.3
9	BI	123	ARG	2.3
13	BM	71	ARG	2.3
3	BC	75	ILE	2.3
41	CO	94	TYR	2.3
9	AI	27	LYS	2.3
7	AG	151	PHE	2.3
16	BP	20	VAL	2.3
44	CR	26	GLY	2.3
35	CH	12	LEU	2.3
53	DI	36	ASP	2.3
20	BT	45	ALA	2.3
19	BS	25	SER	2.3
28	CB	27	C	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	CA	2129	C	2.3
1	BA	1013	G	2.3
1	BA	1144	G	2.3
31	CA	2159	G	2.3
1	BA	101	A	2.3
1	BA	1441	A	2.3
7	BG	131	LYS	2.3
31	CA	2800	A	2.3
22	C1	55	ILE	2.3
36	DJ	8	TYR	2.3
45	CS	55	ASP	2.3
53	DI	120	ALA	2.3
14	BN	24	ARG	2.3
16	BP	45	GLU	2.3
25	C4	2	PRO	2.3
36	CJ	93	PRO	2.3
42	CP	22	GLY	2.3
1	BA	1220	G	2.3
31	CA	1174	U	2.3
54	DA	2107	G	2.3
31	CA	899	A	2.3
9	BI	51	PRO	2.3
19	BS	44	MET	2.3
26	C5	2	LYS	2.3
31	CA	335	C	2.3
35	CH	6	LEU	2.3
14	AN	11	VAL	2.3
34	CG	58	TYR	2.3
34	CG	174	ALA	2.3
1	BA	1041	G	2.3
1	BA	1253	G	2.3
31	CA	2286	G	2.3
31	CA	2405	G	2.3
31	CA	2895	G	2.3
41	CO	93	GLY	2.3
2	AB	44	GLU	2.3
30	CD	74	GLU	2.3
7	AG	45	SER	2.3
26	C5	33	HIS	2.3
33	CF	22	TYR	2.3
31	CA	1454	C	2.3
31	CA	2628	C	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	CW	64	VAL	2.3
39	CM	13	LYS	2.3
40	CN	69	PRO	2.3
31	CA	356	G	2.3
31	CA	2525	G	2.3
26	C5	35	GLN	2.3
32	CE	30	GLN	2.3
42	CP	25	ARG	2.3
32	CE	161	ALA	2.3
35	DH	64	ALA	2.3
42	CP	27	VAL	2.3
47	CU	36	LYS	2.3
13	AM	26	GLY	2.3
36	CJ	37	GLU	2.3
31	CA	328	U	2.3
31	CA	2300	C	2.3
36	DJ	47	ASP	2.3
50	CX	64	ASP	2.3
7	BG	47	LEU	2.3
33	DF	176	PRO	2.3
47	CU	77	ARG	2.3
2	BB	164	ILE	2.3
10	AJ	25	ILE	2.3
24	C3	36	ALA	2.3
34	CG	5	ALA	2.3
1	BA	275	G	2.2
1	BA	976	G	2.2
1	BA	1323	G	2.2
17	BQ	42	THR	2.2
30	CD	42	ASN	2.2
34	CG	101	ASN	2.2
45	CS	94	THR	2.2
13	BM	112	PRO	2.2
33	CF	47	LYS	2.2
43	CQ	5	ILE	2.2
46	CT	6	LYS	2.2
30	CD	90	PHE	2.2
8	BH	130	ALA	2.2
22	C1	5	GLN	2.2
13	AM	99	GLY	2.2
33	CF	54	ALA	2.2
49	CW	33	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	CG	117	LEU	2.2
31	CA	1862	G	2.2
31	CA	1875	G	2.2
49	CW	1	MET	2.2
1	AA	85	U	2.2
1	BA	1281	C	2.2
7	AG	48	GLU	2.2
14	AN	60	GLN	2.2
33	CF	11	GLU	2.2
33	CF	55	ALA	2.2
36	CJ	104	ALA	2.2
39	CM	140	GLY	2.2
44	CR	21	ALA	2.2
2	AB	5	SER	2.2
1	BA	974	A	2.2
1	BA	1246	A	2.2
31	CA	44	A	2.2
32	CE	120	VAL	2.2
35	DH	77	THR	2.2
53	DI	55	VAL	2.2
7	BG	143	ARG	2.2
31	CA	327	G	2.2
33	CF	98	GLU	2.2
34	CG	167	GLU	2.2
54	DA	141	G	2.2
2	AB	15	HIS	2.2
2	AB	64	LYS	2.2
53	DI	3	LEU	2.2
43	CQ	43	PHE	2.2
46	CT	86	MET	2.2
43	CQ	17	VAL	2.2
16	BP	35	ARG	2.2
16	BP	47	GLU	2.2
29	CC	18	LYS	2.2
35	DH	89	LYS	2.2
49	CW	12	GLN	2.2
1	BA	945	G	2.2
17	BQ	69	LYS	2.2
30	CD	103	ASP	2.2
30	CD	200	ASP	2.2
33	CF	134	GLU	2.2
30	CD	209	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	BA	1148	U	2.2
19	AS	57	HIS	2.2
31	CA	1522	A	2.2
31	CA	2305	U	2.2
3	BC	51	SER	2.2
13	BM	75	MET	2.2
20	BT	5	LYS	2.2
23	C2	13	SER	2.2
44	CR	98	ILE	2.2
1	BA	222	C	2.2
1	BA	1237	C	2.2
13	BM	66	GLU	2.2
29	CC	180	GLU	2.2
9	AI	125	PRO	2.2
13	AM	15	ALA	2.2
34	CG	96	ALA	2.2
13	AM	8	ASN	2.2
1	BA	196	A	2.2
14	BN	12	LYS	2.2
35	CH	135	HIS	2.2
44	CR	33	ARG	2.2
31	CA	216	A	2.2
31	CA	1213	A	2.2
48	CV	21	LYS	2.2
35	DH	70	GLU	2.2
43	CQ	19	SER	2.2
10	BJ	12	ALA	2.2
9	AI	126	GLN	2.2
29	CC	251	GLN	2.2
42	CP	32	PRO	2.2
1	BA	1331	G	2.2
35	DH	124	THR	2.2
39	CM	4	ASN	2.2
41	CO	46	ARG	2.2
47	CU	73	ARG	2.2
25	C4	43	HIS	2.2
29	CC	3	VAL	2.2
1	BA	1286	U	2.2
35	CH	137	GLU	2.2
43	CQ	11	GLU	2.2
3	BC	146	ALA	2.2
9	BI	6	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	CG	74	SER	2.2
31	CA	1872	A	2.2
2	AB	74	ARG	2.2
10	BJ	92	LEU	2.2
46	CT	95	ARG	2.2
1	AA	1302	C	2.2
3	BC	120	ILE	2.2
11	BK	110	ILE	2.2
31	CA	334	C	2.2
1	BA	1356	G	2.2
30	CD	76	GLY	2.2
31	CA	291	G	2.2
7	BG	115	SER	2.2
28	CB	32	U	2.2
33	CF	24	SER	2.2
43	CQ	97	LEU	2.2
19	BS	20	GLU	2.2
33	CF	164	GLU	2.2
35	DH	99	ILE	2.2
1	AA	984	C	2.2
14	AN	28	LYS	2.2
30	CD	184	ARG	2.2
31	CA	336	C	2.2
33	CF	5	HIS	2.2
7	BG	108	ALA	2.2
13	AM	23	TYR	2.2
52	CZ	2	LYS	2.2
39	CM	15	ALA	2.2
42	CP	109	ALA	2.2
31	CA	1216	G	2.2
2	AB	47	VAL	2.2
39	CM	143	GLU	2.2
30	CD	44	GLY	2.2
30	CD	56	LYS	2.2
32	CE	21	ARG	2.2
46	CT	100	THR	2.2
31	CA	885	C	2.1
45	CS	103	ALA	2.1
3	AC	103	ILE	2.1
15	BO	26	GLU	2.1
18	AR	20	GLU	2.1
30	CD	9	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	CH	21	VAL	2.1
3	BC	204	LYS	2.1
1	BA	987	G	2.1
31	CA	476	G	2.1
2	AB	117	LEU	2.1
32	CE	13	THR	2.1
35	CH	75	LEU	2.1
48	CV	99	ASN	2.1
20	BT	82	GLN	2.1
2	AB	37	LYS	2.1
2	BB	186	ILE	2.1
13	BM	81	MET	2.1
2	BB	129	LEU	2.1
27	C0	24	LEU	2.1
3	BC	104	ALA	2.1
20	BT	72	ALA	2.1
1	BA	946	A	2.1
13	AM	29	ARG	2.1
28	CB	56	G	2.1
30	CD	179	ARG	2.1
36	DJ	45	LYS	2.1
39	CM	38	GLN	2.1
27	C0	29	LEU	2.1
33	CF	49	LEU	2.1
7	AG	61	ALA	2.1
10	BJ	16	ARG	2.1
34	CG	127	THR	2.1
41	CO	66	ALA	2.1
48	CV	94	ARG	2.1
53	DI	106	PHE	2.1
2	BB	217	VAL	2.1
10	AJ	8	ILE	2.1
29	CC	19	VAL	2.1
1	BA	201	G	2.1
2	AB	124	GLY	2.1
9	AI	88	MET	2.1
22	C1	18	SER	2.1
39	CM	7	SER	2.1
54	DA	2169	A	2.1
3	BC	203	PHE	2.1
32	CE	7	ASP	2.1
31	CA	1320	C	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	CA	1874	C	2.1
35	CH	103	VAL	2.1
52	CZ	58	ASN	2.1
13	AM	63	PHE	2.1
35	CH	68	ARG	2.1
31	CA	2657	A	2.1
43	CQ	95	ALA	2.1
1	BA	1341	U	2.1
31	CA	288	U	2.1
1	BA	972	C	2.1
45	CS	59	ILE	2.1
47	CU	67	VAL	2.1
52	CZ	54	LYS	2.1
7	AG	140	ASP	2.1
20	BT	63	ALA	2.1
29	CC	245	VAL	2.1
32	CE	122	GLU	2.1
1	BA	251	G	2.1
2	AB	36	ASN	2.1
7	BG	9	GLN	2.1
31	CA	185	G	2.1
42	CP	75	GLY	2.1
43	CQ	7	GLN	2.1
2	BB	69	PHE	2.1
16	BP	16	PHE	2.1
25	C4	14	PHE	2.1
34	CG	42	GLU	2.1
36	CJ	39	CYS	2.1
23	C2	42	VAL	2.1
20	BT	60	ARG	2.1
23	C2	44	ARG	2.1
25	C4	41	LYS	2.1
37	CK	93	ILE	2.1
19	AS	71	LEU	2.1
31	CA	1088	A	2.1
31	CA	2796	U	2.1
1	BA	86	G	2.1
31	CA	776	G	2.1
54	DA	2161	C	2.1
35	DH	65	ALA	2.1
48	CV	60	GLU	2.1
2	BB	64	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	BQ	61	ILE	2.1
20	BT	35	VAL	2.1
32	CE	168	ASP	2.1
33	CF	150	ARG	2.1
2	AB	65	GLY	2.1
16	BP	9	HIS	2.1
29	CC	127	GLY	2.1
31	CA	150	U	2.1
31	CA	2629	U	2.1
31	CA	2602	A	2.1
35	CH	109	GLU	2.1
48	CV	75	ALA	2.1
49	CW	28	ALA	2.1
1	AA	1037	C	2.1
1	BA	998	C	2.1
7	BG	7	ILE	2.1
31	CA	1958	C	2.1
35	DH	72	ILE	2.1
7	BG	82	GLY	2.1
13	BM	80	LEU	2.1
31	CA	1869	G	2.1
47	CU	70	HIS	2.1
15	BO	15	PHE	2.1
7	AG	56	LYS	2.1
10	BJ	11	LYS	2.1
1	BA	92	U	2.1
13	BM	86	TYR	2.1
22	C1	6	ASN	2.1
34	CG	44	LYS	2.1
34	DG	177	LYS	2.1
31	CA	1467	U	2.1
50	DX	10	THR	2.1
53	DI	94	ARG	2.1
9	AI	28	ILE	2.1
14	AN	16	LEU	2.1
19	AS	49	ILE	2.1
31	CA	2799	A	2.1
45	CS	15	SER	2.1
2	BB	162	PHE	2.0
20	BT	8	LYS	2.0
22	C1	53	LYS	2.0
24	C3	37	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	CG	22	GLN	2.0
42	CP	97	PHE	2.0
7	BG	63	GLU	2.0
31	CA	1865	U	2.0
42	CP	42	PRO	2.0
45	CS	52	PRO	2.0
31	CA	2835	A	2.0
42	CP	88	LYS	2.0
46	CT	49	LYS	2.0
53	DI	105	LYS	2.0
2	BB	139	ARG	2.0
9	BI	18	ARG	2.0
25	C4	54	ASP	2.0
51	CY	34	HIS	2.0
31	CA	1043	C	2.0
3	BC	39	VAL	2.0
35	DH	56	ALA	2.0
36	DJ	44	ALA	2.0
7	AG	133	THR	2.0
8	BH	55	THR	2.0
31	CA	930	G	2.0
31	CA	1042	G	2.0
31	CA	1212	G	2.0
31	CA	1460	U	2.0
50	CX	68	LYS	2.0
3	BC	107	ARG	2.0
30	CD	24	VAL	2.0
31	CA	514	A	2.0
35	DH	138	VAL	2.0
45	CS	38	VAL	2.0
48	CV	76	ALA	2.0
51	CY	78	TYR	2.0
3	BC	144	LEU	2.0
11	AK	110	ILE	2.0
13	BM	62	LYS	2.0
27	C0	7	ILE	2.0
30	CD	146	ILE	2.0
39	CM	141	LYS	2.0
40	CN	73	ILE	2.0
14	BN	63	ARG	2.0
34	CG	82	GLY	2.0
37	CK	21	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
53	DI	119	PRO	2.0
31	CA	2106	U	2.0
31	CA	488	G	2.0
31	CA	2409	G	2.0
31	CA	2857	G	2.0
17	AQ	83	VAL	2.0
38	CL	56	ASP	2.0
7	BG	50	LEU	2.0
35	DH	141	LYS	2.0
43	CQ	29	LYS	2.0
52	CZ	44	LYS	2.0
52	CZ	56	LEU	2.0
53	DI	92	ALA	2.0
28	CB	50	A	2.0
31	CA	508	A	2.0
54	DA	1090	A	2.0
1	AA	962	C	2.0
1	BA	307	C	2.0
31	CA	357	C	2.0
6	AF	62	MET	2.0
47	CU	33	LYS	2.0
47	CU	61	LEU	2.0
52	CZ	21	LEU	2.0
1	BA	1127	G	2.0
31	CA	1445	G	2.0
53	DI	32	GLY	2.0
26	C5	13	ASN	2.0
31	CA	734	A	2.0
31	CA	1877	A	2.0
31	CA	1053	C	2.0
34	CG	34	THR	2.0
36	CJ	100	LYS	2.0
36	DJ	73	THR	2.0
46	CT	83	LYS	2.0
54	DA	1076	C	2.0
30	CD	203	VAL	2.0
32	CE	157	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
54	1MG	DA	745	24/25	0.99	0.18	-	16,22,28,30	0
31	G7M	CA	2069	24/25	0.93	0.20	-	78,83,88,88	0
30	MEQ	CD	150	9/11	0.89	0.25	-	81,87,117,120	0
1	5MC	AA	967	21/22	0.95	0.16	-	76,93,96,97	0
31	PSU	CA	955	20/21	0.93	0.17	-	84,89,90,90	0
1	PSU	AA	516	20/21	0.98	0.13	-	68,72,78,78	0
1	MA6	AA	1518	24/25	0.98	0.17	-	44,46,50,53	0
30	MEQ	DD	150[B]	10/11	0.98	0.21	-	19,28,34,35	10
31	PSU	CA	746	20/21	0.93	0.15	-	93,99,101,102	0
30	MEQ	DD	150[A]	10/11	0.98	0.21	-	11,18,25,27	10
1	G7M	BA	527	24/25	0.96	0.16	-	80,85,91,93	0
1	MA6	AA	1519	24/25	0.97	0.18	-	46,48,50,54	0
1	2MG	BA	966	24/25	0.84	0.34	-	149,153,160,161	0
31	PSU	CA	2580	20/21	0.94	0.19	-	77,86,88,89	0
54	6MZ	DA	1618	23/24	0.99	0.16	-	17,24,27,28	0
1	2MG	AA	1516	24/25	0.97	0.15	-	44,49,52,53	0
54	5MU	DA	747	21/22	0.99	0.18	-	20,25,31,38	0
1	2MG	BA	1207	24/25	0.84	0.21	-	158,159,162,165	0
54	PSU	DA	2580	20/21	0.99	0.17	-	17,21,28,29	0
54	6MZ	DA	2030	23/24	0.99	0.18	-	15,20,26,28	0
31	3TD	CA	1915	21/22	0.88	0.18	-	146,150,155,155	0
54	PSU	DA	2605	20/21	0.99	0.16	-	26,34,37,38	0
1	UR3	AA	1498	21/22	0.97	0.14	-	51,53,57,59	0
31	PSU	CA	2504	20/21	0.92	0.20	-	78,86,90,91	0
1	4OC	AA	1402	22/23	0.98	0.16	-	48,55,61,62	0
1	2MG	AA	1207	24/25	0.92	0.13	-	113,117,120,122	0
31	2MG	CA	2445	24/25	0.94	0.26	-	66,75,80,83	0
1	5MC	AA	1407	21/22	0.98	0.14	-	43,47,52,53	0
31	PSU	CA	2604	20/21	0.97	0.14	-	65,71,84,84	0
54	PSU	DA	1911	20/21	0.97	0.17	-	67,74,75,75	0
31	OMC	CA	2498	21/22	0.96	0.18	-	77,80,86,87	0
1	PSU	BA	516	20/21	0.89	0.16	-	91,96,99,102	0
31	5MU	CA	747	21/22	0.94	0.17	-	93,100,102,105	0
31	PSU	CA	2605	20/21	0.96	0.15	-	74,75,78,80	0
31	6MZ	CA	1618	23/24	0.94	0.23	-	98,107,108,109	0
31	PSU	CA	2457	20/21	0.95	0.16	-	79,83,85,85	0
1	UR3	BA	1498	21/22	0.96	0.13	-	78,80,84,84	0
31	2MA	CA	2503	23/24	0.90	0.21	-	90,96,102,102	0
54	PSU	DA	955	20/21	0.99	0.19	-	20,23,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	5MU	DA	1939	21/22	0.99	0.18	-	25,30,36,40	0
12	D2T	BL	89	10/11	0.93	0.26	-	81,86,96,96	0
54	OMC	DA	2498	21/22	0.99	0.18	-	18,21,24,27	0
31	PSU	CA	1911	20/21	0.92	0.18	-	111,128,131,132	0
12	D2T	AL	89	10/11	0.94	0.20	-	47,53,67,70	0
1	MA6	BA	1519	24/25	0.96	0.21	-	68,73,77,78	0
1	5MC	BA	1407	21/22	0.93	0.17	-	81,95,99,100	0
40	4D4	DN	81[B]	12/13	0.98	0.21	-	11,21,28,29	9
31	6MZ	CA	2030	23/24	0.92	0.20	-	78,86,97,99	0
54	PSU	DA	746	20/21	0.99	0.17	-	18,23,26,30	0
54	2MA	DA	2503	23/24	0.99	0.18	-	15,28,32,41	0
31	1MG	CA	745	24/25	0.95	0.21	-	85,87,90,93	0
54	5MC	DA	1962	21/22	0.98	0.18	-	28,37,39,42	0
31	2MG	CA	1835	24/25	0.95	0.16	-	60,73,76,78	0
40	4D4	DN	81[A]	12/13	0.98	0.21	-	26,33,49,50	9
54	PSU	DA	1917	20/21	0.96	0.15	-	63,73,79,79	0
54	OMU	DA	2552	21/22	0.99	0.17	-	22,26,30,35	0
1	2MG	BA	1516	24/25	0.95	0.15	-	61,67,78,80	0
54	G7M	DA	2069	24/25	0.99	0.16	-	20,28,31,33	0
31	PSU	CA	1917	20/21	0.87	0.19	-	118,126,134,134	0
31	OMG	CA	2251	24/25	0.95	0.24	-	67,73,75,77	0
31	5MU	CA	1939	21/22	0.97	0.14	-	69,74,80,82	0
54	OMG	DA	2251	24/25	0.99	0.17	-	21,25,34,42	0
1	5MC	BA	967	21/22	0.82	0.31	-	148,154,156,157	0
54	2MG	DA	2445	24/25	0.99	0.18	-	16,22,24,25	0
1	2MG	AA	966	24/25	0.95	0.15	-	78,87,97,97	0
54	PSU	DA	2504	20/21	0.99	0.16	-	31,33,36,38	0
31	OMU	CA	2552	21/22	0.94	0.34	-	78,81,85,89	0
54	2MG	DA	1835	24/25	0.97	0.18	-	31,42,47,48	0
31	5MC	CA	1962	21/22	0.97	0.22	-	67,72,76,76	0
1	G7M	AA	527	24/25	0.98	0.14	-	53,59,62,65	0
54	PSU	DA	2457	20/21	0.99	0.17	-	22,25,26,29	0
54	3TD	DA	1915	21/22	0.94	0.20	-	86,90,102,103	0
1	MA6	BA	1518	24/25	0.95	0.20	-	67,74,79,79	0
54	H2U	DA	2449	20/21	0.99	0.17	-	19,22,24,26	0
1	4OC	BA	1402	22/23	0.96	0.15	-	74,79,81,82	0
54	PSU	DA	2604	20/21	0.99	0.16	-	32,36,47,47	0
40	4D4	CN	81	12/13	0.93	0.27	-	83,89,102,103	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
58	PUT	AA	1674	6/6	0.70	0.73	68.80	128,131,132,133	0
58	PUT	DA	3195	6/6	0.73	0.60	54.59	76,81,86,87	0
58	PUT	DA	3213	6/6	0.86	0.50	32.99	83,85,91,93	0
55	MG	CA	3003	1/1	0.54	1.52	32.28	270,270,270,270	0
61	PEG	D1	103	7/7	0.74	0.46	31.21	76,77,78,78	0
61	PEG	DA	3200	7/7	0.83	0.68	31.07	65,68,77,77	0
64	SPD	DA	3183	10/10	0.93	0.43	30.06	60,70,74,75	0
61	PEG	D3	101	7/7	0.75	1.12	27.39	83,89,94,95	0
57	MPD	DA	3204	8/8	0.81	0.43	22.93	117,118,124,125	0
64	SPD	DA	3206	10/10	0.76	0.32	18.34	86,93,96,96	0
57	MPD	AA	1676	8/8	0.62	0.68	17.63	102,115,118,121	0
55	MG	CA	3133	1/1	0.66	0.50	17.30	83,83,83,83	0
58	PUT	DA	3222	6/6	0.83	0.33	17.07	41,43,47,47	0
63	PGE	DA	3214	10/10	0.93	0.36	16.79	56,58,66,66	0
61	PEG	DA	3218	7/7	0.85	0.33	16.56	99,105,110,112	0
61	PEG	DA	3226	7/7	0.83	0.30	16.12	57,62,74,75	0
63	PGE	DA	3001	10/10	0.79	0.58	15.96	75,85,99,101	0
58	PUT	DA	3184	6/6	0.89	0.29	15.87	53,55,60,60	0
65	1PE	DA	3202	16/16	0.90	0.36	15.22	55,64,72,72	0
63	PGE	DA	3203	10/10	0.91	0.31	14.16	68,72,76,76	0
56	PG4	BA	1642	13/13	0.91	0.42	14.02	84,86,94,96	0
63	PGE	DA	3217	10/10	0.93	0.34	13.91	67,71,76,76	0
63	PGE	D1	102	10/10	0.75	0.65	13.72	107,117,119,119	0
58	PUT	DA	3189	6/6	0.92	0.32	12.25	40,44,47,47	0
56	PG4	DA	3193	13/13	0.85	0.73	11.51	65,77,93,94	0
58	PUT	DA	3219	6/6	0.89	0.29	10.99	63,64,65,66	0
63	PGE	DA	3225	10/10	0.91	0.29	10.77	73,81,92,92	0
62	EDO	DA	3198	4/4	0.90	0.28	10.75	76,79,79,79	0
55	MG	CA	3122	1/1	0.75	0.57	10.68	106,106,106,106	0
61	PEG	DQ	201	7/7	0.58	0.98	10.12	104,108,109,109	0
56	PG4	DA	3216	13/13	0.89	0.27	10.11	77,89,96,96	0
55	MG	AA	1608	1/1	0.87	0.41	9.85	78,78,78,78	0
55	MG	AA	1612	1/1	0.84	0.34	9.39	57,57,57,57	0
57	MPD	DE	301	8/8	0.77	0.81	9.31	123,126,129,129	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	DA	3127	1/1	0.95	0.37	9.00	71,71,71,71	0
55	MG	DA	3037	1/1	0.95	0.24	8.75	22,22,22,22	0
55	MG	CA	3147	1/1	0.93	0.38	8.64	51,51,51,51	1
62	EDO	DA	3209	4/4	0.84	0.42	8.43	93,94,95,95	0
55	MG	DA	3172	1/1	0.83	0.29	8.42	81,81,81,81	0
58	PUT	AA	1672	6/6	0.70	0.51	7.83	90,93,95,95	0
55	MG	DA	3126	1/1	0.95	0.28	7.70	57,57,57,57	0
57	MPD	DA	3207	8/8	0.90	0.32	7.58	86,86,88,89	0
57	MPD	DA	3192	8/8	0.89	0.43	7.29	69,77,79,80	0
59	TAC	BA	1644	32/32	0.74	0.45	7.28	139,152,159,159	0
55	MG	CA	3105	1/1	0.90	0.61	7.25	260,260,260,260	0
58	PUT	AA	1673	6/6	0.89	0.29	6.97	92,93,93,94	0
64	SPD	DA	3224	10/10	0.93	0.23	6.71	30,40,57,60	0
56	PG4	DS	202	13/13	0.92	0.30	6.55	52,54,63,64	0
56	PG4	AA	1670	13/13	0.88	0.25	6.04	64,79,91,92	0
55	MG	DA	3124	1/1	0.93	0.24	6.01	76,76,76,76	0
55	MG	CA	3123	1/1	0.60	0.62	5.62	115,115,115,115	0
66	ACY	DA	3201	4/4	0.95	0.21	5.59	66,68,68,69	0
58	PUT	DA	3205	6/6	0.86	0.33	5.33	77,82,89,91	0
63	PGE	DU	101	10/10	0.92	0.41	5.17	79,84,91,92	0
67	GUN	DA	3211	11/11	0.88	0.36	5.06	82,84,86,86	0
55	MG	BA	1646	1/1	0.88	0.35	4.86	141,141,141,141	0
55	MG	CA	3130	1/1	0.81	0.29	4.65	76,76,76,76	0
62	EDO	D1	101	4/4	0.87	0.24	4.05	56,57,60,60	0
55	MG	BA	1612	1/1	0.75	0.29	3.72	159,159,159,159	0
55	MG	CA	3137	1/1	0.91	0.28	3.55	123,123,123,123	0
63	PGE	DS	201	10/10	0.82	0.39	3.50	65,78,83,83	0
57	MPD	AA	1671	8/8	0.93	0.46	3.45	83,86,89,90	0
61	PEG	DL	201	7/7	0.92	0.25	3.33	66,69,70,71	0
65	1PE	DA	3185	16/16	0.94	0.18	3.31	37,52,80,82	0
55	MG	CA	3151	1/1	0.79	0.30	3.25	81,81,81,81	0
55	MG	CA	3026	1/1	0.95	0.35	2.88	111,111,111,111	0
64	SPD	DA	3187	10/10	0.97	0.20	2.84	30,41,47,48	0
55	MG	BA	1601	1/1	0.98	0.25	2.65	130,130,130,130	0
62	EDO	DA	3197	4/4	0.95	0.22	2.39	51,51,53,53	0
62	EDO	DB	201	4/4	0.94	0.19	2.30	72,75,76,76	0
55	MG	AA	1642	1/1	0.97	0.22	1.96	89,89,89,89	0
55	MG	DA	3093	1/1	0.99	0.18	1.84	23,23,23,23	0
55	MG	CA	3009	1/1	0.84	0.23	1.50	240,240,240,240	0
61	PEG	AL	201	7/7	0.84	0.22	1.49	79,79,85,86	0
55	MG	CA	3037	1/1	0.93	0.30	1.36	146,146,146,146	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3177	1/1	0.96	0.18	1.14	67,67,67,67	0
55	MG	AA	1644	1/1	0.95	0.17	1.11	87,87,87,87	0
55	MG	DD	301	1/1	0.97	0.18	0.62	40,40,40,40	0
55	MG	CA	3136	1/1	0.90	0.22	0.56	87,87,87,87	0
59	TAC	AA	1680	32/32	0.93	0.19	0.44	70,81,96,96	0
55	MG	CA	3155	1/1	0.90	0.22	0.40	152,152,152,152	0
56	PG4	DQ	202	13/13	0.92	0.20	0.39	53,59,69,71	0
55	MG	AA	1661	1/1	0.79	0.20	0.20	139,139,139,139	0
55	MG	DA	3112	1/1	0.99	0.18	0.19	24,24,24,24	0
59	TAC	AA	1681	32/32	0.92	0.21	0.09	94,106,109,110	0
57	MPD	DS	203	8/8	0.98	0.20	-0.01	47,50,57,58	0
55	MG	DA	3024	1/1	0.99	0.18	-0.13	36,36,36,36	0
55	MG	DA	3132	1/1	0.88	0.15	-0.14	54,54,54,54	0
55	MG	AA	1678	1/1	0.64	0.22	-0.18	76,76,76,76	0
55	MG	BA	1614	1/1	0.94	0.15	-0.19	137,137,137,137	0
63	PGE	DA	3186	10/10	0.95	0.16	-0.24	33,40,41,41	0
55	MG	DA	3147	1/1	0.93	0.16	-0.36	104,104,104,104	0
55	MG	CA	3099	1/1	0.93	0.22	-0.47	156,156,156,156	0
55	MG	DA	3013	1/1	0.99	0.19	-0.49	19,19,19,19	0
55	MG	CA	3089	1/1	0.93	0.18	-0.51	54,54,54,54	0
55	MG	DA	3023	1/1	0.99	0.18	-0.51	20,20,20,20	0
55	MG	CA	3094	1/1	0.77	0.23	-0.57	126,126,126,126	0
55	MG	CA	3018	1/1	0.98	0.17	-0.64	90,90,90,90	0
58	PUT	DM	201	6/6	0.97	0.17	-0.69	40,48,52,56	0
55	MG	BA	1624	1/1	0.79	0.29	-0.75	249,249,249,249	0
55	MG	BA	1613	1/1	0.99	0.17	-0.79	79,79,79,79	0
55	MG	DA	3029	1/1	0.99	0.18	-0.83	29,29,29,29	0
55	MG	CA	3019	1/1	0.83	0.18	-0.86	58,58,58,58	0
55	MG	DA	3066	1/1	0.99	0.17	-0.90	40,40,40,40	0
55	MG	CA	3100	1/1	0.97	0.18	-1.04	73,73,73,73	0
55	MG	AA	1657	1/1	0.89	0.20	-1.06	105,105,105,105	0
55	MG	CA	3153	1/1	0.92	0.16	-1.13	59,59,59,59	0
55	MG	AA	1677	1/1	0.93	0.15	-1.20	138,138,138,138	0
55	MG	CA	3102	1/1	0.93	0.10	-1.24	104,104,104,104	0
55	MG	AA	1668	1/1	0.99	0.13	-1.25	59,59,59,59	0
55	MG	AA	1656	1/1	0.98	0.13	-1.35	140,140,140,140	0
55	MG	CA	3061	1/1	0.56	0.07	-1.36	225,225,225,225	0
59	TAC	BA	1643	32/32	0.86	0.16	-1.43	146,150,152,152	0
55	MG	CB	202	1/1	0.94	0.12	-1.45	113,113,113,113	0
55	MG	AA	1611	1/1	0.94	0.15	-1.52	94,94,94,94	0
55	MG	DA	3094	1/1	0.97	0.15	-1.61	20,20,20,20	0
60	ZN	D5	101	1/1	1.00	0.12	-1.61	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	3011	1/1	0.88	0.16	-1.73	70,70,70,70	0
60	ZN	C5	101	1/1	0.89	0.05	-1.85	149,149,149,149	0
55	MG	CA	3103	1/1	0.97	0.11	-2.19	90,90,90,90	0
55	MG	DA	3110	1/1	0.99	0.16	-2.31	35,35,35,35	0
60	ZN	AB	301	1/1	0.97	0.12	-2.34	150,150,150,150	0
55	MG	DA	3022	1/1	0.99	0.15	-2.34	21,21,21,21	0
55	MG	DA	3228	1/1	0.99	0.16	-2.36	36,36,36,36	0
55	MG	CB	201	1/1	0.96	0.06	-2.43	159,159,159,159	0
55	MG	DA	3014	1/1	0.99	0.15	-2.46	14,14,14,14	0
55	MG	BA	1617	1/1	0.91	0.12	-2.63	105,105,105,105	0
55	MG	BA	1632	1/1	0.93	0.11	-2.67	78,78,78,78	0
55	MG	CA	3079	1/1	0.96	0.10	-2.72	116,116,116,116	0
55	MG	CA	3054	1/1	0.83	0.12	-2.76	118,118,118,118	0
55	MG	DA	3018	1/1	0.99	0.07	-2.80	43,43,43,43	0
55	MG	BA	1620	1/1	0.98	0.09	-2.81	113,113,113,113	0
55	MG	AA	1663	1/1	0.96	0.09	-2.81	94,94,94,94	0
55	MG	CA	3024	1/1	0.96	0.12	-2.91	81,81,81,81	0
55	MG	CA	3020	1/1	0.98	0.13	-3.00	86,86,86,86	0
55	MG	DA	3017	1/1	1.00	0.14	-3.01	20,20,20,20	0
55	MG	DA	3009	1/1	0.99	0.12	-3.01	23,23,23,23	0
55	MG	DA	3031	1/1	0.98	0.17	-3.20	27,27,27,27	0
55	MG	DA	3043	1/1	0.97	0.14	-3.25	32,32,32,32	0
55	MG	CA	3101	1/1	0.98	0.08	-3.30	97,97,97,97	0
55	MG	CA	3051	1/1	0.97	0.10	-3.41	73,73,73,73	0
55	MG	CA	3006	1/1	0.92	0.11	-3.41	143,143,143,143	0
55	MG	CA	3041	1/1	0.99	0.05	-3.60	50,50,50,50	0
55	MG	CA	3033	1/1	0.96	0.11	-3.67	91,91,91,91	0
55	MG	CA	3063	1/1	0.93	0.17	-3.73	118,118,118,118	0
55	MG	CA	3088	1/1	0.97	0.08	-3.79	67,67,67,67	0
55	MG	DA	3090	1/1	0.98	0.14	-3.84	30,30,30,30	0
55	MG	CA	3144	1/1	0.92	0.07	-3.98	63,63,63,63	0
55	MG	DA	3095	1/1	0.97	0.12	-4.00	74,74,74,74	0
55	MG	BA	1622	1/1	0.99	0.07	-4.13	99,99,99,99	0
55	MG	BA	1608	1/1	0.93	0.08	-4.16	86,86,86,86	0
55	MG	DA	3064	1/1	0.99	0.12	-4.22	49,49,49,49	0
55	MG	DB	202	1/1	0.96	0.09	-4.27	52,52,52,52	0
55	MG	BA	1626	1/1	0.95	0.10	-4.29	85,85,85,85	0
55	MG	BA	1605	1/1	0.97	0.07	-4.45	146,146,146,146	0
55	MG	AA	1637	1/1	0.99	0.07	-4.49	53,53,53,53	0
55	MG	DA	3097	1/1	0.96	0.07	-4.68	26,26,26,26	0
55	MG	DA	3159	1/1	0.93	0.10	-4.88	76,76,76,76	0
55	MG	AA	1639	1/1	0.99	0.08	-4.88	89,89,89,89	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1659	1/1	0.96	0.07	-4.97	74,74,74,74	0
55	MG	AA	1648	1/1	0.98	0.08	-5.00	60,60,60,60	0
55	MG	DA	3050	1/1	0.99	0.13	-5.16	18,18,18,18	0
55	MG	CA	3013	1/1	0.86	0.15	-5.29	99,99,99,99	0
55	MG	BA	1615	1/1	0.98	0.06	-5.37	65,65,65,65	0
55	MG	BA	1602	1/1	0.91	0.06	-5.42	84,84,84,84	0
55	MG	DA	3084	1/1	0.99	0.11	-5.67	35,35,35,35	0
55	MG	CA	3052	1/1	0.82	0.07	-5.73	71,71,71,71	0
55	MG	DA	3135	1/1	0.96	0.04	-5.86	78,78,78,78	0
55	MG	DA	3109	1/1	1.00	0.16	-6.04	23,23,23,23	0
55	MG	CA	3086	1/1	0.98	0.08	-6.16	59,59,59,59	0
55	MG	DA	3026	1/1	0.95	0.09	-6.19	92,92,92,92	0
55	MG	DA	3092	1/1	0.97	0.10	-6.24	21,21,21,21	0
55	MG	DA	3058	1/1	1.00	0.09	-6.33	32,32,32,32	0
55	MG	AA	1631	1/1	0.96	0.08	-6.54	47,47,47,47	0
55	MG	DA	3150	1/1	0.99	0.10	-6.69	50,50,50,50	0
55	MG	DA	3047	1/1	0.97	0.12	-6.76	58,58,58,58	0
55	MG	DA	3004	1/1	0.99	0.09	-6.85	60,60,60,60	0
55	MG	DA	3071	1/1	0.99	0.10	-7.02	34,34,34,34	0
55	MG	BA	1610	1/1	0.96	0.04	-7.69	93,93,93,93	0
55	MG	CA	3044	1/1	0.96	0.09	-7.84	59,59,59,59	0
55	MG	CA	3040	1/1	0.98	0.07	-7.89	83,83,83,83	0
55	MG	DA	3099	1/1	0.99	0.14	-8.16	23,23,23,23	0
55	MG	DA	3027	1/1	0.98	0.13	-8.36	33,33,33,33	0
55	MG	DA	3046	1/1	1.00	0.13	-9.26	31,31,31,31	0
55	MG	CA	3030	1/1	0.94	0.06	-9.95	64,64,64,64	0
55	MG	DA	3007	1/1	0.95	0.06	-10.03	88,88,88,88	0
55	MG	AA	1653	1/1	0.98	0.07	-10.75	61,61,61,61	0
55	MG	DA	3102	1/1	0.99	0.09	-12.91	30,30,30,30	0
55	MG	AA	1646	1/1	0.99	0.06	-13.53	49,49,49,49	0
55	MG	DA	3063	1/1	0.98	0.07	-14.35	85,85,85,85	0
55	MG	DA	3169	1/1	0.97	0.27	-	66,66,66,66	0
55	MG	DA	3028	1/1	0.98	0.12	-	56,56,56,56	0
55	MG	CA	3115	1/1	0.73	0.23	-	72,72,72,72	0
55	MG	CA	3093	1/1	0.69	0.14	-	84,84,84,84	0
55	MG	DA	3021	1/1	0.98	0.13	-	27,27,27,27	0
55	MG	CA	3124	1/1	0.83	0.20	-	124,124,124,124	0
55	MG	CA	3131	1/1	0.48	0.59	-	83,83,83,83	0
55	MG	BA	1616	1/1	0.95	0.17	-	162,162,162,162	0
55	MG	DA	3152	1/1	0.77	0.30	-	94,94,94,94	0
57	MPD	DN	201	8/8	0.80	0.45	-	84,91,101,101	0
55	MG	DA	3091	1/1	0.99	0.16	-	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	3095	1/1	0.97	0.07	-	69,69,69,69	0
55	MG	DA	3033	1/1	0.97	0.16	-	26,26,26,26	0
55	MG	DA	3088	1/1	0.99	0.10	-	42,42,42,42	0
55	MG	CA	3150	1/1	0.85	0.55	-	74,74,74,74	0
55	MG	DA	3041	1/1	0.99	0.20	-	11,11,11,11	0
68	TRS	DA	3220	8/8	0.83	0.54	-	94,100,107,109	0
57	MPD	DK	201	8/8	0.84	0.32	-	96,98,100,100	0
55	MG	AA	1636	1/1	0.94	0.26	-	113,113,113,113	0
55	MG	DA	3068	1/1	0.99	0.16	-	35,35,35,35	0
55	MG	DA	3154	1/1	0.89	0.34	-	62,62,62,62	0
55	MG	DA	3016	1/1	0.98	0.09	-	43,43,43,43	0
55	MG	CA	3073	1/1	0.96	0.33	-	229,229,229,229	0
55	MG	AA	1604	1/1	0.94	0.29	-	50,50,50,50	0
55	MG	DA	3111	1/1	0.92	0.29	-	292,292,292,292	0
55	MG	DA	3156	1/1	0.91	0.35	-	72,72,72,72	0
55	MG	DA	3180	1/1	0.93	1.60	-	95,95,95,95	0
55	MG	DA	3048	1/1	0.99	0.13	-	26,26,26,26	0
55	MG	DA	3122	1/1	0.97	0.45	-	46,46,46,46	0
55	MG	CA	3043	1/1	0.84	0.08	-	86,86,86,86	0
61	PEG	DA	3227	7/7	0.90	0.33	-	75,79,86,87	0
55	MG	CA	3068	1/1	0.84	0.24	-	205,205,205,205	0
57	MPD	DA	3210	8/8	0.85	0.34	-	87,89,92,94	0
55	MG	CA	3126	1/1	0.90	0.13	-	85,85,85,85	0
55	MG	DA	3065	1/1	0.96	0.15	-	19,19,19,19	0
55	MG	CA	3066	1/1	0.85	0.12	-	110,110,110,110	0
55	MG	DB	208	1/1	0.86	0.80	-	77,77,77,77	0
55	MG	CA	3025	1/1	0.95	0.08	-	87,87,87,87	0
55	MG	DA	3128	1/1	0.92	0.98	-	62,62,62,62	0
55	MG	BA	1633	1/1	0.96	0.13	-	241,241,241,241	0
55	MG	DA	3006	1/1	0.98	0.06	-	75,75,75,75	0
55	MG	AA	1613	1/1	0.90	0.82	-	59,59,59,59	0
55	MG	CA	3135	1/1	0.58	0.57	-	107,107,107,107	0
55	MG	DA	3167	1/1	0.86	0.35	-	90,90,90,90	0
55	MG	CA	3014	1/1	0.67	0.16	-	200,200,200,200	0
55	MG	CA	3156	1/1	0.63	0.17	-	218,218,218,218	0
55	MG	CA	3039	1/1	0.82	0.59	-	158,158,158,158	0
55	MG	AA	1665	1/1	0.94	0.37	-	136,136,136,136	0
55	MG	BA	1637	1/1	0.23	1.04	-	86,86,86,86	0
55	MG	DA	3101	1/1	0.98	0.09	-	45,45,45,45	0
55	MG	CA	3049	1/1	0.96	0.12	-	57,57,57,57	0
55	MG	AA	1655	1/1	0.89	0.14	-	151,151,151,151	0
55	MG	CA	3120	1/1	0.93	0.15	-	137,137,137,137	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1635	1/1	0.99	0.08	-	104,104,104,104	0
55	MG	AA	1602	1/1	0.90	0.19	-	75,75,75,75	0
55	MG	DA	3082	1/1	0.98	0.12	-	72,72,72,72	0
55	MG	DA	3067	1/1	0.99	0.06	-	36,36,36,36	0
55	MG	CA	3114	1/1	0.84	0.31	-	57,57,57,57	0
55	MG	CA	3080	1/1	0.90	0.23	-	119,119,119,119	0
55	MG	DA	3077	1/1	0.99	0.07	-	30,30,30,30	0
55	MG	AA	1651	1/1	0.96	0.09	-	69,69,69,69	0
55	MG	DA	3118	1/1	0.98	0.08	-	36,36,36,36	0
55	MG	AA	1669	1/1	0.98	0.14	-	172,172,172,172	0
55	MG	AA	1614	1/1	0.87	0.10	-	79,79,79,79	0
55	MG	CA	3082	1/1	0.96	0.25	-	112,112,112,112	0
55	MG	DA	3079	1/1	0.98	0.16	-	124,124,124,124	0
55	MG	BA	1623	1/1	0.89	0.58	-	254,254,254,254	0
55	MG	DB	206	1/1	0.92	0.59	-	64,64,64,64	0
62	EDO	DA	3002	4/4	0.91	0.59	-	71,74,79,82	0
55	MG	CA	3008	1/1	0.63	0.10	-	147,147,147,147	0
57	MPD	DA	3190	8/8	0.91	0.30	-	78,82,85,89	0
55	MG	CA	3121	1/1	0.97	0.14	-	65,65,65,65	0
55	MG	CA	3023	1/1	0.93	0.16	-	159,159,159,159	0
55	MG	CA	3092	1/1	0.93	0.06	-	125,125,125,125	0
55	MG	CA	3048	1/1	0.89	0.13	-	91,91,91,91	0
55	MG	AA	1603	1/1	0.76	0.36	-	81,81,81,81	0
55	MG	DA	3040	1/1	0.99	0.08	-	36,36,36,36	0
55	MG	DB	210	1/1	0.90	0.44	-	76,76,76,76	0
55	MG	DR	201	1/1	0.95	0.33	-	32,32,32,32	0
55	MG	DA	3045	1/1	0.99	0.05	-	49,49,49,49	0
55	MG	DB	204	1/1	0.96	0.06	-	37,37,37,37	0
55	MG	CA	3032	1/1	0.92	0.54	-	244,244,244,244	0
55	MG	AA	1622	1/1	0.44	1.00	-	116,116,116,116	0
55	MG	CA	3096	1/1	0.97	0.05	-	64,64,64,64	0
58	PUT	DA	3188	6/6	0.93	0.22	-	43,50,50,51	0
55	MG	CA	3149	1/1	0.87	0.42	-	63,63,63,63	0
62	EDO	DA	3208	4/4	0.91	0.25	-	69,71,72,72	0
55	MG	AA	1623	1/1	0.88	0.27	-	62,62,62,62	0
55	MG	DA	3053	1/1	0.98	0.11	-	44,44,44,44	0
55	MG	CA	3074	1/1	0.88	0.09	-	101,101,101,101	0
55	MG	DA	3019	1/1	0.99	0.28	-	8,8,8,8	0
55	MG	DA	3160	1/1	0.90	0.68	-	81,81,81,81	0
55	MG	DA	3059	1/1	0.99	0.08	-	23,23,23,23	0
55	MG	DA	3130	1/1	0.72	0.39	-	99,99,99,99	0
61	PEG	DP	201	7/7	0.79	0.82	-	90,91,93,95	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3174	1/1	0.94	0.27	-	70,70,70,70	0
55	MG	CA	3001	1/1	0.25	0.27	-	296,296,296,296	0
55	MG	CA	3129	1/1	0.79	0.21	-	89,89,89,89	0
55	MG	CA	3069	1/1	0.92	0.23	-	110,110,110,110	0
55	MG	DA	3025	1/1	0.99	0.10	-	31,31,31,31	0
55	MG	AA	1620	1/1	0.92	0.27	-	63,63,63,63	0
55	MG	DA	3012	1/1	0.95	0.22	-	153,153,153,153	0
55	MG	CA	3047	1/1	0.70	0.18	-	238,238,238,238	0
55	MG	CA	3083	1/1	0.93	0.13	-	203,203,203,203	0
55	MG	DA	3044	1/1	0.96	0.10	-	70,70,70,70	0
55	MG	DA	3131	1/1	0.85	0.22	-	63,63,63,63	0
55	MG	DA	3105	1/1	0.98	0.19	-	31,31,31,31	0
55	MG	DA	3039	1/1	1.00	0.13	-	23,23,23,23	0
62	EDO	DB	211	4/4	0.89	0.32	-	88,88,90,90	0
55	MG	AA	1667	1/1	0.95	0.10	-	41,41,41,41	0
55	MG	CA	3035	1/1	0.85	0.23	-	89,89,89,89	0
55	MG	DA	3137	1/1	0.67	0.30	-	80,80,80,80	0
55	MG	DA	3175	1/1	0.94	0.21	-	68,68,68,68	0
55	MG	CA	3145	1/1	0.91	0.24	-	62,62,62,62	0
55	MG	BA	1634	1/1	0.92	0.09	-	129,129,129,129	0
55	MG	DA	3134	1/1	0.86	0.28	-	95,95,95,95	0
55	MG	CA	3075	1/1	0.45	2.16	-	221,221,221,221	0
55	MG	DA	3075	1/1	0.99	0.15	-	37,37,37,37	0
55	MG	CA	3038	1/1	0.65	0.14	-	258,258,258,258	0
55	MG	CA	3050	1/1	0.98	0.09	-	54,54,54,54	0
55	MG	CA	3128	1/1	0.80	0.43	-	82,82,82,82	0
55	MG	DA	3171	1/1	0.88	0.55	-	74,74,74,74	0
55	MG	DA	3138	1/1	0.81	0.53	-	38,38,38,38	1
55	MG	DA	3081	1/1	0.98	0.09	-	45,45,45,45	0
56	PG4	DR	202	13/13	0.82	0.37	-	97,109,121,121	0
55	MG	CA	3072	1/1	0.94	0.54	-	249,249,249,249	0
55	MG	BA	1638	1/1	0.64	0.65	-	107,107,107,107	0
55	MG	CA	3087	1/1	0.99	0.05	-	59,59,59,59	0
55	MG	DA	3030	1/1	0.95	0.18	-	42,42,42,42	0
55	MG	DA	3073	1/1	1.00	0.13	-	31,31,31,31	0
55	MG	CA	3084	1/1	0.95	0.26	-	167,167,167,167	0
55	MG	AA	1658	1/1	0.76	0.13	-	101,101,101,101	0
55	MG	DA	3141	1/1	0.92	0.23	-	40,40,40,40	0
55	MG	CA	3031	1/1	0.93	0.07	-	73,73,73,73	0
55	MG	DA	3139	1/1	0.97	0.10	-	55,55,55,55	0
55	MG	DA	3085	1/1	0.98	0.12	-	50,50,50,50	0
55	MG	DA	3170	1/1	0.54	0.43	-	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1605	1/1	0.86	0.52	-	80,80,80,80	0
55	MG	CA	3015	1/1	0.98	0.18	-	57,57,57,57	0
55	MG	CA	3012	1/1	0.87	0.12	-	84,84,84,84	0
55	MG	DA	3173	1/1	0.94	0.44	-	100,100,100,100	0
55	MG	BA	1607	1/1	0.94	0.46	-	203,203,203,203	0
55	MG	DA	3114	1/1	0.99	0.12	-	39,39,39,39	0
55	MG	CA	3004	1/1	0.91	0.07	-	106,106,106,106	0
55	MG	AA	1619	1/1	0.88	0.32	-	93,93,93,93	0
55	MG	CA	3148	1/1	0.95	0.60	-	46,46,46,46	1
55	MG	DA	3121	1/1	0.87	0.16	-	70,70,70,70	0
55	MG	DA	3120	1/1	0.94	0.34	-	81,81,81,81	0
55	MG	CA	3060	1/1	0.20	0.45	-	234,234,234,234	0
55	MG	DA	3060	1/1	1.00	0.14	-	21,21,21,21	0
58	PUT	DA	3223	6/6	0.95	0.20	-	54,55,62,64	0
55	MG	BA	1604	1/1	0.73	0.18	-	187,187,187,187	0
55	MG	BA	1647	1/1	0.83	0.11	-	86,86,86,86	0
55	MG	CA	3117	1/1	0.91	0.43	-	69,69,69,69	0
55	MG	DA	3011	1/1	1.00	0.08	-	33,33,33,33	0
55	MG	AA	1641	1/1	0.95	0.07	-	65,65,65,65	0
55	MG	DA	3231	1/1	0.99	0.24	-	36,36,36,36	0
55	MG	DA	3100	1/1	0.98	0.15	-	26,26,26,26	0
55	MG	DA	3106	1/1	0.99	0.17	-	41,41,41,41	0
55	MG	CA	3152	1/1	0.94	0.44	-	145,145,145,145	0
55	MG	DA	3164	1/1	0.96	0.29	-	59,59,59,59	0
55	MG	AA	1664	1/1	0.88	0.18	-	199,199,199,199	0
55	MG	CA	3077	1/1	0.73	0.57	-	232,232,232,232	0
55	MG	BA	1635	1/1	0.92	0.07	-	113,113,113,113	0
55	MG	CA	3116	1/1	0.80	0.45	-	75,75,75,75	0
55	MG	CA	3017	1/1	0.93	0.07	-	75,75,75,75	0
62	EDO	DA	3003	4/4	0.86	0.32	-	89,89,89,89	0
55	MG	BA	1645	1/1	0.91	0.12	-	94,94,94,94	0
55	MG	CA	3127	1/1	0.91	0.08	-	65,65,65,65	0
55	MG	DA	3168	1/1	0.88	0.48	-	106,106,106,106	0
55	MG	AA	1666	1/1	0.96	0.05	-	47,47,47,47	0
55	MG	DA	3162	1/1	0.93	0.12	-	57,57,57,57	0
55	MG	BA	1630	1/1	0.81	0.10	-	160,160,160,160	0
55	MG	BA	1631	1/1	0.93	0.06	-	45,45,45,45	0
55	MG	BA	1629	1/1	0.81	0.38	-	184,184,184,184	0
55	MG	AA	1638	1/1	0.98	0.07	-	86,86,86,86	0
55	MG	DA	3074	1/1	0.97	0.04	-	47,47,47,47	0
55	MG	DA	3005	1/1	0.99	0.12	-	60,60,60,60	0
55	MG	DA	3096	1/1	0.99	0.12	-	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	3002	1/1	0.83	0.19	-	258,258,258,258	0
55	MG	DA	3020	1/1	1.00	0.05	-	45,45,45,45	0
55	MG	DA	3161	1/1	0.91	0.28	-	62,62,62,62	0
55	MG	CA	3036	1/1	0.95	0.14	-	133,133,133,133	0
55	MG	CA	3021	1/1	0.94	0.82	-	261,261,261,261	0
55	MG	DA	3115	1/1	0.99	0.16	-	37,37,37,37	0
55	MG	DA	3038	1/1	0.99	0.09	-	19,19,19,19	0
55	MG	CA	3065	1/1	0.93	0.11	-	72,72,72,72	0
55	MG	DA	3107	1/1	0.98	0.14	-	35,35,35,35	0
55	MG	CA	3125	1/1	0.86	0.25	-	98,98,98,98	0
55	MG	CA	3104	1/1	0.84	0.21	-	254,254,254,254	0
55	MG	CA	3113	1/1	0.76	0.57	-	79,79,79,79	0
55	MG	CA	3071	1/1	0.85	0.09	-	152,152,152,152	0
55	MG	DA	3103	1/1	0.99	0.12	-	35,35,35,35	0
55	MG	BA	1639	1/1	0.38	0.49	-	93,93,93,93	0
55	MG	DA	3148	1/1	0.93	0.20	-	62,62,62,62	0
55	MG	AA	1621	1/1	0.78	0.61	-	97,97,97,97	0
55	MG	CA	3016	1/1	0.96	0.50	-	164,164,164,164	0
55	MG	CA	3142	1/1	0.95	0.10	-	71,71,71,71	0
55	MG	AA	1628	1/1	0.78	0.22	-	110,110,110,110	0
55	MG	CA	3059	1/1	0.99	0.09	-	74,74,74,74	0
55	MG	DA	3015	1/1	0.98	0.10	-	40,40,40,40	0
55	MG	CA	3042	1/1	0.98	0.10	-	82,82,82,82	0
55	MG	DA	3104	1/1	0.99	0.19	-	34,34,34,34	0
55	MG	CA	3005	1/1	0.45	0.72	-	239,239,239,239	0
55	MG	DA	3032	1/1	0.99	0.18	-	23,23,23,23	0
55	MG	AA	1649	1/1	0.95	0.07	-	57,57,57,57	0
55	MG	BA	1619	1/1	0.96	0.19	-	79,79,79,79	0
55	MG	CA	3110	1/1	0.78	0.23	-	102,102,102,102	0
57	MPD	DT	201	8/8	0.79	0.37	-	84,87,99,100	0
55	MG	AA	1634	1/1	0.90	0.18	-	144,144,144,144	0
55	MG	BA	1603	1/1	0.81	0.50	-	279,279,279,279	0
55	MG	AA	1607	1/1	0.96	0.48	-	70,70,70,70	0
55	MG	AA	1632	1/1	0.95	0.04	-	65,65,65,65	0
55	MG	CA	3028	1/1	0.70	0.23	-	274,274,274,274	0
55	MG	DA	3061	1/1	0.99	0.14	-	30,30,30,30	0
55	MG	CA	3143	1/1	0.94	0.14	-	67,67,67,67	0
55	MG	DA	3098	1/1	0.97	0.10	-	87,87,87,87	0
55	MG	CA	3055	1/1	0.97	0.07	-	135,135,135,135	0
55	MG	CA	3010	1/1	0.94	0.34	-	245,245,245,245	0
55	MG	DA	3145	1/1	0.99	0.11	-	78,78,78,78	0
55	MG	DA	3036	1/1	0.99	0.19	-	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1624	1/1	0.64	0.49	-	93,93,93,93	0
55	MG	DA	3166	1/1	0.82	0.65	-	88,88,88,88	0
55	MG	DA	3076	1/1	1.00	0.13	-	23,23,23,23	0
55	MG	AA	1626	1/1	0.36	1.73	-	113,113,113,113	0
55	MG	BA	1648	1/1	0.97	0.35	-	68,68,68,68	0
55	MG	AA	1647	1/1	0.96	0.09	-	149,149,149,149	0
55	MG	DA	3056	1/1	0.99	0.17	-	42,42,42,42	0
55	MG	DA	3153	1/1	0.90	0.23	-	53,53,53,53	0
55	MG	BA	1628	1/1	0.93	0.12	-	92,92,92,92	0
55	MG	DA	3083	1/1	0.97	0.05	-	45,45,45,45	0
55	MG	CA	3112	1/1	0.89	0.17	-	62,62,62,62	0
55	MG	CA	3132	1/1	0.92	0.46	-	97,97,97,97	0
55	MG	DB	207	1/1	0.89	0.57	-	80,80,80,80	0
55	MG	DA	3052	1/1	0.97	0.10	-	70,70,70,70	0
55	MG	DA	3057	1/1	0.99	0.08	-	13,13,13,13	0
55	MG	CA	3111	1/1	0.83	0.24	-	76,76,76,76	0
55	MG	DA	3176	1/1	0.93	0.32	-	97,97,97,97	0
55	MG	CA	3057	1/1	0.91	0.10	-	106,106,106,106	0
55	MG	DA	3179	1/1	0.83	0.36	-	101,101,101,101	0
55	MG	DA	3034	1/1	0.99	0.13	-	16,16,16,16	0
55	MG	CA	3034	1/1	0.50	0.16	-	244,244,244,244	0
55	MG	DA	3151	1/1	0.97	0.25	-	30,30,30,30	0
55	MG	AA	1610	1/1	0.93	0.44	-	95,95,95,95	0
55	MG	CA	3106	1/1	0.91	0.17	-	75,75,75,75	0
55	MG	CB	203	1/1	0.73	0.09	-	133,133,133,133	0
55	MG	AA	1643	1/1	0.99	0.13	-	53,53,53,53	0
55	MG	DA	3049	1/1	0.97	0.10	-	39,39,39,39	0
55	MG	BA	1625	1/1	0.91	0.23	-	251,251,251,251	0
55	MG	DR	203	1/1	0.96	0.12	-	140,140,140,140	0
57	MPD	DE	302	8/8	0.88	0.57	-	71,76,83,85	0
55	MG	AA	1616	1/1	0.55	0.50	-	87,87,87,87	0
55	MG	CA	3119	1/1	0.81	0.35	-	86,86,86,86	0
55	MG	CA	3022	1/1	0.93	0.84	-	206,206,206,206	0
55	MG	DA	3163	1/1	0.60	0.34	-	84,84,84,84	0
55	MG	DA	3157	1/1	0.98	0.14	-	54,54,54,54	0
55	MG	CA	3108	1/1	0.95	0.21	-	73,73,73,73	0
55	MG	CA	3062	1/1	0.89	0.11	-	190,190,190,190	0
55	MG	DA	3010	1/1	1.00	0.11	-	17,17,17,17	0
55	MG	AA	1633	1/1	0.98	0.23	-	128,128,128,128	0
55	MG	CA	3081	1/1	0.98	0.06	-	84,84,84,84	0
55	MG	DA	3119	1/1	0.99	0.31	-	69,69,69,69	0
55	MG	CA	3139	1/1	0.56	0.37	-	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	3107	1/1	0.95	0.37	-	65,65,65,65	0
55	MG	DA	3146	1/1	0.87	0.24	-	70,70,70,70	0
55	MG	CA	3134	1/1	0.65	0.46	-	126,126,126,126	0
55	MG	DA	3144	1/1	0.70	1.09	-	107,107,107,107	0
55	MG	AA	1618	1/1	0.85	1.19	-	86,86,86,86	0
55	MG	DA	3165	1/1	0.85	0.19	-	47,47,47,47	0
55	MG	DA	3070	1/1	0.98	0.07	-	62,62,62,62	0
55	MG	CA	3029	1/1	0.92	0.27	-	114,114,114,114	0
55	MG	CA	3141	1/1	0.89	0.28	-	66,66,66,66	0
55	MG	DA	3062	1/1	0.80	0.10	-	211,211,211,211	0
55	MG	CA	3076	1/1	0.85	0.18	-	132,132,132,132	0
55	MG	DA	3129	1/1	0.89	0.16	-	67,67,67,67	0
55	MG	DA	3078	1/1	0.98	0.07	-	52,52,52,52	0
55	MG	AA	1630	1/1	0.91	0.15	-	105,105,105,105	0
55	MG	AA	1654	1/1	0.82	0.35	-	259,259,259,259	0
55	MG	CA	3067	1/1	0.88	0.46	-	277,277,277,277	0
55	MG	CA	3085	1/1	0.91	0.08	-	69,69,69,69	0
55	MG	AA	1617	1/1	0.08	0.29	-	147,147,147,147	0
55	MG	BA	1640	1/1	0.91	0.22	-	94,94,94,94	0
55	MG	CA	3070	1/1	0.86	0.09	-	87,87,87,87	0
55	MG	DA	3089	1/1	0.98	0.18	-	23,23,23,23	0
66	ACY	DA	3196	4/4	0.78	0.31	-	72,76,77,77	0
55	MG	DA	3182	1/1	0.87	0.28	-	52,52,52,52	0
55	MG	BA	1627	1/1	0.90	0.30	-	126,126,126,126	0
55	MG	AA	1609	1/1	0.90	0.20	-	88,88,88,88	0
55	MG	AA	1640	1/1	0.97	0.09	-	52,52,52,52	0
55	MG	CA	3090	1/1	0.90	0.40	-	170,170,170,170	0
55	MG	CA	3078	1/1	0.90	0.06	-	153,153,153,153	0
55	MG	CA	3146	1/1	0.87	0.16	-	164,164,164,164	0
55	MG	BA	1618	1/1	0.98	0.07	-	69,69,69,69	0
55	MG	DA	3080	1/1	0.98	0.14	-	149,149,149,149	0
55	MG	CA	3109	1/1	0.92	0.24	-	62,62,62,62	0
55	MG	CA	3138	1/1	0.86	0.11	-	84,84,84,84	0
55	MG	CA	3097	1/1	0.96	0.08	-	83,83,83,83	0
55	MG	CA	3140	1/1	0.88	0.22	-	75,75,75,75	0
55	MG	AA	1662	1/1	0.98	0.15	-	73,73,73,73	0
55	MG	AA	1627	1/1	0.80	0.22	-	72,72,72,72	0
55	MG	CA	3058	1/1	0.95	0.22	-	138,138,138,138	0
55	MG	AA	1660	1/1	0.92	0.27	-	281,281,281,281	0
55	MG	DA	3054	1/1	0.98	0.10	-	70,70,70,70	0
55	MG	DA	3008	1/1	0.95	0.09	-	87,87,87,87	0
55	MG	DB	205	1/1	0.99	0.13	-	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3123	1/1	0.90	0.32	-	81,81,81,81	0
55	MG	DA	3158	1/1	0.91	0.38	-	63,63,63,63	0
55	MG	DA	3181	1/1	0.94	0.31	-	70,70,70,70	0
55	MG	DA	3035	1/1	0.99	0.20	-	32,32,32,32	0
55	MG	DA	3178	1/1	0.95	0.21	-	69,69,69,69	0
55	MG	CA	3118	1/1	0.91	0.30	-	64,64,64,64	0
55	MG	AA	1601	1/1	0.83	0.87	-	76,76,76,76	0
55	MG	DA	3087	1/1	0.98	0.14	-	34,34,34,34	0
55	MG	DB	203	1/1	1.00	0.10	-	30,30,30,30	0
55	MG	DA	3155	1/1	0.97	0.19	-	60,60,60,60	0
55	MG	AA	1629	1/1	0.98	0.10	-	71,71,71,71	0
62	EDO	DA	3194	4/4	0.88	0.24	-	61,63,64,65	0
55	MG	CA	3056	1/1	0.86	0.36	-	78,78,78,78	0
55	MG	DM	202	1/1	0.99	0.04	-	34,34,34,34	0
55	MG	CA	3045	1/1	0.94	0.11	-	107,107,107,107	0
55	MG	DA	3042	1/1	0.99	0.10	-	29,29,29,29	0
57	MPD	DT	202	8/8	0.80	0.35	-	105,107,109,109	0
62	EDO	DA	3215	4/4	0.90	0.24	-	67,71,74,74	0
55	MG	DA	3136	1/1	0.94	0.20	-	43,43,43,43	0
55	MG	DA	3149	1/1	0.94	0.11	-	47,47,47,47	0
55	MG	AA	1606	1/1	0.88	0.23	-	83,83,83,83	0
58	PUT	AA	1675	6/6	0.76	0.47	-	106,107,108,109	0
55	MG	DA	3086	1/1	1.00	0.11	-	29,29,29,29	0
55	MG	CA	3154	1/1	-0.24	1.40	-	136,136,136,136	0
55	MG	DB	209	1/1	0.97	0.23	-	65,65,65,65	0
55	MG	DA	3117	1/1	0.97	0.20	-	62,62,62,62	0
55	MG	DA	3108	1/1	0.99	0.09	-	30,30,30,30	0
55	MG	CA	3046	1/1	0.81	0.12	-	117,117,117,117	0
58	PUT	DA	3212	6/6	0.85	0.28	-	54,63,66,70	0
55	MG	BA	1609	1/1	0.88	0.16	-	168,168,168,168	0
55	MG	AA	1625	1/1	0.91	0.38	-	68,68,68,68	0
55	MG	DA	3055	1/1	0.99	0.21	-	24,24,24,24	0
55	MG	DA	3072	1/1	0.98	0.19	-	55,55,55,55	0
55	MG	BA	1636	1/1	0.95	0.45	-	91,91,91,91	0
55	MG	DA	3143	1/1	0.94	0.18	-	50,50,50,50	0
55	MG	BA	1606	1/1	0.85	0.18	-	251,251,251,251	0
55	MG	CA	3064	1/1	0.96	0.28	-	260,260,260,260	0
55	MG	DA	3051	1/1	0.99	0.09	-	14,14,14,14	0
55	MG	DA	3142	1/1	0.95	0.38	-	84,84,84,84	0
55	MG	DA	3113	1/1	0.98	0.09	-	52,52,52,52	0
55	MG	BA	1641	1/1	0.66	0.27	-	121,121,121,121	0
66	ACY	DA	3191	4/4	0.91	0.28	-	80,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	PEG	DA	3199	7/7	0.87	0.41	-	79,84,92,93	0
55	MG	CA	3053	1/1	0.95	0.15	-	81,81,81,81	0
55	MG	BA	1621	1/1	0.98	0.22	-	36,36,36,36	0
55	MG	DA	3125	1/1	0.98	0.19	-	58,58,58,58	0
55	MG	AA	1645	1/1	0.97	0.07	-	46,46,46,46	0
55	MG	CA	3091	1/1	0.96	0.09	-	80,80,80,80	0
55	MG	DA	3229	1/1	0.99	0.07	-	36,36,36,36	0
55	MG	CA	3027	1/1	0.95	0.14	-	68,68,68,68	0
58	PUT	DA	3221	6/6	0.86	0.40	-	113,116,117,118	0
55	MG	AA	1615	1/1	0.86	0.48	-	84,84,84,84	0
55	MG	AA	1679	1/1	0.98	0.21	-	62,62,62,62	0
55	MG	DA	3069	1/1	0.99	0.15	-	46,46,46,46	0
55	MG	BA	1611	1/1	0.99	0.10	-	56,56,56,56	0
55	MG	AA	1652	1/1	0.98	0.25	-	21,21,21,21	0
55	MG	CA	3007	1/1	0.72	0.40	-	214,214,214,214	0
55	MG	DA	3140	1/1	0.96	0.20	-	68,68,68,68	0
55	MG	DA	3230	1/1	0.98	0.07	-	48,48,48,48	0
55	MG	CA	3098	1/1	0.96	0.07	-	78,78,78,78	0
55	MG	DA	3116	1/1	0.97	0.13	-	34,34,34,34	0
55	MG	AA	1650	1/1	0.97	0.07	-	79,79,79,79	0
62	EDO	DB	212	4/4	0.95	0.24	-	70,72,73,73	0
55	MG	DA	3133	1/1	0.62	0.23	-	78,78,78,78	0

6.5 Other polymers

There are no such residues in this entry.