



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2016 – 05:54 PM EDT

PDB ID : 5J5B
Title : Structure of the WT E coli ribosome bound to tetracycline
Authors : Cocozaki, A.; Ferguson, A.
Deposited on : 2016-04-01
Resolution : 2.80 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

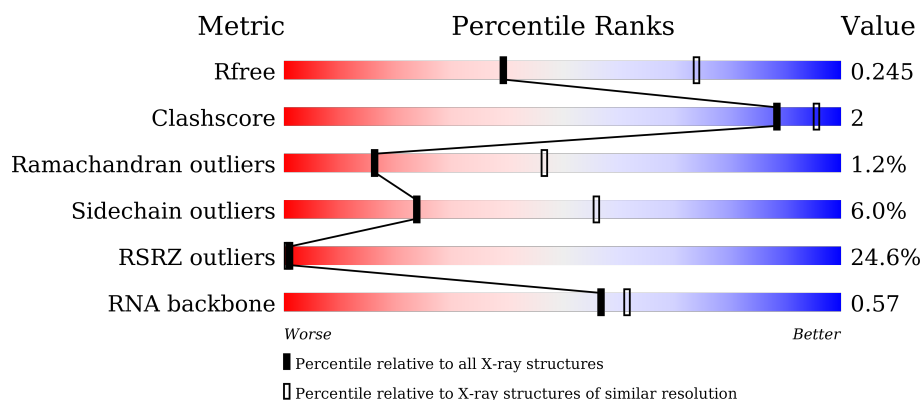
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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

Mol	Chain	Length	Quality of chain
1	AA	1534	<div> <div>3%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
1	BA	1534	<div> <div>25%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>
2	AB	224	<div> <div>35%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
2	BB	224	<div> <div>38%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	206	<div> <div>9%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
3	BC	206	<div> <div>40%</div> <div>83%</div> <div>17%</div> </div>
4	AD	205	<div> <div>3%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
4	BD	205	<div> <div>%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
5	AE	155	<div> <div>4%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>
5	BE	155	<div> <div>12%</div> <div>63%</div> <div>29%</div> <div>5%</div> <div>..</div> </div>
6	AF	106	<div> <div>12%</div> <div>85%</div> <div>15%</div> </div>
6	BF	106	<div> <div>8%</div> <div>72%</div> <div>22%</div> <div>.</div> <div>6%</div> </div>
7	AG	151	<div> <div>28%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
7	BG	151	<div> <div>72%</div> <div>86%</div> <div>14%</div> </div>
8	AH	129	<div> <div>5%</div> <div>81%</div> <div>19%</div> </div>
8	BH	129	<div> <div>15%</div> <div>85%</div> <div>15%</div> </div>
9	AI	127	<div> <div>35%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
9	BI	127	<div> <div>61%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
10	AJ	99	<div> <div>21%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
10	BJ	99	<div> <div>74%</div> <div>73%</div> <div>23%</div> <div>..</div> </div>
11	AK	117	<div> <div>24%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
11	BK	117	<div> <div>21%</div> <div>74%</div> <div>22%</div> <div>.</div> </div>
12	AL	123	<div> <div>2%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
12	BL	123	<div> <div>24%</div> <div>81%</div> <div>13%</div> <div>6%</div> </div>
13	AM	114	<div> <div>41%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
13	BM	114	<div> <div>93%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
14	AN	100	<div> <div>21%</div> <div>88%</div> <div>12%</div> </div>
14	BN	100	<div> <div>73%</div> <div>88%</div> <div>12%</div> </div>
15	AO	88	<div> <div>8%</div> <div>92%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
15	BO	88	
16	AP	82	
16	BP	82	
17	AQ	80	
17	BQ	80	
18	AR	55	
18	BR	55	
19	AS	79	
19	BS	79	
20	AT	86	
20	BT	86	
21	AU	56	
21	BU	56	
22	C1	56	
22	D1	56	
23	C2	51	
23	D2	51	
24	C3	46	
24	D3	46	
25	C4	64	
25	D4	64	
26	C5	38	
26	D5	38	
27	C0	58	
27	D0	58	

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Mol	Chain	Length	Quality of chain
28	CB	120	<div> <div>33%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
28	DB	120	<div> <div>91%</div> <div>8%</div> <div>.</div> </div>
29	CC	271	<div> <div>29%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
29	DC	271	<div> <div>91%</div> <div>8%</div> <div>.</div> </div>
30	CD	209	<div> <div>49%</div> <div>89%</div> <div>11%</div> <div>.</div> </div>
30	DD	209	<div> <div>89%</div> <div>11%</div> </div>
31	CA	2904	<div> <div>31%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>
32	CE	201	<div> <div>62%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
32	DE	201	<div> <div>3%</div> <div>91%</div> <div>9%</div> </div>
33	CF	177	<div> <div>86%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
33	DF	177	<div> <div>4%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
34	CG	176	<div> <div>76%</div> <div>88%</div> <div>12%</div> </div>
34	DG	176	<div> <div>3%</div> <div>88%</div> <div>12%</div> </div>
35	CH	149	<div> <div>50%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
35	DH	149	<div> <div>42%</div> <div>83%</div> <div>17%</div> <div>.</div> </div>
36	CJ	134	<div> <div>97%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
36	DJ	134	<div> <div>83%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
37	CK	142	<div> <div>37%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
37	DK	142	<div> <div>94%</div> <div>5%</div> <div>.</div> </div>
38	CL	123	<div> <div>19%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>
38	DL	123	<div> <div>90%</div> <div>8%</div> <div>.</div> </div>
39	CM	144	<div> <div>74%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
39	DM	144	<div> <div>%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
40	CN	136	<div> <div>28%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
40	DN	136	<div> <div>92%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
41	CO	125	<div> <div>44%</div> <div>84%</div> <div>10%</div> <div>.</div> <div>.</div> </div>
41	DO	125	<div> <div>93%</div> <div>7%</div> </div>
42	CP	117	<div> <div>79%</div> <div>88%</div> <div>9%</div> <div>.</div> <div>.</div> </div>
42	DP	117	<div> <div>90%</div> <div>8%</div> <div>.</div> </div>
43	CQ	114	<div> <div>41%</div> <div>89%</div> <div>11%</div> <div>.</div> </div>
43	DQ	114	<div> <div>3%</div> <div>90%</div> <div>10%</div> </div>
44	CR	117	<div> <div>49%</div> <div>88%</div> <div>12%</div> </div>
44	DR	117	<div> <div>%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
45	CS	103	<div> <div>77%</div> <div>85%</div> <div>13%</div> <div>.</div> <div>.</div> </div>
45	DS	103	<div> <div>92%</div> <div>7%</div> <div>.</div> </div>
46	CT	110	<div> <div>50%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
46	DT	110	<div> <div>86%</div> <div>14%</div> </div>
47	CU	93	<div> <div>72%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
47	DU	93	<div> <div>5%</div> <div>90%</div> <div>10%</div> </div>
48	CV	102	<div> <div>83%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
48	DV	102	<div> <div>10%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
49	CW	94	<div> <div>52%</div> <div>89%</div> <div>11%</div> </div>
49	DW	94	<div> <div>91%</div> <div>9%</div> </div>
50	CX	76	<div> <div>54%</div> <div>95%</div> <div>.</div> <div>.</div> </div>
50	DX	76	<div> <div>%</div> <div>91%</div> <div>9%</div> </div>
51	CY	77	<div> <div>40%</div> <div>83%</div> <div>17%</div> </div>
51	DY	77	<div> <div>%</div> <div>90%</div> <div>10%</div> </div>
52	CZ	62	<div> <div>79%</div> <div>92%</div> <div>8%</div> </div>
52	DZ	62	<div> <div>10%</div> <div>94%</div> <div>6%</div> </div>
53	DI	135	<div> <div>51%</div> <div>71%</div> <div>27%</div> <div>.</div> </div>

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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	1607	-	-	-	X
55	MG	AA	1612	-	-	-	X
55	MG	AA	1642	-	-	-	X
55	MG	AA	1661	-	-	-	X
55	MG	BA	1603	-	-	-	X
55	MG	CA	3002	-	-	-	X
55	MG	CA	3021	-	-	-	X
55	MG	CA	3025	-	-	-	X
55	MG	CA	3031	-	-	-	X
55	MG	CA	3104	-	-	-	X
55	MG	CA	3109	-	-	-	X
55	MG	CA	3130	-	-	-	X
55	MG	CA	3132	-	-	-	X
55	MG	CA	3136	-	-	-	X
55	MG	CA	3146	-	-	-	X
55	MG	CA	3150	-	-	-	X
55	MG	DA	3014	-	-	-	X
55	MG	DA	3027	-	-	-	X
55	MG	DA	3038	-	-	-	X
55	MG	DA	3065	-	-	-	X
55	MG	DA	3125	-	-	-	X
55	MG	DA	3127	-	-	-	X
55	MG	DA	3133	-	-	-	X
55	MG	DA	3163	-	-	-	X
55	MG	DA	3172	-	-	-	X
55	MG	DA	3177	-	-	-	X
55	MG	DA	3182	-	-	-	X
56	PG4	AA	1670	-	-	-	X
56	PG4	BA	1601	-	-	-	X
56	PG4	DA	3193	-	-	-	X
56	PG4	DA	3215	-	-	-	X
56	PG4	DS	202	-	-	-	X
57	MPD	AA	1671	-	-	-	X
57	MPD	AA	1676	-	-	-	X
57	MPD	DA	3192	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MPD	DA	3203	-	-	-	X
57	MPD	DA	3206	-	-	-	X
57	MPD	DE	301	-	-	-	X
57	MPD	DE	302	-	-	-	X
58	PUT	AA	1672	-	-	-	X
58	PUT	AA	1673	-	-	-	X
58	PUT	AA	1674	-	-	-	X
58	PUT	DA	3189	-	-	-	X
58	PUT	DA	3195	-	-	-	X
58	PUT	DA	3204	-	-	-	X
58	PUT	DA	3211	-	-	-	X
58	PUT	DA	3212	-	-	-	X
58	PUT	DA	3218	-	-	-	X
58	PUT	DA	3220	-	-	-	X
58	PUT	DA	3221	-	-	-	X
61	PEG	AL	201	-	-	-	X
61	PEG	D1	103	-	-	-	X
61	PEG	D3	102	-	-	-	X
61	PEG	DA	3200	-	-	-	X
61	PEG	DA	3217	-	-	-	X
61	PEG	DQ	201	-	-	-	X
62	EDO	D1	101	-	-	-	X
62	EDO	DA	3001	-	-	-	X
62	EDO	DA	3197	-	-	-	X
62	EDO	DA	3198	-	-	-	X
63	PGE	D1	102	-	-	-	X
63	PGE	D3	101	-	-	-	X
63	PGE	DA	3213	-	-	-	X
63	PGE	DA	3224	-	-	-	X
63	PGE	DD	301	-	-	-	X
63	PGE	DS	201	-	-	-	X
63	PGE	DU	101	-	-	-	X
64	SPD	DA	3183	-	-	-	X
64	SPD	DA	3187	-	-	-	X
64	SPD	DA	3205	-	-	-	X
64	SPD	DA	3223	-	-	-	X
65	1PE	DA	3185	-	-	-	X
65	1PE	DA	3202	-	-	-	X
66	ACY	DA	3201	-	-	-	X
67	GUN	DA	3210	-	-	-	X

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295188 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CC	271	Total	C	N	O	S	0	0	0
			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			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	1723	G	A	conflict	GB 939731527
CA	1725	U	C	conflict	GB 939731527
CA	1726	C	G	conflict	GB 939731527
CA	1727	C	A	conflict	GB 939731527
CA	1730	C	U	conflict	GB 939731527
CA	1733	G	U	conflict	GB 939731527
CA	1734	G	C	conflict	GB 939731527
CA	1735	A	G	conflict	GB 939731527

- 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			

There are 2 discrepancies between the modelled and reference sequences:

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

- 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	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	0
			917	574	179	163	1			
43	DQ	114	Total	C	N	O	S	0	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	0
			816	516	153	145	2			
45	DS	103	Total	C	N	O	S	0	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	0
			857	532	166	156	3			
46	DT	110	Total	C	N	O	S	0	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	0
			739	466	139	132	2			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			

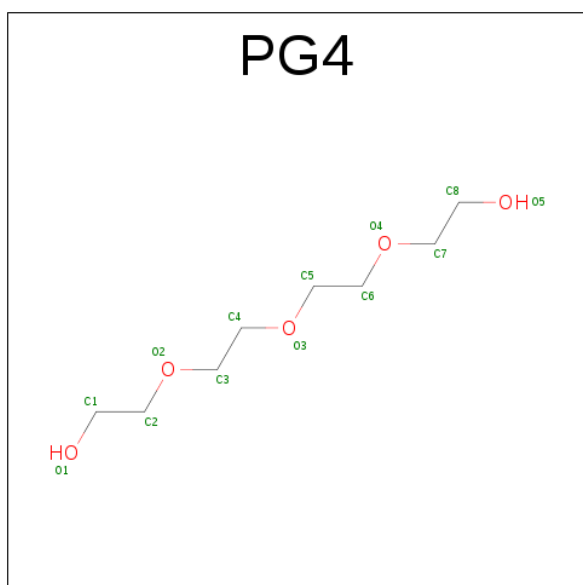
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	1723	G	A	conflict	GB 939731527
DA	1725	U	C	conflict	GB 939731527
DA	1726	C	G	conflict	GB 939731527
DA	1727	C	A	conflict	GB 939731527
DA	1730	C	U	conflict	GB 939731527
DA	1733	G	U	conflict	GB 939731527
DA	1734	G	C	conflict	GB 939731527
DA	1735	A	G	conflict	GB 939731527

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	BA	43	Total 43 Mg 43	0	0
55	CA	155	Total 155 Mg 155	0	0
55	CB	3	Total 3 Mg 3	0	0
55	DM	1	Total 1 Mg 1	0	0
55	DR	2	Total 2 Mg 2	0	0
55	AA	71	Total 71 Mg 71	0	0
55	DA	182	Total 182 Mg 182	0	0
55	C3	1	Total 1 Mg 1	0	0
55	DB	9	Total 9 Mg 9	0	0
55	DD	2	Total 2 Mg 2	0	0

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



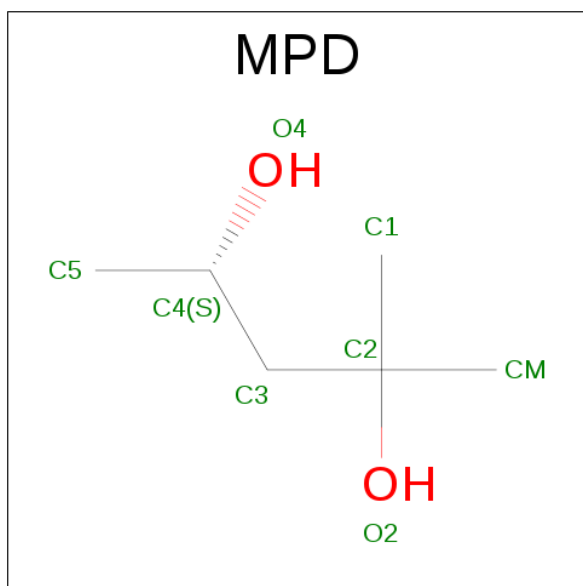
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AA	1	Total 13 C 8 O 5	0	0
56	BA	1	Total 13 C 8 O 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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: $C_6H_{14}O_2$).



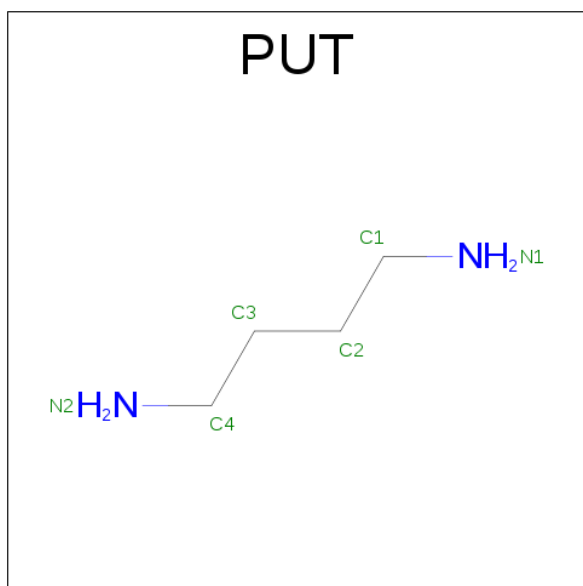
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			8	6	2		
57	AA	1	Total	C	O	0	0
			8	6	2		
57	DE	1	Total	C	O	0	0
			8	6	2		
57	DE	1	Total	C	O	0	0
			8	6	2		
57	DK	1	Total	C	O	0	0
			8	6	2		
57	DN	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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-DIAMINOBTUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



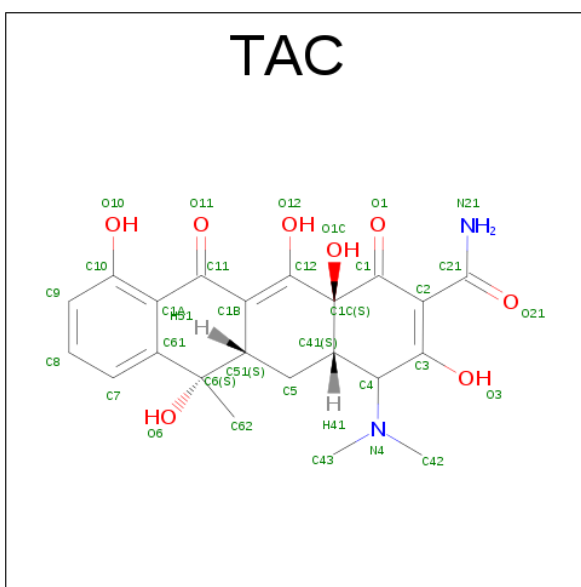
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AA	1	Total	C	N	0	0
			6	4	2		
58	AA	1	Total	C	N	0	0
			6	4	2		
58	AA	1	Total	C	N	0	0
			6	4	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AA	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		
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: $C_{22}H_{24}N_2O_8$).

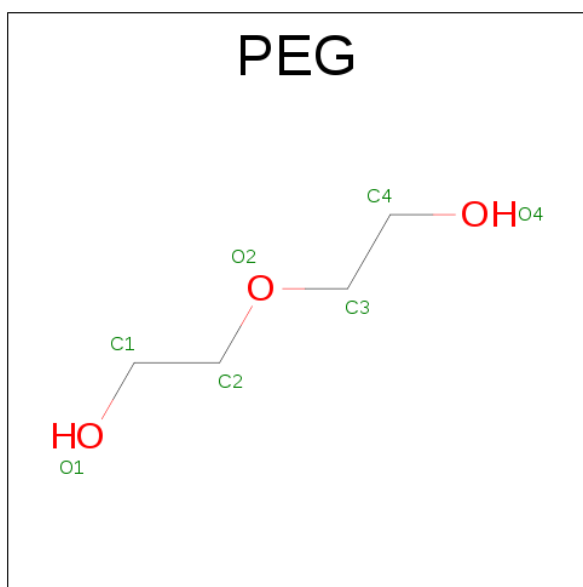


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	AA	1	Total	C	N	O	0	0
			32	22	2	8		
59	BA	1	Total	C	N	O	0	0
			32	22	2	8		

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

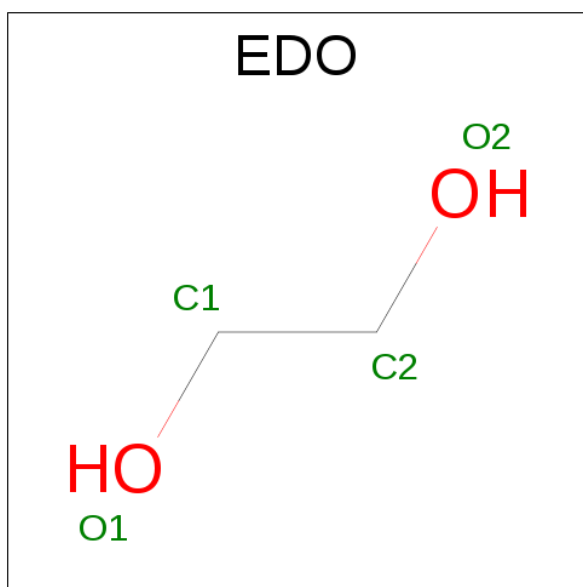
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	C5	1	Total	Zn	0	0
			1	1		
60	AB	1	Total	Zn	0	0
			1	1		
60	D5	1	Total	Zn	0	0
			1	1		

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



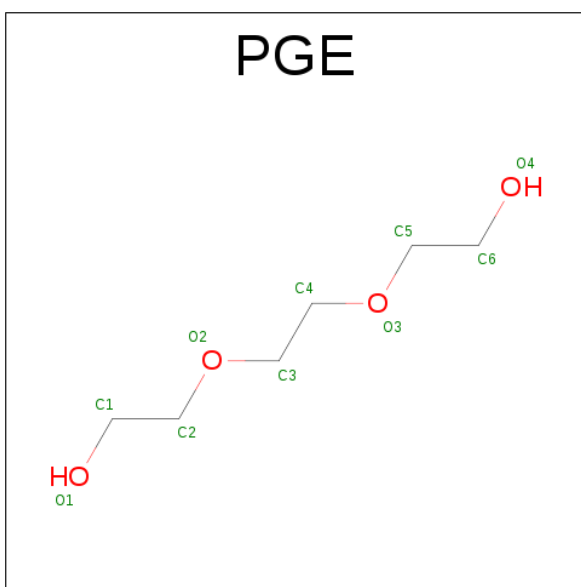
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	D1	1	Total	C	O	0	0
			7	4	3		
61	D3	1	Total	C	O	0	0
			7	4	3		
61	DL	1	Total	C	O	0	0
			7	4	3		
61	DP	1	Total	C	O	0	0
			7	4	3		
61	DQ	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7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

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



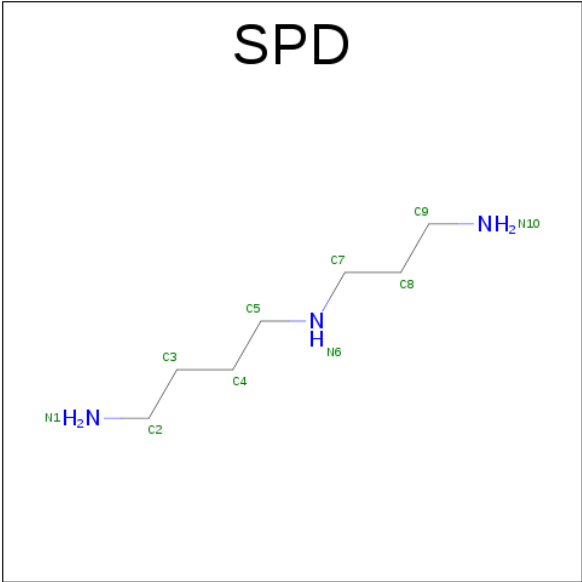
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	D1	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4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

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



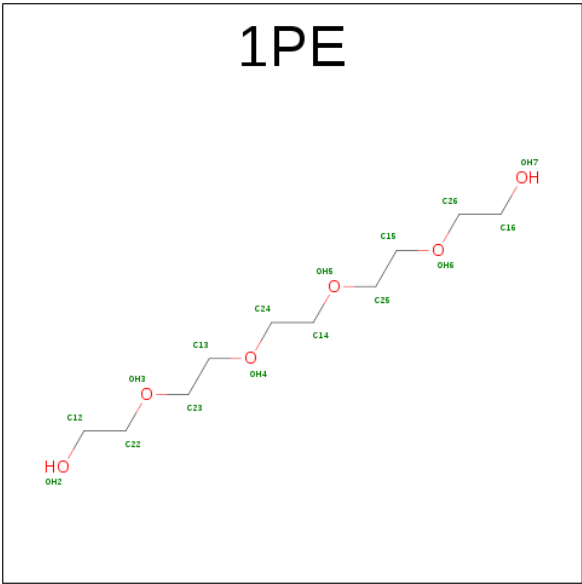
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			10	6	4		
63	D3	1	Total	C	O	0	0
			10	6	4		
63	DD	1	Total	C	O	0	0
			10	6	4		
63	DS	1	Total	C	O	0	0
			10	6	4		
63	DU	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0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

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



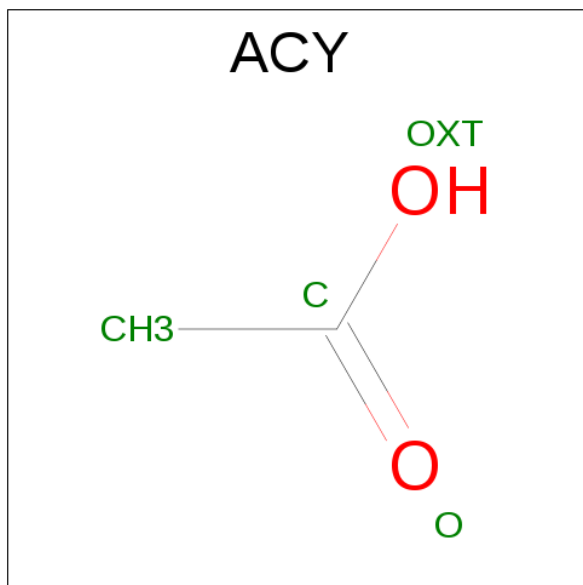
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		

- Molecule 65 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



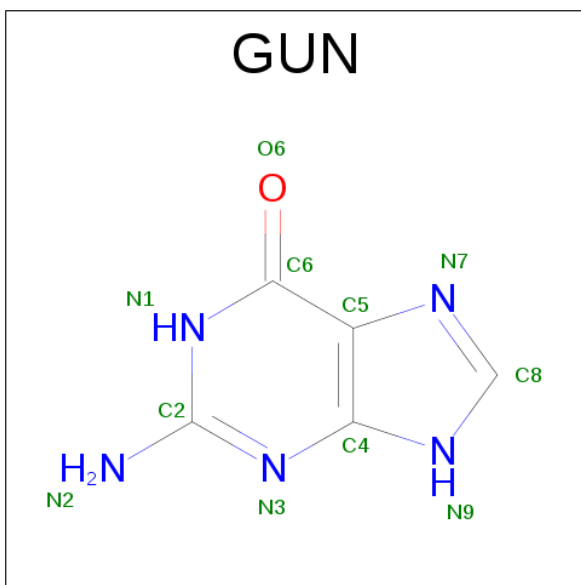
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
65	DA	1	Total	C	O	0	0
			16	10	6		
65	DA	1	Total	C	O	0	0
			16	10	6		

- Molecule 66 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



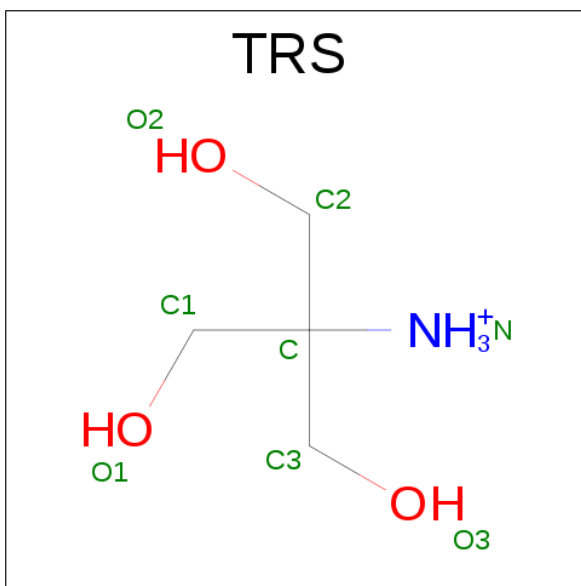
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 67 is GUANINE (three-letter code: GUN) (formula: $C_5H_5N_5O$).



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	507	Total 507	O 507	0	0
69	AC	4	Total 4	O 4	0	0
69	AD	2	Total 2	O 2	0	0
69	AE	4	Total 4	O 4	0	0
69	AF	1	Total 1	O 1	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	5	Total 5	O 5	0	0
69	AL	8	Total 8	O 8	0	0
69	AM	4	Total 4	O 4	0	0
69	AN	5	Total 5	O 5	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	AS	1	Total 1	O 1	0	0
69	AT	2	Total 2	O 2	0	0
69	AU	3	Total 3	O 3	0	0
69	C3	3	Total 3	O 3	0	0
69	C4	2	Total 2	O 2	0	0
69	BA	287	Total 287	O 287	0	0
69	BD	13	Total 13	O 13	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	BE	1	Total 1	O 1	0	0
69	BF	1	Total 1	O 1	0	0
69	BK	1	Total 1	O 1	0	0
69	BL	3	Total 3	O 3	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	BR	1	Total 1	O 1	0	0
69	BT	4	Total 4	O 4	0	0
69	BU	2	Total 2	O 2	0	0
69	D1	42	Total 42	O 42	0	0
69	D2	7	Total 7	O 7	0	0
69	D3	24	Total 24	O 24	0	0
69	D4	33	Total 33	O 33	0	0
69	D5	13	Total 13	O 13	0	0
69	D0	27	Total 27	O 27	0	0
69	CB	13	Total 13	O 13	0	0
69	CC	10	Total 10	O 10	0	0
69	CD	5	Total 5	O 5	0	0
69	CA	692	Total 692	O 692	0	0
69	DC	102	Total 102	O 102	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DD	105	Total 105	O 105	0	0
69	CE	7	Total 7	O 7	0	0
69	CL	1	Total 1	O 1	0	0
69	CM	3	Total 3	O 3	0	0
69	CO	1	Total 1	O 1	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	63	Total 63	O 63	0	0
69	DF	14	Total 14	O 14	0	0
69	DG	6	Total 6	O 6	0	0
69	DH	2	Total 2	O 2	0	0
69	DK	58	Total 58	O 58	0	0
69	DL	51	Total 51	O 51	0	0
69	DM	62	Total 62	O 62	0	0
69	DN	71	Total 71	O 71	0	0
69	DO	44	Total 44	O 44	0	0
69	DP	35	Total 35	O 35	0	0
69	DQ	27	Total 27	O 27	0	0
69	DR	64	Total 64	O 64	0	0

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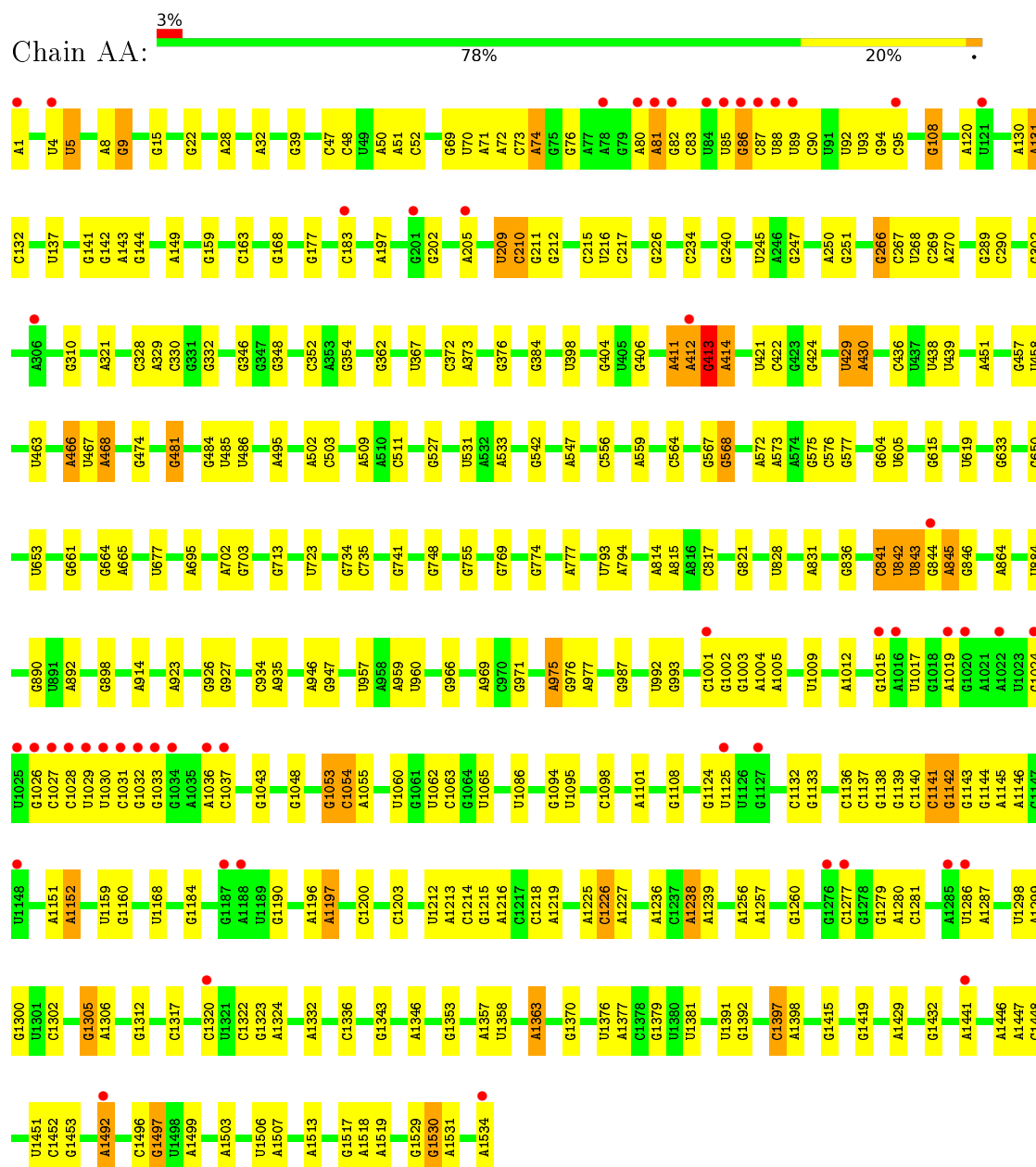
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DS	51	Total 51	O 51	0	0
69	DT	69	Total 69	O 69	0	0
69	DU	17	Total 17	O 17	0	0
69	DV	19	Total 19	O 19	0	0
69	DW	31	Total 31	O 31	0	0
69	DX	30	Total 30	O 30	0	0
69	DY	9	Total 9	O 9	0	0
69	DZ	7	Total 7	O 7	0	0
69	DB	212	Total 212	O 212	0	0
69	DA	4834	Total 4834	O 4834	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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

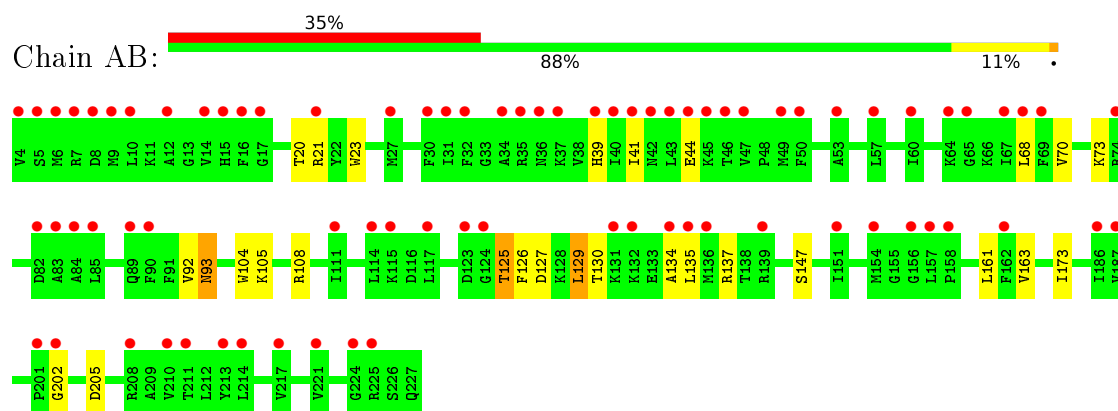
- Molecule 1: 16S rRNA



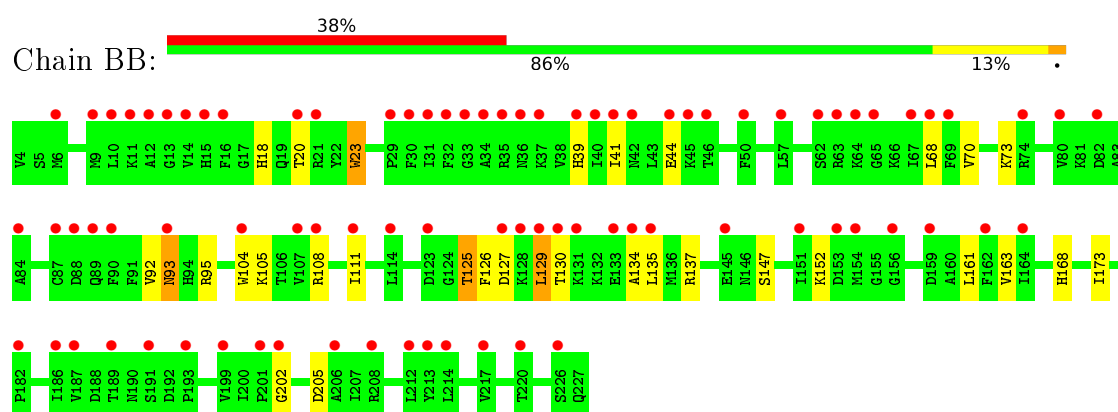
- Molecule 1: 16S rRNA



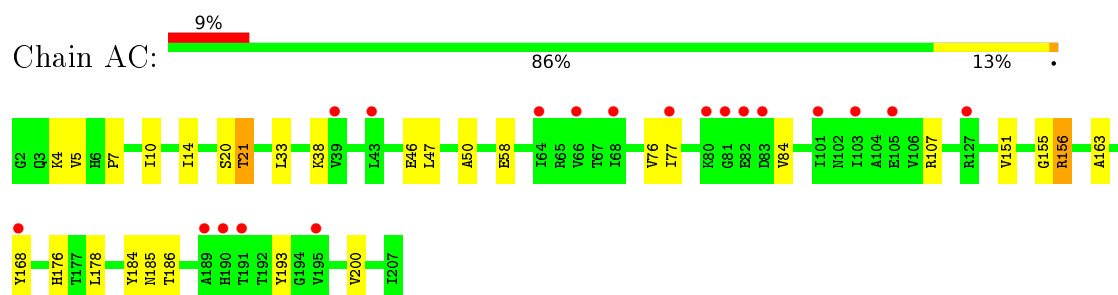
- Molecule 2: 30S ribosomal protein S2



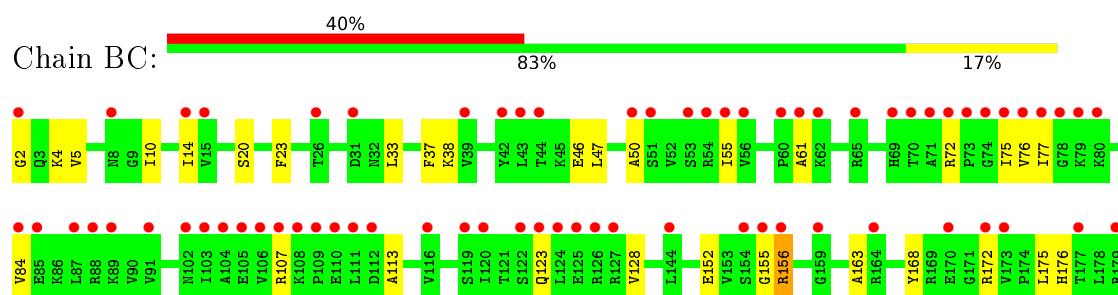
- Molecule 2: 30S ribosomal protein S2

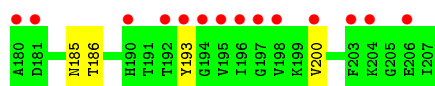


- Molecule 3: 30S ribosomal protein S3

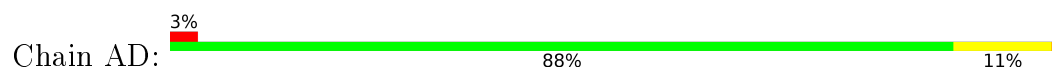


- Molecule 3: 30S ribosomal protein S3

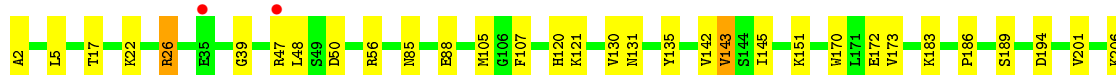
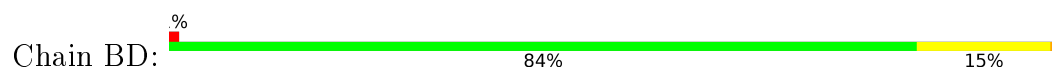




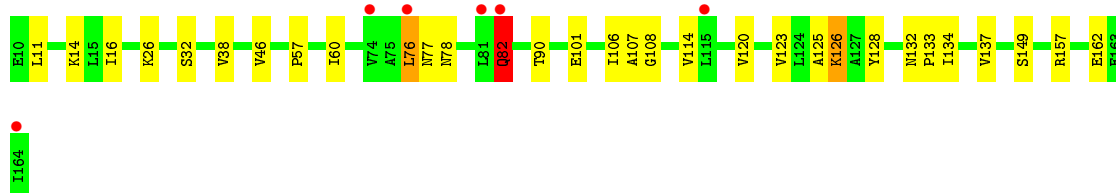
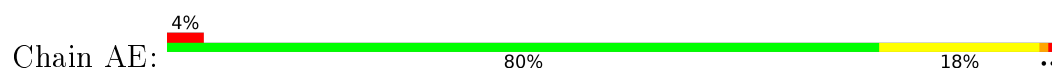
- Molecule 4: 30S ribosomal protein S4



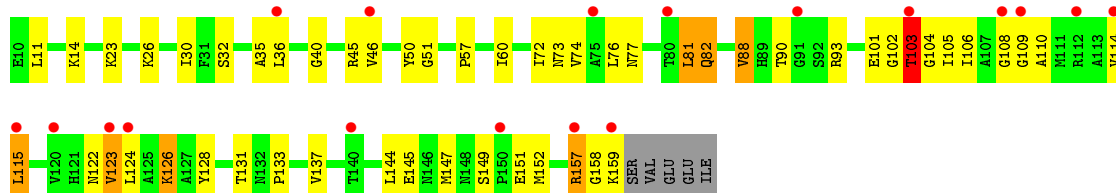
- Molecule 4: 30S ribosomal protein S4



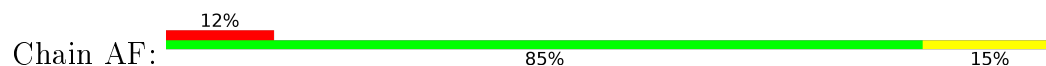
- Molecule 5: 30S ribosomal protein S5



- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6

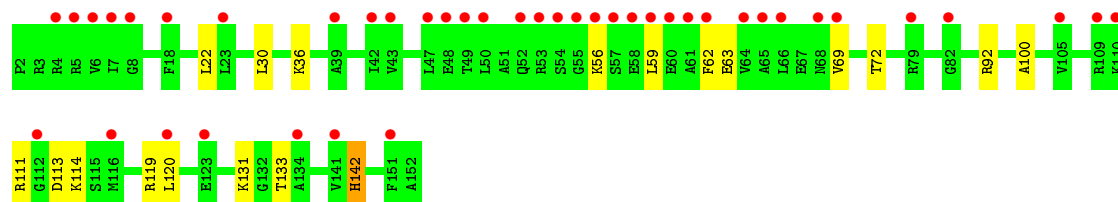
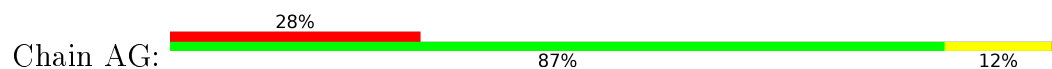


- Molecule 6: 30S ribosomal protein S6

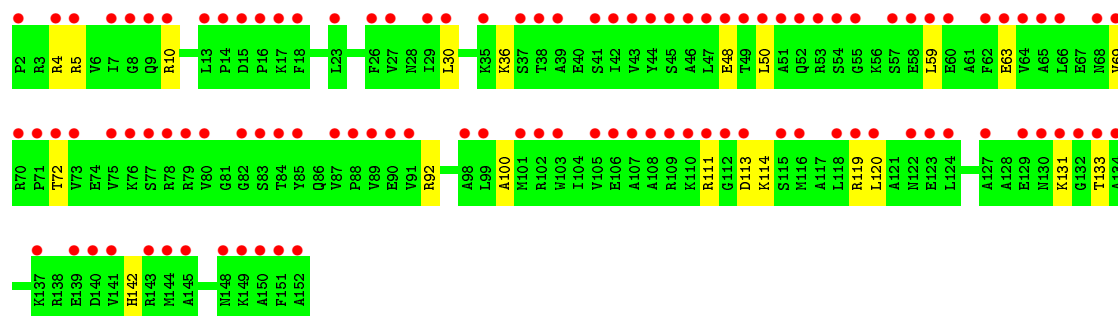
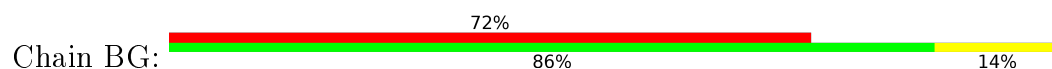




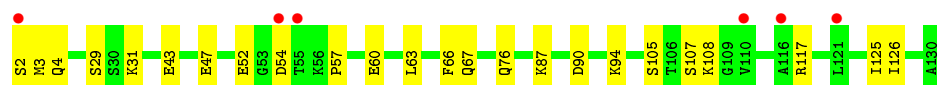
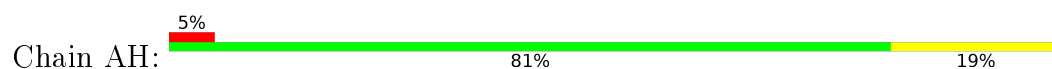
- Molecule 7: 30S ribosomal protein S7



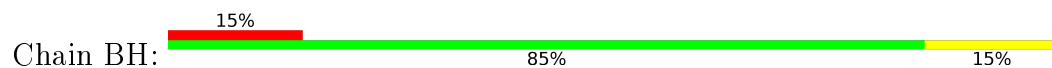
- Molecule 7: 30S ribosomal protein S7



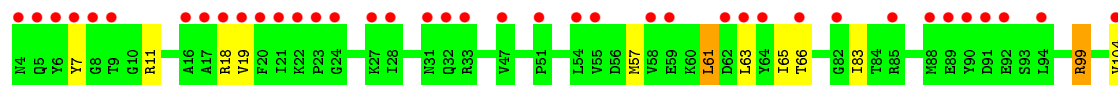
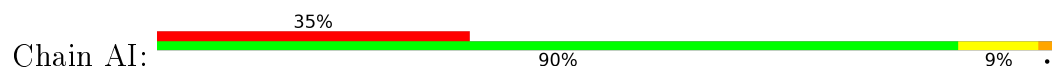
- Molecule 8: 30S ribosomal protein S8

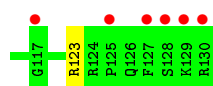


- Molecule 8: 30S ribosomal protein S8

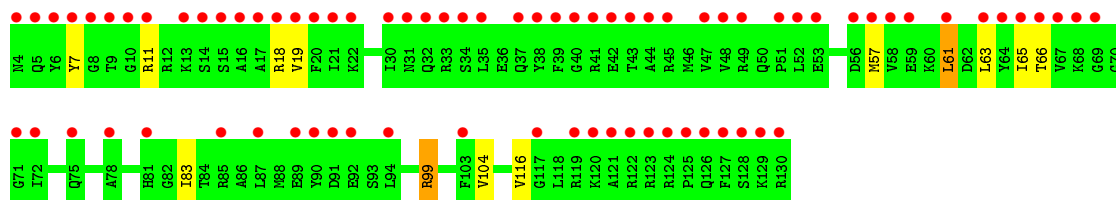
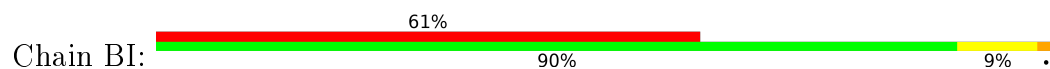


- Molecule 9: 30S ribosomal protein S9

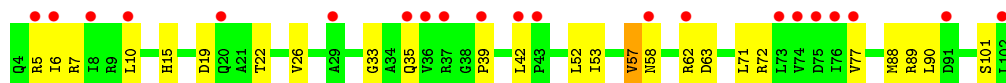
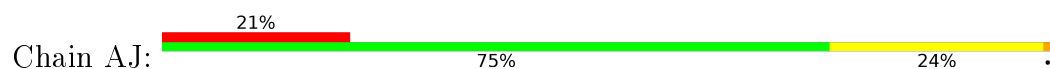




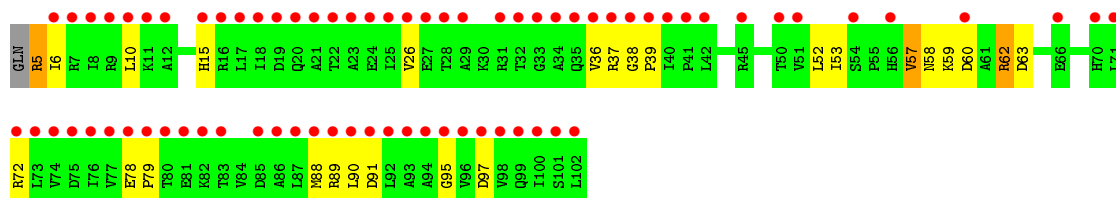
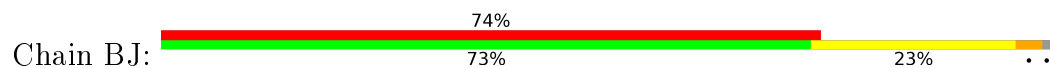
• Molecule 9: 30S ribosomal protein S9



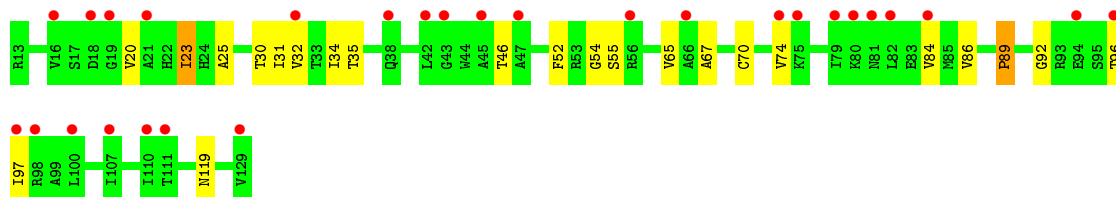
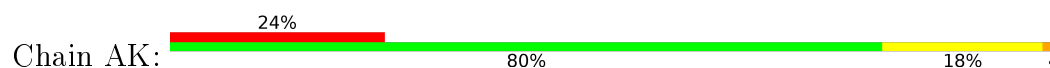
• Molecule 10: 30S ribosomal protein S10



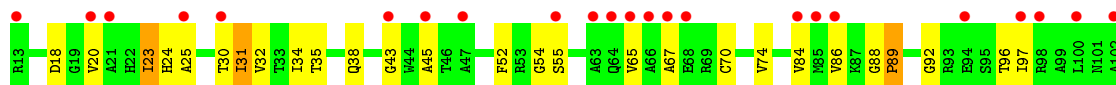
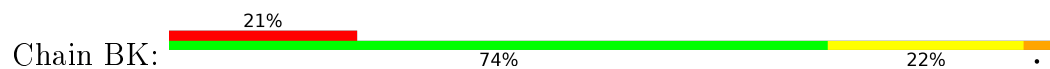
• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

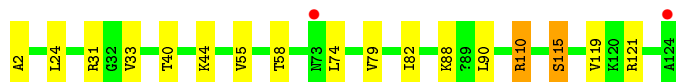
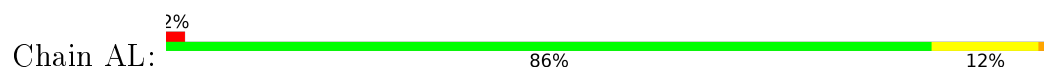


• Molecule 11: 30S ribosomal protein S11

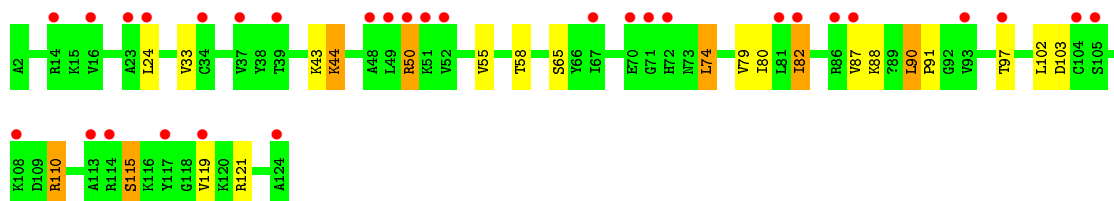
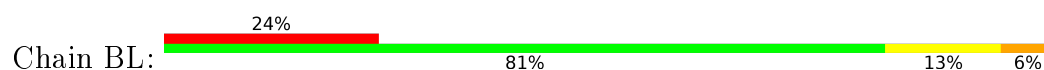




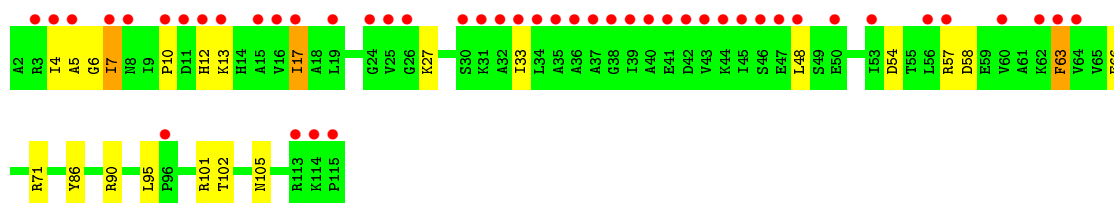
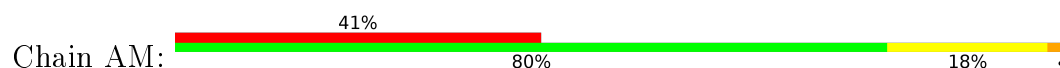
- Molecule 12: 30S ribosomal protein S12



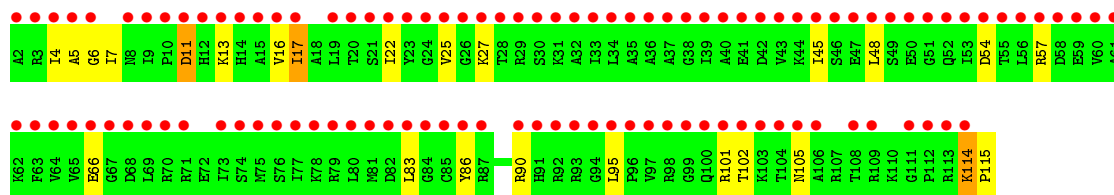
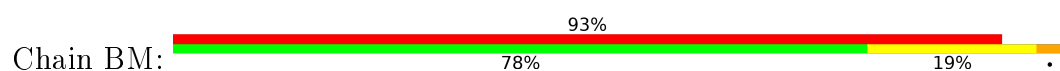
- Molecule 12: 30S ribosomal protein S12



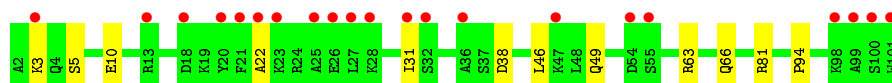
- Molecule 13: 30S ribosomal protein S13



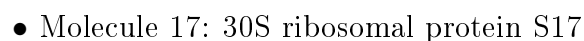
- Molecule 13: 30S ribosomal protein S13

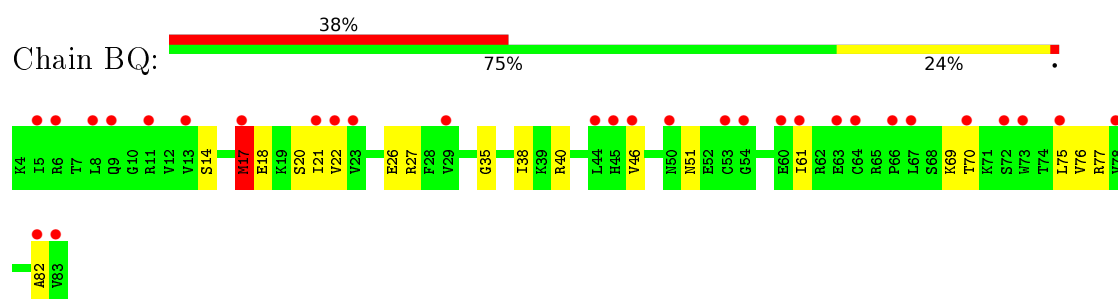


- Molecule 14: 30S ribosomal protein S14

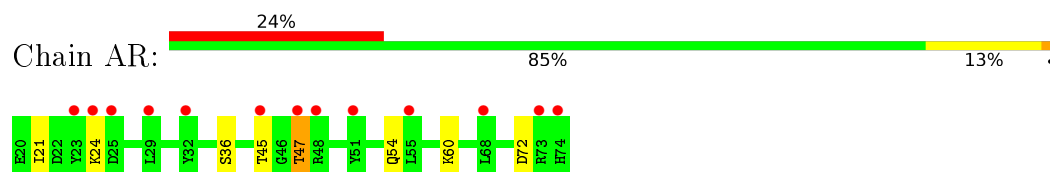


- Molecule 14: 30S ribosomal protein S14

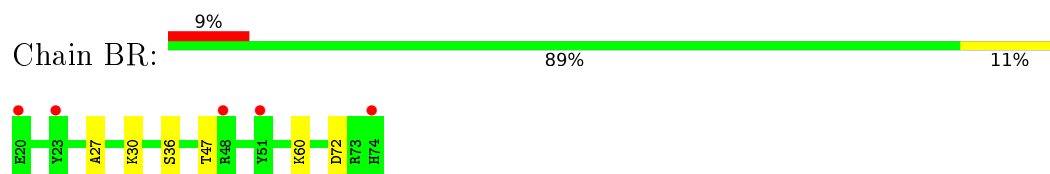




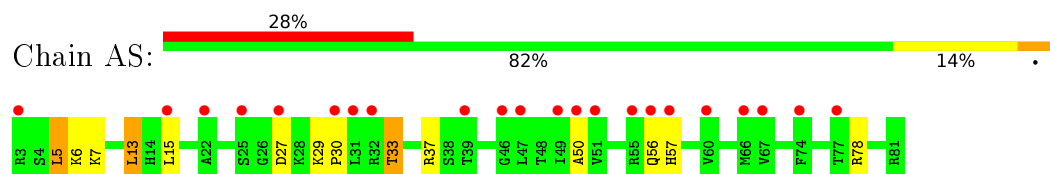
- Molecule 18: 30S ribosomal protein S18



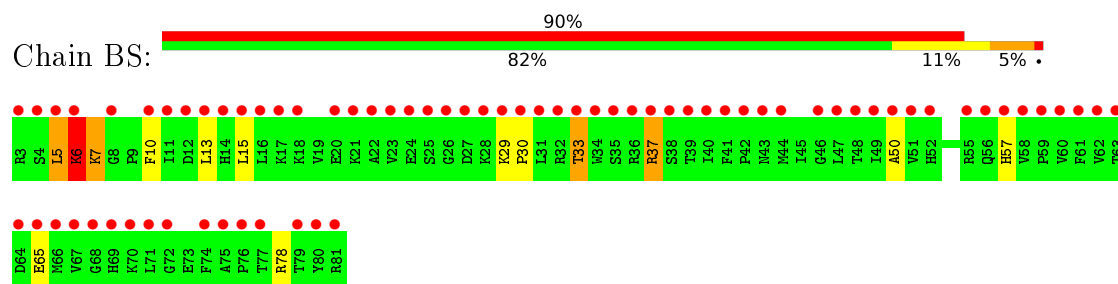
- Molecule 18: 30S ribosomal protein S18



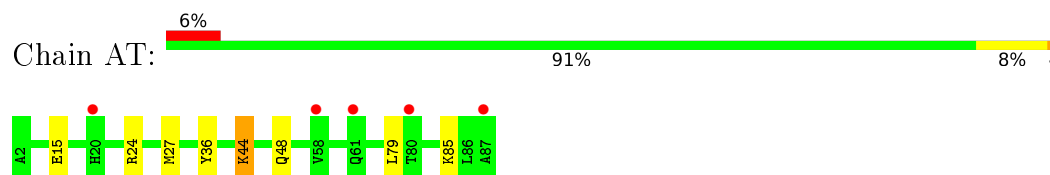
- Molecule 19: 30S ribosomal protein S19



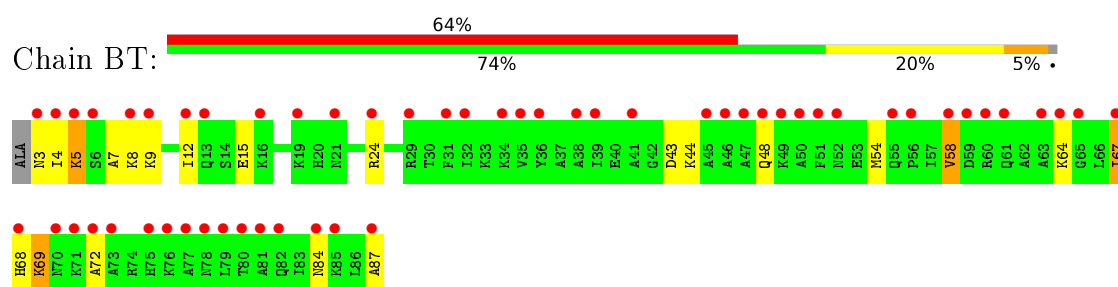
- Molecule 19: 30S ribosomal protein S19



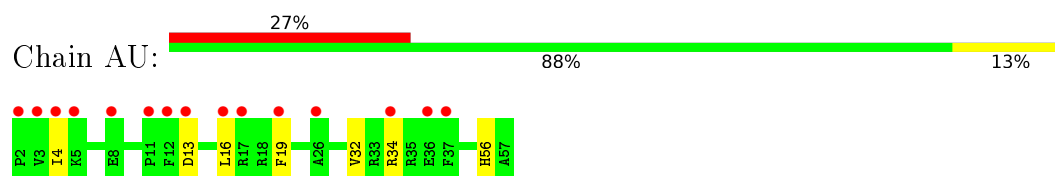
- Molecule 20: 30S ribosomal protein S20



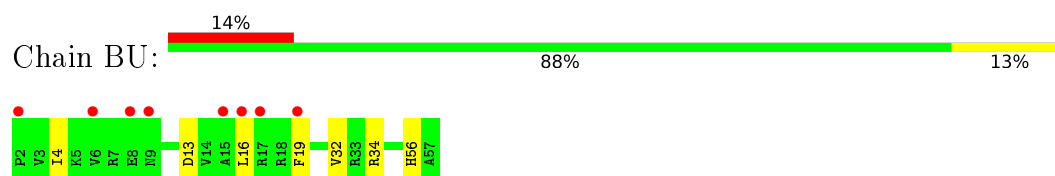
- Molecule 20: 30S ribosomal protein S20



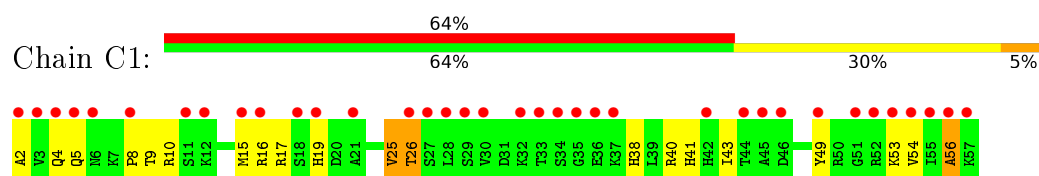
- Molecule 21: 30S ribosomal protein S21



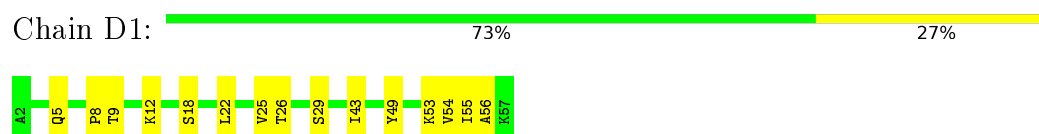
- Molecule 21: 30S ribosomal protein S21



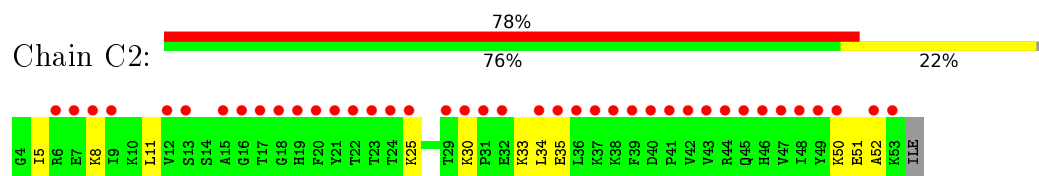
- Molecule 22: 50S ribosomal protein L32



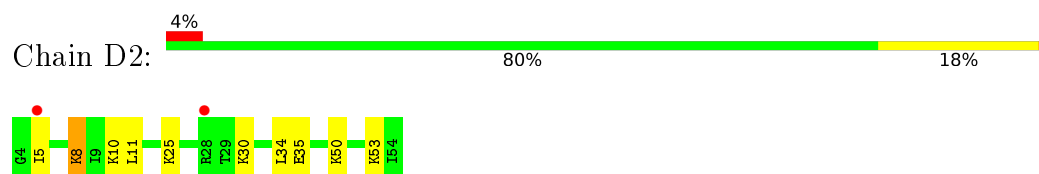
- Molecule 22: 50S ribosomal protein L32



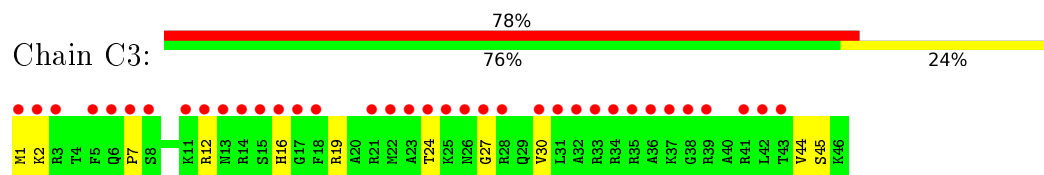
- Molecule 23: 50S ribosomal protein L33



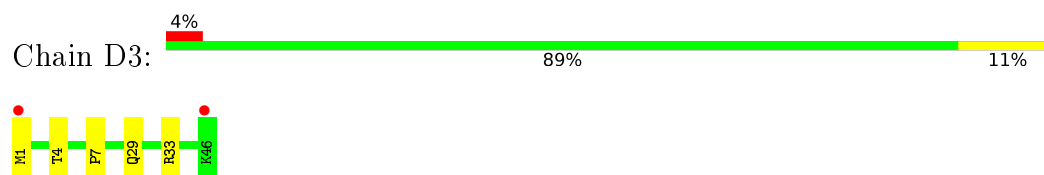
- Molecule 23: 50S ribosomal protein L33



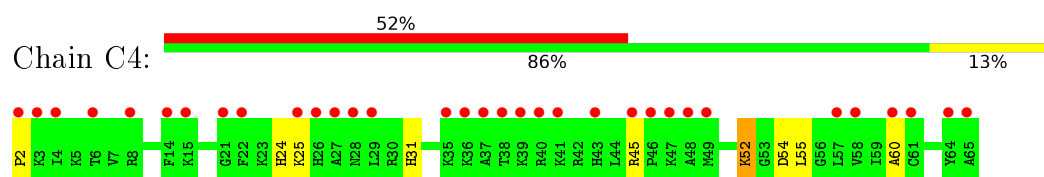
- Molecule 24: 50S ribosomal protein L34



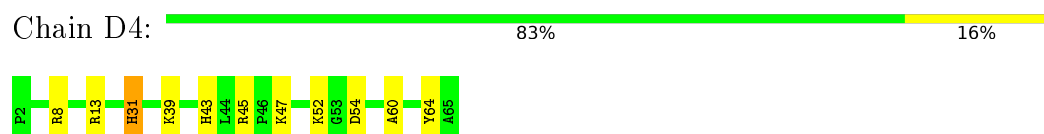
- Molecule 24: 50S ribosomal protein L34



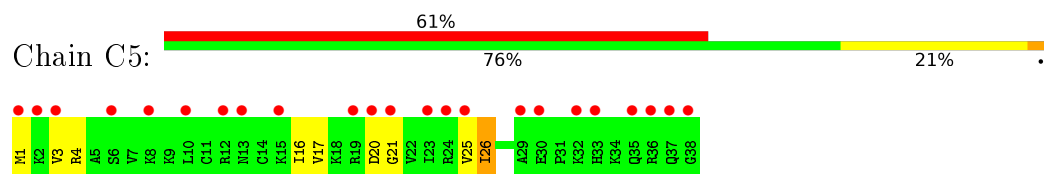
- Molecule 25: 50S ribosomal protein L35



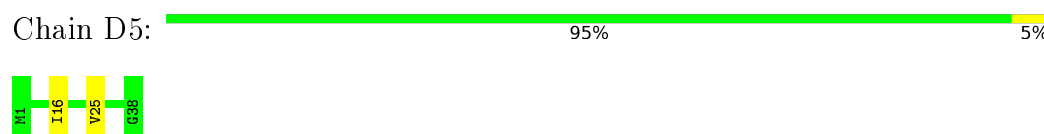
- Molecule 25: 50S ribosomal protein L35



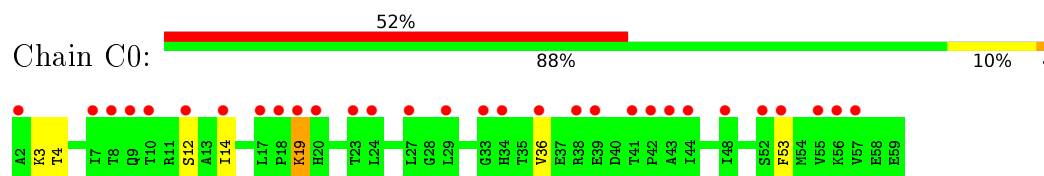
- Molecule 26: 50S ribosomal protein L36



- Molecule 26: 50S ribosomal protein L36



- Molecule 27: 50S ribosomal protein L30




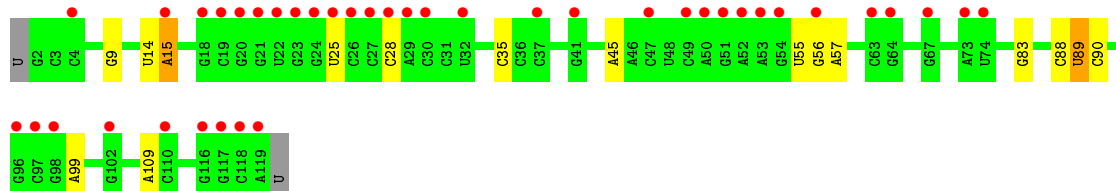
- Molecule 27: 50S ribosomal protein L30

Chain D0:  91% 9%



- Molecule 28: 5S rRNA

Chain CB:  33% 85% 12%




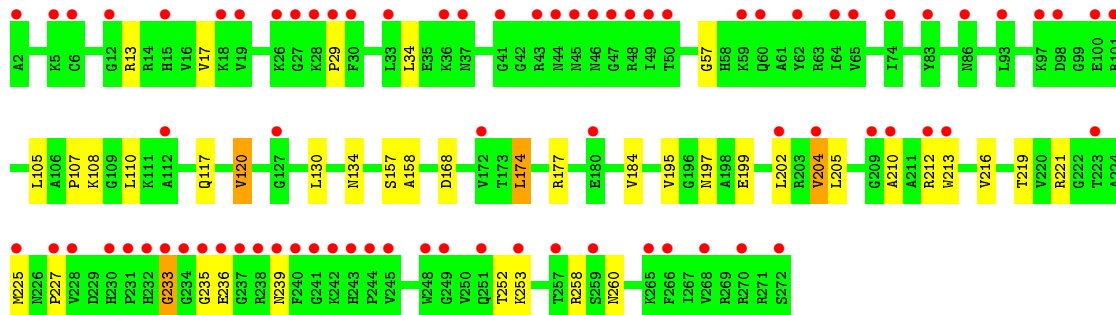
- Molecule 28: 5S rRNA

Chain DB:  91% 8%



- Molecule 29: 50S ribosomal protein L2

Chain CC:  29% 85% 14%



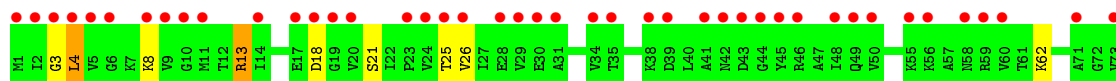
- Molecule 29: 50S ribosomal protein L2

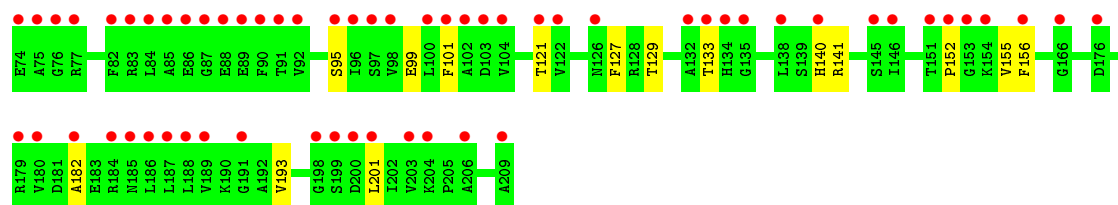
Chain DC:  91% 8%



- Molecule 30: 50S ribosomal protein L3

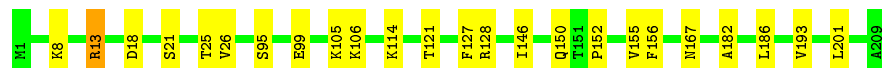
Chain CD:  49% 89% 11%





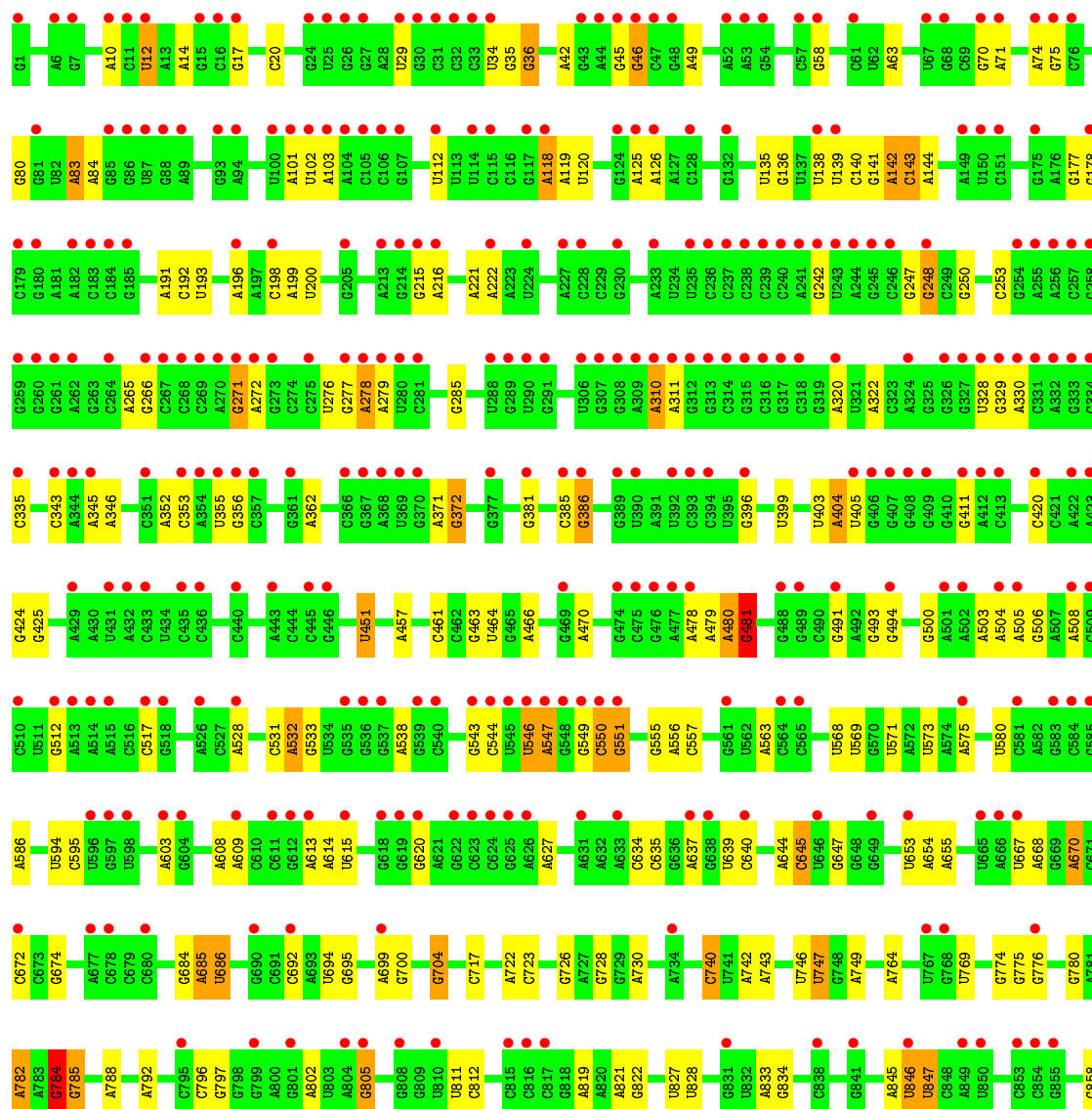
• Molecule 30: 50S ribosomal protein L3

Chain DD: 89% 11%

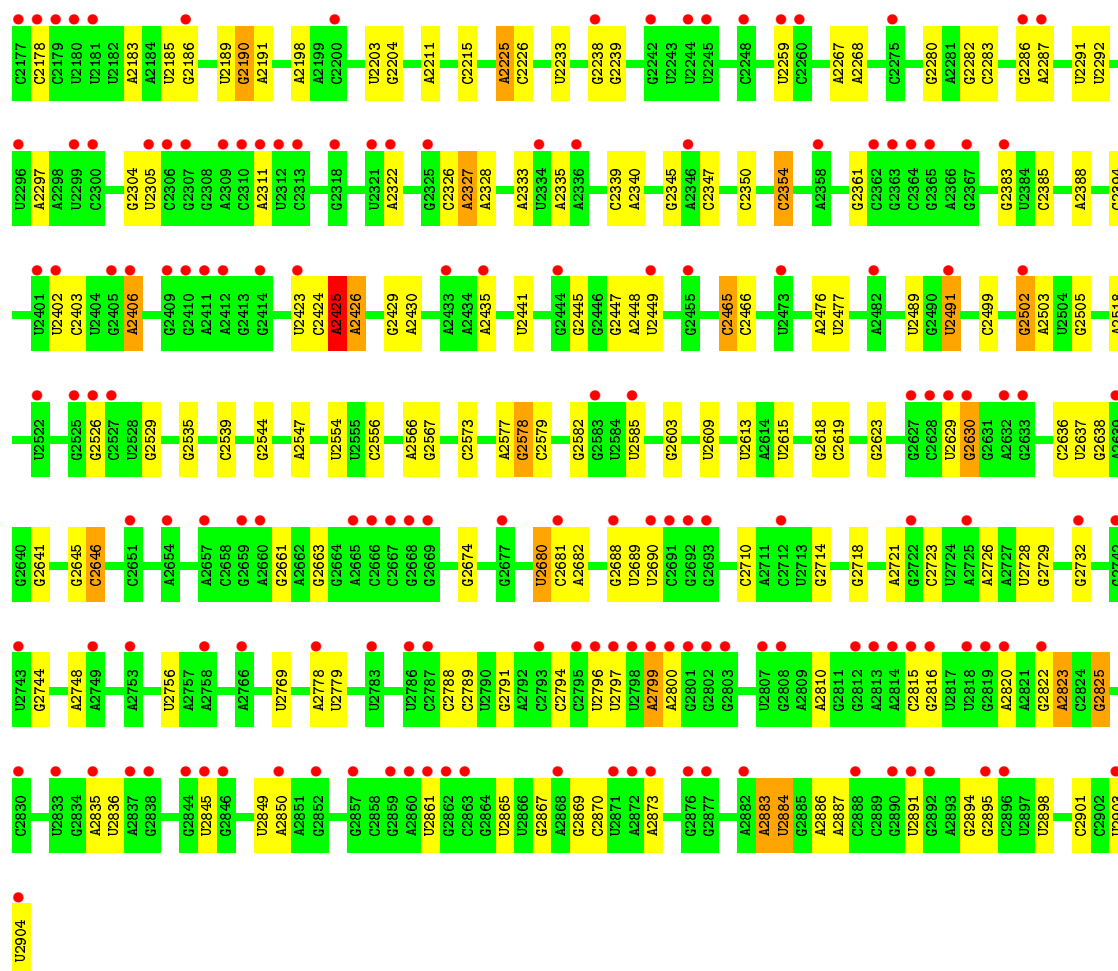


• Molecule 31: 23S rRNA

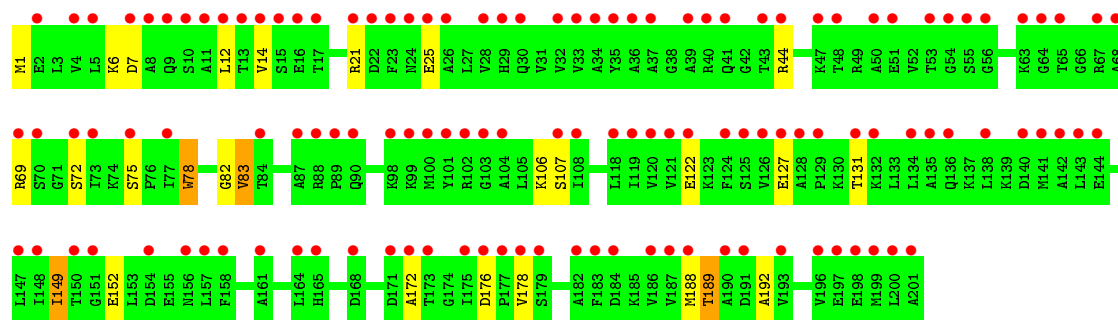
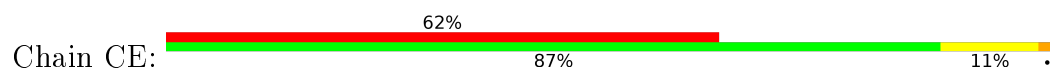
Chain CA: 31% 76% 21%



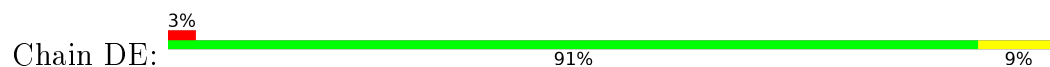




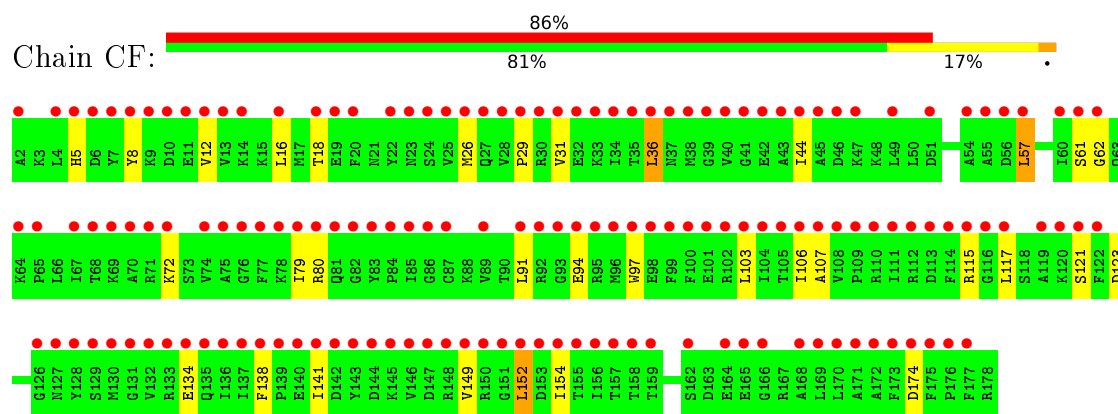
- Molecule 32: 50S ribosomal protein L4



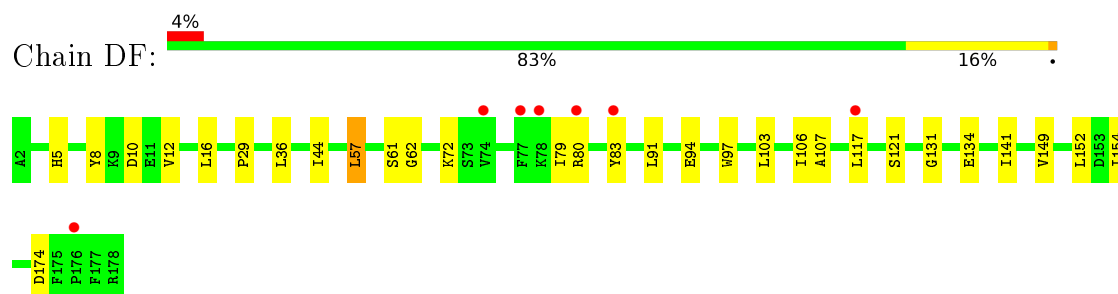
- Molecule 32: 50S ribosomal protein L4



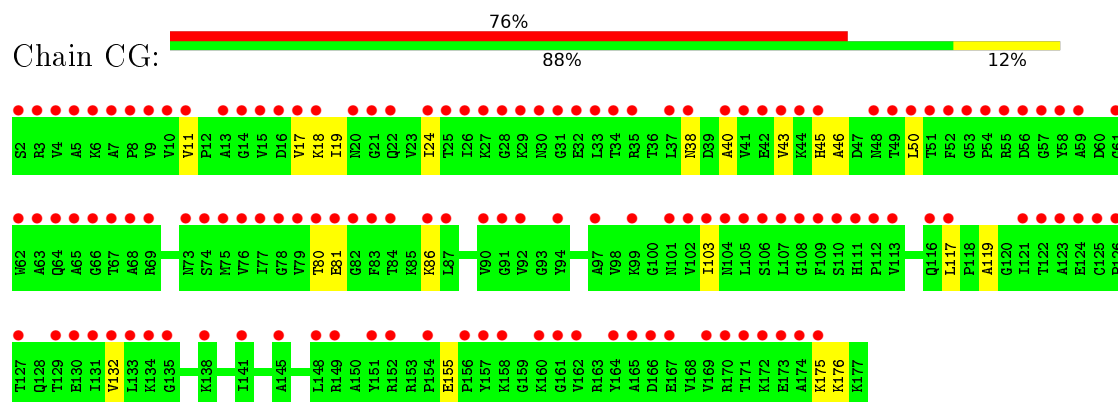
- Molecule 33: 50S ribosomal protein L5



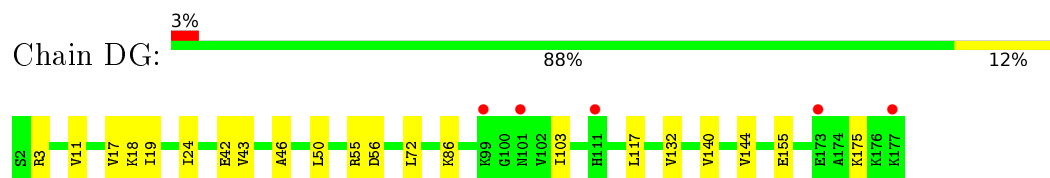
• Molecule 33: 50S ribosomal protein L5



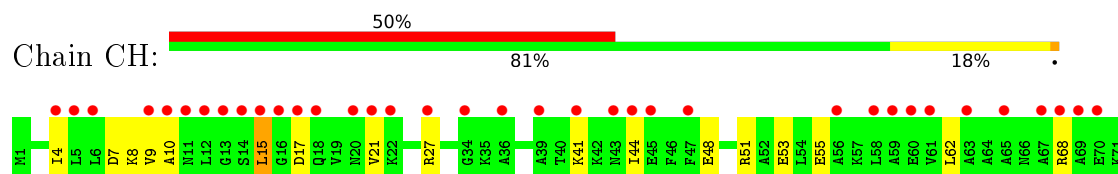
• Molecule 34: 50S ribosomal protein L6



• Molecule 34: 50S ribosomal protein L6

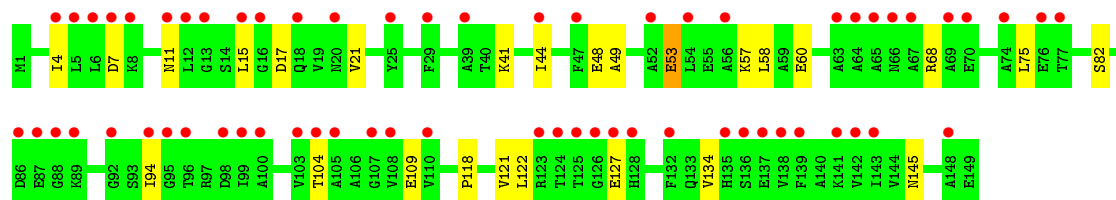
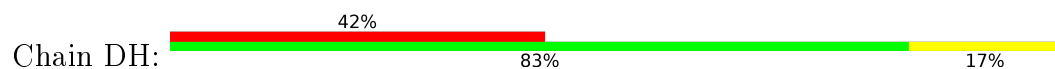


• Molecule 35: 50S ribosomal protein L9

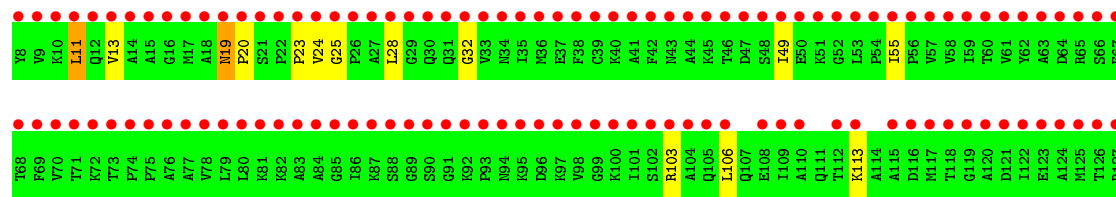
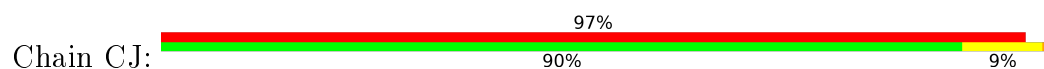




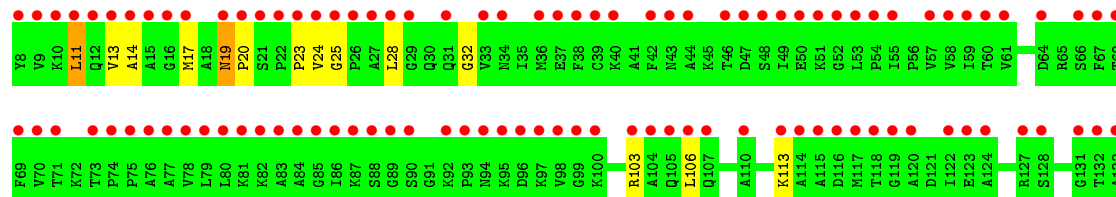
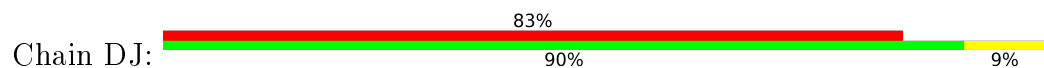
- Molecule 35: 50S ribosomal protein L9



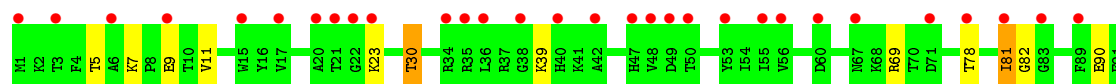
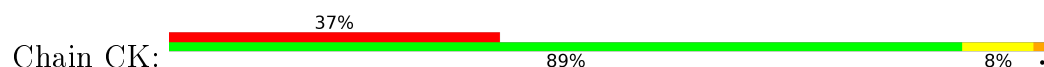
- Molecule 36: 50S ribosomal protein L11

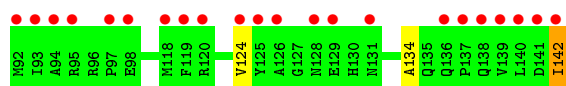


- Molecule 36: 50S ribosomal protein L11



- Molecule 37: 50S ribosomal protein L13





- Molecule 37: 50S ribosomal protein L13

Chain DK: 94% 5% .



- Molecule 38: 50S ribosomal protein L14

Chain CL: 19% 87% 11% ..



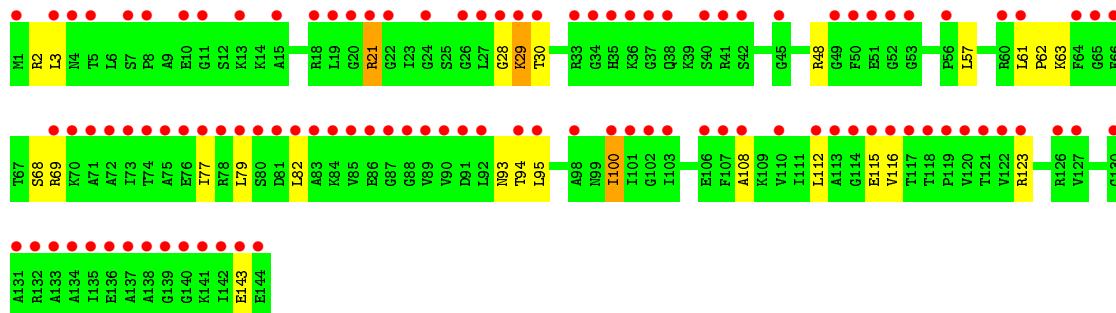
- Molecule 38: 50S ribosomal protein L14

Chain DL: 90% 8% .



- Molecule 39: 50S ribosomal protein L15

Chain CM: 74% 82% 16% .



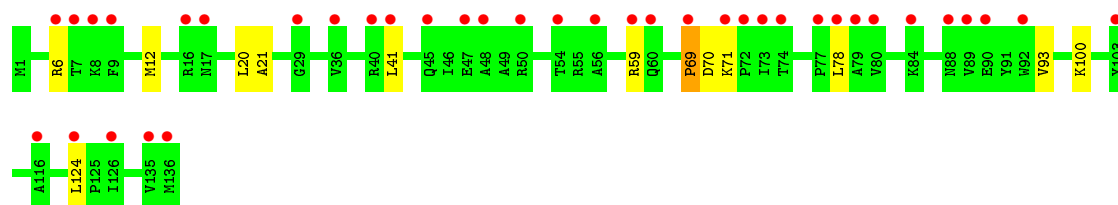
- Molecule 39: 50S ribosomal protein L15

Chain DM: 84% 15% .



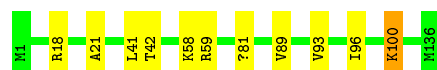
- Molecule 40: 50S ribosomal protein L16

Chain CN: 28% 90% 9% .



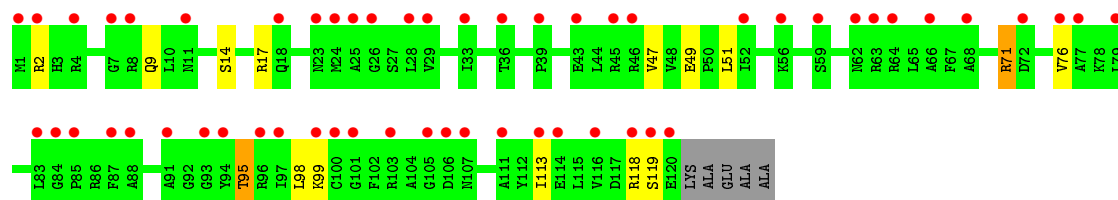
- Molecule 40: 50S ribosomal protein L16

Chain DN: 92% 7% .



- Molecule 41: 50S ribosomal protein L17

Chain CO: 44% 84% 10% . .



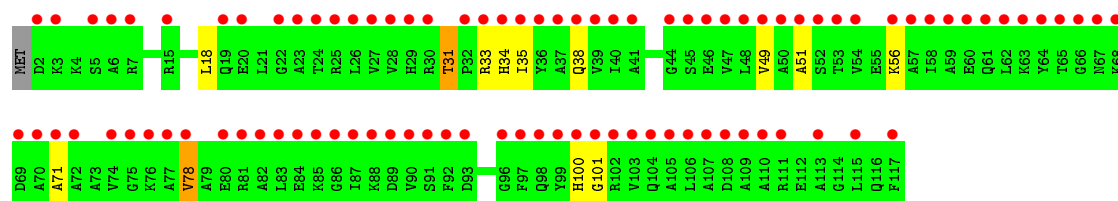
- Molecule 41: 50S ribosomal protein L17

Chain DO: 93% 7%



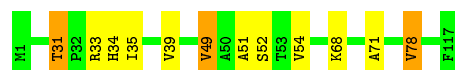
- Molecule 42: 50S ribosomal protein L18

Chain CP: 79% 88% 9% . .

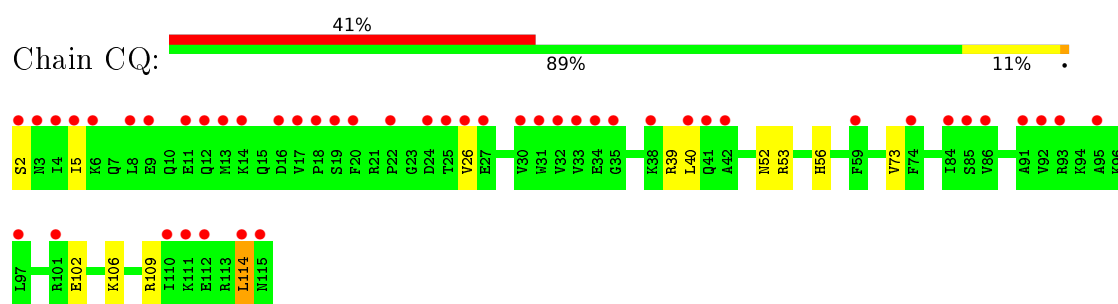


- Molecule 42: 50S ribosomal protein L18

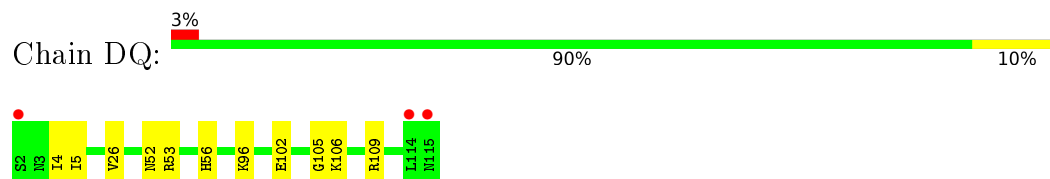
Chain DP: 90% 8% .



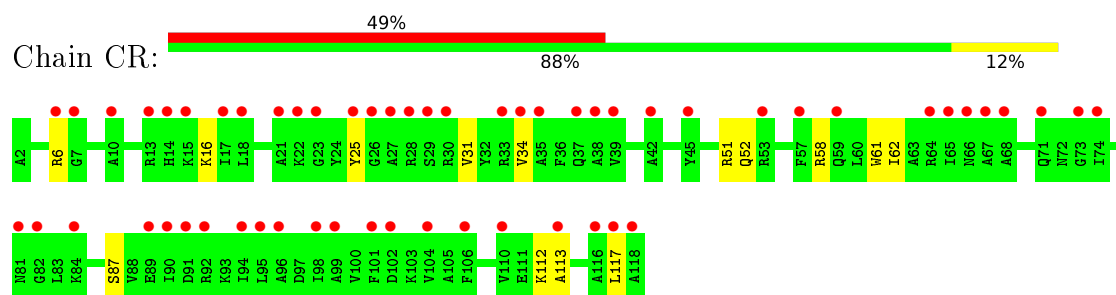
- Molecule 43: 50S ribosomal protein L19



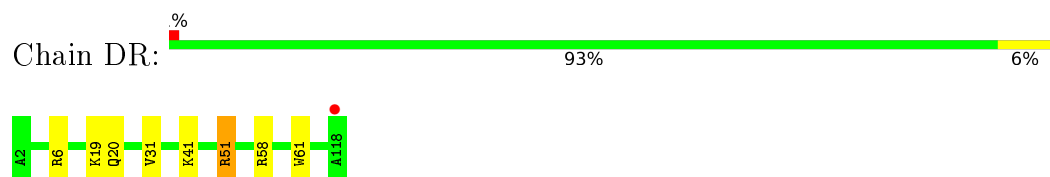
- Molecule 43: 50S ribosomal protein L19



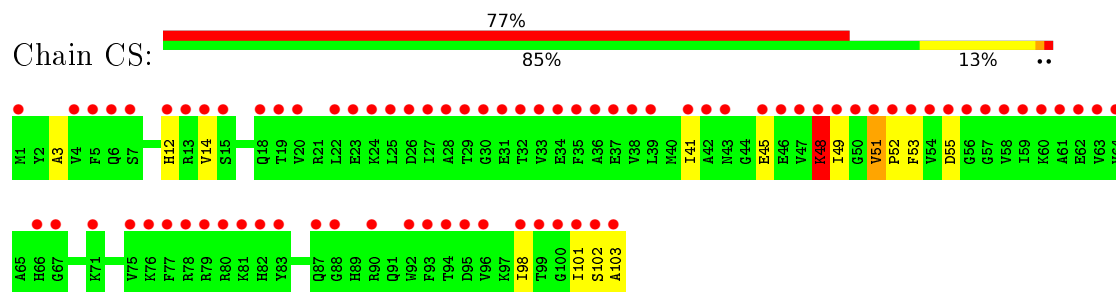
- Molecule 44: 50S ribosomal protein L20



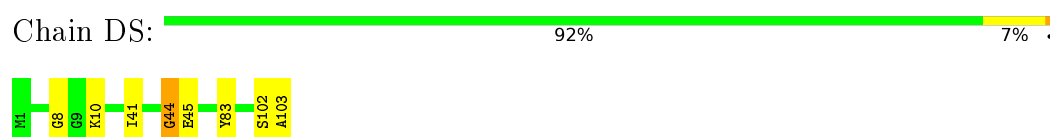
- Molecule 44: 50S ribosomal protein L20



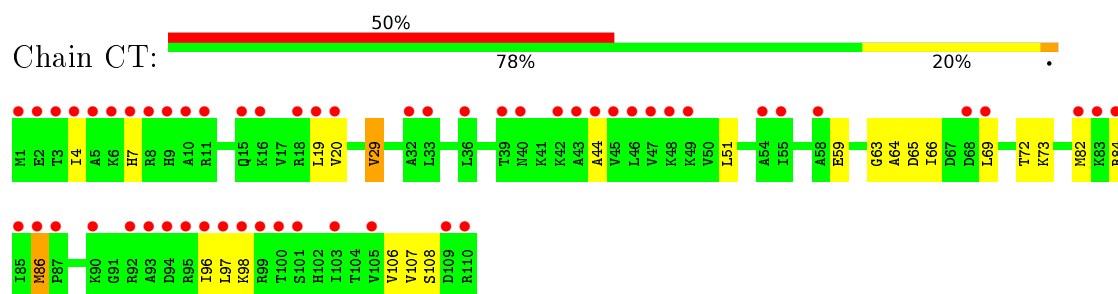
- Molecule 45: 50S ribosomal protein L21



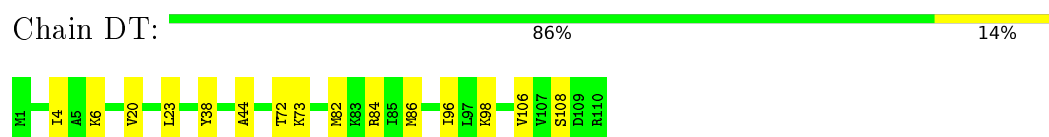
- Molecule 45: 50S ribosomal protein L21



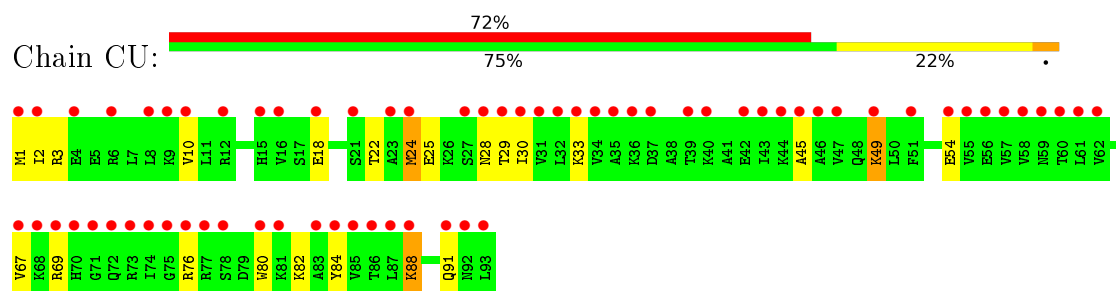
- Molecule 46: 50S ribosomal protein L22



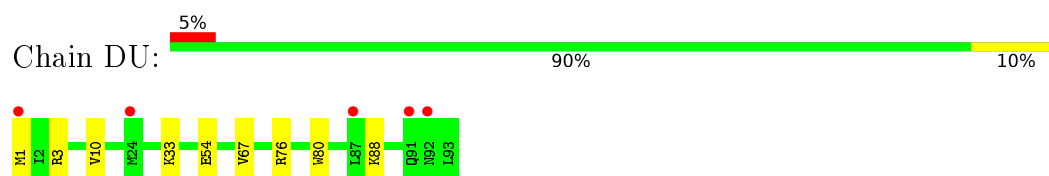
- Molecule 46: 50S ribosomal protein L22



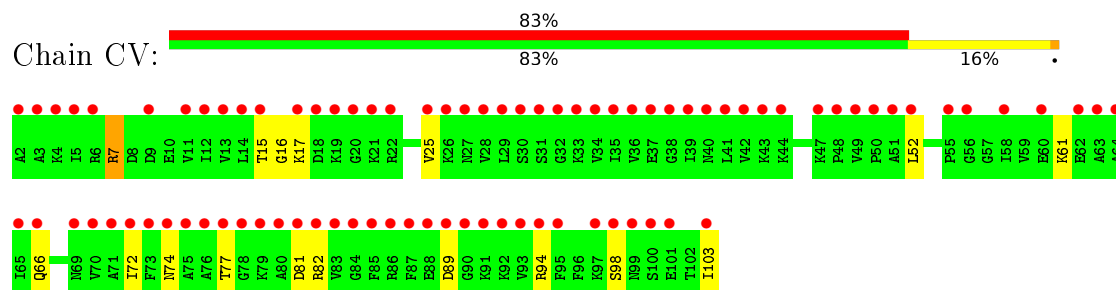
- Molecule 47: 50S ribosomal protein L23



- Molecule 47: 50S ribosomal protein L23

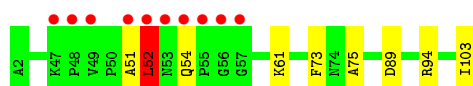


- Molecule 48: 50S ribosomal protein L24

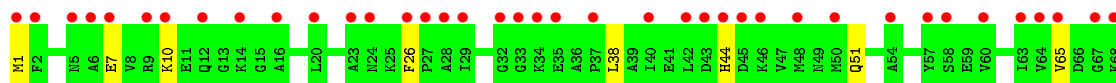
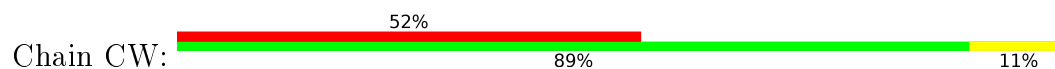


- Molecule 48: 50S ribosomal protein L24





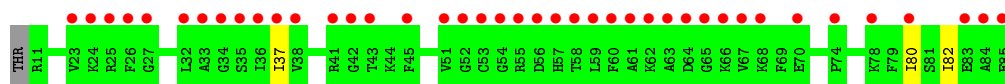
- Molecule 49: 50S ribosomal protein L25



- Molecule 49: 50S ribosomal protein L25



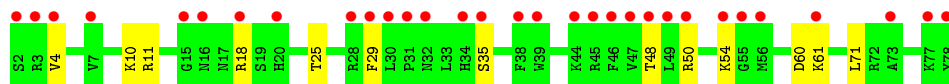
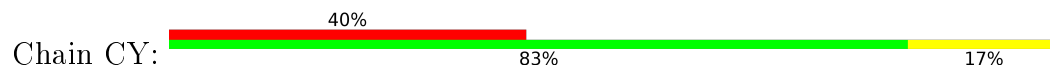
- Molecule 50: 50S ribosomal protein L27



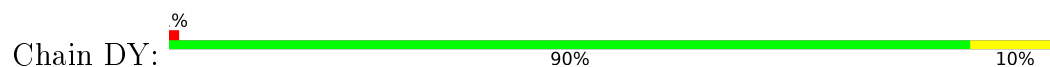
- Molecule 50: 50S ribosomal protein L27



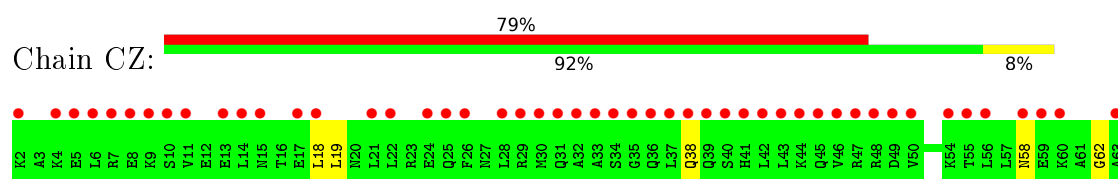
- Molecule 51: 50S ribosomal protein L28



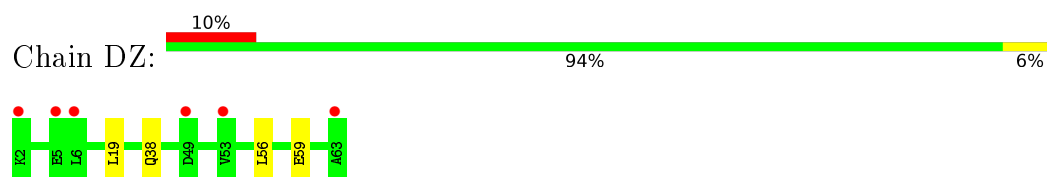
- Molecule 51: 50S ribosomal protein L28



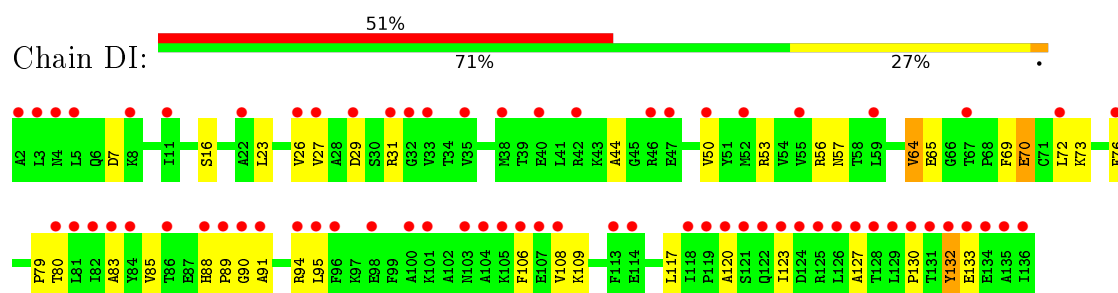
- Molecule 52: 50S ribosomal protein L29



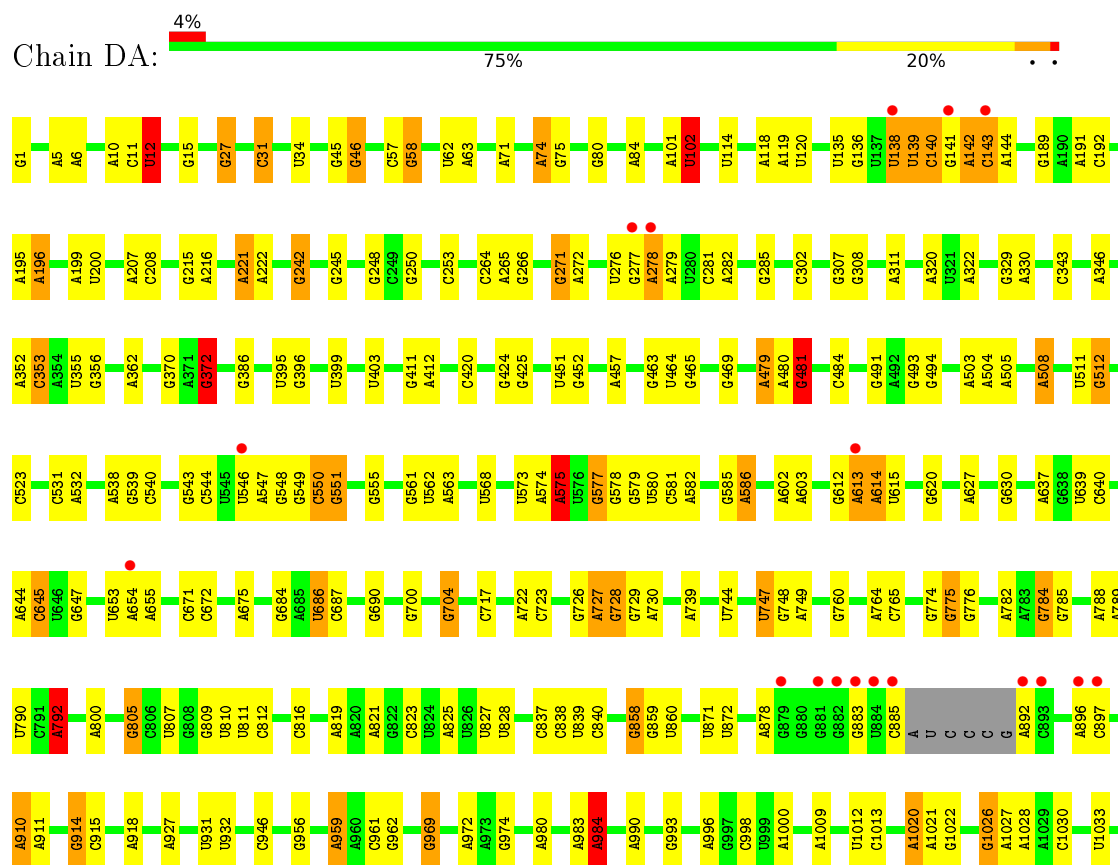
- Molecule 52: 50S ribosomal protein L29



- Molecule 53: 50S ribosomal protein L10



- Molecule 54: 23S rRNA



C2730	C2573	C2424	G2087	G1971	U1779	G1631	A1453	A1286	A1134	A1040
G2731	G2574	A2425	A2037	G1972	U1779	A1635	U1460	U1294	C1135	G1047
G2732	C2575	C2426	G2100	G1975	U1782	U1636	U1636	U1137	C1136	
G2744	G2576	C2427	G2101	U1991	A1787	A1637	G1478	G1300	U1141	A1057
A2748	G2577	U2431	G2102	G1992	A1794	C1644	G1482	A1301	A1142	U1058
U2756	G2581	A2435	U2105	U1993	C1795	C1645	A1490	C1306	C1161	U1059
G2765	G2582	U2441	U2106	C1997	A1795	C1646	G1491	G1309	U1142	U1060
A2766	U2585	G2444	G2107	A1998	C1800	U1647	G1492	G1310	C1164	U1061
	G2595	G2445	A2108	C1999	A1801	U1648	C1493	G1311	A1165	G1062
U2778	G2596	G2446	U2109	A2014	A1802	G1649	A1494	C1320	U1065	U1064
C2788	G2597	A2448	G2110	A1852	A1808	A1652	U1497	A1321	G1168	U1066
C2789	G2603	U2449	U2111	G1653	C1816	G1653	A1508	A1324	U1067	U1068
U2790	U2609	G2455	G2112	A1854	U1847	G1654	A1509	A1070	A1069	U1069
G2791	U2613	U2324	U2113	G1660	U1820	G1660	G1510	U1329	G1071	G1071
U2796	G2623	G2325	G2114	A1664	A1829	A1664	G1511	U1330	C1072	C1072
U2797	G2628	G2326	U2115	A1665	C1830	A1665	G1512	G1331	U1174	U1174
U2798	G2630	A2327	G2116	G1666	A1871	G1666	U1513	U1332	A1175	C1073
A2799	G2633	G2328	G2117	G1667	C1831	G1667	G1514	C1335	G1177	C1074
A2800	U2629	U2329	G2118	A1672	A1847	A1672	A1515	G1343	U1180	C1075
G2811	U2636	G2330	U2119	G1673	A1848	G1673	A1516	U1349	U1181	C1076
A2820	U2637	A2331	U2120	C2032	U1848	G1674	U1523	U1352	G1182	U1077
G2822	U2638	G2332	U2121	A2033	A1853	C1675	A1532	U1357	U1183	U1078
A2823	G2645	U2333	G2122	C2036	A1853	C1675	C1532	A1365	U1187	C1079
A2826	G2661	G2334	G2123	A2037	G1869	G1681	C1533	U1362	U1188	U1083
U2836	G2662	A2335	A2126	G2038	C1870	G1682	U1534	A1383	U1189	A1084
U2845	G2663	C2339	G2127	U2039	A1871	G1682	A1535	U1391	G1202	A1088
G2848	G2674	U2340	C2129	C2043	A1872	U1693	C1536	U1394	G1236	A1089
U2849	G2681	G2341	U2130	C2044	G1873	C1704	G1537	G1416	A1237	A1090
A2868	G2684	G2342	U2131	G2048	G1906	G1715	G1555	C1417	G1238	G1091
A2873	G2688	G2343	G2132	C2050	G1907	G1715	A1566	U1394	G1250	C1092
G2885	U2690	G2344	A2134	A2051	A1913	C1727	A1569	G1418	A1253	U1093
A2886	G2691	G2345	A2135	A2052	C1914	C1728	A1578	G1424	U1263	U1101
U2891	G2692	G2346	G2140	G2053	C1920	U1729	A1579	A1264	C1102	C1102
G2895	G2708	G2347	G2141	A2054	G1930	C1730	U1578	A1265	U1096	A1096
G2901	G2714	G2348	A2142	C2055	U1931	G1731	A1593	A1266	U1097	U1097
C2901	G2717	G2349	G2143	G2056	G1939	C1732	A1593	U1267	A1098	A1098
G2902	A2726	A2407	G2144	A2060	U1937	G1733	A1583	G1428	U1105	U1105
U	A2727	G2420	C2145	A2061	A1932	G1738	U1584	A1268	G1106	G1106
			G2146	A2062	G1933	A1739	C1585	A1269	G1107	G1107
			G2147	G2069	A1936	A1744	G1586	G1429	U1267	U1267
			G2148	A2070	A1937	A1744	G1588	A1430	A1268	A1268
			G2152	A2071	A1938	G1763	A1603	A1431	A1269	A1269
			C2153	C2072	U1955	C1761	C1607	G1432	G1271	G1271
			U2155	G2073	U1955	C1761	A1608	A1433	A1272	A1272
			G2156	U2074	C1965	C1764	A1608	A1434	U1273	G1125
			A2158	A2077	A1966	A1773	C1611	A1435	A1274	G1125
			C2159	C2078	C1967	A1773	A1616	G1436	G1283	G1283
			C2160	U2086	A1970	G1776	A1616	C1437	A1284	U1132
			C2161					G1452	A1285	A1133

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.31Å 434.58Å 624.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.16 – 2.80 48.14 – 2.80	Depositor EDS
% Data completeness (in resolution range)	85.7 (48.16-2.80) 85.7 (48.14-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	19.79 (at 2.81Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.209 , 0.219 0.235 , 0.245	Depositor DCC
R_{free} test set	4734 reflections (0.40%)	DCC
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 80.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	295188	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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	1.04	7/36593 (0.0%)	0.86	5/57081 (0.0%)
1	BA	1.05	10/36568 (0.0%)	0.86	5/57042 (0.0%)
2	AB	0.48	0/1784	0.65	0/2403
2	BB	0.48	0/1784	0.65	0/2403
3	AC	0.48	0/1652	0.67	0/2225
3	BC	0.47	0/1652	0.67	0/2225
4	AD	0.44	0/1665	0.69	0/2227
4	BD	0.43	0/1665	0.70	0/2227
5	AE	0.48	0/1157	0.77	0/1557
5	BE	0.51	0/1118	0.81	0/1504
6	AF	0.46	0/881	0.69	0/1189
6	BF	0.47	0/835	0.77	0/1128
7	AG	0.45	0/1196	0.61	0/1602
7	BG	0.46	0/1196	0.62	0/1602
8	AH	0.46	0/989	0.71	0/1326
8	BH	0.46	0/989	0.69	0/1326
9	AI	0.44	0/1034	0.66	0/1375
9	BI	0.44	0/1034	0.65	0/1375
10	AJ	0.44	0/806	0.67	0/1089
10	BJ	0.48	0/797	0.71	0/1077
11	AK	0.46	0/893	0.65	0/1205
11	BK	0.45	0/893	0.68	0/1205
12	AL	0.44	0/960	0.74	0/1286
12	BL	0.47	0/960	0.74	0/1286
13	AM	0.51	0/893	0.72	0/1193
13	BM	0.49	0/893	0.71	0/1193
14	AN	0.46	0/817	0.63	0/1088
14	BN	0.44	0/817	0.63	0/1088
15	AO	0.48	0/722	0.60	0/964
15	BO	0.47	0/722	0.63	0/964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	AP	0.48	0/659	0.70	0/884
16	BP	0.50	0/659	0.76	0/884
17	AQ	0.48	0/658	0.73	0/881
17	BQ	0.51	0/658	0.78	0/881
18	AR	0.53	0/463	0.65	0/621
18	BR	0.50	0/463	0.64	0/621
19	AS	0.47	0/653	0.59	0/877
19	BS	0.45	0/653	0.60	0/877
20	AT	0.48	0/676	0.66	0/895
20	BT	0.52	0/671	0.68	0/888
21	AU	0.45	0/472	0.61	0/627
21	BU	0.43	0/472	0.63	0/627
22	C1	0.49	0/450	0.71	0/599
22	D1	0.61	0/450	0.79	0/599
23	C2	0.46	0/416	0.73	0/554
23	D2	0.51	0/421	0.73	0/561
24	C3	0.46	0/380	0.69	0/498
24	D3	0.55	0/380	0.76	0/498
25	C4	0.46	0/513	0.67	0/676
25	D4	0.56	0/513	0.71	0/676
26	C5	0.43	0/303	0.77	0/397
26	D5	0.53	0/303	0.76	0/397
27	C0	0.52	0/453	0.77	0/605
27	D0	0.62	0/467	0.81	0/623
28	CB	0.98	0/2828	0.88	2/4410 (0.0%)
28	DB	1.12	1/2872 (0.0%)	0.90	0/4478
29	CC	0.45	0/2122	0.76	0/2852
29	DC	0.50	0/2122	0.76	1/2852 (0.0%)
30	CD	0.43	0/1576	0.70	0/2119
30	DD	0.54	0/1576	0.73	0/2119
31	CA	1.07	44/69165 (0.1%)	0.87	17/107896 (0.0%)
32	CE	0.45	0/1571	0.72	0/2113
32	DE	0.52	0/1571	0.72	0/2113
33	CF	0.43	0/1435	0.68	0/1926
33	DF	0.46	0/1435	0.70	0/1926
34	CG	0.42	0/1343	0.66	0/1816
34	DG	0.44	0/1343	0.64	0/1816
35	CH	0.48	0/1121	0.68	0/1515
35	DH	0.48	0/1121	0.68	0/1515
36	CJ	0.48	0/993	0.62	0/1341
36	DJ	0.48	0/993	0.62	0/1341
37	CK	0.43	0/1152	0.70	0/1551
37	DK	0.56	0/1152	0.74	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	CL	0.47	0/947	0.74	0/1268
38	DL	0.54	0/955	0.75	0/1279
39	CM	0.46	0/1062	0.74	1/1413 (0.1%)
39	DM	0.50	0/1062	0.75	1/1413 (0.1%)
40	CN	0.45	0/1081	0.75	1/1443 (0.1%)
40	DN	0.59	0/1092	0.81	0/1457
41	CO	0.46	0/973	0.72	0/1301
41	DO	0.58	0/1006	0.81	0/1345
42	CP	0.43	0/902	0.73	0/1209
42	DP	0.47	0/910	0.73	0/1219
43	CQ	0.41	0/929	0.71	0/1242
43	DQ	0.48	0/929	0.72	0/1242
44	CR	0.48	0/960	0.69	0/1278
44	DR	0.62	0/960	0.76	0/1278
45	CS	0.44	0/829	0.73	0/1107
45	DS	0.55	0/829	0.78	0/1107
46	CT	0.43	0/864	0.74	0/1156
46	DT	0.55	0/864	0.75	0/1156
47	CU	0.44	0/745	0.72	0/994
47	DU	0.48	0/745	0.72	0/994
48	CV	0.45	0/788	0.77	0/1051
48	DV	0.49	0/788	0.77	0/1051
49	CW	0.40	0/766	0.65	0/1025
49	DW	0.50	0/766	0.69	0/1025
50	CX	0.39	0/576	0.65	0/762
50	DX	0.53	0/598	0.73	0/790
51	CY	0.43	0/635	0.73	0/848
51	DY	0.46	0/635	0.72	0/848
52	CZ	0.42	0/502	0.60	0/667
52	DZ	0.43	0/502	0.60	0/667
53	DI	0.51	0/1037	0.74	1/1402 (0.1%)
54	DA	1.27	154/69364 (0.2%)	0.97	25/108207 (0.0%)
All	All	0.98	216/309263 (0.1%)	0.85	59/462195 (0.0%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	AE	0	1
10	BJ	0	1
31	CA	0	12
54	DA	0	89
All	All	0	110

All (216) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	DA	1020	A	N3-C4	9.99	1.40	1.34
31	CA	1936	A	N9-C4	-9.12	1.32	1.37
31	CA	2095	A	O5'-C5'	-9.03	1.28	1.42
54	DA	539	G	N7-C5	7.80	1.44	1.39
54	DA	195	A	N9-C4	7.60	1.42	1.37
54	DA	12	U	C1'-N1	7.56	1.60	1.48
54	DA	2097	A	O5'-C5'	-7.34	1.31	1.42
54	DA	2050	C	N1-C6	7.33	1.41	1.37
31	CA	769	U	C1'-N1	7.13	1.59	1.48
54	DA	2520	C	N1-C6	7.12	1.41	1.37
54	DA	1286	A	N3-C4	7.07	1.39	1.34
31	CA	12	U	C1'-N1	7.05	1.59	1.48
54	DA	2585	U	C1'-N1	6.98	1.59	1.48
54	DA	2060	A	N3-C4	6.97	1.39	1.34
31	CA	2425	A	C3'-O3'	6.94	1.51	1.42
54	DA	484	C	C1'-N1	6.79	1.58	1.48
1	BA	1493	A	C3'-O3'	6.79	1.51	1.42
31	CA	546	U	C1'-N1	6.78	1.58	1.48
54	DA	1665	A	N7-C5	6.69	1.43	1.39
54	DA	1787	A	N9-C4	6.63	1.41	1.37
1	BA	5	U	C1'-N1	6.53	1.58	1.48
1	BA	1397	C	N1-C2	6.52	1.46	1.40
1	BA	28	A	O5'-C5'	-6.49	1.32	1.42
54	DA	959	A	N3-C4	6.38	1.38	1.34
54	DA	2053	G	C6-N1	6.37	1.44	1.39
54	DA	671	C	C1'-N1	6.34	1.58	1.48
54	DA	1306	C	C1'-N1	6.31	1.58	1.48
31	CA	2225	A	C3'-O3'	6.30	1.50	1.42
54	DA	582	A	N9-C4	6.30	1.41	1.37
54	DA	2547	A	O5'-C5'	-6.23	1.32	1.42
54	DA	998	C	C1'-N1	6.21	1.58	1.48
54	DA	31	C	N1-C6	6.15	1.40	1.37
54	DA	2023	C	N1-C6	6.13	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	28	A	O5'-C5'	-6.11	1.33	1.42
54	DA	1000	A	N3-C4	6.10	1.38	1.34
28	DB	90	C	O5'-C5'	-6.09	1.33	1.42
54	DA	372	G	C3'-O3'	6.09	1.50	1.42
54	DA	727	A	N3-C4	6.08	1.38	1.34
54	DA	2867	G	C3'-O3'	6.07	1.50	1.42
54	DA	579	G	C2'-C1'	-6.04	1.46	1.53
1	BA	1008	U	O5'-C5'	-6.00	1.33	1.42
54	DA	972	A	C6-N6	5.98	1.38	1.33
54	DA	102	U	N1-C2	5.98	1.44	1.38
54	DA	1635	A	N3-C4	5.97	1.38	1.34
54	DA	578	G	N3-C4	5.97	1.39	1.35
54	DA	2547	A	P-O5'	-5.93	1.53	1.59
1	AA	5	U	C1'-N1	5.93	1.57	1.48
54	DA	2518	A	N9-C4	5.93	1.41	1.37
54	DA	2717	C	N1-C6	5.91	1.40	1.37
54	DA	1294	U	O5'-C5'	-5.90	1.33	1.42
54	DA	2297	A	O5'-C5'	-5.90	1.33	1.42
54	DA	984	A	N3-C4	5.90	1.38	1.34
31	CA	253	C	C1'-N1	5.88	1.57	1.48
54	DA	1137	G	N3-C4	5.86	1.39	1.35
54	DA	2756	U	C3'-O3'	5.86	1.50	1.42
54	DA	2044	C	N1-C6	5.85	1.40	1.37
54	DA	1965	C	C1'-N1	5.84	1.57	1.48
1	AA	1397	C	N1-C6	5.82	1.40	1.37
54	DA	2036	C	N1-C6	5.81	1.40	1.37
54	DA	2127	G	C3'-O3'	5.80	1.50	1.42
31	CA	1788	C	C1'-N1	5.80	1.57	1.48
54	DA	2447	G	N3-C4	5.80	1.39	1.35
54	DA	2521	C	N1-C6	5.78	1.40	1.37
31	CA	2619	C	C1'-N1	5.78	1.57	1.48
54	DA	838	C	N1-C6	5.77	1.40	1.37
54	DA	2766	A	N9-C4	5.76	1.41	1.37
54	DA	575	A	N9-C4	5.76	1.41	1.37
54	DA	969	G	C8-N7	-5.76	1.27	1.30
54	DA	1267	U	C2-N3	5.73	1.41	1.37
31	CA	2579	C	C1'-N1	5.73	1.57	1.48
54	DA	1164	C	N1-C6	5.72	1.40	1.37
31	CA	1306	C	C1'-N1	5.72	1.57	1.48
54	DA	2446	G	N3-C4	5.68	1.39	1.35
1	BA	290	C	C1'-N1	5.68	1.57	1.48
54	DA	990	A	N7-C5	5.68	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	DA	1534	U	C1'-N1	5.67	1.57	1.48
31	CA	1314	C	C1'-N1	5.65	1.57	1.48
54	DA	1189	A	N9-C4	5.64	1.41	1.37
54	DA	457	A	N3-C4	5.64	1.38	1.34
54	DA	744	U	N1-C6	5.63	1.43	1.38
54	DA	12	U	N1-C2	5.62	1.43	1.38
54	DA	1311	G	C6-N1	5.62	1.43	1.39
54	DA	508	A	N3-C4	5.61	1.38	1.34
54	DA	2426	A	N3-C4	5.61	1.38	1.34
54	DA	1021	A	N9-C4	5.58	1.41	1.37
54	DA	1660	G	O5'-C5'	-5.58	1.33	1.42
31	CA	1658	C	C1'-N1	5.57	1.57	1.48
54	DA	1965	C	C3'-O3'	-5.56	1.34	1.42
54	DA	823	C	N1-C6	5.56	1.40	1.37
1	BA	485	U	N1-C2	5.55	1.43	1.38
54	DA	2576	G	O3'-P	-5.53	1.54	1.61
54	DA	1920	C	C1'-N1	5.53	1.57	1.48
54	DA	2425	A	C3'-O3'	5.52	1.49	1.42
54	DA	2444	G	N7-C5	5.51	1.42	1.39
31	CA	2680	U	C3'-O3'	5.50	1.49	1.42
54	DA	739	A	N3-C4	5.50	1.38	1.34
54	DA	2056	G	C6-N1	5.50	1.43	1.39
1	BA	575	G	C3'-O3'	5.50	1.49	1.42
54	DA	821	A	N3-C4	5.48	1.38	1.34
31	CA	2006	C	C1'-N1	5.46	1.56	1.48
54	DA	2821	A	N3-C4	5.45	1.38	1.34
54	DA	613	A	N9-C4	5.43	1.41	1.37
31	CA	995	C	O5'-C5'	-5.42	1.34	1.42
31	CA	2233	U	C1'-N1	5.42	1.56	1.48
54	DA	561	G	N3-C4	5.41	1.39	1.35
54	DA	810	U	N1-C2	5.39	1.43	1.38
54	DA	1133	A	O5'-C5'	-5.39	1.34	1.42
31	CA	2146	C	C3'-O3'	5.39	1.49	1.42
54	DA	12	U	P-O5'	5.38	1.65	1.59
31	CA	946	C	C1'-N1	5.38	1.56	1.48
31	CA	2823	A	C3'-O3'	5.38	1.49	1.42
1	AA	1203	C	C1'-N1	5.37	1.56	1.48
54	DA	918	A	N3-C4	5.36	1.38	1.34
54	DA	962	G	N3-C4	5.36	1.39	1.35
54	DA	1274	A	N7-C5	-5.36	1.36	1.39
54	DA	469	G	N3-C4	5.36	1.39	1.35
54	DA	196	A	N9-C4	5.35	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	DA	816	C	N1-C6	5.35	1.40	1.37
54	DA	1270	C	N1-C6	5.35	1.40	1.37
54	DA	2692	G	N3-C4	5.35	1.39	1.35
31	CA	1825	U	C1'-N1	5.35	1.56	1.48
31	CA	404	A	C3'-O3'	5.34	1.49	1.42
54	DA	809	G	N7-C5	5.34	1.42	1.39
54	DA	2730	C	N1-C6	5.34	1.40	1.37
54	DA	653	U	C1'-N1	5.33	1.56	1.48
54	DA	959	A	N9-C4	5.33	1.41	1.37
54	DA	819	A	N3-C4	5.31	1.38	1.34
54	DA	1268	A	N3-C4	5.31	1.38	1.34
54	DA	1664	A	N9-C4	5.31	1.41	1.37
54	DA	613	A	C3'-O3'	5.31	1.49	1.42
31	CA	451	U	C1'-N1	5.30	1.56	1.48
54	DA	2036	C	C1'-N1	5.29	1.56	1.48
31	CA	461	C	C1'-N1	5.29	1.56	1.48
31	CA	653	U	C1'-N1	5.29	1.56	1.48
31	CA	1629	U	C1'-N1	5.27	1.56	1.48
54	DA	1265	A	N9-C4	5.27	1.41	1.37
1	BA	842	U	C3'-O3'	5.27	1.49	1.42
54	DA	2273	A	N3-C4	5.27	1.38	1.34
31	CA	480	A	N9-C4	5.26	1.41	1.37
31	CA	2723	C	C1'-N1	5.26	1.56	1.48
31	CA	557	C	C1'-N1	5.25	1.56	1.48
54	DA	271	G	C3'-O3'	5.25	1.49	1.42
54	DA	27	G	C6-N1	5.23	1.43	1.39
54	DA	2521	C	C1'-N1	5.22	1.56	1.48
1	AA	575	G	C3'-O3'	5.22	1.49	1.42
54	DA	2288	A	N3-C4	5.22	1.38	1.34
54	DA	512	G	N9-C4	5.22	1.42	1.38
31	CA	198	C	C1'-N1	5.21	1.56	1.48
54	DA	264	C	N1-C2	5.20	1.45	1.40
54	DA	2211	A	C3'-O3'	5.20	1.49	1.42
54	DA	1675	C	N1-C6	5.19	1.40	1.37
54	DA	2585	U	N1-C2	5.19	1.43	1.38
31	CA	1771	C	C1'-N1	5.19	1.56	1.48
31	CA	2646	C	C1'-N1	5.18	1.56	1.48
54	DA	2033	A	P-O5'	5.18	1.65	1.59
31	CA	672	C	C1'-N1	5.18	1.56	1.48
54	DA	2901	C	C1'-N1	5.18	1.56	1.48
1	BA	291	U	C1'-N1	5.17	1.56	1.48
31	CA	1971	U	C1'-N1	5.17	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	DA	2354	C	O5'-C5'	-5.17	1.34	1.42
54	DA	1776	G	O5'-C5'	-5.16	1.34	1.42
54	DA	1284	A	N3-C4	5.15	1.38	1.34
54	DA	1965	C	O5'-C5'	-5.15	1.34	1.42
54	DA	2077	A	N3-C4	5.15	1.38	1.34
54	DA	2427	C	N1-C6	5.15	1.40	1.37
54	DA	1584	U	C1'-N1	5.14	1.56	1.48
54	DA	577	G	N3-C4	5.13	1.39	1.35
54	DA	562	U	N1-C6	5.13	1.42	1.38
54	DA	792	A	N3-C4	5.12	1.38	1.34
54	DA	2581	G	C3'-O3'	5.12	1.49	1.42
54	DA	911	A	N3-C4	5.12	1.38	1.34
54	DA	2496	C	O5'-C5'	-5.11	1.34	1.42
54	DA	1030	C	N1-C6	5.11	1.40	1.37
54	DA	581	C	C1'-N1	5.10	1.56	1.48
54	DA	2301	C	C1'-N1	5.10	1.56	1.48
54	DA	585	G	N9-C4	5.10	1.42	1.38
31	CA	2354	C	C1'-N1	5.10	1.56	1.48
31	CA	2465	C	C1'-N1	5.10	1.56	1.48
54	DA	2708	G	N3-C4	5.10	1.39	1.35
54	DA	1704	C	C1'-N1	5.09	1.56	1.48
54	DA	684	G	N3-C4	5.09	1.39	1.35
54	DA	1331	G	N3-C4	5.08	1.39	1.35
1	AA	290	C	C1'-N1	5.08	1.56	1.48
54	DA	353	C	C1'-N1	5.08	1.56	1.48
54	DA	1607	C	N1-C6	5.08	1.40	1.37
31	CA	2756	U	C3'-O3'	5.08	1.49	1.42
54	DA	1335	C	C1'-N1	5.08	1.56	1.48
54	DA	1611	C	N1-C6	5.08	1.40	1.37
54	DA	195	A	N3-C4	5.07	1.37	1.34
31	CA	2215	C	C1'-N1	5.07	1.56	1.48
54	DA	1253	A	O5'-C5'	-5.07	1.34	1.42
54	DA	2406	A	P-O5'	5.07	1.64	1.59
31	CA	2901	C	C1'-N1	5.07	1.56	1.48
54	DA	1644	C	C1'-N1	5.07	1.56	1.48
54	DA	114	U	C1'-N1	5.06	1.56	1.48
54	DA	2455	G	C3'-O3'	-5.06	1.35	1.42
54	DA	465	G	N3-C4	5.06	1.39	1.35
54	DA	2471	A	N3-C4	5.05	1.37	1.34
54	DA	1637	A	N7-C5	5.05	1.42	1.39
31	CA	692	C	C1'-N1	5.04	1.56	1.48
54	DA	12	U	C3'-O3'	5.04	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	15	G	N3-C4	5.04	1.39	1.35
31	CA	2044	C	C1'-N1	5.03	1.56	1.48
31	CA	20	C	C1'-N1	5.03	1.56	1.48
31	CA	1704	C	C1'-N1	5.03	1.56	1.48
54	DA	672	C	N1-C6	5.02	1.40	1.37
54	DA	140	C	C1'-N1	5.01	1.56	1.48
54	DA	1437	C	O5'-C5'	-5.01	1.34	1.42
54	DA	2158	A	C3'-O3'	5.01	1.49	1.42
54	DA	511	U	C1'-N1	5.01	1.56	1.48
54	DA	2585	U	C3'-O3'	5.01	1.49	1.42
54	DA	1999	C	N1-C6	5.01	1.40	1.37
54	DA	2826	A	C8-N7	-5.00	1.28	1.31
54	DA	574	A	O5'-C5'	-5.00	1.34	1.42
54	DA	1020	A	C6-N1	5.00	1.39	1.35
54	DA	2402	U	P-O5'	5.00	1.64	1.59

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	CB	15	A	O4'-C1'-N9	10.09	116.27	108.20
54	DA	512	G	O4'-C1'-N9	8.48	114.99	108.20
1	AA	413	G	C1'-O4'-C4'	-8.21	103.34	109.90
54	DA	784	G	P-O3'-C3'	7.87	129.15	119.70
40	CN	69	PRO	C-N-CA	7.39	140.17	121.70
54	DA	1936	A	O4'-C1'-N9	7.29	114.03	108.20
1	AA	1	A	OP1-P-OP2	-7.17	108.84	119.60
54	DA	2820	A	P-O3'-C3'	7.12	128.24	119.70
54	DA	892	A	OP1-P-OP2	-7.03	109.05	119.60
53	DI	132	TYR	C-N-CA	7.00	139.21	121.70
31	CA	892	A	OP1-P-OP2	-6.96	109.16	119.60
54	DA	1	G	OP1-P-OP2	-6.87	109.30	119.60
1	BA	1362	A	C1'-O4'-C4'	-6.83	104.44	109.90
31	CA	974	G	N9-C1'-C2'	6.74	122.76	114.00
1	BA	2	A	OP1-P-OP2	-6.69	109.56	119.60
31	CA	271	G	P-O3'-C3'	6.45	127.44	119.70
54	DA	271	G	P-O3'-C3'	6.44	127.42	119.70
1	AA	413	G	O4'-C1'-N9	6.41	113.33	108.20
54	DA	2848	G	O4'-C1'-N9	6.25	113.20	108.20
54	DA	1311	G	O4'-C1'-N9	6.14	113.11	108.20
31	CA	2425	A	P-O3'-C3'	5.95	126.84	119.70
31	CA	512	G	O4'-C1'-N9	5.88	112.90	108.20
31	CA	451	U	C1'-O4'-C4'	-5.87	105.21	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	842	U	P-O3'-C3'	5.84	126.71	119.70
54	DA	1379	U	P-O3'-C3'	5.78	126.63	119.70
39	DM	60	ARG	CG-CD-NE	5.73	123.84	111.80
1	BA	485	U	O4'-C1'-N1	5.70	112.76	108.20
31	CA	1379	U	P-O3'-C3'	5.69	126.53	119.70
31	CA	784	G	P-O3'-C3'	5.69	126.53	119.70
54	DA	704	G	O4'-C1'-N9	5.61	112.69	108.20
54	DA	242	G	C3'-C2'-C1'	-5.59	97.03	101.50
54	DA	2406	A	C5'-C4'-O4'	-5.57	102.41	109.10
54	DA	1434	A	O4'-C1'-N9	5.41	112.53	108.20
54	DA	27	G	O4'-C1'-N9	5.37	112.50	108.20
1	BA	1397	C	C2-N1-C1'	5.35	124.69	118.80
29	DC	156	ARG	CB-CG-CD	-5.33	97.73	111.60
54	DA	1165	A	O4'-C1'-N9	5.33	112.46	108.20
31	CA	2035	G	C1'-O4'-C4'	-5.29	105.67	109.90
31	CA	2095	A	C5'-C4'-C3'	-5.28	107.55	116.00
31	CA	2225	A	P-O3'-C3'	5.25	126.01	119.70
31	CA	704	G	O4'-C1'-N9	5.25	112.40	108.20
31	CA	2825	G	O4'-C1'-N9	5.21	112.37	108.20
54	DA	512	G	C1'-O4'-C4'	-5.20	105.74	109.90
54	DA	2280	G	C4'-C3'-C2'	-5.20	97.40	102.60
31	CA	242	G	C3'-C2'-C1'	-5.19	97.35	101.50
39	CM	68	SER	C-N-CA	5.19	134.67	121.70
54	DA	479	A	C3'-C2'-C1'	-5.18	97.35	101.50
54	DA	2645	G	O4'-C1'-N9	5.18	112.35	108.20
31	CA	2406	A	C5'-C4'-O4'	5.18	115.31	109.10
54	DA	807	U	C4'-C3'-C2'	-5.17	97.43	102.60
1	AA	841	C	P-O3'-C3'	5.14	125.87	119.70
54	DA	1238	G	C4'-C3'-C2'	-5.12	97.48	102.60
28	CB	89	U	O4'-C1'-N1	5.10	112.28	108.20
54	DA	1997	C	C4'-C3'-C2'	-5.10	97.50	102.60
54	DA	2048	G	C8-N9-C4	-5.09	104.36	106.40
31	CA	2447	G	C3'-C2'-C1'	-5.06	97.45	101.50
1	AA	890	G	C3'-C2'-C1'	-5.05	97.46	101.50
54	DA	2447	G	C3'-C2'-C1'	-5.04	97.47	101.50
31	CA	974	G	C3'-C2'-C1'	-5.03	97.47	101.50

There are no chirality outliers.

All (110) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1432	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	362	G	Sidechain
1	AA	898	G	Sidechain
5	AE	82	GLN	Sidechain
1	BA	1432	G	Sidechain
1	BA	362	G	Sidechain
1	BA	575	G	Sidechain
1	BA	898	G	Sidechain
10	BJ	37	ARG	Mainchain
31	CA	1693	U	Sidechain
31	CA	1777	U	Sidechain
31	CA	1936	A	Sidechain
31	CA	1937	A	Sidechain
31	CA	2267	A	Sidechain
31	CA	2638	G	Sidechain
31	CA	2732	G	Sidechain
31	CA	463	G	Sidechain
31	CA	481	G	Sidechain
31	CA	704	G	Sidechain
31	CA	726	G	Sidechain
31	CA	805	G	Sidechain
54	DA	1009	A	Sidechain
54	DA	1142	A	Sidechain
54	DA	1236	G	Sidechain
54	DA	1253	A	Sidechain
54	DA	1283	G	Sidechain
54	DA	1311	G	Sidechain
54	DA	1324	G	Sidechain
54	DA	1343	G	Sidechain
54	DA	1425	G	Sidechain
54	DA	15	G	Sidechain
54	DA	1631	G	Sidechain
54	DA	1645	G	Sidechain
54	DA	1666	G	Sidechain
54	DA	1667	G	Sidechain
54	DA	1672	A	Sidechain
54	DA	1681	G	Sidechain
54	DA	1682	G	Sidechain
54	DA	1693	U	Sidechain
54	DA	1753	G	Sidechain
54	DA	1761	C	Sidechain
54	DA	1779	U	Sidechain
54	DA	1802	A	Sidechain

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Mol	Chain	Res	Type	Group
54	DA	1938	A	Sidechain
54	DA	2029	G	Sidechain
54	DA	2037	A	Sidechain
54	DA	2048	G	Sidechain
54	DA	2074	U	Sidechain
54	DA	2078	C	Sidechain
54	DA	221	A	Sidechain
54	DA	2250	G	Sidechain
54	DA	2266	A	Sidechain
54	DA	2267	A	Sidechain
54	DA	2282	G	Sidechain
54	DA	2328	A	Sidechain
54	DA	2375	G	Sidechain
54	DA	2382	G	Sidechain
54	DA	2405	G	Sidechain
54	DA	2468	A	Sidechain
54	DA	2481	G	Sidechain
54	DA	2489	U	Sidechain
54	DA	2497	A	Sidechain
54	DA	250	G	Sidechain
54	DA	2516	A	Sidechain
54	DA	2517	C	Sidechain
54	DA	2529	G	Sidechain
54	DA	2564	A	Sidechain
54	DA	2566	A	Sidechain
54	DA	2581	G	Sidechain
54	DA	2582	G	Sidechain
54	DA	2595	G	Sidechain
54	DA	2597	G	Sidechain
54	DA	2638	G	Sidechain
54	DA	2645	G	Sidechain
54	DA	2688	G	Sidechain
54	DA	27	G	Sidechain
54	DA	2727	A	Sidechain
54	DA	2732	G	Sidechain
54	DA	2848	G	Sidechain
54	DA	307	G	Sidechain
54	DA	308	G	Sidechain
54	DA	395	U	Sidechain
54	DA	452	G	Sidechain
54	DA	463	G	Sidechain
54	DA	464	U	Sidechain

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Mol	Chain	Res	Type	Group
54	DA	481	G	Sidechain
54	DA	512	G	Sidechain
54	DA	555	G	Sidechain
54	DA	575	A	Sidechain
54	DA	577	G	Sidechain
54	DA	58	G	Sidechain
54	DA	630	G	Sidechain
54	DA	675	A	Sidechain
54	DA	690	G	Sidechain
54	DA	700	G	Sidechain
54	DA	704	G	Sidechain
54	DA	726	G	Sidechain
54	DA	727	A	Sidechain
54	DA	728	G	Sidechain
54	DA	748	G	Sidechain
54	DA	774	G	Sidechain
54	DA	775	G	Sidechain
54	DA	800	A	Sidechain
54	DA	805	G	Sidechain
54	DA	858	G	Sidechain
54	DA	910	A	Sidechain
54	DA	956	G	Sidechain
54	DA	959	A	Sidechain
54	DA	980	A	Sidechain
54	DA	984	A	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32930	0	16591	90	0
1	BA	32908	0	16580	98	0
2	AB	1753	0	1780	10	0
2	BB	1753	0	1780	14	0
3	AC	1625	0	1696	14	0
3	BC	1625	0	1696	18	0
4	AD	1643	0	1707	13	0
4	BD	1643	0	1707	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AE	1144	0	1185	15	0
5	BE	1105	0	1148	30	0
6	AF	862	0	864	7	0
6	BF	817	0	808	8	0
7	AG	1182	0	1238	7	0
7	BG	1182	0	1238	4	0
8	AH	979	0	1031	8	0
8	BH	979	0	1031	4	0
9	AI	1022	0	1070	6	0
9	BI	1022	0	1070	6	0
10	AJ	796	0	836	11	0
10	BJ	787	0	828	10	0
11	AK	877	0	887	14	0
11	BK	877	0	887	17	0
12	AL	957	0	1017	7	0
12	BL	957	0	1017	10	0
13	AM	884	0	941	10	0
13	BM	884	0	941	11	0
14	AN	805	0	844	8	0
14	BN	805	0	844	8	0
15	AO	714	0	734	1	0
15	BO	714	0	734	0	0
16	AP	649	0	666	3	0
16	BP	649	0	666	5	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	5	0
18	AR	456	0	478	5	0
18	BR	456	0	478	3	0
19	AS	638	0	665	7	0
19	BS	638	0	665	9	0
20	AT	670	0	719	2	0
20	BT	665	0	714	8	0
21	AU	465	0	491	2	0
21	BU	465	0	491	2	0
22	C1	444	0	458	21	0
22	D1	444	0	458	13	0
23	C2	409	0	440	4	0
23	D2	414	0	442	5	0
24	C3	377	0	418	9	0
24	D3	377	0	418	5	0
25	C4	504	0	572	7	0
25	D4	504	0	572	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	C5	302	0	340	7	0
26	D5	302	0	340	1	0
27	C0	449	0	488	3	0
27	D0	463	0	504	1	0
28	CB	2529	0	1281	5	0
28	DB	2569	0	1301	5	0
29	CC	2083	0	2154	17	0
29	DC	2083	0	2154	11	0
30	CD	1565	0	1614	16	0
30	DD	1576	0	1627	16	0
31	CA	62229	0	31318	213	0
32	CE	1552	0	1619	13	0
32	DE	1552	0	1619	11	0
33	CF	1411	0	1444	15	0
33	DF	1411	0	1444	11	0
34	CG	1323	0	1371	9	0
34	DG	1323	0	1371	9	0
35	CH	1110	0	1148	7	0
35	DH	1110	0	1148	6	0
36	CJ	979	0	1028	5	0
36	DJ	979	0	1028	4	0
37	CK	1129	0	1162	10	0
37	DK	1129	0	1162	4	0
38	CL	938	0	1012	8	0
38	DL	946	0	1023	6	0
39	CM	1053	0	1129	16	0
39	DM	1053	0	1129	15	0
40	CN	1075	0	1154	5	0
40	DN	1092	0	1177	7	0
41	CO	960	0	1000	7	0
41	DO	993	0	1034	5	0
42	CP	892	0	923	6	0
42	DP	900	0	935	9	0
43	CQ	917	0	962	7	0
43	DQ	917	0	962	7	0
44	CR	947	0	1019	13	0
44	DR	947	0	1019	9	0
45	CS	816	0	839	8	0
45	DS	816	0	839	5	0
46	CT	857	0	922	12	0
46	DT	857	0	922	10	0
47	CU	739	0	807	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	DU	739	0	807	4	0
48	CV	780	0	831	6	0
48	DV	780	0	831	4	0
49	CW	753	0	780	5	0
49	DW	753	0	780	3	0
50	CX	569	0	581	1	0
50	DX	591	0	606	7	0
51	CY	625	0	652	7	0
51	DY	625	0	652	4	0
52	CZ	501	0	531	0	0
52	DZ	501	0	531	1	0
53	DI	1023	0	1052	19	0
54	DA	62423	0	31411	171	0
55	AA	71	0	0	0	0
55	BA	43	0	0	0	0
55	C3	1	0	0	0	0
55	CA	155	0	0	0	0
55	CB	3	0	0	0	0
55	DA	182	0	0	0	0
55	DB	9	0	0	0	0
55	DD	2	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	0	0
56	DA	26	0	36	2	0
56	DQ	13	0	18	0	0
56	DR	13	0	18	5	0
56	DS	13	0	18	1	0
57	AA	16	0	28	0	0
57	DA	40	0	70	5	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	72	0	144	10	0
59	AA	32	0	21	1	0
59	BA	32	0	21	1	0
60	AB	1	0	0	0	0
60	C5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
61	DA	35	0	50	1	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
62	DA	36	0	54	2	0
62	DB	8	0	12	1	0
63	D1	10	0	14	2	0
63	D3	10	0	14	0	0
63	DA	40	0	56	5	0
63	DD	10	0	14	2	0
63	DS	10	0	14	0	0
63	DU	10	0	14	1	0
64	DA	40	0	76	4	0
65	DA	32	0	44	0	0
66	DA	12	0	11	0	0
67	DA	11	0	5	0	0
68	DA	8	0	12	1	0
69	AA	507	0	0	0	0
69	AC	4	0	0	0	0
69	AD	2	0	0	0	0
69	AE	4	0	0	0	0
69	AF	1	0	0	0	0
69	AG	1	0	0	0	0
69	AH	1	0	0	0	0
69	AJ	2	0	0	0	0
69	AK	5	0	0	0	0
69	AL	8	0	0	0	0
69	AM	4	0	0	1	0
69	AN	5	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	AS	1	0	0	0	0
69	AT	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	BE	1	0	0	0	0
69	BF	1	0	0	0	0
69	BK	1	0	0	0	0
69	BL	3	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	BR	1	0	0	0	0
69	BT	4	0	0	0	0
69	BU	2	0	0	0	0
69	C3	3	0	0	1	0
69	C4	2	0	0	0	0
69	CA	692	0	0	1	0
69	CB	13	0	0	0	0
69	CC	10	0	0	0	0
69	CD	5	0	0	0	0
69	CE	7	0	0	0	0
69	CL	1	0	0	0	0
69	CM	3	0	0	0	0
69	CO	1	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	27	0	0	0	0
69	D1	42	0	0	0	0
69	D2	7	0	0	0	0
69	D3	24	0	0	0	0
69	D4	33	0	0	1	0
69	D5	13	0	0	0	0
69	DA	4834	0	0	7	0
69	DB	212	0	0	0	0
69	DC	102	0	0	0	0
69	DD	105	0	0	1	0
69	DE	63	0	0	0	0
69	DF	14	0	0	0	0
69	DG	6	0	0	0	0
69	DH	2	0	0	0	0
69	DK	58	0	0	0	0
69	DL	51	0	0	0	0
69	DM	62	0	0	0	0
69	DN	71	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	DO	44	0	0	0	0
69	DP	35	0	0	0	0
69	DQ	27	0	0	1	0
69	DR	64	0	0	0	0
69	DS	51	0	0	0	0
69	DT	69	0	0	1	0
69	DU	17	0	0	0	0
69	DV	19	0	0	0	0
69	DW	31	0	0	0	0
69	DX	30	0	0	1	0
69	DY	9	0	0	0	0
69	DZ	7	0	0	0	0
All	All	295188	0	194452	1182	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 2.

All (1182) 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	1.32	1.05
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.43	0.98
31:CA:1936:A:H2	31:CA:1943:U:H3	1.01	0.98
47:CU:28:ASN:HD21	47:CU:91:GLN:HB3	1.29	0.96
14:AN:66:GLN:HB2	69:AN:205:HOH:O	1.67	0.95
26:C5:3:VAL:HG11	31:CA:2539:C:H5'	1.50	0.93
39:CM:82:LEU:HD11	39:CM:116:VAL:HG23	1.52	0.92
45:CS:14:VAL:CG2	45:CS:98:ILE:HG13	1.99	0.90
5:AE:77:ASN:HB2	5:AE:82:GLN:NE2	1.86	0.90
39:CM:77:ILE:HD11	39:CM:108:ALA:HB1	1.55	0.89
8:BH:87:LYS:HB2	8:BH:125:ILE:HD11	1.55	0.87
31:CA:1005:C:O2'	37:CK:30:THR:HG21	1.75	0.86
5:BE:77:ASN:HB2	5:BE:82:GLN:NE2	1.91	0.86
8:AH:87:LYS:HB2	8:AH:125:ILE:HD11	1.58	0.85
31:CA:2796:U:H3	31:CA:2799:A:H61	1.22	0.85
31:CA:1779:U:H5	31:CA:1784:A:N7	1.74	0.85
1:BA:1305:G:H21	1:BA:1332:A:H2	1.24	0.83
54:DA:2796:U:H3	54:DA:2799:A:H61	1.21	0.83
11:BK:88:GLY:H	11:BK:114:THR:HG22	1.43	0.83
2:BB:23:TRP:HB3	2:BB:39:HIS:CE1	2.14	0.82
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1305:G:H21	1:AA:1332:A:H2	1.23	0.81
31:CA:740:C:H5'	31:CA:1784:A:H3'	1.62	0.81
32:CE:149:ILE:HG12	32:CE:188:MET:HG2	1.62	0.81
12:BL:65:SER:HB2	12:BL:82:ILE:HD11	1.62	0.81
13:BM:114:LYS:HB3	13:BM:115:PRO:HD3	1.62	0.80
54:DA:2033:A:H5'	69:DA:4112:HOH:O	1.81	0.80
45:CS:14:VAL:HG21	45:CS:98:ILE:CG1	2.11	0.79
2:BB:20:THR:HA	2:BB:39:HIS:CE1	2.18	0.79
1:BA:9:G:H5'	5:BE:108:GLY:HA3	1.63	0.79
44:DR:20:GLN:CG	56:DR:202:PG4:H42	2.12	0.79
40:DN:18[A]:ARG:HG2	28:DB:90:C:H5'	1.64	0.78
44:DR:20:GLN:HG3	56:DR:202:PG4:H42	1.64	0.78
54:DA:135:U:H3	54:DA:144:A:H61	1.32	0.77
34:DG:24:ILE:HD11	34:DG:43:VAL:HG11	1.66	0.77
22:C1:38:HIS:HE1	31:CA:2884:U:O4	1.67	0.77
34:CG:24:ILE:HD11	34:CG:43:VAL:HG11	1.66	0.77
31:CA:135:U:H3	31:CA:144:A:H61	1.33	0.77
13:BM:22:ILE:HB	13:BM:25:VAL:CG1	2.15	0.77
54:DA:568:U:H1'	54:DA:2030:6MZ:H9C1	1.66	0.77
22:C1:4:GLN:HA	31:CA:2615:U:C2	2.20	0.76
1:BA:664:G:H22	1:BA:741:G:H1	1.34	0.76
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.66	0.76
38:CL:38:ILE:HD11	38:CL:112:PHE:HZ	1.49	0.76
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.68	0.75
1:AA:664:G:H22	1:AA:741:G:H1	1.34	0.75
10:AJ:7:ARG:HB3	10:AJ:101:SER:HB2	1.69	0.74
4:AD:107:PHE:HB3	4:AD:145:ILE:HD11	1.70	0.74
4:BD:107:PHE:HB3	4:BD:145:ILE:HD11	1.70	0.73
13:BM:83:LEU:HD21	19:BS:65:GLU:HB2	1.70	0.73
31:CA:528:A:C2	31:CA:2043:C:H4'	2.23	0.73
3:BC:123:GLN:HB3	3:BC:128:VAL:HG21	1.69	0.73
1:AA:842:U:H4'	1:AA:843:U:OP1	1.88	0.73
1:BA:522:C:H5	12:BL:50:ARG:HH12	1.37	0.73
1:BA:1060:U:C5	3:BC:2:GLY:HA3	2.23	0.73
13:BM:6:GLY:HA3	13:BM:66:GLU:HG3	1.69	0.73
24:C3:7:PRO:HB2	31:CA:1309:G:H4'	1.71	0.72
54:DA:2127:G:H4'	54:DA:2128:G:OP1	1.90	0.72
1:AA:1492:A:H5''	12:AL:44:LYS:HG2	1.71	0.71
38:DL:38:ILE:HD11	38:DL:112:PHE:HZ	1.53	0.71
1:AA:73:C:HO2'	1:AA:74:A:H8	1.38	0.70
1:BA:202:G:HO2'	1:BA:468:A:H8	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:CT:86:MET:HB2	46:CT:96:ILE:HD11	1.73	0.70
54:DA:1913:A:H4'	54:DA:1913:A:OP1	1.90	0.70
54:DA:2255:G:H21	68:DA:3219:TRS:H12	1.56	0.70
31:CA:1936:A:H2	31:CA:1943:U:N3	1.83	0.70
31:CA:846:U:H1'	31:CA:847:U:H5	1.56	0.70
25:D4:54:ASP:HB3	39:DM:57:LEU:HD22	1.74	0.70
54:DA:2628:C:H5'	58:DA:3195:PUT:H12	1.73	0.69
31:CA:1478:G:H1	31:CA:1513:U:H3	1.39	0.69
53:DI:64:VAL:HG22	53:DI:69:PHE:HB2	1.75	0.69
54:DA:1478:G:H1	54:DA:1513:U:H3	1.38	0.68
2:BB:23:TRP:HB3	2:BB:39:HIS:HE1	1.56	0.68
33:CF:36:LEU:HD21	33:CF:91:LEU:HD11	1.76	0.68
25:C4:60:ALA:O	39:CM:48:ARG:HD2	1.94	0.68
58:DA:3195:PUT:H11	69:DA:5709:HOH:O	1.94	0.68
4:BD:201:VAL:HG11	5:BE:103:THR:HB	1.76	0.67
11:BK:88:GLY:N	11:BK:114:THR:HG22	2.09	0.67
22:C1:15:MET:HB3	31:CA:2045:C:O3'	1.94	0.67
51:CY:4:VAL:HG22	51:CY:11:ARG:HG3	1.75	0.67
38:DL:30:ARG:HD2	54:DA:2674:G:H4'	1.76	0.67
48:DV:52:LEU:HB3	48:DV:54:GLN:HB2	1.77	0.67
31:CA:674:G:H1'	32:CE:69:ARG:HD2	1.77	0.67
31:CA:45:G:H5''	31:CA:46:G:H5'	1.76	0.67
42:DP:39:VAL:HB	42:DP:49:VAL:HG23	1.76	0.66
1:BA:73:C:HO2'	1:BA:74:A:H8	1.43	0.66
1:BA:502:A:OP1	12:BL:115:SER:HB2	1.95	0.66
1:BA:451:A:H2'	69:BA:1701:HOH:O	1.94	0.66
22:D1:55:ILE:HD12	41:DO:33:ILE:HD11	1.78	0.66
1:AA:202:G:HO2'	1:AA:468:A:H8	1.44	0.66
39:CM:79:LEU:HD11	39:CM:112:LEU:HD12	1.77	0.66
34:CG:80:THR:HG23	34:CG:81:GLU:H	1.60	0.65
54:DA:45:G:H5''	54:DA:46:G:H5'	1.77	0.65
30:CD:133:THR:HG22	31:CA:1993:U:H4'	1.78	0.65
24:D3:7:PRO:HB2	54:DA:1309:G:H4'	1.78	0.65
31:CA:1250:G:H5''	44:CR:6:ARG:HD3	1.79	0.65
12:BL:110:ARG:HB2	12:BL:119:VAL:HG21	1.78	0.64
31:CA:974:G:H8	31:CA:990:A:H62	1.46	0.64
1:AA:502:A:OP1	12:AL:115:SER:HB2	1.97	0.64
1:AA:412:A:H3'	1:AA:413:G:H5'	1.79	0.64
1:BA:841:C:H3'	1:BA:842:U:C5'	2.27	0.64
33:DF:61:SER:HB2	33:DF:91:LEU:HD21	1.79	0.64
12:BL:43:LYS:HD2	12:BL:91:PRO:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C3:12:ARG:HD2	24:C3:44:VAL:HG11	1.80	0.64
22:C1:43:ILE:HG22	22:C1:49:TYR:HB2	1.80	0.63
33:CF:61:SER:HB2	33:CF:91:LEU:HD21	1.80	0.63
31:CA:1105:U:H2'	31:CA:1106:G:C8	2.33	0.63
29:CC:29:PRO:HG2	29:CC:34:LEU:HD11	1.80	0.63
54:DA:1105:U:H2'	54:DA:1106:G:C8	2.33	0.63
54:DA:31:C:O3'	54:DA:1238:G:H5''	1.98	0.63
17:BQ:14:SER:HB3	17:BQ:22:VAL:HG12	1.80	0.63
38:CL:76:VAL:HG12	43:CQ:73:VAL:HB	1.81	0.63
46:CT:82:MET:HB2	46:CT:98:LYS:HB2	1.79	0.63
54:DA:2256:G:H21	56:DA:3193:PG4:H31	1.63	0.63
39:DM:77:ILE:HD11	39:DM:101:ILE:CG2	2.29	0.63
20:BT:9:LYS:O	20:BT:12:ILE:HG13	1.98	0.62
31:CA:17:G:H4'	44:CR:25:TYR:HE2	1.62	0.62
44:DR:20:GLN:HG2	56:DR:202:PG4:H51	1.81	0.62
54:DA:1482:G:H1'	54:DA:1509:A:H61	1.65	0.62
31:CA:2728:U:HO2'	31:CA:2729:G:H8	1.47	0.62
17:AQ:17:MET:HG2	17:AQ:20:SER:HB2	1.82	0.62
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	1.80	0.62
29:DC:29:PRO:HG2	29:DC:34:LEU:HD11	1.82	0.62
5:BE:72:ILE:HG12	5:BE:145:GLU:HG3	1.80	0.62
24:C3:30:VAL:HG13	31:CA:466:A:H5''	1.81	0.62
54:DA:788:A:H3'	58:DA:3221:PUT:H41	1.82	0.62
42:DP:31:THR:HG21	28:DB:28:C:OP1	2.00	0.62
1:BA:209:U:H4'	1:BA:210:C:OP2	2.01	0.61
5:AE:77:ASN:HB2	5:AE:82:GLN:HE22	1.61	0.61
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.82	0.61
22:D1:43:ILE:HG22	22:D1:49:TYR:HB2	1.82	0.61
16:BP:20:VAL:HG13	16:BP:32:PHE:HB2	1.82	0.61
19:BS:6:LYS:HD2	19:BS:7:LYS:H	1.65	0.61
54:DA:1847:A:HO2'	54:DA:1848:A:H8	1.48	0.61
63:DD:301:PGE:H12	54:DA:2623:G:OP1	2.01	0.61
2:BB:41:ILE:HD13	2:BB:202:GLY:HA2	1.83	0.61
35:CH:15:LEU:HD22	35:CH:15:LEU:H	1.66	0.61
25:C4:54:ASP:HB3	39:CM:57:LEU:HD22	1.82	0.61
44:DR:20:GLN:HG2	56:DR:202:PG4:H42	1.81	0.60
32:DE:48:THR:HG23	32:DE:88:ARG:NH1	2.16	0.60
12:AL:110:ARG:HB2	12:AL:119:VAL:HG21	1.81	0.60
33:CF:31:VAL:CG1	33:CF:97:TRP:CH2	2.84	0.60
29:CC:17:VAL:HB	29:CC:204:VAL:HG13	1.83	0.60
46:DT:82:MET:HB2	46:DT:98:LYS:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1323:G:H2'	1:BA:1324:A:C8	2.36	0.60
31:CA:1482:G:H1'	31:CA:1509:A:H61	1.66	0.60
47:DU:80:TRP:HB3	63:DU:101:PGE:H32	1.84	0.60
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.49	0.60
13:AM:33:ILE:HD11	13:AM:63:PHE:HE1	1.66	0.60
46:CT:59:GLU:HA	46:CT:64:ALA:HA	1.82	0.60
1:BA:843:U:H5''	1:BA:843:U:H6	1.67	0.59
22:C1:25:VAL:HG13	22:C1:26:THR:H	1.67	0.59
31:CA:528:A:H3'	31:CA:528:A:H8	1.67	0.59
1:BA:978:A:HO2'	1:BA:1322:C:H5	1.51	0.59
1:BA:9:G:H4'	5:BE:109:GLY:H	1.66	0.59
31:CA:1779:U:C5	31:CA:1784:A:N7	2.64	0.59
1:AA:1238:A:H5'	1:AA:1336:C:H41	1.68	0.59
2:AB:41:ILE:HD13	2:AB:202:GLY:HA2	1.82	0.59
5:BE:104:GLY:HA3	5:BE:122:ASN:HA	1.83	0.59
44:DR:31:VAL:HG13	54:DA:580:U:O3'	2.02	0.59
1:BA:1141:C:HO2'	1:BA:1142:G:H8	1.51	0.59
31:CA:528:A:H3'	31:CA:528:A:C8	2.38	0.59
32:DE:33:VAL:HG22	57:DA:3192:MPD:H12	1.84	0.59
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.38	0.59
1:AA:451:A:H61	1:AA:481:G:H5'	1.67	0.59
31:CA:1847:A:HO2'	31:CA:1848:A:H8	1.48	0.59
1:AA:202:G:H21	1:AA:466:A:H61	1.51	0.58
26:C5:16:ILE:HD13	26:C5:25:VAL:HG22	1.85	0.58
31:CA:372:G:H5''	51:CY:61:LYS:HD3	1.83	0.58
44:DR:19:LYS:HB3	56:DR:202:PG4:H41	1.85	0.58
31:CA:2728:U:O2'	31:CA:2729:G:H5''	2.04	0.58
1:BA:841:C:H3'	1:BA:842:U:H5''	1.85	0.58
54:DA:2128:G:H1	54:DA:2160:C:H42	1.52	0.58
11:AK:34:ILE:HG12	11:AK:70:CYS:SG	2.43	0.58
13:BM:22:ILE:HB	13:BM:25:VAL:HG12	1.86	0.58
5:BE:133:PRO:O	5:BE:137:VAL:HG12	2.02	0.58
22:C1:38:HIS:CE1	31:CA:2884:U:O4	2.54	0.58
54:DA:12:U:O2	54:DA:12:U:H2'	2.04	0.58
1:BA:946:A:H2'	1:BA:947:G:C8	2.38	0.58
41:CO:49:GLU:OE2	41:CO:95:THR:HG22	2.04	0.58
1:AA:946:A:H2'	1:AA:947:G:C8	2.39	0.58
54:DA:1105:U:H2'	54:DA:1106:G:H8	1.68	0.58
30:DD:114:LYS:HE2	54:DA:2681:C:OP2	2.04	0.58
23:C2:35:GLU:HG2	23:C2:50:LYS:HG2	1.86	0.58
35:CH:41:LYS:HA	35:CH:44:ILE:HG12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:120:VAL:HG12	29:CC:134:ASN:ND2	2.19	0.57
18:AR:36:SER:HA	18:AR:72:ASP:HB3	1.87	0.57
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.86	0.57
1:BA:209:U:O2	1:BA:209:U:H2'	2.03	0.57
7:BG:113:ASP:HB2	7:BG:119:ARG:HG3	1.86	0.57
1:AA:1492:A:C5'	12:AL:44:LYS:HG2	2.33	0.57
31:CA:550:C:H2'	31:CA:551:G:H5''	1.86	0.57
26:D5:16:ILE:HD13	26:D5:25:VAL:HG22	1.86	0.57
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.86	0.57
31:CA:1105:U:H2'	31:CA:1106:G:H8	1.68	0.57
31:CA:1703:G:H2'	31:CA:1704:C:C6	2.40	0.57
33:CF:36:LEU:HD21	33:CF:91:LEU:CD1	2.34	0.57
35:CH:27:ARG:HH11	51:CY:60:ASP:HA	1.70	0.57
32:DE:189:THR:HG22	32:DE:192:ALA:H	1.69	0.57
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.86	0.57
1:BA:1238:A:H5'	1:BA:1336:C:H41	1.68	0.57
39:CM:28:GLY:O	39:CM:29:LYS:O	2.21	0.57
46:CT:66:ILE:HA	46:CT:69:LEU:HD22	1.87	0.57
47:CU:24:MET:HG2	47:CU:29:THR:O	2.05	0.57
34:DG:42:GLU:HG2	34:DG:55:ARG:HH21	1.68	0.57
1:AA:1141:C:HO2'	1:AA:1142:G:H8	1.52	0.57
29:DC:120:VAL:HG12	29:DC:134:ASN:ND2	2.20	0.57
35:DH:41:LYS:HA	35:DH:44:ILE:HG12	1.86	0.57
1:AA:81:A:H61	1:AA:86:G:H1	1.53	0.56
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.87	0.56
7:AG:22:LEU:HD12	7:AG:62:PHE:HE2	1.69	0.56
1:BA:451:A:H61	1:BA:481:G:H5'	1.69	0.56
22:C1:49:TYR:OH	31:CA:2883:A:OP1	2.22	0.56
22:D1:8:PRO:HG2	54:DA:1264:A:H5'	1.86	0.56
22:C1:19:HIS:CD2	31:CA:2046:G:H1'	2.41	0.56
32:CE:189:THR:HG22	32:CE:192:ALA:H	1.71	0.56
31:CA:2394:C:H5''	39:CM:63:LYS:HE2	1.88	0.56
30:DD:146:ILE:HD12	30:DD:155:VAL:HG21	1.87	0.56
40:DN:18[B]:ARG:HG3	28:DB:90:C:H5'	1.88	0.56
5:BE:77:ASN:HB2	5:BE:82:GLN:HE22	1.69	0.56
31:CA:2095:A:H8	31:CA:2095:A:H5''	1.70	0.56
54:DA:62:U:O4'	57:DA:3203:MPD:H31	2.05	0.56
39:DM:77:ILE:HD11	39:DM:101:ILE:HG21	1.87	0.56
1:AA:8:A:C6	4:AD:206:LYS:HB3	2.40	0.56
1:BA:1012:A:H61	1:BA:1017:U:H3	1.54	0.56
54:DA:550:C:H2'	54:DA:551:G:H5''	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:DQ:96:LYS:HE3	69:DQ:306:HOH:O	2.04	0.56
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.36	0.56
1:AA:1277:C:HO2'	1:AA:1279:G:H8	1.53	0.56
11:AK:67:ALA:HB2	11:AK:96:THR:HG23	1.88	0.56
23:D2:35:GLU:HG2	23:D2:50:LYS:HG2	1.86	0.56
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.36	0.55
13:BM:86:TYR:CZ	13:BM:90:ARG:HD2	2.41	0.55
31:CA:2304:G:H5'	33:CF:121:SER:HB2	1.88	0.55
24:D3:4:THR:HG22	54:DA:687:C:H1'	1.88	0.55
1:AA:1012:A:H61	1:AA:1017:U:H3	1.55	0.55
1:BA:619:U:H3	4:BD:131:ASN:HB3	1.71	0.55
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.89	0.55
24:C3:30:VAL:CG1	31:CA:466:A:H5''	2.36	0.55
31:CA:457:A:N1	31:CA:470:A:H5''	2.21	0.55
10:AJ:5:ARG:HE	10:AJ:77:VAL:HG22	1.70	0.55
1:BA:1106:G:H5''	3:BC:172:ARG:HG3	1.87	0.55
54:DA:31:C:O2'	54:DA:1238:G:H5'	2.06	0.55
8:AH:29:SER:HB3	8:AH:57:PRO:HB2	1.88	0.55
3:BC:77:ILE:HA	3:BC:84:VAL:HG23	1.88	0.55
1:AA:412:A:H3'	1:AA:413:G:C5'	2.37	0.55
10:AJ:35:GLN:HB2	10:AJ:77:VAL:HB	1.88	0.55
1:BA:1151:A:HO2'	1:BA:1152:A:H8	1.53	0.55
4:BD:85:ASN:HB3	4:BD:88:GLU:HB2	1.89	0.55
5:BE:72:ILE:HG13	5:BE:73:ASN:H	1.72	0.55
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	1.89	0.55
31:CA:2822:G:H2'	31:CA:2823:A:H5''	1.88	0.55
54:DA:2297:A:H5''	54:DA:2297:A:C8	2.42	0.55
13:AM:86:TYR:CZ	13:AM:90:ARG:HD2	2.41	0.55
47:CU:22:THR:HA	47:CU:25:GLU:HG2	1.87	0.55
11:BK:89:PRO:HG3	21:BU:32:VAL:HG11	1.88	0.54
31:CA:2502:G:H5''	31:CA:2503:2MA:H5''	1.89	0.54
28:CB:55:U:H1'	33:CF:26:MET:HG3	1.89	0.54
11:BK:67:ALA:HB2	11:BK:96:THR:HG23	1.88	0.54
11:AK:31:ILE:HG12	11:AK:46:THR:HG22	1.88	0.54
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.89	0.54
27:C0:12:SER:HB3	31:CA:988:A:P	2.47	0.54
43:DQ:106:LYS:HA	43:DQ:109:ARG:HD3	1.90	0.54
1:BA:108:G:N3	1:BA:108:G:H5''	2.23	0.54
16:BP:4:ILE:HG12	16:BP:21:VAL:HG22	1.90	0.54
26:C5:17:VAL:CG1	26:C5:26:ILE:HD12	2.38	0.54
64:DA:3223:SPD:H92	64:DA:3223:SPD:H52	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:76:LEU:HD11	5:AE:120:VAL:HG22	1.90	0.54
24:C3:2:LYS:NZ	69:C3:201:HOH:O	2.40	0.54
25:D4:8:ARG:HD3	54:DA:245:G:O6	2.08	0.54
1:AA:404:G:N7	4:AD:2:ALA:HB3	2.23	0.54
44:CR:87:SER:HB3	45:CS:52:PRO:HD3	1.90	0.54
5:BE:35:ALA:O	5:BE:50:TYR:O	2.26	0.54
10:BJ:5:ARG:HG2	10:BJ:79:PRO:HG3	1.90	0.54
13:AM:33:ILE:HD11	13:AM:63:PHE:CE1	2.42	0.54
1:BA:769:G:H4'	1:BA:1513:A:H4'	1.88	0.54
5:BE:72:ILE:HG13	5:BE:73:ASN:N	2.22	0.54
11:BK:52:PHE:HE2	11:BK:65:VAL:HG21	1.73	0.54
31:CA:1394:U:H4'	31:CA:1603:A:H4'	1.90	0.54
47:DU:67:VAL:HG22	47:DU:76:ARG:HG3	1.90	0.54
1:AA:108:G:H5''	1:AA:108:G:N3	2.22	0.53
5:BE:126:LYS:HG2	5:BE:128:TYR:CZ	2.43	0.53
43:CQ:106:LYS:HA	43:CQ:109:ARG:HD3	1.90	0.53
1:AA:1144:G:H21	1:AA:1146:A:H62	1.56	0.53
4:AD:85:ASN:HB3	4:AD:88:GLU:HB2	1.90	0.53
1:BA:374:A:OP1	1:BA:452:A:N1	2.42	0.53
32:CE:149:ILE:HD12	32:CE:172:ALA:HA	1.89	0.53
33:CF:31:VAL:HG11	33:CF:97:TRP:CH2	2.43	0.53
1:AA:209:U:H4'	1:AA:210:C:OP2	2.08	0.53
39:CM:82:LEU:HD11	39:CM:116:VAL:CG2	2.32	0.53
1:BA:1144:G:H21	1:BA:1146:A:H62	1.56	0.53
63:D1:102:PGE:H42	46:DT:23:LEU:HD23	1.91	0.53
3:BC:5:VAL:HG21	3:BC:10:ILE:HD13	1.91	0.53
6:BF:45:ARG:O	6:BF:56:LYS:HA	2.08	0.53
12:BL:33:VAL:HG22	12:BL:79:VAL:HG22	1.90	0.53
35:CH:4:ILE:HD11	35:CH:44:ILE:HG22	1.90	0.53
11:AK:52:PHE:HE2	11:AK:65:VAL:HG21	1.73	0.53
8:BH:29:SER:HB3	8:BH:57:PRO:HB2	1.91	0.53
31:CA:2845:U:H5''	43:CQ:52:ASN:O	2.09	0.53
54:DA:2796:U:H3	54:DA:2799:A:N6	1.97	0.53
2:BB:129:LEU:HD13	2:BB:134:ALA:HB2	1.91	0.53
53:DI:69:PHE:HB3	53:DI:72:LEU:HD12	1.91	0.53
38:DL:76:VAL:CG2	54:DA:2684:U:H4'	2.38	0.53
1:AA:735:C:H5'	18:AR:60:LYS:HD3	1.91	0.53
2:AB:129:LEU:HD13	2:AB:134:ALA:HB2	1.91	0.53
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.90	0.53
6:BF:38:ARG:HH12	6:BF:99:ALA:HB3	1.74	0.53
10:BJ:26:VAL:HG21	10:BJ:39:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:328:U:O3'	48:CV:66:GLN:HG3	2.09	0.53
43:DQ:52:ASN:O	54:DA:2845:U:H5''	2.09	0.53
10:AJ:42:LEU:HB2	10:AJ:71:LEU:HB3	1.91	0.53
19:AS:29:LYS:HB3	19:AS:30:PRO:HD2	1.91	0.53
22:C1:17:ARG:NH2	31:CA:1266:G:OP2	2.42	0.53
31:CA:1936:A:C2	31:CA:1943:U:N3	2.59	0.53
25:D4:64:TYR:CE2	54:DA:242:G:H5''	2.44	0.53
23:D2:8:LYS:HE3	54:DA:2420:C:H5''	1.91	0.52
3:AC:5:VAL:HG21	3:AC:10:ILE:HD13	1.92	0.52
6:AF:45:ARG:O	6:AF:56:LYS:HA	2.08	0.52
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	1.91	0.52
31:CA:1847:A:O2'	31:CA:1848:A:H8	1.92	0.52
34:DG:175:LYS:HG3	54:DA:2529:G:H4'	1.91	0.52
6:BF:3:HIS:H	6:BF:92:THR:HG23	1.73	0.52
31:CA:2037:A:H2'	31:CA:2038:G:C8	2.44	0.52
8:AH:2:SER:HB2	8:AH:4:GLN:HE21	1.75	0.52
31:CA:118:A:N3	31:CA:178:G:H1'	2.25	0.52
31:CA:2796:U:H3	31:CA:2799:A:N6	1.99	0.52
30:DD:128:ARG:HG3	69:DA:7413:HOH:O	2.09	0.52
31:CA:2297:A:C8	31:CA:2297:A:H5''	2.45	0.52
54:DA:74:A:N3	54:DA:74:A:H5''	2.25	0.52
34:DG:86:LYS:HG2	34:DG:132:VAL:HG22	1.91	0.52
1:BA:404:G:N7	4:BD:2:ALA:HB3	2.24	0.52
31:CA:668:A:H2'	31:CA:670:A:H62	1.75	0.52
34:CG:86:LYS:HG2	34:CG:132:VAL:HG22	1.92	0.52
42:CP:100:HIS:CD2	42:CP:101:GLY:H	2.28	0.52
1:AA:86:G:H21	1:AA:87:C:H41	1.58	0.52
23:C2:11:LEU:HD21	23:C2:34:LEU:HD23	1.91	0.52
64:DA:3223:SPD:H92	64:DA:3223:SPD:C5	2.40	0.52
47:DU:54:GLU:HB3	47:DU:88:LYS:HD2	1.92	0.52
1:AA:845:A:O4'	1:AA:845:A:P	2.68	0.52
11:AK:23:ILE:HD11	11:AK:86:VAL:HG13	1.92	0.52
6:BF:38:ARG:NH1	6:BF:99:ALA:HB3	2.24	0.52
31:CA:699:A:H2'	31:CA:700:G:O4'	2.10	0.52
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.45	0.52
1:AA:1277:C:O2'	1:AA:1279:G:H8	1.93	0.52
10:AJ:26:VAL:HG21	10:AJ:39:PRO:HD3	1.91	0.52
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.74	0.52
32:CE:21:ARG:HD3	32:CE:106:LYS:HB3	1.92	0.52
32:DE:21:ARG:HD3	32:DE:106:LYS:HB3	1.91	0.52
53:DI:44:ALA:HB1	53:DI:95:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:DM:79:LEU:HD11	39:DM:112:LEU:HD12	1.92	0.52
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.92	0.51
42:CP:51:ALA:HB3	42:CP:78:VAL:HG13	1.92	0.51
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.76	0.51
1:BA:350:G:H5''	20:BT:3:ASN:HD22	1.76	0.51
29:CC:13:ARG:HD3	31:CA:728:G:H4'	1.92	0.51
4:BD:48:LEU:HD21	4:BD:56:ARG:HG3	1.93	0.51
19:BS:29:LYS:HB3	19:BS:30:PRO:HD2	1.93	0.51
46:CT:69:LEU:HG	46:CT:107:VAL:HG22	1.92	0.51
54:DA:1853:A:N1	54:DA:2087:G:H1'	2.25	0.51
30:DD:25:THR:HG21	30:DD:193:VAL:HG22	1.92	0.51
7:BG:111:ARG:HB3	7:BG:119:ARG:HG2	1.93	0.51
11:BK:23:ILE:HD11	11:BK:86:VAL:HG13	1.91	0.51
31:CA:532:A:N1	31:CA:2020:A:H1'	2.25	0.51
25:D4:60:ALA:O	39:DM:48:ARG:HD2	2.10	0.51
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.92	0.51
1:BA:374:A:H5''	1:BA:452:A:N1	2.25	0.51
31:CA:569:U:H5''	31:CA:821:A:C2	2.46	0.51
47:CU:54:GLU:HB3	47:CU:88:LYS:HD2	1.92	0.51
22:D1:22:LEU:HD23	61:D1:103:PEG:H31	1.91	0.51
38:DL:38:ILE:HD11	38:DL:112:PHE:CZ	2.42	0.51
11:AK:23:ILE:HG22	11:AK:32:VAL:HG13	1.92	0.51
1:BA:1218:C:H2'	1:BA:1219:A:C8	2.46	0.51
31:CA:12:U:H2'	31:CA:12:U:O2	2.11	0.51
31:CA:1447:C:H2'	31:CA:1448:G:C8	2.46	0.51
1:BA:1277:C:O2'	1:BA:1279:G:H8	1.93	0.51
30:CD:25:THR:HG21	30:CD:193:VAL:HG22	1.93	0.51
42:DP:51:ALA:HB3	42:DP:78:VAL:HG13	1.93	0.51
5:AE:126:LYS:HG2	5:AE:128:TYR:CZ	2.46	0.51
31:CA:2025:C:H2'	31:CA:2026:U:C6	2.46	0.51
30:CD:4:LEU:HD22	30:CD:101:PHE:CE2	2.45	0.51
22:C1:8:PRO:HG2	31:CA:1264:A:H5'	1.93	0.51
31:CA:2189:U:H2'	31:CA:2190:G:H8	1.76	0.51
30:CD:129:THR:HG23	30:CD:140:HIS:O	2.11	0.51
31:CA:674:G:H1'	32:CE:69:ARG:HH11	1.76	0.51
54:DA:1847:A:O2'	54:DA:1848:A:H8	1.93	0.51
5:BE:106:ILE:HD11	5:BE:124:LEU:HD23	1.93	0.50
47:CU:18:GLU:H	47:CU:18:GLU:CD	2.15	0.50
35:DH:4:ILE:HD11	35:DH:44:ILE:HG22	1.93	0.50
1:AA:774:G:H21	56:AA:1670:PG4:H51	1.75	0.50
31:CA:784:G:H5'	31:CA:785:G:OP1	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:CT:73:LYS:HB2	46:CT:106:VAL:HB	1.92	0.50
12:AL:33:VAL:HG22	12:AL:79:VAL:HG22	1.92	0.50
20:BT:4:ILE:HA	20:BT:8:LYS:HE2	1.93	0.50
22:C1:15:MET:SD	31:CA:2045:C:H5''	2.51	0.50
37:CK:81:ILE:HG23	37:CK:82:GLY:H	1.77	0.50
53:DI:57:ASN:HB3	53:DI:76:PHE:HB3	1.93	0.50
25:D4:31:HIS:HB2	69:D4:103:HOH:O	2.11	0.50
54:DA:1026:G:H2'	54:DA:1027:A:C8	2.46	0.50
33:DF:131:GLY:HA3	54:DA:2305:U:H5''	1.94	0.50
34:DG:19:ILE:HG12	34:DG:24:ILE:HG12	1.93	0.50
11:BK:23:ILE:HG22	11:BK:32:VAL:HG13	1.93	0.50
1:AA:1358:U:H3	1:AA:1363:A:H62	1.59	0.50
19:AS:15:LEU:HD13	19:AS:33:THR:HG21	1.93	0.50
17:BQ:17:MET:HB3	17:BQ:20:SER:HB3	1.93	0.50
1:BA:1003:G:H21	1:BA:1005:A:H5'	1.77	0.50
22:C1:16:ARG:HA	31:CA:2046:G:C5'	2.41	0.50
31:CA:17:G:H4'	44:CR:25:TYR:CE2	2.44	0.50
25:D4:8:ARG:CD	54:DA:245:G:O6	2.60	0.50
7:AG:111:ARG:HB3	7:AG:119:ARG:HG2	1.93	0.50
3:AC:20:SER:HB3	14:AN:94:PRO:HG3	1.92	0.50
8:BH:2:SER:HB2	8:BH:4:GLN:HE21	1.76	0.50
9:BI:19:VAL:HG22	9:BI:65:ILE:HG22	1.92	0.50
11:BK:43:GLY:HA3	11:BK:74:VAL:HG12	1.93	0.50
31:CA:1638:C:H5''	31:CA:2710:C:O2'	2.12	0.50
24:C3:16:HIS:CD2	31:CA:464:U:HO2'	2.29	0.50
23:D2:25:LYS:HE2	23:D2:30:LYS:O	2.12	0.50
18:AR:45:THR:OG1	18:AR:47:THR:HG22	2.12	0.50
31:CA:532:A:H2'	31:CA:532:A:N3	2.26	0.50
31:CA:70:G:H5''	31:CA:112:U:O2	2.12	0.50
54:DA:1536:C:H4'	54:DA:1537:G:H5''	1.93	0.50
42:DP:68:LYS:HB3	61:DP:201:PEG:H22	1.93	0.50
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.94	0.49
9:AI:19:VAL:HG22	9:AI:65:ILE:HG22	1.93	0.49
9:BI:57:MET:HG3	9:BI:61:LEU:HG	1.93	0.49
30:CD:99:GLU:HG2	30:CD:182:ALA:HB2	1.94	0.49
50:DX:41[A]:ARG:HG3	54:DA:2386:A:N3	2.26	0.49
54:DA:479:A:N3	54:DA:481:G:H5''	2.26	0.49
40:DN:81[B]:4D4:H9	54:DA:2496:C:OP2	2.12	0.49
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	1.94	0.49
1:BA:374:A:H5''	1:BA:452:A:C2	2.47	0.49
1:BA:735:C:H5'	18:BR:60:LYS:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:CF:44:ILE:HG21	33:CF:79:ILE:HG22	1.94	0.49
54:DA:914:G:H8	54:DA:914:G:H5'	1.78	0.49
7:BG:69:VAL:HG23	7:BG:100:ALA:HB1	1.94	0.49
18:BR:36:SER:HA	18:BR:72:ASP:HB3	1.93	0.49
24:C3:24:THR:HG23	24:C3:27:GLY:H	1.78	0.49
31:CA:2445:2MG:HM21	31:CA:2449:U:O4	2.11	0.49
29:CC:210:ALA:HA	29:CC:213:TRP:CE2	2.47	0.49
40:CN:21:ALA:HB1	40:CN:100:LYS:HG2	1.94	0.49
29:DC:227:PRO:HA	29:DC:233:GLY:HA2	1.95	0.49
53:DI:31:ARG:HB2	53:DI:79:PRO:HG2	1.93	0.49
6:AF:16:GLU:HB3	4:BD:189:SER:HA	1.93	0.49
31:CA:2185:U:H2'	31:CA:2186:G:C8	2.47	0.49
54:DA:1433:A:O2'	54:DA:1434:A:H5'	2.12	0.49
1:BA:202:G:H1	1:BA:215:C:H42	1.59	0.49
34:CG:19:ILE:HG12	34:CG:24:ILE:HG12	1.93	0.49
54:DA:2441:U:O2'	64:DA:3223:SPD:H91	2.13	0.49
54:DA:789:A:OP1	58:DA:3221:PUT:H12	2.12	0.49
1:AA:411:A:P	4:AD:26:ARG:HH12	2.36	0.49
11:AK:84:VAL:HG21	11:AK:97:ILE:HG23	1.95	0.49
29:CC:227:PRO:HA	29:CC:233:GLY:HA2	1.95	0.49
1:BA:76:G:H1	1:BA:93:U:H3	1.61	0.49
3:BC:113:ALA:O	3:BC:200:VAL:HG11	2.12	0.49
31:CA:1587:G:H2'	31:CA:1588:G:H8	1.78	0.49
28:CB:14:U:H2'	28:CB:15:A:H2	1.76	0.49
1:BA:202:G:O2'	1:BA:468:A:H8	1.95	0.49
25:C4:25:LYS:HB3	39:CM:62:PRO:HG2	1.94	0.49
31:CA:2019:A:H4'	44:CR:34:VAL:HG21	1.94	0.49
1:AA:1003:G:H21	1:AA:1005:A:H5'	1.77	0.49
26:C5:1:MET:HB2	31:CA:2526:G:O2'	2.13	0.49
39:DM:21:ARG:HA	54:DA:811:U:H2'	1.95	0.49
1:AA:202:G:O2'	1:AA:468:A:H8	1.95	0.49
11:AK:34:ILE:HB	11:AK:74:VAL:HG11	1.95	0.49
38:CL:43:ILE:HD12	38:CL:56:ASP:HB2	1.94	0.49
46:CT:4:ILE:HG12	46:CT:106:VAL:HG22	1.94	0.49
1:BA:840:C:H2'	1:BA:841:C:O4'	2.13	0.48
3:BC:47:LEU:HB3	3:BC:50:ALA:HB3	1.95	0.48
3:BC:20:SER:HB3	14:BN:94:PRO:HG3	1.93	0.48
31:CA:1182:G:H2'	31:CA:1183:U:O4'	2.13	0.48
28:DB:84:G:H21	62:DB:211:EDO:H11	1.78	0.48
5:AE:107:ALA:HB2	5:AE:125:ALA:HB3	1.94	0.48
15:AO:82:ILE:HG21	15:AO:89:ARG:OXT	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2623:G:H4'	31:CA:2825:G:H8	1.78	0.48
31:CA:2630:G:O4'	31:CA:2894:G:H1'	2.13	0.48
31:CA:381:G:OP1	51:CY:18:ARG:HD3	2.12	0.48
31:CA:479:A:N3	31:CA:481:G:H5''	2.28	0.48
31:CA:998:C:OP2	44:CR:58:ARG:NH2	2.46	0.48
32:CE:75:SER:O	32:CE:78:TRP:HB2	2.13	0.48
54:DA:837:C:H5	69:DA:6714:HOH:O	1.95	0.48
30:DD:13:ARG:NH1	69:DD:401:HOH:O	2.44	0.48
4:AD:48:LEU:HD21	4:AD:56:ARG:HG3	1.95	0.48
2:BB:73:LYS:HD2	2:BB:168:HIS:HD2	1.77	0.48
3:BC:72:ARG:HB3	3:BC:75:ILE:HG22	1.94	0.48
22:C1:16:ARG:HA	31:CA:2046:G:H5'	1.95	0.48
34:CG:80:THR:HG23	34:CG:81:GLU:N	2.24	0.48
33:DF:121:SER:HB2	54:DA:2304:G:H5'	1.95	0.48
30:DD:99:GLU:HG2	30:DD:182:ALA:HB2	1.94	0.48
31:CA:914:G:H8	31:CA:914:G:H5''	1.79	0.48
29:CC:177:ARG:HG2	31:CA:1820:U:OP1	2.14	0.48
63:D1:102:PGE:H4	69:DT:313:HOH:O	2.13	0.48
11:BK:30:THR:HG21	11:BK:92:GLY:HA3	1.96	0.48
1:AA:413:G:H5''	1:AA:414:A:H5'	1.96	0.48
1:BA:677:U:H3	1:BA:713:G:H22	1.61	0.48
28:CB:14:U:H2'	28:CB:15:A:C2	2.49	0.48
42:DP:31:THR:HG22	42:DP:33:ARG:H	1.79	0.48
5:AE:38:VAL:HG11	5:AE:114:VAL:HG22	1.96	0.48
9:AI:57:MET:HG3	9:AI:61:LEU:HG	1.94	0.48
11:AK:30:THR:HG21	11:AK:92:GLY:HA3	1.95	0.48
31:CA:634:C:H2'	31:CA:635:C:C6	2.49	0.48
46:DT:4:ILE:HG12	46:DT:106:VAL:HG22	1.94	0.48
1:BA:975:A:H8	1:BA:1357:A:HO2'	1.61	0.48
38:CL:38:ILE:HD11	38:CL:112:PHE:CZ	2.38	0.48
23:D2:11:LEU:HD21	23:D2:34:LEU:HD23	1.93	0.48
53:DI:50:VAL:HG13	53:DI:85:VAL:HG22	1.96	0.48
40:DN:41:LEU:HG	40:DN:96:ILE:HG13	1.96	0.48
46:DT:72:THR:HG21	46:DT:108:SER:HB3	1.95	0.48
1:AA:975:A:H8	1:AA:1357:A:HO2'	1.60	0.48
2:AB:20:THR:HG22	2:AB:39:HIS:CE1	2.49	0.48
31:CA:247:G:H4'	31:CA:386:G:C5	2.49	0.48
7:AG:22:LEU:HD12	7:AG:62:PHE:CE2	2.48	0.48
5:BE:36:LEU:HD21	5:BE:137:VAL:HG11	1.95	0.48
54:DA:1587:G:H2'	54:DA:1588:G:H8	1.79	0.48
30:DD:150[B]:MEQ:HE2	54:DA:2033:A:O5'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DF:44:ILE:HG21	33:DF:79:ILE:HG22	1.95	0.48
46:DT:73:LYS:HB2	46:DT:106:VAL:HB	1.95	0.48
1:AA:542:G:H5'	4:AD:39:GLY:HA3	1.96	0.47
36:CJ:19:ASN:H	36:CJ:20:PRO:HD2	1.79	0.47
54:DA:1172:C:C5	54:DA:1173:U:H1'	2.49	0.47
54:DA:11:C:H2'	54:DA:12:U:H5'	1.95	0.47
5:AE:133:PRO:O	5:AE:137:VAL:HG13	2.14	0.47
1:BA:542:G:H5'	4:BD:39:GLY:HA3	1.96	0.47
33:CF:36:LEU:HB2	33:CF:57:LEU:HD21	1.97	0.47
54:DA:1975:G:H21	63:DA:3224:PGE:C2	2.27	0.47
1:AA:1055:A:H2'	3:AC:156:ARG:HD2	1.96	0.47
6:AF:38:ARG:HE	6:AF:63:ASN:ND2	2.12	0.47
1:BA:1391:U:H2'	1:BA:1392:G:C8	2.49	0.47
17:BQ:76:VAL:HG12	17:BQ:77:ARG:HG3	1.97	0.47
23:C2:25:LYS:HE2	23:C2:30:LYS:O	2.14	0.47
30:DD:8:LYS:HB2	30:DD:201:LEU:HD11	1.96	0.47
13:AM:4:ILE:HD12	13:AM:10:PRO:HG2	1.95	0.47
1:BA:1190:G:H5'	3:BC:176:HIS:NE2	2.29	0.47
44:DR:6:ARG:HD3	54:DA:1250:G:H5''	1.95	0.47
30:DD:105:LYS:NZ	30:DD:106:LYS:HE3	2.30	0.47
38:DL:43:ILE:HD12	38:DL:56:ASP:HB2	1.96	0.47
11:BK:84:VAL:HG21	11:BK:97:ILE:HG23	1.97	0.47
31:CA:1141:U:H4'	31:CA:1142:A:O4'	2.15	0.47
31:CA:2185:U:H2'	31:CA:2186:G:H8	1.79	0.47
33:CF:8:TYR:HA	33:CF:12:VAL:HB	1.97	0.47
51:CY:10:LYS:HE3	51:CY:54:LYS:HG2	1.96	0.47
22:D1:9:THR:HG21	54:DA:2020:A:H5'	1.96	0.47
54:DA:2291:U:H2'	54:DA:2292:U:C6	2.49	0.47
36:DJ:103:ARG:HA	36:DJ:106:LEU:HD12	1.96	0.47
54:DA:789:A:OP1	58:DA:3221:PUT:C1	2.63	0.47
1:AA:269:C:H2'	1:AA:270:A:C8	2.50	0.47
1:BA:1493:A:H1'	31:CA:1913:A:H61	1.79	0.47
31:CA:2030:6MZ:C2	31:CA:2499:C:H5''	2.45	0.47
54:DA:644:A:H2'	54:DA:645:C:O4'	2.14	0.47
33:DF:8:TYR:HA	33:DF:12:VAL:HB	1.97	0.47
42:DP:52:SER:OG	42:DP:54:VAL:HG22	2.14	0.47
48:DV:73:PHE:CE2	48:DV:75:ALA:HA	2.49	0.47
1:AA:677:U:H3	1:AA:713:G:H22	1.63	0.47
1:BA:846:G:H2'	1:BA:847:G:H8	1.79	0.47
54:DA:1975:G:H21	63:DA:3224:PGE:H2	1.79	0.47
33:DF:36:LEU:HB2	33:DF:57:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DH:49:ALA:O	35:DH:53:GLU:HB3	2.15	0.47
51:DY:10:LYS:HE3	51:DY:54:LYS:HG2	1.97	0.47
1:BA:269:C:H2'	1:BA:270:A:C8	2.50	0.47
32:CE:1:MET:HG2	32:CE:14:VAL:HG23	1.97	0.47
54:DA:1182:G:H2'	54:DA:1183:U:O4'	2.15	0.47
36:DJ:19:ASN:H	36:DJ:20:PRO:HD2	1.80	0.47
31:CA:2291:U:H2'	31:CA:2292:U:C6	2.50	0.47
30:CD:155:VAL:HG21	31:CA:2618:G:H21	1.79	0.47
31:CA:396:G:H1'	51:CY:29:PHE:HB3	1.95	0.47
31:CA:608:A:H2'	31:CA:609:A:C8	2.50	0.47
48:CV:74:ASN:HD22	48:CV:77:THR:H	1.63	0.47
22:D1:55:ILE:HD12	41:DO:33:ILE:CD1	2.45	0.47
54:DA:1236:G:N7	58:DA:3189:PUT:H41	2.30	0.47
42:DP:31:THR:HG21	28:DB:28:C:P	2.54	0.47
2:BB:73:LYS:HD2	2:BB:168:HIS:CD2	2.51	0.47
5:BE:57:PRO:O	5:BE:60:ILE:HG13	2.15	0.47
22:C1:41:HIS:O	41:CO:99:LYS:HE2	2.14	0.47
24:C3:19:ARG:NH2	31:CA:125:A:OP2	2.38	0.47
31:CA:1936:A:H62	31:CA:1963:U:H3	1.60	0.47
27:C0:19:LYS:HE3	31:CA:920:A:OP1	2.14	0.47
31:CA:310:A:H5''	48:CV:15:THR:HG23	1.96	0.47
37:DK:69:ARG:O	37:DK:90:GLU:HB2	2.15	0.47
1:AA:310:G:H5''	16:AP:31:ARG:HB2	1.97	0.46
1:BA:1055:A:H2'	3:BC:156:ARG:HD2	1.97	0.46
31:CA:193:U:H5	69:CA:3370:HOH:O	1.98	0.46
33:CF:103:LEU:HA	33:CF:107:ALA:HB3	1.97	0.46
54:DA:1180:U:H5''	54:DA:1180:U:H6	1.80	0.46
54:DA:749:A:H4'	54:DA:1271:G:N3	2.29	0.46
32:DE:176:ASP:OD2	32:DE:178:VAL:HG12	2.15	0.46
1:AA:73:C:O2'	1:AA:74:A:H8	1.97	0.46
21:AU:4:ILE:HG13	21:AU:19:PHE:HA	1.97	0.46
1:BA:23:C:H5	1:BA:561:U:O4	1.98	0.46
22:C1:2:ALA:N	31:CA:2577:A:H2	2.13	0.46
41:CO:47:VAL:O	41:CO:51:LEU:HD23	2.15	0.46
33:DF:103:LEU:HA	33:DF:107:ALA:HB3	1.97	0.46
1:AA:1197:A:H5''	59:AA:1678:TAC:O12	2.15	0.46
1:BA:202:G:H21	1:BA:466:A:H61	1.62	0.46
31:CA:846:U:H1'	31:CA:847:U:C5	2.44	0.46
42:CP:31:THR:HG22	42:CP:33:ARG:H	1.79	0.46
48:CV:7:ARG:O	48:CV:25:VAL:HB	2.15	0.46
22:D1:25:VAL:HG11	46:DT:38:TYR:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BS:15:LEU:HD13	19:BS:33:THR:HG21	1.95	0.46
30:CD:62:LYS:HE2	31:CA:2810:A:H5''	1.98	0.46
30:CD:152:PRO:HG3	30:CD:156:PHE:CZ	2.51	0.46
51:DY:61:LYS:HD3	54:DA:372:G:H5''	1.98	0.46
50:DX:39:ARG:NH1	69:DX:101:HOH:O	2.48	0.46
1:AA:76:G:H1	1:AA:93:U:H3	1.62	0.46
6:AF:47:LEU:HD13	6:AF:51:ILE:HG12	1.97	0.46
30:CD:3:GLY:O	30:CD:4:LEU:HD13	2.15	0.46
39:CM:77:ILE:CD1	39:CM:108:ALA:HB1	2.36	0.46
54:DA:102:U:H2'	54:DA:102:U:O2	2.15	0.46
25:D4:64:TYR:CZ	54:DA:242:G:H5''	2.51	0.46
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.50	0.46
1:BA:1001:C:H2'	1:BA:1002:G:H8	1.81	0.46
30:CD:133:THR:CG2	31:CA:1993:U:H4'	2.45	0.46
31:CA:740:C:H5'	31:CA:1784:A:C3'	2.38	0.46
31:CA:749:A:H4'	31:CA:1271:G:N3	2.29	0.46
29:CC:219:THR:O	31:CA:1789:A:H5''	2.15	0.46
54:DA:57:C:H2'	54:DA:58:G:O4'	2.16	0.46
29:DC:207:LYS:HB2	54:DA:729:G:C6	2.51	0.46
1:AA:1190:G:H5'	3:AC:176:HIS:NE2	2.31	0.46
21:BU:4:ILE:HG13	21:BU:19:PHE:HA	1.97	0.46
43:CQ:114:LEU:H	43:CQ:114:LEU:HD23	1.81	0.46
47:CU:45:ALA:O	47:CU:49:LYS:HG2	2.14	0.46
22:D1:5:GLN:O	54:DA:2017:U:H4'	2.16	0.46
1:BA:376:G:H5''	16:BP:5:ARG:HB2	1.97	0.46
31:CA:2489:U:HO2'	31:CA:2491:U:H5	1.64	0.46
31:CA:948:C:H1'	31:CA:984:A:C8	2.50	0.46
29:CC:235:GLY:HA3	29:CC:239:ASN:HB2	1.97	0.46
34:CG:80:THR:CG2	34:CG:81:GLU:H	2.27	0.46
44:CR:58:ARG:HA	44:CR:61:TRP:CE3	2.50	0.46
31:CA:1250:G:C5'	44:CR:6:ARG:HD3	2.45	0.46
1:AA:1054:C:H5''	1:AA:1054:C:H6	1.80	0.46
1:AA:438:U:H5'	4:AD:120:HIS:HB3	1.98	0.46
5:AE:16:ILE:HD13	5:AE:137:VAL:HG11	1.97	0.46
17:AQ:76:VAL:HG12	17:AQ:77:ARG:HG3	1.97	0.46
1:BA:1496:C:H2'	1:BA:1497:G:O4'	2.16	0.46
1:BA:310:G:H5''	16:BP:31:ARG:HB2	1.97	0.46
1:BA:438:U:H5'	4:BD:120:HIS:HB3	1.97	0.46
18:BR:27:ALA:O	18:BR:30:LYS:HG2	2.16	0.46
23:D2:10:LYS:HE3	23:D2:53:LYS:O	2.16	0.46
54:DA:871:U:H2'	54:DA:872:U:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:DD:186:LEU:HD21	43:DQ:4:ILE:HG21	1.97	0.46
1:AA:216:U:H2'	1:AA:217:C:C6	2.50	0.46
5:AE:57:PRO:O	5:AE:60:ILE:HG13	2.15	0.46
31:CA:833:A:H2'	31:CA:834:G:C8	2.51	0.46
47:CU:67:VAL:HG22	47:CU:76:ARG:HG3	1.98	0.46
54:DA:2800:A:C2	54:DA:2895:G:H1'	2.51	0.46
54:DA:722:A:H2'	54:DA:723:C:O4'	2.16	0.46
1:BA:846:G:H2'	1:BA:847:G:C8	2.51	0.45
9:BI:7:TYR:HE1	9:BI:18:ARG:HB2	1.80	0.45
31:CA:594:U:H2'	31:CA:595:C:C6	2.51	0.45
31:CA:694:U:OP1	31:CA:1569:A:H1'	2.16	0.45
36:CJ:103:ARG:HA	36:CJ:106:LEU:HD12	1.96	0.45
31:CA:1131:G:OP1	37:CK:82:GLY:HA2	2.16	0.45
54:DA:2070:A:H2'	54:DA:2071:A:O4'	2.16	0.45
10:AJ:52:LEU:HB2	14:AN:81:ARG:HD2	1.99	0.45
1:BA:1053:G:N7	1:BA:1200:C:H5''	2.32	0.45
30:CD:8:LYS:HB2	30:CD:201:LEU:HD11	1.97	0.45
40:CN:69:PRO:O	40:CN:93:VAL:O	2.34	0.45
42:CP:31:THR:HG22	42:CP:34:HIS:H	1.81	0.45
54:DA:2086:U:H2'	54:DA:2087:G:C8	2.51	0.45
54:DA:2117:A:H61	54:DA:2171:A:H61	1.63	0.45
64:DA:3223:SPD:H82	69:DA:4264:HOH:O	2.16	0.45
35:DH:104:THR:HG22	35:DH:109:GLU:HA	1.97	0.45
1:BA:411:A:P	4:BD:26:ARG:HH12	2.39	0.45
2:BB:163:VAL:HG11	2:BB:173:ILE:HD11	1.99	0.45
1:BA:1108:G:H5''	3:BC:176:HIS:CE1	2.52	0.45
54:DA:2628:C:C5'	58:DA:3195:PUT:H12	2.42	0.45
29:DC:177:ARG:HG2	54:DA:1820:U:OP1	2.17	0.45
29:DC:235:GLY:HA3	29:DC:239:ASN:HB2	1.99	0.45
32:DE:1:MET:HG2	32:DE:14:VAL:HG23	1.97	0.45
41:DO:9:GLN:O	41:DO:17:ARG:HD3	2.17	0.45
1:AA:923:A:OP1	5:AE:26:LYS:HG2	2.16	0.45
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	1.97	0.45
1:BA:216:U:H2'	1:BA:217:C:C6	2.51	0.45
31:CA:1326:U:H2'	31:CA:1327:A:H8	1.81	0.45
26:C5:4:ARG:NH1	31:CA:2477:U:O2	2.44	0.45
31:CA:320:A:H2'	32:CE:131:THR:HG21	1.99	0.45
31:CA:1251:C:OP2	44:CR:6:ARG:HD2	2.17	0.45
45:DS:8:GLY:HA2	54:DA:1161:C:O2'	2.16	0.45
30:DD:152:PRO:HG3	30:DD:156:PHE:CZ	2.52	0.45
50:DX:37:ILE:HG21	50:DX:80:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:DY:7:VAL:HG23	51:DY:51:VAL:HG12	1.98	0.45
1:AA:845:A:H2'	1:AA:846:G:O4'	2.17	0.45
1:AA:376:G:H5''	16:AP:5:ARG:HB2	1.98	0.45
1:BA:8:A:H1'	5:BE:108:GLY:HA2	1.97	0.45
22:C1:5:GLN:NE2	31:CA:2056:G:H4'	2.31	0.45
31:CA:722:A:H2'	31:CA:723:C:O4'	2.16	0.45
37:CK:69:ARG:O	37:CK:90:GLU:HB3	2.16	0.45
54:DA:1133:A:N3	58:DA:3212:PUT:H22	2.32	0.45
44:DR:58:ARG:HA	44:DR:61:TRP:CE3	2.51	0.45
2:AB:93:ASN:H	2:AB:93:ASN:HD22	1.65	0.45
31:CA:191:A:H2'	31:CA:192:C:C6	2.51	0.45
31:CA:871:U:H2'	31:CA:872:U:C6	2.51	0.45
31:CA:2674:G:H4'	38:CL:30:ARG:HD2	1.99	0.45
44:CR:112:LYS:HD3	45:CS:48:LYS:HG3	1.99	0.45
46:CT:84:ARG:HB2	46:CT:96:ILE:HB	1.99	0.45
54:DA:1509:A:HO2'	54:DA:1510:G:H8	1.65	0.45
34:DG:103:ILE:HD11	34:DG:117:LEU:HD21	1.99	0.45
32:DE:32:VAL:HG21	39:DM:6:LEU:HD13	1.99	0.45
42:DP:35:ILE:HG21	42:DP:71:ALA:HA	1.98	0.45
43:DQ:52:ASN:O	43:DQ:53:ARG:HD3	2.16	0.45
4:AD:172:GLU:HG2	4:AD:183:LYS:HD2	1.99	0.45
2:BB:93:ASN:H	2:BB:93:ASN:HD22	1.65	0.45
31:CA:248:G:H5'	31:CA:250:G:N7	2.31	0.45
31:CA:2544:G:H5'	31:CA:2645:G:C2	2.51	0.45
32:CE:176:ASP:OD2	32:CE:178:VAL:HG12	2.16	0.45
45:CS:49:ILE:HB	45:CS:51:VAL:O	2.17	0.45
47:CU:28:ASN:ND2	47:CU:91:GLN:HB3	2.14	0.45
54:DA:136:G:H1	54:DA:143:C:H42	1.65	0.45
53:DI:70:GLU:HG2	53:DI:73:LYS:HE3	1.98	0.45
1:BA:923:A:OP1	5:BE:26:LYS:HG2	2.17	0.45
54:DA:1168:G:H5''	54:DA:1168:G:H8	1.81	0.45
54:DA:2609:U:C5	62:DA:3194:EDO:H12	2.51	0.45
53:DI:132:TYR:H	53:DI:133:GLU:HB2	1.81	0.45
1:AA:202:G:H1	1:AA:215:C:H42	1.64	0.45
8:AH:105:SER:HB2	8:AH:126:ILE:HD11	1.98	0.45
31:CA:1810:A:H2'	31:CA:1811:G:O4'	2.17	0.45
31:CA:1965:C:H5''	31:CA:1966:A:H2'	1.99	0.45
25:C4:25:LYS:O	39:CM:62:PRO:HD2	2.16	0.45
46:CT:72:THR:HG21	46:CT:108:SER:HB3	1.98	0.45
24:D3:33:ARG:HG3	61:D3:102:PEG:H31	1.99	0.45
54:DA:355:U:H2'	54:DA:356:G:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:DK:7:LYS:O	37:DK:11:VAL:HG23	2.17	0.45
49:DW:38:LEU:HD21	49:DW:65:VAL:HG11	1.99	0.45
4:BD:172:GLU:HG2	4:BD:183:LYS:HD2	1.99	0.45
31:CA:1775:U:O4	31:CA:1789:A:H2	2.00	0.45
31:CA:278:A:N3	31:CA:278:A:H2'	2.32	0.45
54:DA:612:G:H2'	54:DA:614:A:C8	2.52	0.45
29:DC:199:GLU:O	29:DC:202:LEU:HB2	2.17	0.45
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.82	0.44
24:C3:19:ARG:HG3	31:CA:126:A:O5'	2.17	0.44
31:CA:320:A:H4'	31:CA:322:A:N7	2.32	0.44
31:CA:478:A:H61	31:CA:500:G:H4'	1.81	0.44
54:DA:1283:G:H1'	54:DA:1329:U:O2	2.17	0.44
54:DA:1349:C:O2'	56:DA:3215:PG4:H82	2.16	0.44
2:BB:68:LEU:HD11	2:BB:92:VAL:HG23	2.00	0.44
25:C4:2:PRO:HD2	31:CA:667:U:O2	2.17	0.44
30:CD:13:ARG:HH11	43:CQ:56:HIS:HA	1.83	0.44
54:DA:1738:G:HO2'	54:DA:1739:A:H8	1.62	0.44
54:DA:278:A:H2'	54:DA:278:A:N3	2.32	0.44
54:DA:760:G:H4'	54:DA:1776:G:OP1	2.18	0.44
29:DC:212:ARG:HD2	29:DC:216:VAL:O	2.18	0.44
33:DF:16:LEU:HD13	33:DF:29:PRO:HD2	1.99	0.44
1:AA:957:U:O2	1:AA:959:A:H8	2.01	0.44
2:AB:68:LEU:HD11	2:AB:92:VAL:HG23	1.99	0.44
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.81	0.44
1:BA:957:U:O2	1:BA:959:A:H8	2.01	0.44
31:CA:1556:C:H2'	31:CA:1557:C:C6	2.51	0.44
31:CA:639:U:H2'	31:CA:640:C:C6	2.52	0.44
50:CX:37:ILE:HG21	50:CX:80:ILE:HG21	1.98	0.44
42:DP:31:THR:HG22	42:DP:34:HIS:H	1.80	0.44
1:AA:1053:G:N7	1:AA:1200:C:H5''	2.33	0.44
1:BA:1054:C:H6	1:BA:1054:C:H5''	1.83	0.44
1:BA:1226:C:H2'	13:BM:102:THR:HB	1.99	0.44
6:BF:47:LEU:HD13	6:BF:51:ILE:HG12	1.99	0.44
22:C1:53:LYS:HE3	22:C1:56:ALA:HA	1.99	0.44
1:AA:9:G:H5'	5:AE:108:GLY:HA3	1.99	0.44
2:AB:129:LEU:H	2:AB:129:LEU:HG	1.51	0.44
9:AI:99:ARG:HG2	9:AI:104:VAL:HG21	1.99	0.44
1:BA:73:C:O2'	1:BA:74:A:H8	1.97	0.44
11:BK:84:VAL:HG11	11:BK:97:ILE:HG12	2.00	0.44
14:BN:31:ILE:HG23	14:BN:42:TRP:CZ2	2.53	0.44
33:CF:16:LEU:HD13	33:CF:29:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D1:9:THR:CG2	54:DA:2020:A:H5'	2.48	0.44
24:D3:4:THR:HA	54:DA:687:C:O4'	2.16	0.44
54:DA:1321:A:C2	63:DA:3216:PGE:H12	2.53	0.44
29:DC:13:ARG:HD3	54:DA:728:G:H4'	2.00	0.44
29:DC:203:ARG:HH21	29:DC:205:LEU:HD21	1.82	0.44
27:C0:53:PHE:CG	28:CB:83:G:H4'	2.53	0.44
31:CA:747:5MU:O2	31:CA:2014:A:H1'	2.18	0.44
31:CA:863:A:H2'	31:CA:864:G:C8	2.53	0.44
35:CH:104:THR:HG22	35:CH:109:GLU:HA	1.98	0.44
49:CW:38:LEU:HD21	49:CW:65:VAL:HG11	1.98	0.44
27:D0:15:GLY:HA2	54:DA:969:G:O3'	2.17	0.44
39:DM:60:ARG:HD2	54:DA:2360:G:H1'	2.00	0.44
54:DA:639:U:H2'	54:DA:640:C:C6	2.53	0.44
1:AA:864:A:H4'	5:AE:90:THR:HG23	2.00	0.44
3:AC:21:THR:HG23	3:AC:58:GLU:HB3	1.99	0.44
8:AH:87:LYS:HB2	8:AH:125:ILE:CD1	2.41	0.44
13:AM:12:HIS:HB3	69:AM:302:HOH:O	2.18	0.44
13:AM:17:ILE:H	13:AM:17:ILE:HD12	1.83	0.44
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	2.00	0.44
20:BT:58:VAL:HG13	20:BT:72:ALA:HB1	2.00	0.44
42:CP:35:ILE:HG21	42:CP:71:ALA:HA	1.99	0.44
54:DA:493:G:H2'	54:DA:494:G:O4'	2.18	0.44
11:AK:84:VAL:HG11	11:AK:97:ILE:HG12	1.99	0.44
20:BT:5:LYS:HB3	20:BT:7:ALA:H	1.82	0.44
31:CA:2051:A:H5'	31:CA:2578:G:O4'	2.18	0.44
29:CC:199:GLU:O	29:CC:202:LEU:HB2	2.18	0.44
29:CC:212:ARG:HD2	29:CC:216:VAL:O	2.18	0.44
54:DA:1831:G:H1'	63:DA:3224:PGE:H22	1.98	0.44
54:DA:62:U:H5'	57:DA:3203:MPD:H53	2.00	0.44
1:BA:1060:U:H5	3:BC:2:GLY:HA3	1.81	0.44
23:C2:33:LYS:HA	23:C2:52:ALA:HB3	2.00	0.44
31:CA:1469:A:H2'	31:CA:1470:A:C8	2.53	0.44
37:CK:7:LYS:O	37:CK:11:VAL:HG23	2.17	0.44
49:CW:51:GLN:HG2	49:CW:86:LEU:HD11	2.00	0.44
53:DI:85:VAL:HG21	53:DI:90:GLY:O	2.17	0.44
36:DJ:11:LEU:HD22	36:DJ:24:VAL:HG23	2.00	0.44
45:DS:41:ILE:HD13	45:DS:103:ALA:HA	1.99	0.44
48:DV:94:ARG:HB3	48:DV:103:ILE:HD12	1.99	0.44
1:AA:1496:C:H2'	1:AA:1497:G:O4'	2.18	0.43
4:BD:85:ASN:HA	5:BE:102:GLY:CA	2.31	0.43
6:BF:70:VAL:HA	6:BF:73:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BN:10:GLU:HG3	14:BN:63:ARG:HD2	2.00	0.43
31:CA:1274:A:N3	31:CA:1297:C:H1'	2.33	0.43
31:CA:1991:U:H2'	31:CA:1992:G:H5''	2.00	0.43
22:C1:5:GLN:HG3	31:CA:2054:A:C2	2.53	0.43
31:CA:528:A:C8	31:CA:528:A:C3'	3.00	0.43
30:CD:13:ARG:HD3	30:CD:21:SER:OG	2.18	0.43
44:CR:113:ALA:O	44:CR:117:LEU:HD12	2.18	0.43
40:DN:42:THR:HG22	40:DN:93:VAL:HG12	1.99	0.43
2:AB:163:VAL:HG11	2:AB:173:ILE:HD11	2.00	0.43
14:AN:46:LEU:HA	14:AN:49:GLN:HE21	1.83	0.43
17:AQ:8:LEU:HD13	17:AQ:25:ILE:HG13	2.00	0.43
1:BA:1060:U:H4'	10:BJ:53:ILE:HG23	2.00	0.43
10:BJ:52:LEU:HB2	14:BN:81:ARG:HD2	2.00	0.43
16:BP:20:VAL:CG1	16:BP:32:PHE:HB2	2.47	0.43
31:CA:2623:G:H4'	31:CA:2825:G:C8	2.53	0.43
31:CA:355:U:H2'	31:CA:356:G:H8	1.83	0.43
33:CF:5:HIS:HB2	33:CF:97:TRP:CD1	2.53	0.43
54:DA:1394:U:H4'	54:DA:1603:A:H4'	2.00	0.43
32:DE:84:THR:HG21	54:DA:586:A:H5'	1.99	0.43
1:AA:1060:U:H4'	10:AJ:53:ILE:HG23	2.00	0.43
14:AN:10:GLU:HG3	14:AN:63:ARG:HD2	2.00	0.43
1:BA:10:A:OP2	5:BE:131:THR:HG21	2.18	0.43
31:CA:532:A:H4'	31:CA:533:G:C8	2.54	0.43
30:CD:26:VAL:HG21	43:CQ:5:ILE:HG12	2.00	0.43
33:DF:80:ARG:HB3	33:DF:83:TYR:CE1	2.53	0.43
1:AA:604:G:H2'	1:AA:605:U:O4'	2.19	0.43
2:AB:70:VAL:HB	2:AB:163:VAL:HG22	2.00	0.43
10:AJ:10:LEU:HB2	10:AJ:72:ARG:HB2	2.00	0.43
1:BA:1277:C:HO2'	1:BA:1279:G:H8	1.62	0.43
31:CA:2688:G:H1'	31:CA:2721:A:N6	2.34	0.43
34:CG:17:VAL:HG11	34:CG:50:LEU:HD21	2.01	0.43
48:CV:94:ARG:HB3	48:CV:103:ILE:HD12	1.99	0.43
54:DA:1424:G:H21	63:DA:3213:PGE:H32	1.84	0.43
54:DA:142:A:H2'	54:DA:143:C:C6	2.53	0.43
54:DA:2031:A:C6	54:DA:2498:OMC:H1'	2.53	0.43
33:DF:5:HIS:HB2	33:DF:97:TRP:CD1	2.54	0.43
12:AL:31:ARG:O	12:AL:58:THR:HG23	2.18	0.43
1:AA:1226:C:H2'	13:AM:102:THR:HB	2.00	0.43
17:AQ:15:ASP:HA	17:AQ:21:ILE:HG22	1.99	0.43
11:BK:24:HIS:HB3	11:BK:31:ILE:HG23	2.00	0.43
26:C5:17:VAL:HG12	26:C5:26:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:142:A:H2'	31:CA:143:C:C6	2.53	0.43
30:CD:121:THR:HB	30:CD:127:PHE:CD2	2.54	0.43
36:CJ:11:LEU:HD22	36:CJ:24:VAL:HG23	2.00	0.43
38:CL:113:MET:O	38:CL:116:ILE:HG13	2.18	0.43
54:DA:191:A:H2'	54:DA:192:C:C6	2.53	0.43
54:DA:523:C:H4'	54:DA:540:C:O2	2.19	0.43
20:AT:44:LYS:H	20:AT:44:LYS:HG3	1.61	0.43
3:BC:23:PHE:CD2	10:BJ:97:ASP:HB2	2.54	0.43
8:BH:105:SER:HB2	8:BH:126:ILE:HD11	1.99	0.43
13:BM:54:ASP:HA	13:BM:57:ARG:HD2	2.00	0.43
17:BQ:46:VAL:HG11	17:BQ:61:ILE:CG2	2.48	0.43
31:CA:528:A:C2	31:CA:2042:A:H2'	2.54	0.43
29:CC:225:MET:O	29:CC:233:GLY:O	2.36	0.43
38:CL:103:VAL:O	38:CL:122:VAL:HB	2.18	0.43
39:CM:95:LEU:HD22	39:CM:100:ILE:HG12	1.99	0.43
41:CO:71:ARG:HG3	41:CO:71:ARG:O	2.19	0.43
22:C1:54:VAL:HG21	41:CO:98:LEU:HD22	2.00	0.43
22:D1:53:LYS:HE3	22:D1:56:ALA:HA	2.00	0.43
54:DA:2849:U:H4'	54:DA:2868:A:C2	2.54	0.43
53:DI:27:VAL:HG13	53:DI:80:THR:HG23	2.00	0.43
53:DI:50:VAL:HG22	53:DI:85:VAL:HG13	2.00	0.43
45:DS:44:GLY:O	45:DS:45:GLU:HG2	2.17	0.43
1:BA:502:A:H2'	1:BA:503:C:O4'	2.19	0.43
1:BA:1152:A:H5'	10:BJ:15:HIS:HB2	2.01	0.43
31:CA:2636:C:H2'	31:CA:2637:U:C6	2.54	0.43
31:CA:2728:U:O2'	31:CA:2729:G:H8	2.01	0.43
31:CA:493:G:H2'	31:CA:494:G:O4'	2.18	0.43
31:CA:335:C:H5''	48:CV:82:ARG:HD3	2.01	0.43
54:DA:1028:A:N6	54:DA:1125:G:H2'	2.34	0.43
54:DA:1654:A:H1'	54:DA:2823:A:H5'	2.00	0.43
54:DA:5:A:H2'	54:DA:6:A:C8	2.53	0.43
53:DI:56:ARG:HA	54:DA:1107:G:OP1	2.19	0.43
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.54	0.43
1:AA:892:A:O2'	1:AA:1415:G:H4'	2.19	0.43
3:AC:7:PRO:HD2	3:AC:184:TYR:CD1	2.54	0.43
6:AF:70:VAL:HA	6:AF:73:GLU:HG2	2.00	0.43
1:BA:1493:A:H8	1:BA:1493:A:OP2	2.01	0.43
31:CA:580:U:O3'	44:CR:31:VAL:HG13	2.19	0.43
31:CA:685:A:H5''	31:CA:774:G:O6	2.19	0.43
31:CA:83:A:H2	31:CA:103:A:N7	2.17	0.43
54:DA:2233:U:H2'	54:DA:2234:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DF:36:LEU:HD22	33:DF:154:ILE:HG12	2.01	0.43
53:DI:26:VAL:HB	53:DI:83:ALA:HB3	2.01	0.43
37:DK:23:LYS:HE2	37:DK:142:ILE:OXT	2.19	0.43
47:DU:33:LYS:HG3	47:DU:80:TRP:CE3	2.53	0.43
4:BD:105:MET:SD	4:BD:143:VAL:HG22	2.59	0.43
5:BE:40:GLY:HA2	5:BE:45:ARG:O	2.19	0.43
5:BE:88:VAL:HG12	5:BE:93:ARG:HG2	2.00	0.43
31:CA:1168:G:H5''	31:CA:1168:G:H8	1.83	0.43
28:CB:28:C:OP1	42:CP:31:THR:HG21	2.17	0.43
41:CO:9:GLN:O	41:CO:17:ARG:HD3	2.17	0.43
45:CS:3:ALA:HB3	45:CS:101:ILE:HD12	2.01	0.43
45:DS:83:TYR:CE1	54:DA:1187:G:H5''	2.54	0.43
30:DD:121:THR:HB	30:DD:127:PHE:CD2	2.54	0.43
45:DS:10:LYS:HE3	56:DS:202:PG4:H21	2.00	0.43
8:AH:66:PHE:CD2	8:AH:67:GLN:HG2	2.54	0.43
13:BM:90:ARG:HH21	13:BM:95:LEU:HB3	1.84	0.43
31:CA:1936:A:N6	31:CA:1963:U:H3	2.16	0.43
31:CA:2106:U:H2'	31:CA:2107:G:H8	1.84	0.43
31:CA:35:G:H2'	31:CA:36:G:O4'	2.19	0.43
34:CG:103:ILE:HD11	34:CG:117:LEU:HD21	2.01	0.43
24:D3:29:GLN:HG2	61:D3:102:PEG:H21	2.01	0.43
54:DA:1101:U:H2'	54:DA:1102:C:C6	2.54	0.43
37:DK:7:LYS:HG2	54:DA:538:A:H4'	2.01	0.43
49:DW:51:GLN:HG2	49:DW:86:LEU:HD11	2.01	0.43
1:AA:1376:U:H2'	1:AA:1377:A:C8	2.55	0.42
3:AC:151:VAL:HG12	3:AC:200:VAL:HG22	2.00	0.42
2:BB:104:TRP:O	2:BB:108:ARG:HB2	2.19	0.42
9:BI:99:ARG:HG2	9:BI:104:VAL:HG21	2.00	0.42
54:DA:2326:C:H3'	69:DA:7768:HOH:O	2.18	0.42
54:DA:2636:C:H2'	54:DA:2637:U:C6	2.53	0.42
61:DA:3200:PEG:H32	69:DA:3799:HOH:O	2.19	0.42
34:DG:17:VAL:HG11	34:DG:50:LEU:HD21	2.00	0.42
40:DN:21:ALA:HB1	40:DN:100:LYS:HG2	2.00	0.42
1:BA:978:A:O2'	1:BA:1322:C:H5	2.00	0.42
1:BA:864:A:H4'	5:BE:90:THR:HG23	2.00	0.42
5:BE:74:VAL:HG11	5:BE:144:LEU:HB3	2.01	0.42
5:BE:81:LEU:HB3	5:BE:147:MET:SD	2.58	0.42
31:CA:136:G:H1	31:CA:143:C:H42	1.65	0.42
31:CA:822:G:O6	31:CA:943:A:H2	2.01	0.42
33:CF:36:LEU:HD12	33:CF:154:ILE:HG12	2.01	0.42
37:CK:23:LYS:HE3	37:CK:142:ILE:OXT	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:CU:33:LYS:HG3	47:CU:80:TRP:CE3	2.55	0.42
49:CW:26:PHE:CE1	49:CW:44:HIS:HA	2.53	0.42
22:D1:54:VAL:HG23	22:D1:55:ILE:HG12	2.00	0.42
54:DA:1510:G:H2'	54:DA:1511:G:O4'	2.18	0.42
54:DA:2051:A:H5'	54:DA:2578:G:O4'	2.19	0.42
30:DD:13:ARG:HD3	30:DD:21:SER:OG	2.18	0.42
49:DW:26:PHE:CE2	49:DW:44:HIS:HA	2.54	0.42
1:AA:619:U:C2	4:AD:132:ILE:HD11	2.54	0.42
8:AH:94:LYS:HB3	8:AH:117:ARG:HH22	1.84	0.42
12:BL:80:ILE:HD12	12:BL:97:THR:HG22	2.01	0.42
31:CA:2815:C:H2'	31:CA:2816:G:O4'	2.19	0.42
31:CA:2869:G:H2'	31:CA:2870:C:O4'	2.19	0.42
29:CC:105:LEU:H	29:CC:105:LEU:HD12	1.85	0.42
45:CS:41:ILE:HD13	45:CS:103:ALA:HA	2.00	0.42
54:DA:1654:A:C1'	54:DA:2823:A:H5'	2.50	0.42
30:DD:167:ASN:O	63:DD:301:PGE:H52	2.20	0.42
32:DE:48:THR:HG23	32:DE:88:ARG:HH12	1.82	0.42
1:BA:49:U:O2	1:BA:362:G:H1'	2.20	0.42
2:BB:70:VAL:HB	2:BB:163:VAL:HG22	2.00	0.42
54:DA:1932:A:H2'	54:DA:1933:G:O4'	2.20	0.42
54:DA:189:G:N7	62:DA:3197:EDO:H21	2.35	0.42
1:BA:604:G:H2'	1:BA:605:U:O4'	2.20	0.42
3:BC:47:LEU:HD22	3:BC:76:VAL:HG22	2.00	0.42
10:BJ:10:LEU:HB2	10:BJ:72:ARG:HB2	2.00	0.42
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	2.01	0.42
31:CA:1028:A:N6	31:CA:1125:G:H2'	2.34	0.42
3:AC:47:LEU:HD22	3:AC:76:VAL:HG22	2.01	0.42
5:AE:132:ASN:OD1	5:AE:134:ILE:HG22	2.20	0.42
2:BB:129:LEU:H	2:BB:129:LEU:HG	1.53	0.42
11:BK:25:ALA:HA	11:BK:30:THR:HG22	2.01	0.42
13:BM:11:ASP:HA	13:BM:45:ILE:HD13	2.01	0.42
22:C1:9:THR:CG2	31:CA:2020:A:H5'	2.49	0.42
31:CA:1430:G:H2'	31:CA:1431:A:O4'	2.20	0.42
31:CA:538:A:H4'	37:CK:7:LYS:HG2	2.02	0.42
31:CA:686:U:H2'	31:CA:788:A:N1	2.34	0.42
29:CC:57:GLY:HA2	29:CC:213:TRP:HA	2.00	0.42
38:CL:121:GLU:HG2	38:CL:122:VAL:HG23	2.02	0.42
29:DC:225:MET:O	29:DC:233:GLY:O	2.38	0.42
41:DO:67:PHE:O	41:DO:71:ARG:HD2	2.20	0.42
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.55	0.42
1:AA:502:A:H2'	1:AA:503:C:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BM:17:ILE:HD12	13:BM:17:ILE:H	1.85	0.42
31:CA:1510:G:H2'	31:CA:1511:G:O4'	2.20	0.42
31:CA:2800:A:C2	31:CA:2895:G:H1'	2.54	0.42
33:CF:138:PHE:HE1	33:CF:152:LEU:HD21	1.85	0.42
37:CK:81:ILE:HG23	37:CK:82:GLY:N	2.35	0.42
54:DA:2445:2MG:HM21	54:DA:2449:H2U:O4	2.20	0.42
54:DA:825:A:H5''	58:DA:3222:PUT:H12	2.02	0.42
54:DA:984:A:N3	54:DA:984:A:H2'	2.33	0.42
1:AA:1305:G:HO2'	1:AA:1306:A:H8	1.65	0.42
4:AD:105:MET:SD	4:AD:143:VAL:HG22	2.60	0.42
20:AT:36:TYR:CE2	20:AT:79:LEU:HD21	2.55	0.42
1:BA:1322:C:O2	1:BA:1322:C:OP1	2.38	0.42
1:BA:1530:G:H2'	1:BA:1531:A:C8	2.55	0.42
35:CH:68:ARG:HB3	35:CH:134:VAL:HG21	2.02	0.42
46:CT:20:VAL:HG11	46:CT:44:ALA:HA	2.02	0.42
49:CW:86:LEU:HD13	49:CW:89:ILE:HD11	2.01	0.42
54:DA:355:U:H2'	54:DA:356:G:C8	2.55	0.42
48:DV:51:ALA:O	48:DV:52:LEU:HB2	2.19	0.42
2:AB:104:TRP:O	2:AB:108:ARG:HB2	2.20	0.42
5:AE:77:ASN:HB2	5:AE:82:GLN:HE21	1.74	0.42
5:BE:157:ARG:HG2	5:BE:158:GLY:N	2.35	0.42
12:BL:102:LEU:HB3	12:BL:103:ASP:H	1.78	0.42
31:CA:2074:U:H2'	31:CA:2075:U:C6	2.55	0.42
31:CA:796:C:H2'	31:CA:797:G:C8	2.54	0.42
31:CA:2060:A:N6	32:CE:69:ARG:NH2	2.67	0.42
32:CE:178:VAL:HG23	39:CM:3:LEU:HD21	2.02	0.42
54:DA:1794:A:H2'	54:DA:1795:C:C6	2.54	0.42
39:DM:109:LYS:HG2	39:DM:126:ARG:HB2	2.02	0.42
1:AA:1298:U:H3	7:AG:114:LYS:HA	1.85	0.42
1:AA:1152:A:H5'	10:AJ:15:HIS:HB2	2.02	0.42
1:AA:1322:C:P	19:AS:78:ARG:HH22	2.43	0.42
35:CH:82:SER:HB2	35:CH:94:ILE:HD11	2.02	0.42
49:CW:26:PHE:HE1	49:CW:44:HIS:HA	1.85	0.42
54:DA:1555:G:OP1	58:DA:3218:PUT:H41	2.20	0.42
54:DA:747:5MU:O2	54:DA:2014:A:H1'	2.20	0.42
54:DA:2406:A:H5'	54:DA:2406:A:C8	2.55	0.42
25:D4:8:ARG:HG3	54:DA:253:C:N4	2.35	0.42
3:AC:156:ARG:HD3	3:AC:193:TYR:O	2.20	0.41
7:AG:72:THR:HG22	7:AG:142:HIS:CE1	2.55	0.41
5:BE:115:LEU:HG	5:BE:123:VAL:HG21	2.01	0.41
11:BK:45:ALA:HB3	11:BK:70:CYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C1:4:GLN:HB3	31:CA:2615:U:H1'	2.02	0.41
31:CA:1101:U:H2'	31:CA:1102:C:C6	2.54	0.41
25:D4:39:LYS:O	25:D4:43:HIS:HD2	2.03	0.41
54:DA:320:A:H4'	54:DA:322:A:N7	2.35	0.41
1:AA:131:A:H2'	1:AA:132:C:C6	2.56	0.41
11:AK:25:ALA:HA	11:AK:30:THR:HG22	2.02	0.41
19:AS:30:PRO:HB2	19:AS:50:ALA:HB2	2.03	0.41
5:BE:23:LYS:HB3	5:BE:30:ILE:HG23	2.01	0.41
31:CA:2425:A:H4'	31:CA:2426:A:O5'	2.20	0.41
40:CN:41:LEU:HD21	40:CN:124:LEU:HD22	2.02	0.41
43:CQ:52:ASN:O	43:CQ:53:ARG:HD3	2.20	0.41
54:DA:136:G:H1	54:DA:143:C:N4	2.18	0.41
46:DT:6:LYS:HB2	54:DA:494:G:H4'	2.02	0.41
1:AA:1108:G:H5''	3:AC:176:HIS:ND1	2.36	0.41
1:AA:302:G:O2'	1:AA:556:C:H5''	2.20	0.41
14:BN:31:ILE:HG23	14:BN:42:TRP:HZ2	1.85	0.41
1:BA:1048:G:H4'	14:BN:3:LYS:HE2	2.02	0.41
31:CA:136:G:H1	31:CA:143:C:N4	2.19	0.41
29:CC:221:ARG:NH1	31:CA:1789:A:OP2	2.53	0.41
31:CA:2106:U:H2'	31:CA:2107:G:C8	2.55	0.41
40:CN:71:LYS:HB3	40:CN:93:VAL:O	2.21	0.41
47:CU:82:LYS:HD3	47:CU:84:TYR:CE1	2.55	0.41
54:DA:1418:G:H2'	54:DA:1579:A:N6	2.35	0.41
54:DA:1417:C:H5'	54:DA:1588:G:H1'	2.01	0.41
44:DR:51:ARG:HH22	54:DA:993:G:P	2.43	0.41
1:AA:1048:G:H4'	14:AN:3:LYS:HE2	2.02	0.41
1:BA:429:U:H1'	1:BA:430:A:H5''	2.03	0.41
20:BT:67:ILE:O	20:BT:68:HIS:HB2	2.20	0.41
31:CA:1794:A:H2'	31:CA:1795:C:C6	2.56	0.41
31:CA:2339:C:H2'	31:CA:2340:A:C8	2.56	0.41
31:CA:355:U:H2'	31:CA:356:G:C8	2.56	0.41
31:CA:742:A:H2'	31:CA:743:A:C8	2.55	0.41
54:DA:1202:G:H1'	57:DA:3192:MPD:HM1	2.02	0.41
54:DA:1430:G:H2'	54:DA:1431:A:O4'	2.20	0.41
53:DI:94:ARG:HG2	53:DI:127:ALA:HA	2.02	0.41
4:AD:170:TRP:CD2	4:AD:186:PRO:HB3	2.56	0.41
19:AS:5:LEU:HG	19:AS:5:LEU:H	1.75	0.41
1:BA:131:A:H2'	1:BA:132:C:C6	2.55	0.41
14:BN:53:ARG:HH21	19:BS:37:ARG:HH22	1.69	0.41
31:CA:2043:C:H5''	31:CA:2043:C:C6	2.55	0.41
31:CA:2060:A:N6	32:CE:69:ARG:HH21	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:174:LEU:CD2	29:CC:184:VAL:HB	2.50	0.41
39:CM:123:ARG:HG3	39:CM:143:GLU:HG3	2.03	0.41
46:CT:29:VAL:HG22	46:CT:51:LEU:HD11	2.02	0.41
25:D4:47:LYS:HE3	39:DM:64:PHE:CD1	2.55	0.41
54:DA:138:U:H5'	54:DA:139:U:H5'	2.03	0.41
54:DA:2128:G:H1	54:DA:2160:C:N4	2.18	0.41
25:D4:13:ARG:HH11	54:DA:2394:C:H5'	1.84	0.41
54:DA:602:A:C6	57:DA:3190:MPD:H31	2.56	0.41
54:DA:686:U:H2'	54:DA:788:A:N1	2.35	0.41
54:DA:792:A:N3	54:DA:2072:C:O2'	2.48	0.41
41:DO:8:ARG:HD3	54:DA:1652:A:OP1	2.19	0.41
1:AA:1343:G:O2'	9:AI:123:ARG:HD2	2.20	0.41
1:AA:439:U:H5''	4:AD:121:LYS:HD2	2.02	0.41
13:AM:54:ASP:HA	13:AM:57:ARG:HD2	2.02	0.41
4:BD:130:VAL:HG11	4:BD:135:TYR:CG	2.56	0.41
11:BK:20:VAL:HB	11:BK:35:THR:HG23	2.02	0.41
12:BL:87:VAL:HG11	12:BL:90:LEU:HD22	2.02	0.41
31:CA:1722:A:N6	31:CA:1738:G:H1'	2.36	0.41
30:CD:141:ARG:HB2	31:CA:1656:C:H5''	2.01	0.41
46:CT:69:LEU:HG	46:CT:107:VAL:CG2	2.50	0.41
31:CA:1364:G:P	51:CY:50:ARG:HH22	2.43	0.41
54:DA:2097:A:H8	54:DA:2097:A:H5''	1.85	0.41
35:DH:82:SER:HB2	35:DH:94:ILE:HD11	2.02	0.41
1:AA:429:U:H1'	1:AA:430:A:H5''	2.02	0.41
6:AF:102:MET:CE	18:AR:24:LYS:HB3	2.50	0.41
1:BA:1376:U:H2'	1:BA:1377:A:C8	2.55	0.41
5:BE:82:GLN:HG2	5:BE:149:SER:HA	2.01	0.41
1:BA:1298:U:H3	7:BG:114:LYS:HA	1.86	0.41
9:BI:19:VAL:HG11	9:BI:83:ILE:HA	2.03	0.41
20:BT:44:LYS:HB3	20:BT:87:ALA:HB2	2.03	0.41
31:CA:2114:A:N6	31:CA:2119:A:H62	2.18	0.41
31:CA:2788:C:H2'	31:CA:2789:C:C6	2.55	0.41
31:CA:811:U:H2'	39:CM:21:ARG:HA	2.02	0.41
41:CO:95:THR:HG21	41:CO:113:ILE:HD11	2.02	0.41
54:DA:1515:A:H2'	54:DA:1516:G:O4'	2.20	0.41
54:DA:2038:G:H2'	54:DA:2039:U:O4'	2.21	0.41
34:DG:140:VAL:O	34:DG:144:VAL:HG23	2.20	0.41
46:DT:20:VAL:HG11	46:DT:44:ALA:HA	2.03	0.41
4:BD:170:TRP:CD2	4:BD:186:PRO:HB3	2.56	0.41
5:BE:77:ASN:HB2	5:BE:82:GLN:HE21	1.79	0.41
31:CA:2095:A:H5''	31:CA:2095:A:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2898:U:O2	37:CK:134:ALA:HB1	2.20	0.41
31:CA:910:A:H62	40:CN:12:MET:HA	1.85	0.41
54:DA:1020:A:C2	54:DA:1141:U:C2	3.08	0.41
54:DA:2324:U:H3'	54:DA:2325:G:H5''	2.03	0.41
50:DX:41[A]:ARG:HD2	54:DA:2387:U:H1'	2.03	0.41
35:DH:68:ARG:HB3	35:DH:134:VAL:HG21	2.03	0.41
50:DX:41[B]:ARG:HA	50:DX:41[B]:ARG:HD3	1.94	0.41
9:AI:19:VAL:HG11	9:AI:83:ILE:HA	2.03	0.41
1:BA:841:C:H3'	1:BA:842:U:C4'	2.51	0.41
19:BS:30:PRO:HB2	19:BS:50:ALA:HB2	2.03	0.41
31:CA:2038:G:H2'	31:CA:2039:U:O4'	2.21	0.41
31:CA:2641:G:H5''	37:CK:78:THR:HB	2.03	0.41
31:CA:547:A:H2'	31:CA:547:A:N3	2.36	0.41
54:DA:2133:G:H21	54:DA:2158:A:N6	2.18	0.41
32:DE:178:VAL:HG23	39:DM:3:LEU:HD21	2.01	0.41
32:DE:23:PHE:HE2	32:DE:25:GLU:HG3	1.86	0.41
50:DX:38:VAL:HG12	50:DX:59:LEU:HB2	2.02	0.41
5:AE:157:ARG:CD	8:AH:43:GLU:O	2.69	0.41
11:AK:20:VAL:HB	11:AK:35:THR:HG23	2.03	0.41
1:BA:567:G:H2'	1:BA:568:G:O4'	2.20	0.41
11:BK:34:ILE:HG12	11:BK:70:CYS:SG	2.60	0.41
25:C4:24:HIS:CG	39:CM:61:LEU:HD13	2.56	0.41
31:CA:1636:U:H2'	31:CA:1637:A:C8	2.55	0.41
34:CG:38:ASN:HD22	34:CG:40:ALA:HB3	1.86	0.41
36:CJ:49:ILE:HG13	36:CJ:55:ILE:HD13	2.03	0.41
53:DI:132:TYR:N	53:DI:133:GLU:HB2	2.35	0.41
30:DD:13:ARG:HH11	43:DQ:56:HIS:HA	1.86	0.41
10:AJ:19:ASP:HA	10:AJ:22:THR:HB	2.03	0.41
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.85	0.41
1:BA:439:U:H5''	4:BD:121:LYS:HD2	2.02	0.41
1:BA:216:U:H4'	1:BA:464:U:H4'	2.02	0.41
26:C5:4:ARG:HB2	31:CA:2466:C:OP1	2.21	0.41
31:CA:29:U:O5'	31:CA:29:U:H6	2.02	0.41
31:CA:780:G:H2'	31:CA:782:A:N7	2.36	0.41
29:CC:107:PRO:HD2	29:CC:110:LEU:HD22	2.03	0.41
54:DA:1306:C:H5''	54:DA:1306:C:H6	1.85	0.41
54:DA:207:A:H2'	54:DA:208:C:O4'	2.20	0.41
51:DY:29:PHE:HB3	54:DA:396:G:H1'	2.03	0.41
53:DI:29:ASP:HB3	53:DI:106:PHE:HB2	2.02	0.41
36:DJ:14:ALA:HB3	36:DJ:17:MET:HB2	2.03	0.41
39:DM:74:THR:HG23	39:DM:107:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:DN:89:VAL:CG1	57:DN:201:MPD:HM3	2.50	0.41
46:DT:84:ARG:HB2	46:DT:96:ILE:HB	2.02	0.41
1:AA:1141:C:O2'	1:AA:1142:G:H8	2.03	0.40
1:AA:568:G:O6	12:AL:2:ALA:HB2	2.21	0.40
1:AA:1216:A:H5''	14:AN:5:SER:HB3	2.02	0.40
6:BF:22:ILE:HG23	6:BF:39:LEU:HD11	2.02	0.40
10:BJ:59:LYS:HD2	10:BJ:60:ASP:OD1	2.21	0.40
20:BT:69:LYS:H	20:BT:69:LYS:HG3	1.60	0.40
54:DA:281:C:H2'	54:DA:282:A:C8	2.56	0.40
54:DA:839:U:H2'	54:DA:840:C:C6	2.56	0.40
30:DD:26:VAL:HG21	43:DQ:5:ILE:HG12	2.03	0.40
34:DG:50:LEU:HD13	34:DG:72:LEU:HD23	2.02	0.40
53:DI:23:LEU:HD13	53:DI:89:PRO:HD3	2.03	0.40
39:DM:123:ARG:HG3	39:DM:143:GLU:HG3	2.03	0.40
50:DX:41[A]:ARG:HH12	54:DA:2262:U:H5''	1.85	0.40
1:AA:831:A:H5''	2:AB:21:ARG:HD3	2.03	0.40
14:AN:46:LEU:HD22	19:AS:13:LEU:HG	2.02	0.40
1:BA:1197:A:H5''	59:BA:1602:TAC:O12	2.21	0.40
1:BA:268:U:H2'	1:BA:269:C:C6	2.56	0.40
1:BA:1108:G:H5''	3:BC:176:HIS:ND1	2.36	0.40
9:BI:116:VAL:HG21	10:BJ:62:ARG:HD3	2.04	0.40
1:BA:718:A:H5'	11:BK:119:ASN:HB2	2.04	0.40
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.56	0.40
54:DA:2273:A:H2'	54:DA:2274:A:C8	2.55	0.40
53:DI:120:ALA:HA	53:DI:123:ILE:HD11	2.03	0.40
53:DI:65:GLU:HA	53:DI:70:GLU:HG3	2.02	0.40
52:DZ:56:LEU:HA	52:DZ:59:GLU:HG2	2.03	0.40
1:AA:268:U:H2'	1:AA:269:C:C6	2.56	0.40
11:AK:31:ILE:HG12	11:AK:46:THR:CG2	2.51	0.40
25:C4:52:LYS:HA	25:C4:55:LEU:HD12	2.03	0.40
31:CA:1306:C:H5''	31:CA:1306:C:H6	1.86	0.40
31:CA:1418:G:H2'	31:CA:1579:A:N6	2.36	0.40
54:DA:1532:A:H5''	54:DA:1532:A:H8	1.86	0.40
54:DA:2339:C:H2'	54:DA:2340:A:C8	2.57	0.40
39:DM:77:ILE:CD1	39:DM:101:ILE:CG2	2.97	0.40
39:DM:95:LEU:HD11	39:DM:125:LEU:HD21	2.03	0.40
46:DT:72:THR:CG2	46:DT:108:SER:HB3	2.52	0.40
1:AA:234:C:H4'	17:AQ:66:PRO:HG3	2.03	0.40
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	2.04	0.40
12:BL:74:LEU:HD21	12:BL:80:ILE:HG21	2.03	0.40
1:BA:1322:C:P	19:BS:78:ARG:HH22	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1509:A:HO2'	31:CA:1510:G:H8	1.70	0.40
31:CA:2327:A:H2'	31:CA:2328:A:C8	2.56	0.40
31:CA:644:A:H2'	31:CA:645:C:O4'	2.22	0.40
36:CJ:19:ASN:N	36:CJ:20:PRO:HD2	2.37	0.40
44:CR:58:ARG:HH11	44:CR:62:ILE:HD11	1.86	0.40
22:D1:12:LYS:HD2	22:D1:12:LYS:HA	1.86	0.40
22:D1:8:PRO:HD2	54:DA:1263:U:O2'	2.22	0.40
54:DA:2788:C:H2'	54:DA:2789:C:C6	2.57	0.40
38:DL:113:MET:O	38:DL:116:ILE:HG13	2.19	0.40
1:AA:567:G:H2'	1:AA:568:G:O4'	2.21	0.40
1:BA:580:C:H2'	1:BA:581:G:O4'	2.22	0.40
19:BS:5:LEU:CD2	19:BS:10:PHE:HB2	2.51	0.40
31:CA:1072:C:H2'	31:CA:1093:G:O6	2.21	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%)	210 (95%)	9 (4%)	3 (1%)	14	42
2	BB	222/224 (99%)	211 (95%)	7 (3%)	4 (2%)	11	34
3	AC	204/206 (99%)	192 (94%)	11 (5%)	1 (0%)	34	69
3	BC	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	19	52
4	AD	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
4	BD	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
5	AE	153/155 (99%)	147 (96%)	5 (3%)	1 (1%)	26	62
5	BE	148/155 (96%)	132 (89%)	12 (8%)	4 (3%)	6	21
6	AF	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
6	BF	98/106 (92%)	91 (93%)	5 (5%)	2 (2%)	9	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	149/151 (99%)	137 (92%)	11 (7%)	1 (1%)	26	62
7	BG	149/151 (99%)	140 (94%)	9 (6%)	0	100	100
8	AH	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
8	BH	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
9	AI	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
9	BI	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
10	AJ	97/99 (98%)	88 (91%)	7 (7%)	2 (2%)	9	29
10	BJ	96/99 (97%)	77 (80%)	14 (15%)	5 (5%)	2	7
11	AK	115/117 (98%)	107 (93%)	6 (5%)	2 (2%)	11	36
11	BK	115/117 (98%)	104 (90%)	9 (8%)	2 (2%)	11	36
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
12	BL	120/123 (98%)	114 (95%)	5 (4%)	1 (1%)	24	58
13	AM	112/114 (98%)	103 (92%)	6 (5%)	3 (3%)	6	21
13	BM	112/114 (98%)	102 (91%)	5 (4%)	5 (4%)	3	10
14	AN	98/100 (98%)	88 (90%)	8 (8%)	2 (2%)	9	30
14	BN	98/100 (98%)	90 (92%)	6 (6%)	2 (2%)	9	30
15	AO	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
15	BO	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	16	47
16	AP	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
16	BP	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	7	24
17	AQ	78/80 (98%)	70 (90%)	7 (9%)	1 (1%)	15	44
17	BQ	78/80 (98%)	68 (87%)	5 (6%)	5 (6%)	2	4
18	AR	53/55 (96%)	53 (100%)	0	0	100	100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	15	44
19	BS	77/79 (98%)	68 (88%)	7 (9%)	2 (3%)	7	22
20	AT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
20	BT	83/86 (96%)	79 (95%)	3 (4%)	1 (1%)	16	47
21	AU	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
21	BU	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
22	C1	54/56 (96%)	47 (87%)	4 (7%)	3 (6%)	2	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	D1	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	3	11
23	D2	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
24	C3	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	8	26
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	C4	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
25	D4	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
26	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	6	21
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	54 (96%)	0	2 (4%)	4	14
27	D0	57/58 (98%)	56 (98%)	1 (2%)	0	100	100
29	CC	269/271 (99%)	252 (94%)	12 (4%)	5 (2%)	10	32
29	DC	269/271 (99%)	257 (96%)	10 (4%)	2 (1%)	26	62
30	CD	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
30	DD	206/209 (99%)	202 (98%)	4 (2%)	0	100	100
32	CE	199/201 (99%)	191 (96%)	5 (2%)	3 (2%)	13	40
32	DE	199/201 (99%)	194 (98%)	4 (2%)	1 (0%)	34	69
33	CF	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	30	65
33	DF	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	30	65
34	CG	174/176 (99%)	162 (93%)	7 (4%)	5 (3%)	6	19
34	DG	174/176 (99%)	165 (95%)	8 (5%)	1 (1%)	30	65
35	CH	147/149 (99%)	136 (92%)	6 (4%)	5 (3%)	5	16
35	DH	147/149 (99%)	138 (94%)	6 (4%)	3 (2%)	9	30
36	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	5	18
36	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	5	18
37	CK	140/142 (99%)	135 (96%)	4 (3%)	1 (1%)	26	62
37	DK	140/142 (99%)	137 (98%)	2 (1%)	1 (1%)	26	62
38	CL	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	11	36
38	DL	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	24	58
39	CM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	9	29
39	DM	142/144 (99%)	136 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	CN	133/136 (98%)	125 (94%)	7 (5%)	1 (1%)	24	58
40	DN	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
41	CO	118/125 (94%)	111 (94%)	5 (4%)	2 (2%)	11	36
41	DO	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
42	CP	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
42	DP	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
43	CQ	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
43	DQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	21	55
44	CR	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
44	DR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
45	CS	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	5	18
45	DS	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	19	52
46	CT	108/110 (98%)	101 (94%)	5 (5%)	2 (2%)	10	32
46	DT	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
47	CU	91/93 (98%)	86 (94%)	4 (4%)	1 (1%)	17	50
47	DU	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
48	CV	100/102 (98%)	91 (91%)	4 (4%)	5 (5%)	3	8
48	DV	100/102 (98%)	96 (96%)	2 (2%)	2 (2%)	9	30
49	CW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
49	DW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
50	CX	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
50	DX	75/76 (99%)	74 (99%)	1 (1%)	0	100	100
51	CY	75/77 (97%)	74 (99%)	1 (1%)	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	36
52	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
53	DI	133/135 (98%)	114 (86%)	13 (10%)	6 (4%)	3	10
All	All	11406/11629 (98%)	10790 (95%)	484 (4%)	132 (1%)	16	47

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE

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

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

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Mol	Chain	Res	Type
32	DE	6	LYS
35	DH	118	PRO
38	DL	108	ARG
45	DS	44	GLY
48	DV	89	ASP
53	DI	91	ALA
53	DI	109	LYS
53	DI	130	PRO
5	AE	162	GLU
10	BJ	36	VAL
13	BM	4	ILE
35	CH	9	VAL
39	CM	30	THR
41	CO	119	SER
45	CS	55	ASP
46	CT	63	GLY
35	DH	11	ASN
53	DI	70	GLU
53	DI	88	HIS
19	AS	6	LYS
2	BB	95	ARG
5	BE	105	ILE
14	BN	22	ALA
35	CH	8	LYS
35	CH	122	LEU
36	CJ	23	PRO
45	CS	48	LYS
45	CS	53	PHE
35	DH	122	LEU
36	DJ	23	PRO
43	DQ	105	GLY
53	DI	108	VAL
14	AN	22	ALA
16	BP	44	SER
34	CG	45	HIS
38	CL	110	GLU
46	CT	65	ASP
48	CV	52	LEU
52	CZ	62	GLY
37	DK	83	GLY
26	C5	21	GLY
33	CF	62	GLY

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Mol	Chain	Res	Type
36	CJ	32	GLY
33	DF	62	GLY
36	DJ	32	GLY
17	BQ	35	GLY
10	AJ	33	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/186 (100%)	173 (93%)	13 (7%)	19	47
2	BB	186/186 (100%)	173 (93%)	13 (7%)	19	47
3	AC	170/170 (100%)	159 (94%)	11 (6%)	21	52
3	BC	170/170 (100%)	156 (92%)	14 (8%)	14	38
4	AD	172/172 (100%)	163 (95%)	9 (5%)	29	62
4	BD	172/172 (100%)	160 (93%)	12 (7%)	19	47
5	AE	118/118 (100%)	106 (90%)	12 (10%)	9	26
5	BE	113/118 (96%)	95 (84%)	18 (16%)	3	9
6	AF	92/92 (100%)	86 (94%)	6 (6%)	21	52
6	BF	87/92 (95%)	77 (88%)	10 (12%)	7	21
7	AG	124/124 (100%)	115 (93%)	9 (7%)	17	44
7	BG	124/124 (100%)	109 (88%)	15 (12%)	6	18
8	AH	104/104 (100%)	93 (89%)	11 (11%)	8	24
8	BH	104/104 (100%)	93 (89%)	11 (11%)	8	24
9	AI	105/105 (100%)	100 (95%)	5 (5%)	31	66
9	BI	105/105 (100%)	100 (95%)	5 (5%)	31	66
10	AJ	87/87 (100%)	81 (93%)	6 (7%)	19	48
10	BJ	86/87 (99%)	78 (91%)	8 (9%)	11	32
11	AK	90/90 (100%)	87 (97%)	3 (3%)	45	79
11	BK	90/90 (100%)	83 (92%)	7 (8%)	16	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	102/102 (100%)	92 (90%)	10 (10%)	10	28
12	BL	102/102 (100%)	90 (88%)	12 (12%)	6	19
13	AM	92/92 (100%)	83 (90%)	9 (10%)	10	28
13	BM	92/92 (100%)	85 (92%)	7 (8%)	16	42
14	AN	83/83 (100%)	82 (99%)	1 (1%)	78	95
14	BN	83/83 (100%)	82 (99%)	1 (1%)	78	95
15	AO	76/76 (100%)	71 (93%)	5 (7%)	21	51
15	BO	76/76 (100%)	65 (86%)	11 (14%)	4	11
16	AP	65/65 (100%)	64 (98%)	1 (2%)	72	93
16	BP	65/65 (100%)	63 (97%)	2 (3%)	47	81
17	AQ	74/74 (100%)	67 (90%)	7 (10%)	11	30
17	BQ	74/74 (100%)	66 (89%)	8 (11%)	8	23
18	AR	48/48 (100%)	47 (98%)	1 (2%)	61	90
18	BR	48/48 (100%)	47 (98%)	1 (2%)	61	90
19	AS	70/70 (100%)	63 (90%)	7 (10%)	9	27
19	BS	70/70 (100%)	65 (93%)	5 (7%)	18	46
20	AT	65/65 (100%)	59 (91%)	6 (9%)	11	32
20	BT	65/65 (100%)	55 (85%)	10 (15%)	3	10
21	AU	48/48 (100%)	44 (92%)	4 (8%)	14	38
21	BU	48/48 (100%)	44 (92%)	4 (8%)	14	38
22	C1	47/47 (100%)	45 (96%)	2 (4%)	35	70
22	D1	47/47 (100%)	44 (94%)	3 (6%)	22	52
23	C2	45/46 (98%)	44 (98%)	1 (2%)	60	89
23	D2	45/46 (98%)	43 (96%)	2 (4%)	35	69
24	C3	38/38 (100%)	37 (97%)	1 (3%)	54	86
24	D3	38/38 (100%)	37 (97%)	1 (3%)	54	86
25	C4	51/51 (100%)	48 (94%)	3 (6%)	24	57
25	D4	51/51 (100%)	48 (94%)	3 (6%)	24	57
26	C5	34/34 (100%)	32 (94%)	2 (6%)	24	57
26	D5	34/34 (100%)	34 (100%)	0	100	100
27	C0	48/48 (100%)	45 (94%)	3 (6%)	22	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	D0	49/48 (102%)	45 (92%)	4 (8%)	14	38
29	CC	216/216 (100%)	203 (94%)	13 (6%)	24	56
29	DC	216/216 (100%)	210 (97%)	6 (3%)	51	84
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%)	152 (92%)	13 (8%)	15	40
32	DE	165/165 (100%)	161 (98%)	4 (2%)	57	87
33	CF	148/148 (100%)	133 (90%)	15 (10%)	9	27
33	DF	148/148 (100%)	137 (93%)	11 (7%)	17	43
34	CG	137/137 (100%)	134 (98%)	3 (2%)	60	89
34	DG	137/137 (100%)	132 (96%)	5 (4%)	42	76
35	CH	114/114 (100%)	101 (89%)	13 (11%)	7	21
35	DH	114/114 (100%)	101 (89%)	13 (11%)	7	21
36	CJ	104/104 (100%)	100 (96%)	4 (4%)	40	74
36	DJ	104/104 (100%)	100 (96%)	4 (4%)	40	74
37	CK	116/116 (100%)	110 (95%)	6 (5%)	29	62
37	DK	116/116 (100%)	114 (98%)	2 (2%)	68	92
38	CL	103/104 (99%)	99 (96%)	4 (4%)	39	74
38	DL	104/104 (100%)	99 (95%)	5 (5%)	31	66
39	CM	103/103 (100%)	97 (94%)	6 (6%)	25	57
39	DM	103/103 (100%)	99 (96%)	4 (4%)	39	74
40	CN	108/108 (100%)	104 (96%)	4 (4%)	41	76
40	DN	109/108 (101%)	106 (97%)	3 (3%)	51	84
41	CO	100/102 (98%)	95 (95%)	5 (5%)	30	64
41	DO	102/102 (100%)	99 (97%)	3 (3%)	50	83
42	CP	86/87 (99%)	80 (93%)	6 (7%)	19	47
42	DP	87/87 (100%)	84 (97%)	3 (3%)	44	78
43	CQ	99/99 (100%)	93 (94%)	6 (6%)	23	55
43	DQ	99/99 (100%)	97 (98%)	2 (2%)	63	90
44	CR	89/89 (100%)	86 (97%)	3 (3%)	44	78
44	DR	89/89 (100%)	87 (98%)	2 (2%)	60	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	CS	84/84 (100%)	79 (94%)	5 (6%)	24	56
45	DS	84/84 (100%)	83 (99%)	1 (1%)	78	95
46	CT	93/93 (100%)	88 (95%)	5 (5%)	27	60
46	DT	93/93 (100%)	92 (99%)	1 (1%)	80	95
47	CU	80/80 (100%)	72 (90%)	8 (10%)	9	27
47	DU	80/80 (100%)	77 (96%)	3 (4%)	40	74
48	CV	83/83 (100%)	79 (95%)	4 (5%)	31	66
48	DV	83/83 (100%)	81 (98%)	2 (2%)	57	87
49	CW	78/78 (100%)	75 (96%)	3 (4%)	40	74
49	DW	78/78 (100%)	76 (97%)	2 (3%)	54	86
50	CX	56/58 (97%)	55 (98%)	1 (2%)	66	91
50	DX	58/58 (100%)	57 (98%)	1 (2%)	68	92
51	CY	67/67 (100%)	63 (94%)	4 (6%)	24	56
51	DY	67/67 (100%)	65 (97%)	2 (3%)	48	82
52	CZ	54/54 (100%)	50 (93%)	4 (7%)	17	43
52	DZ	54/54 (100%)	52 (96%)	2 (4%)	41	76
53	DI	103/103 (100%)	98 (95%)	5 (5%)	31	65
All	All	9460/9477 (100%)	8897 (94%)	563 (6%)	24	56

All (563) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	23	TRP
2	AB	44	GLU
2	AB	73	LYS
2	AB	93	ASN
2	AB	105	LYS
2	AB	125	THR
2	AB	129	LEU
2	AB	130	THR
2	AB	135	LEU
2	AB	137	ARG
2	AB	147	SER
2	AB	161	LEU
2	AB	205	ASP
3	AC	4	LYS

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Mol	Chain	Res	Type
3	AC	14	ILE
3	AC	21	THR
3	AC	33	LEU
3	AC	38	LYS
3	AC	46	GLU
3	AC	107	ARG
3	AC	168	TYR
3	AC	178	LEU
3	AC	185	ASN
3	AC	186	THR
4	AD	5	LEU
4	AD	17	THR
4	AD	22	LYS
4	AD	26	ARG
4	AD	50	ASP
4	AD	132	ILE
4	AD	142	VAL
4	AD	143	VAL
4	AD	194	ASP
5	AE	11	LEU
5	AE	14	LYS
5	AE	32	SER
5	AE	46	VAL
5	AE	76	LEU
5	AE	78	ASN
5	AE	82	GLN
5	AE	101	GLU
5	AE	106	ILE
5	AE	123	VAL
5	AE	126	LYS
5	AE	149	SER
6	AF	36	ILE
6	AF	69	GLU
6	AF	71	ILE
6	AF	74	LEU
6	AF	89	VAL
6	AF	93	LYS
7	AG	30	LEU
7	AG	36	LYS
7	AG	59	LEU
7	AG	63	GLU
7	AG	92	ARG

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Mol	Chain	Res	Type
7	AG	120	LEU
7	AG	131	LYS
7	AG	133	THR
7	AG	142	HIS
8	AH	3	MET
8	AH	31	LYS
8	AH	47	GLU
8	AH	52	GLU
8	AH	54	ASP
8	AH	60	GLU
8	AH	63	LEU
8	AH	76	GLN
8	AH	90	ASP
8	AH	107	SER
8	AH	108	LYS
9	AI	11	ARG
9	AI	61	LEU
9	AI	63	LEU
9	AI	66	THR
9	AI	99	ARG
10	AJ	6	ILE
10	AJ	62	ARG
10	AJ	63	ASP
10	AJ	88	MET
10	AJ	89	ARG
10	AJ	90	LEU
11	AK	23	ILE
11	AK	55	SER
11	AK	119	ASN
12	AL	24	LEU
12	AL	40	THR
12	AL	55	VAL
12	AL	74	LEU
12	AL	82	ILE
12	AL	88	LYS
12	AL	90	LEU
12	AL	110	ARG
12	AL	115	SER
12	AL	121	ARG
13	AM	7	ILE
13	AM	13	LYS
13	AM	17	ILE

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Mol	Chain	Res	Type
13	AM	27	LYS
13	AM	48	LEU
13	AM	58	ASP
13	AM	63	PHE
13	AM	71	ARG
13	AM	101	ARG
14	AN	31	ILE
15	AO	2	SER
15	AO	24	SER
15	AO	40	GLN
15	AO	70	LEU
15	AO	84	ARG
16	AP	48	GLU
17	AQ	5	ILE
17	AQ	16	LYS
17	AQ	27	ARG
17	AQ	38	ILE
17	AQ	40	ARG
17	AQ	75	LEU
17	AQ	83	VAL
18	AR	47	THR
19	AS	5	LEU
19	AS	7	LYS
19	AS	13	LEU
19	AS	27	ASP
19	AS	33	THR
19	AS	37	ARG
19	AS	56	GLN
20	AT	15	GLU
20	AT	24	ARG
20	AT	27	MET
20	AT	44	LYS
20	AT	48	GLN
20	AT	85	LYS
21	AU	13	ASP
21	AU	16	LEU
21	AU	34	ARG
21	AU	56	HIS
22	C1	10	ARG
22	C1	40	ARG
23	C2	8	LYS
24	C3	1	MET

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Mol	Chain	Res	Type
25	C4	31	HIS
25	C4	45	ARG
25	C4	52	LYS
26	C5	20	ASP
26	C5	26	ILE
27	C0	3	LYS
27	C0	19	LYS
27	C0	36	VAL
2	BB	18	HIS
2	BB	23	TRP
2	BB	44	GLU
2	BB	93	ASN
2	BB	105	LYS
2	BB	125	THR
2	BB	129	LEU
2	BB	130	THR
2	BB	135	LEU
2	BB	137	ARG
2	BB	147	SER
2	BB	161	LEU
2	BB	205	ASP
3	BC	4	LYS
3	BC	14	ILE
3	BC	33	LEU
3	BC	37	PHE
3	BC	38	LYS
3	BC	46	GLU
3	BC	55	ILE
3	BC	107	ARG
3	BC	152	GLU
3	BC	168	TYR
3	BC	175	LEU
3	BC	185	ASN
3	BC	186	THR
3	BC	193	TYR
4	BD	5	LEU
4	BD	17	THR
4	BD	22	LYS
4	BD	26	ARG
4	BD	47	ARG
4	BD	50	ASP
4	BD	142	VAL

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Mol	Chain	Res	Type
4	BD	143	VAL
4	BD	151	LYS
4	BD	173	VAL
4	BD	194	ASP
4	BD	206	LYS
5	BE	11	LEU
5	BE	14	LYS
5	BE	32	SER
5	BE	46	VAL
5	BE	76	LEU
5	BE	81	LEU
5	BE	82	GLN
5	BE	88	VAL
5	BE	101	GLU
5	BE	103	THR
5	BE	114	VAL
5	BE	115	LEU
5	BE	123	VAL
5	BE	126	LYS
5	BE	151	GLU
5	BE	152	MET
5	BE	157	ARG
5	BE	159	LYS
6	BF	9	MET
6	BF	14	GLN
6	BF	16	GLU
6	BF	36	ILE
6	BF	53	LYS
6	BF	68	GLN
6	BF	69	GLU
6	BF	71	ILE
6	BF	89	VAL
6	BF	93	LYS
7	BG	4	ARG
7	BG	5	ARG
7	BG	10	ARG
7	BG	30	LEU
7	BG	36	LYS
7	BG	48	GLU
7	BG	50	LEU
7	BG	59	LEU
7	BG	63	GLU

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Mol	Chain	Res	Type
7	BG	72	THR
7	BG	92	ARG
7	BG	120	LEU
7	BG	131	LYS
7	BG	133	THR
7	BG	142	HIS
8	BH	3	MET
8	BH	47	GLU
8	BH	52	GLU
8	BH	60	GLU
8	BH	76	GLN
8	BH	77	ARG
8	BH	80	ARG
8	BH	83	LEU
8	BH	90	ASP
8	BH	107	SER
8	BH	108	LYS
9	BI	11	ARG
9	BI	61	LEU
9	BI	63	LEU
9	BI	66	THR
9	BI	99	ARG
10	BJ	5	ARG
10	BJ	6	ILE
10	BJ	62	ARG
10	BJ	63	ASP
10	BJ	78	GLU
10	BJ	88	MET
10	BJ	89	ARG
10	BJ	90	LEU
11	BK	18	ASP
11	BK	23	ILE
11	BK	31	ILE
11	BK	38	GLN
11	BK	55	SER
11	BK	118	HIS
11	BK	119	ASN
12	BL	24	LEU
12	BL	44	LYS
12	BL	50	ARG
12	BL	55	VAL
12	BL	58	THR

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Mol	Chain	Res	Type
12	BL	74	LEU
12	BL	82	ILE
12	BL	88	LYS
12	BL	90	LEU
12	BL	110	ARG
12	BL	115	SER
12	BL	121	ARG
13	BM	11	ASP
13	BM	13	LYS
13	BM	16	VAL
13	BM	17	ILE
13	BM	27	LYS
13	BM	48	LEU
13	BM	101	ARG
14	BN	26	GLU
15	BO	2	SER
15	BO	13	SER
15	BO	17	ARG
15	BO	24	SER
15	BO	40	GLN
15	BO	64	ARG
15	BO	66	LEU
15	BO	84	ARG
15	BO	87	LEU
15	BO	88	ARG
15	BO	89	ARG
16	BP	20	VAL
16	BP	46	LYS
17	BQ	17	MET
17	BQ	21	ILE
17	BQ	26	GLU
17	BQ	27	ARG
17	BQ	38	ILE
17	BQ	40	ARG
17	BQ	51	ASN
17	BQ	75	LEU
18	BR	47	THR
19	BS	6	LYS
19	BS	7	LYS
19	BS	13	LEU
19	BS	33	THR
19	BS	37	ARG

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Mol	Chain	Res	Type
20	BT	15	GLU
20	BT	24	ARG
20	BT	43	ASP
20	BT	48	GLN
20	BT	54	MET
20	BT	58	VAL
20	BT	64	LYS
20	BT	67	ILE
20	BT	69	LYS
20	BT	84	ASN
21	BU	13	ASP
21	BU	16	LEU
21	BU	34	ARG
21	BU	56	HIS
22	D1	18	SER
22	D1	26	THR
22	D1	29	SER
23	D2	5	ILE
23	D2	8	LYS
24	D3	1	MET
25	D4	31	HIS
25	D4	45	ARG
25	D4	52	LYS
27	D0	10	THR
27	D0	19	LYS
27	D0	25	LEU
27	D0	36	VAL
29	CC	117	GLN
29	CC	120	VAL
29	CC	130	LEU
29	CC	157	SER
29	CC	168	ASP
29	CC	174	LEU
29	CC	195	VAL
29	CC	204	VAL
29	CC	205	LEU
29	CC	236	GLU
29	CC	252	THR
29	CC	258	ARG
29	CC	260	ASN
30	CD	4	LEU
30	CD	13	ARG

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Mol	Chain	Res	Type
30	CD	18	ASP
30	CD	95	SER
29	DC	70	ASN
29	DC	117	GLN
29	DC	120	VAL
29	DC	130	LEU
29	DC	236	GLU
29	DC	252	THR
30	DD	13	ARG
30	DD	18	ASP
30	DD	95	SER
32	CE	7	ASP
32	CE	12	LEU
32	CE	25	GLU
32	CE	44	ARG
32	CE	72	SER
32	CE	78	TRP
32	CE	83	VAL
32	CE	107	SER
32	CE	122	GLU
32	CE	127	GLU
32	CE	149	ILE
32	CE	152	GLU
32	CE	189	THR
33	CF	18	THR
33	CF	36	LEU
33	CF	57	LEU
33	CF	72	LYS
33	CF	80	ARG
33	CF	94	GLU
33	CF	106	ILE
33	CF	115	ARG
33	CF	117	LEU
33	CF	123	ASP
33	CF	134	GLU
33	CF	141	ILE
33	CF	149	VAL
33	CF	152	LEU
33	CF	174	ASP
34	CG	11	VAL
34	CG	18	LYS
34	CG	155	GLU

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Mol	Chain	Res	Type
35	CH	7	ASP
35	CH	15	LEU
35	CH	17	ASP
35	CH	21	VAL
35	CH	48	GLU
35	CH	51	ARG
35	CH	53	GLU
35	CH	55	GLU
35	CH	62	LEU
35	CH	75	LEU
35	CH	121	VAL
35	CH	127	GLU
35	CH	145	ASN
36	CJ	11	LEU
36	CJ	13	VAL
36	CJ	28	LEU
36	CJ	113	LYS
37	CK	5	THR
37	CK	9	GLU
37	CK	30	THR
37	CK	39	LYS
37	CK	124	VAL
37	CK	142	ILE
38	CL	35	VAL
38	CL	58	LEU
38	CL	98	ARG
38	CL	113	MET
39	CM	2	ARG
39	CM	21	ARG
39	CM	93	ASN
39	CM	94	THR
39	CM	100	ILE
39	CM	115	GLU
40	CN	6	ARG
40	CN	20	LEU
40	CN	59	ARG
40	CN	78	LEU
41	CO	2	ARG
41	CO	14	SER
41	CO	71	ARG
41	CO	76	VAL
41	CO	95	THR

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Mol	Chain	Res	Type
42	CP	18	LEU
42	CP	31	THR
42	CP	38	GLN
42	CP	49	VAL
42	CP	56	LYS
42	CP	78	VAL
43	CQ	2	SER
43	CQ	26	VAL
43	CQ	39	ARG
43	CQ	40	LEU
43	CQ	102	GLU
43	CQ	114	LEU
44	CR	16	LYS
44	CR	51	ARG
44	CR	52	GLN
45	CS	12	HIS
45	CS	45	GLU
45	CS	48	LYS
45	CS	51	VAL
45	CS	102	SER
46	CT	7	HIS
46	CT	19	LEU
46	CT	29	VAL
46	CT	86	MET
46	CT	97	LEU
47	CU	1	MET
47	CU	2	ILE
47	CU	3	ARG
47	CU	10	VAL
47	CU	24	MET
47	CU	30	ILE
47	CU	49	LYS
47	CU	69	ARG
48	CV	61	LYS
48	CV	72	ILE
48	CV	81	ASP
48	CV	98	SER
49	CW	1	MET
49	CW	7	GLU
49	CW	10	LYS
50	CX	82	ILE
51	CY	25	THR

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Mol	Chain	Res	Type
51	CY	35	SER
51	CY	48	THR
51	CY	71	LEU
52	CZ	18	LEU
52	CZ	19	LEU
52	CZ	38	GLN
52	CZ	58	ASN
32	DE	12	LEU
32	DE	107	SER
32	DE	127	GLU
32	DE	189	THR
33	DF	10	ASP
33	DF	57	LEU
33	DF	72	LYS
33	DF	94	GLU
33	DF	106	ILE
33	DF	117	LEU
33	DF	134	GLU
33	DF	141	ILE
33	DF	149	VAL
33	DF	152	LEU
33	DF	174	ASP
34	DG	3	ARG
34	DG	11	VAL
34	DG	18	LYS
34	DG	56	ASP
34	DG	155	GLU
35	DH	7	ASP
35	DH	15	LEU
35	DH	17	ASP
35	DH	21	VAL
35	DH	48	GLU
35	DH	53	GLU
35	DH	57	LYS
35	DH	58	LEU
35	DH	60	GLU
35	DH	75	LEU
35	DH	121	VAL
35	DH	127	GLU
35	DH	145	ASN
36	DJ	11	LEU
36	DJ	13	VAL

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Mol	Chain	Res	Type
36	DJ	28	LEU
36	DJ	113	LYS
37	DK	124	VAL
37	DK	142	ILE
38	DL	58	LEU
38	DL	76	VAL
38	DL	110	GLU
38	DL	113	MET
38	DL	123	LEU
39	DM	2	ARG
39	DM	91	ASP
39	DM	94	THR
39	DM	115	GLU
40	DN	58	LYS
40	DN	59	ARG
40	DN	100	LYS
41	DO	2	ARG
41	DO	14	SER
41	DO	76	VAL
42	DP	31	THR
42	DP	49	VAL
42	DP	78	VAL
43	DQ	26	VAL
43	DQ	102	GLU
44	DR	41	LYS
44	DR	51	ARG
45	DS	102	SER
46	DT	86	MET
47	DU	1	MET
47	DU	3	ARG
47	DU	10	VAL
48	DV	52	LEU
48	DV	61	LYS
49	DW	7	GLU
49	DW	53	LYS
50	DX	82	ILE
51	DY	25	THR
51	DY	35	SER
52	DZ	19	LEU
52	DZ	38	GLN
53	DI	7	ASP
53	DI	16	SER

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Mol	Chain	Res	Type
53	DI	53	ARG
53	DI	64	VAL
53	DI	117	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	18	HIS
2	AB	93	ASN
2	AB	94	HIS
2	AB	120	GLN
4	AD	136	GLN
5	AE	89	HIS
6	AF	63	ASN
7	AG	97	ASN
7	AG	142	HIS
8	AH	4	GLN
10	AJ	58	ASN
20	AT	48	GLN
20	AT	78	ASN
22	C1	6	ASN
22	C1	38	HIS
2	BB	39	HIS
2	BB	93	ASN
2	BB	94	HIS
2	BB	120	GLN
2	BB	168	HIS
4	BD	131	ASN
5	BE	70	ASN
5	BE	89	HIS
5	BE	122	ASN
7	BG	97	ASN
8	BH	4	GLN
8	BH	38	ASN
17	BQ	51	ASN
20	BT	3	ASN
24	D3	26	ASN
25	D4	43	HIS
29	CC	142	HIS
29	DC	142	HIS
32	CE	115	GLN
33	CF	27	GLN

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Mol	Chain	Res	Type
34	CG	38	ASN
37	CK	138	GLN
42	CP	29	HIS
42	CP	100	HIS
47	CU	28	ASN
48	CV	74	ASN
50	CX	57	HIS
52	CZ	45	GLN
48	DV	54	GLN
53	DI	122	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	239 (15%)	27 (1%)
1	BA	1529/1534 (99%)	246 (16%)	28 (1%)
28	CB	117/120 (97%)	11 (9%)	0
28	DB	119/120 (99%)	9 (7%)	0
31	CA	2892/2904 (99%)	425 (14%)	72 (2%)
54	DA	2880/2904 (99%)	367 (12%)	57 (1%)
All	All	9067/9116 (99%)	1297 (14%)	184 (2%)

All (1297) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	69	G
1	AA	71	A
1	AA	72	A
1	AA	74	A
1	AA	80	A

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Mol	Chain	Res	Type
1	AA	81	A
1	AA	82	G
1	AA	83	C
1	AA	85	U
1	AA	86	G
1	AA	88	U
1	AA	89	U
1	AA	90	C
1	AA	92	U
1	AA	94	G
1	AA	95	C
1	AA	108	G
1	AA	120	A
1	AA	130	A
1	AA	131	A
1	AA	137	U
1	AA	141	G
1	AA	142	G
1	AA	143	A
1	AA	144	G
1	AA	149	A
1	AA	159	G
1	AA	163	C
1	AA	168	G
1	AA	177	G
1	AA	183	C
1	AA	197	A
1	AA	205	A
1	AA	210	C
1	AA	211	G
1	AA	212	G
1	AA	226	G
1	AA	240	G
1	AA	245	U
1	AA	247	G
1	AA	250	A
1	AA	251	G
1	AA	266	G
1	AA	267	C
1	AA	289	G
1	AA	321	A
1	AA	328	C

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Mol	Chain	Res	Type
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	346	G
1	AA	348	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	384	G
1	AA	398	U
1	AA	406	G
1	AA	411	A
1	AA	412	A
1	AA	413	G
1	AA	414	A
1	AA	421	U
1	AA	422	C
1	AA	424	G
1	AA	429	U
1	AA	430	A
1	AA	436	C
1	AA	457	G
1	AA	458	U
1	AA	463	U
1	AA	466	A
1	AA	467	U
1	AA	468	A
1	AA	474	G
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	509	A
1	AA	511	C
1	AA	527	G7M
1	AA	531	U
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	564	C

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Mol	Chain	Res	Type
1	AA	568	G
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	615	G
1	AA	633	G
1	AA	650	G
1	AA	653	U
1	AA	661	G
1	AA	665	A
1	AA	695	A
1	AA	702	A
1	AA	703	G
1	AA	723	U
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	814	A
1	AA	815	A
1	AA	817	C
1	AA	821	G
1	AA	828	U
1	AA	836	G
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	934	C
1	AA	935	A
1	AA	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	971	G
1	AA	975	A

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Mol	Chain	Res	Type
1	AA	976	G
1	AA	977	A
1	AA	987	G
1	AA	993	G
1	AA	1004	A
1	AA	1009	U
1	AA	1015	G
1	AA	1019	A
1	AA	1024	G
1	AA	1026	G
1	AA	1027	C
1	AA	1028	C
1	AA	1029	U
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	G
1	AA	1036	A
1	AA	1037	C
1	AA	1043	G
1	AA	1053	G
1	AA	1054	C
1	AA	1065	U
1	AA	1086	U
1	AA	1094	G
1	AA	1095	U
1	AA	1098	C
1	AA	1101	A
1	AA	1124	G
1	AA	1125	U
1	AA	1132	C
1	AA	1133	G
1	AA	1136	C
1	AA	1137	C
1	AA	1138	G
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1142	G
1	AA	1143	G
1	AA	1145	A
1	AA	1152	A

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Mol	Chain	Res	Type
1	AA	1159	U
1	AA	1160	G
1	AA	1168	U
1	AA	1184	G
1	AA	1196	A
1	AA	1197	A
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1236	A
1	AA	1238	A
1	AA	1239	A
1	AA	1256	A
1	AA	1257	A
1	AA	1260	G
1	AA	1280	A
1	AA	1281	C
1	AA	1286	U
1	AA	1287	A
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1312	G
1	AA	1317	C
1	AA	1320	C
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1379	G
1	AA	1381	U
1	AA	1398	A
1	AA	1419	G
1	AA	1429	A
1	AA	1441	A
1	AA	1446	A
1	AA	1447	A
1	AA	1448	C

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Mol	Chain	Res	Type
1	AA	1451	U
1	AA	1452	C
1	AA	1453	G
1	AA	1492	A
1	AA	1497	G
1	AA	1499	A
1	AA	1503	A
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1534	A
1	BA	4	U
1	BA	5	U
1	BA	9	G
1	BA	22	G
1	BA	32	A
1	BA	39	G
1	BA	47	C
1	BA	48	C
1	BA	50	A
1	BA	51	A
1	BA	52	C
1	BA	69	G
1	BA	71	A
1	BA	72	A
1	BA	74	A
1	BA	80	A
1	BA	82	G
1	BA	83	C
1	BA	84	U
1	BA	85	U
1	BA	86	G
1	BA	87	C
1	BA	88	U
1	BA	89	U
1	BA	90	C
1	BA	92	U
1	BA	94	G
1	BA	95	C
1	BA	108	G

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Mol	Chain	Res	Type
1	BA	120	A
1	BA	130	A
1	BA	131	A
1	BA	137	U
1	BA	141	G
1	BA	142	G
1	BA	143	A
1	BA	144	G
1	BA	149	A
1	BA	159	G
1	BA	163	C
1	BA	168	G
1	BA	177	G
1	BA	183	C
1	BA	197	A
1	BA	200	G
1	BA	205	A
1	BA	210	C
1	BA	211	G
1	BA	212	G
1	BA	226	G
1	BA	245	U
1	BA	247	G
1	BA	250	A
1	BA	251	G
1	BA	266	G
1	BA	267	C
1	BA	289	G
1	BA	321	A
1	BA	328	C
1	BA	329	A
1	BA	330	C
1	BA	332	G
1	BA	346	G
1	BA	348	G
1	BA	352	C
1	BA	354	G
1	BA	367	U
1	BA	372	C
1	BA	373	A
1	BA	384	G
1	BA	398	U

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Mol	Chain	Res	Type
1	BA	406	G
1	BA	412	A
1	BA	413	G
1	BA	414	A
1	BA	421	U
1	BA	422	C
1	BA	424	G
1	BA	429	U
1	BA	430	A
1	BA	436	C
1	BA	457	G
1	BA	458	U
1	BA	463	U
1	BA	467	U
1	BA	468	A
1	BA	474	G
1	BA	481	G
1	BA	484	G
1	BA	486	U
1	BA	495	A
1	BA	509	A
1	BA	511	C
1	BA	527	G7M
1	BA	531	U
1	BA	532	A
1	BA	533	A
1	BA	547	A
1	BA	559	A
1	BA	564	C
1	BA	568	G
1	BA	572	A
1	BA	573	A
1	BA	576	C
1	BA	577	G
1	BA	615	G
1	BA	633	G
1	BA	650	G
1	BA	653	U
1	BA	661	G
1	BA	665	A
1	BA	695	A
1	BA	702	A

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Mol	Chain	Res	Type
1	BA	703	G
1	BA	723	U
1	BA	734	G
1	BA	748	G
1	BA	755	G
1	BA	777	A
1	BA	793	U
1	BA	794	A
1	BA	814	A
1	BA	815	A
1	BA	817	C
1	BA	821	G
1	BA	828	U
1	BA	836	G
1	BA	839	C
1	BA	840	C
1	BA	841	C
1	BA	842	U
1	BA	843	U
1	BA	844	G
1	BA	845	A
1	BA	846	G
1	BA	914	A
1	BA	926	G
1	BA	927	G
1	BA	934	C
1	BA	935	A
1	BA	960	U
1	BA	966	2MG
1	BA	969	A
1	BA	971	G
1	BA	975	A
1	BA	976	G
1	BA	977	A
1	BA	987	G
1	BA	993	G
1	BA	1004	A
1	BA	1008	U
1	BA	1009	U
1	BA	1015	G
1	BA	1019	A
1	BA	1024	G

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Mol	Chain	Res	Type
1	BA	1026	G
1	BA	1027	C
1	BA	1028	C
1	BA	1029	U
1	BA	1030	U
1	BA	1031	C
1	BA	1032	G
1	BA	1033	G
1	BA	1036	A
1	BA	1037	C
1	BA	1043	G
1	BA	1046	A
1	BA	1053	G
1	BA	1054	C
1	BA	1065	U
1	BA	1070	U
1	BA	1086	U
1	BA	1094	G
1	BA	1095	U
1	BA	1098	C
1	BA	1101	A
1	BA	1124	G
1	BA	1125	U
1	BA	1132	C
1	BA	1133	G
1	BA	1136	C
1	BA	1137	C
1	BA	1138	G
1	BA	1139	G
1	BA	1140	C
1	BA	1141	C
1	BA	1142	G
1	BA	1143	G
1	BA	1145	A
1	BA	1152	A
1	BA	1159	U
1	BA	1160	G
1	BA	1168	U
1	BA	1196	A
1	BA	1197	A
1	BA	1212	U
1	BA	1213	A

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Mol	Chain	Res	Type
1	BA	1214	C
1	BA	1215	G
1	BA	1225	A
1	BA	1226	C
1	BA	1227	A
1	BA	1236	A
1	BA	1238	A
1	BA	1239	A
1	BA	1256	A
1	BA	1257	A
1	BA	1260	G
1	BA	1280	A
1	BA	1281	C
1	BA	1286	U
1	BA	1287	A
1	BA	1300	G
1	BA	1302	C
1	BA	1305	G
1	BA	1312	G
1	BA	1317	C
1	BA	1320	C
1	BA	1346	A
1	BA	1353	G
1	BA	1362	A
1	BA	1363	A
1	BA	1370	G
1	BA	1379	G
1	BA	1381	U
1	BA	1398	A
1	BA	1419	G
1	BA	1429	A
1	BA	1441	A
1	BA	1446	A
1	BA	1447	A
1	BA	1448	C
1	BA	1451	U
1	BA	1452	C
1	BA	1453	G
1	BA	1492	A
1	BA	1493	A
1	BA	1497	G
1	BA	1499	A

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Mol	Chain	Res	Type
1	BA	1503	A
1	BA	1506	U
1	BA	1507	A
1	BA	1517	G
1	BA	1529	G
1	BA	1530	G
1	BA	1534	A
28	CB	9	G
28	CB	25	U
28	CB	35	C
28	CB	45	A
28	CB	56	G
28	CB	57	A
28	CB	88	C
28	CB	89	U
28	CB	90	C
28	CB	99	A
28	CB	109	A
31	CA	10	A
31	CA	14	A
31	CA	34	U
31	CA	36	G
31	CA	42	A
31	CA	46	G
31	CA	49	A
31	CA	58	G
31	CA	63	A
31	CA	71	A
31	CA	74	A
31	CA	75	G
31	CA	80	G
31	CA	83	A
31	CA	84	A
31	CA	101	A
31	CA	102	U
31	CA	118	A
31	CA	119	A
31	CA	120	U
31	CA	138	U
31	CA	139	U
31	CA	140	C
31	CA	141	G

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Mol	Chain	Res	Type
31	CA	142	A
31	CA	143	C
31	CA	196	A
31	CA	199	A
31	CA	200	U
31	CA	215	G
31	CA	216	A
31	CA	221	A
31	CA	222	A
31	CA	248	G
31	CA	265	A
31	CA	266	G
31	CA	272	A
31	CA	276	U
31	CA	277	G
31	CA	278	A
31	CA	279	A
31	CA	285	G
31	CA	311	A
31	CA	329	G
31	CA	330	A
31	CA	343	C
31	CA	346	A
31	CA	352	A
31	CA	353	C
31	CA	362	A
31	CA	371	A
31	CA	372	G
31	CA	385	C
31	CA	386	G
31	CA	399	U
31	CA	404	A
31	CA	405	U
31	CA	411	G
31	CA	420	C
31	CA	424	G
31	CA	425	G
31	CA	451	U
31	CA	480	A
31	CA	481	G
31	CA	491	G
31	CA	503	A

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Mol	Chain	Res	Type
31	CA	504	A
31	CA	505	A
31	CA	508	A
31	CA	517	C
31	CA	531	C
31	CA	532	A
31	CA	543	G
31	CA	544	C
31	CA	546	U
31	CA	547	A
31	CA	549	G
31	CA	550	C
31	CA	551	G
31	CA	555	G
31	CA	556	A
31	CA	563	A
31	CA	571	U
31	CA	573	U
31	CA	575	A
31	CA	586	A
31	CA	603	A
31	CA	613	A
31	CA	614	A
31	CA	615	U
31	CA	627	A
31	CA	637	A
31	CA	645	C
31	CA	647	G
31	CA	654	A
31	CA	655	A
31	CA	670	A
31	CA	684	G
31	CA	685	A
31	CA	686	U
31	CA	695	G
31	CA	717	C
31	CA	730	A
31	CA	740	C
31	CA	746	PSU
31	CA	747	5MU
31	CA	775	G
31	CA	776	G

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Mol	Chain	Res	Type
31	CA	782	A
31	CA	784	G
31	CA	785	G
31	CA	792	A
31	CA	802	A
31	CA	805	G
31	CA	812	C
31	CA	819	A
31	CA	827	U
31	CA	828	U
31	CA	845	A
31	CA	846	U
31	CA	847	U
31	CA	858	G
31	CA	859	G
31	CA	878	A
31	CA	883	G
31	CA	896	A
31	CA	897	C
31	CA	910	A
31	CA	914	G
31	CA	915	C
31	CA	931	U
31	CA	932	U
31	CA	941	A
31	CA	946	C
31	CA	953	G
31	CA	961	C
31	CA	974	G
31	CA	983	A
31	CA	984	A
31	CA	985	C
31	CA	995	C
31	CA	996	A
31	CA	1012	U
31	CA	1013	C
31	CA	1022	G
31	CA	1026	G
31	CA	1033	U
31	CA	1040	A
31	CA	1045	C
31	CA	1046	A

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Mol	Chain	Res	Type
31	CA	1047	G
31	CA	1057	A
31	CA	1061	U
31	CA	1070	A
31	CA	1083	U
31	CA	1088	A
31	CA	1089	A
31	CA	1090	A
31	CA	1091	G
31	CA	1096	A
31	CA	1097	U
31	CA	1111	A
31	CA	1112	G
31	CA	1128	G
31	CA	1129	A
31	CA	1132	U
31	CA	1133	A
31	CA	1135	C
31	CA	1136	G
31	CA	1142	A
31	CA	1168	G
31	CA	1169	A
31	CA	1170	C
31	CA	1171	G
31	CA	1172	C
31	CA	1175	A
31	CA	1176	U
31	CA	1177	G
31	CA	1179	G
31	CA	1180	U
31	CA	1186	G
31	CA	1210	G
31	CA	1212	G
31	CA	1236	G
31	CA	1238	G
31	CA	1253	A
31	CA	1256	G
31	CA	1266	G
31	CA	1271	G
31	CA	1272	A
31	CA	1273	U
31	CA	1300	G

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Mol	Chain	Res	Type
31	CA	1301	A
31	CA	1313	U
31	CA	1320	C
31	CA	1321	A
31	CA	1328	A
31	CA	1352	U
31	CA	1365	A
31	CA	1376	C
31	CA	1379	U
31	CA	1380	G
31	CA	1383	A
31	CA	1391	U
31	CA	1395	A
31	CA	1416	G
31	CA	1417	C
31	CA	1419	A
31	CA	1420	A
31	CA	1428	C
31	CA	1437	C
31	CA	1452	G
31	CA	1453	A
31	CA	1460	U
31	CA	1482	G
31	CA	1490	A
31	CA	1491	G
31	CA	1493	C
31	CA	1494	A
31	CA	1497	U
31	CA	1509	A
31	CA	1510	G
31	CA	1515	A
31	CA	1523	U
31	CA	1532	A
31	CA	1534	U
31	CA	1535	A
31	CA	1536	C
31	CA	1537	G
31	CA	1565	C
31	CA	1566	A
31	CA	1569	A
31	CA	1578	U
31	CA	1583	A

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Mol	Chain	Res	Type
31	CA	1585	C
31	CA	1607	C
31	CA	1608	A
31	CA	1647	U
31	CA	1648	U
31	CA	1649	G
31	CA	1674	G
31	CA	1695	G
31	CA	1715	G
31	CA	1729	U
31	CA	1730	C
31	CA	1731	G
31	CA	1732	C
31	CA	1738	G
31	CA	1744	A
31	CA	1750	G
31	CA	1764	C
31	CA	1773	A
31	CA	1782	U
31	CA	1800	C
31	CA	1801	A
31	CA	1808	A
31	CA	1816	C
31	CA	1822	C
31	CA	1829	A
31	CA	1869	G
31	CA	1870	C
31	CA	1871	A
31	CA	1872	A
31	CA	1873	G
31	CA	1900	A
31	CA	1906	G
31	CA	1907	G
31	CA	1914	C
31	CA	1929	G
31	CA	1930	G
31	CA	1931	U
31	CA	1937	A
31	CA	1938	A
31	CA	1955	U
31	CA	1967	C
31	CA	1970	A

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Mol	Chain	Res	Type
31	CA	1972	G
31	CA	1991	U
31	CA	1993	U
31	CA	1997	C
31	CA	2022	U
31	CA	2023	C
31	CA	2031	A
31	CA	2033	A
31	CA	2036	C
31	CA	2043	C
31	CA	2055	C
31	CA	2056	G
31	CA	2060	A
31	CA	2061	G
31	CA	2062	A
31	CA	2069	G7M
31	CA	2072	C
31	CA	2080	A
31	CA	2093	G
31	CA	2095	A
31	CA	2100	G
31	CA	2102	G
31	CA	2108	A
31	CA	2110	G
31	CA	2111	U
31	CA	2112	G
31	CA	2113	U
31	CA	2115	G
31	CA	2117	A
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

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Mol	Chain	Res	Type
31	CA	2157	G
31	CA	2158	A
31	CA	2159	G
31	CA	2160	C
31	CA	2162	G
31	CA	2164	C
31	CA	2165	C
31	CA	2171	A
31	CA	2172	U
31	CA	2173	A
31	CA	2174	C
31	CA	2178	C
31	CA	2183	A
31	CA	2190	G
31	CA	2198	A
31	CA	2203	U
31	CA	2204	G
31	CA	2211	A
31	CA	2225	A
31	CA	2226	C
31	CA	2238	G
31	CA	2239	G
31	CA	2259	U
31	CA	2268	A
31	CA	2280	G
31	CA	2283	C
31	CA	2287	A
31	CA	2305	U
31	CA	2311	A
31	CA	2322	A
31	CA	2326	C
31	CA	2327	A
31	CA	2333	A
31	CA	2335	A
31	CA	2345	G
31	CA	2347	C
31	CA	2350	C
31	CA	2354	C
31	CA	2361	G
31	CA	2383	G
31	CA	2385	C
31	CA	2388	A

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Mol	Chain	Res	Type
31	CA	2402	U
31	CA	2403	C
31	CA	2406	A
31	CA	2423	U
31	CA	2424	C
31	CA	2425	A
31	CA	2426	A
31	CA	2429	G
31	CA	2430	A
31	CA	2435	A
31	CA	2441	U
31	CA	2448	A
31	CA	2465	C
31	CA	2476	A
31	CA	2491	U
31	CA	2502	G
31	CA	2505	G
31	CA	2518	A
31	CA	2529	G
31	CA	2535	G
31	CA	2547	A
31	CA	2554	U
31	CA	2556	C
31	CA	2566	A
31	CA	2567	G
31	CA	2573	C
31	CA	2578	G
31	CA	2582	G
31	CA	2585	U
31	CA	2603	G
31	CA	2609	U
31	CA	2613	U
31	CA	2629	U
31	CA	2630	G
31	CA	2646	C
31	CA	2661	G
31	CA	2663	G
31	CA	2681	C
31	CA	2682	A
31	CA	2689	U
31	CA	2690	U
31	CA	2714	G

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Mol	Chain	Res	Type
31	CA	2718	G
31	CA	2726	A
31	CA	2744	G
31	CA	2748	A
31	CA	2769	U
31	CA	2778	A
31	CA	2791	G
31	CA	2794	C
31	CA	2799	A
31	CA	2820	A
31	CA	2835	A
31	CA	2836	U
31	CA	2850	A
31	CA	2861	U
31	CA	2865	U
31	CA	2867	G
31	CA	2883	A
31	CA	2884	U
31	CA	2886	A
31	CA	2887	A
31	CA	2891	U
31	CA	2903	U
31	CA	2904	U
28	DB	25	U
28	DB	35	C
28	DB	45	A
28	DB	56	G
28	DB	57	A
28	DB	88	C
28	DB	89	U
28	DB	90	C
28	DB	109	A
54	DA	10	A
54	DA	12	U
54	DA	34	U
54	DA	46	G
54	DA	63	A
54	DA	71	A
54	DA	74	A
54	DA	75	G
54	DA	80	G
54	DA	84	A

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Mol	Chain	Res	Type
54	DA	101	A
54	DA	102	U
54	DA	118	A
54	DA	119	A
54	DA	120	U
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	196	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	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	346	A
54	DA	352	A
54	DA	353	C
54	DA	362	A
54	DA	370	G
54	DA	372	G
54	DA	386	G
54	DA	399	U
54	DA	411	G
54	DA	412	A

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Mol	Chain	Res	Type
54	DA	420	C
54	DA	424	G
54	DA	425	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	531	C
54	DA	532	A
54	DA	543	G
54	DA	544	C
54	DA	546	U
54	DA	547	A
54	DA	548	G
54	DA	549	G
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	654	A
54	DA	655	A
54	DA	686	U
54	DA	717	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

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Mol	Chain	Res	Type
54	DA	782	A
54	DA	784	G
54	DA	785	G
54	DA	790	U
54	DA	792	A
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	860	U
54	DA	878	A
54	DA	883	G
54	DA	885	C
54	DA	896	A
54	DA	897	C
54	DA	910	A
54	DA	914	G
54	DA	915	C
54	DA	927	A
54	DA	931	U
54	DA	932	U
54	DA	946	C
54	DA	961	C
54	DA	974	G
54	DA	983	A
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	1070	A
54	DA	1083	U
54	DA	1088	A
54	DA	1089	A
54	DA	1090	A

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Mol	Chain	Res	Type
54	DA	1091	G
54	DA	1096	A
54	DA	1097	U
54	DA	1112	G
54	DA	1132	U
54	DA	1133	A
54	DA	1135	C
54	DA	1136	G
54	DA	1142	A
54	DA	1168	G
54	DA	1172	C
54	DA	1174	U
54	DA	1175	A
54	DA	1176	U
54	DA	1177	G
54	DA	1180	U
54	DA	1187	G
54	DA	1237	A
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	1329	U
54	DA	1352	U
54	DA	1365	A
54	DA	1379	U
54	DA	1383	A
54	DA	1391	U
54	DA	1416	G
54	DA	1417	C
54	DA	1427	A
54	DA	1428	C
54	DA	1434	A
54	DA	1435	G
54	DA	1452	G
54	DA	1453	A
54	DA	1460	U
54	DA	1482	G

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Mol	Chain	Res	Type
54	DA	1490	A
54	DA	1491	G
54	DA	1493	C
54	DA	1494	A
54	DA	1497	U
54	DA	1508	A
54	DA	1509	A
54	DA	1510	G
54	DA	1515	A
54	DA	1523	U
54	DA	1532	A
54	DA	1534	U
54	DA	1535	A
54	DA	1536	C
54	DA	1537	G
54	DA	1566	A
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	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	1731	G
54	DA	1732	C
54	DA	1738	G
54	DA	1744	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	1816	C
54	DA	1829	A

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Mol	Chain	Res	Type
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
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	2097	A
54	DA	2100	G
54	DA	2102	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

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Mol	Chain	Res	Type
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
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	2177	C
54	DA	2178	C
54	DA	2179	C
54	DA	2181	U
54	DA	2183	A
54	DA	2185	U
54	DA	2190	G
54	DA	2198	A
54	DA	2204	G
54	DA	2211	A
54	DA	2225	A
54	DA	2238	G
54	DA	2239	G

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Mol	Chain	Res	Type
54	DA	2268	A
54	DA	2283	C
54	DA	2286	G
54	DA	2287	A
54	DA	2305	U
54	DA	2308	G
54	DA	2312	U
54	DA	2324	U
54	DA	2325	G
54	DA	2333	A
54	DA	2335	A
54	DA	2347	C
54	DA	2383	G
54	DA	2385	C
54	DA	2402	U
54	DA	2403	C
54	DA	2406	A
54	DA	2407	A
54	DA	2423	U
54	DA	2424	C
54	DA	2425	A
54	DA	2431	U
54	DA	2435	A
54	DA	2441	U
54	DA	2448	A
54	DA	2476	A
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	2574	G
54	DA	2585	U
54	DA	2603	G
54	DA	2609	U
54	DA	2613	U

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Mol	Chain	Res	Type
54	DA	2629	U
54	DA	2630	G
54	DA	2661	G
54	DA	2663	G
54	DA	2689	U
54	DA	2690	U
54	DA	2714	G
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	2811	G
54	DA	2820	A
54	DA	2821	A
54	DA	2836	U
54	DA	2867	G
54	DA	2891	U

All (184) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	70	U
1	AA	88	U
1	AA	89	U
1	AA	209	U
1	AA	413	G
1	AA	429	U
1	AA	485	U
1	AA	576	C
1	AA	653	U
1	AA	702	A
1	AA	793	U
1	AA	841	C
1	AA	842	U
1	AA	884	U
1	AA	992	U
1	AA	1086	U

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Mol	Chain	Res	Type
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1225	A
1	AA	1281	C
1	AA	1299	A
1	AA	1397	C
1	AA	1447	A
1	AA	1452	C
1	BA	5	U
1	BA	70	U
1	BA	86	G
1	BA	89	U
1	BA	209	U
1	BA	429	U
1	BA	485	U
1	BA	576	C
1	BA	653	U
1	BA	702	A
1	BA	793	U
1	BA	842	U
1	BA	844	G
1	BA	884	U
1	BA	992	U
1	BA	1008	U
1	BA	1086	U
1	BA	1137	C
1	BA	1139	G
1	BA	1140	C
1	BA	1141	C
1	BA	1225	A
1	BA	1281	C
1	BA	1299	A
1	BA	1362	A
1	BA	1397	C
1	BA	1447	A
1	BA	1452	C
31	CA	83	A
31	CA	101	A
31	CA	138	U
31	CA	141	G

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Mol	Chain	Res	Type
31	CA	177	G
31	CA	196	A
31	CA	199	A
31	CA	221	A
31	CA	271	G
31	CA	278	A
31	CA	310	A
31	CA	345	A
31	CA	403	U
31	CA	404	A
31	CA	451	U
31	CA	503	A
31	CA	506	G
31	CA	555	G
31	CA	620	G
31	CA	764	A
31	CA	784	G
31	CA	846	U
31	CA	973	A
31	CA	984	A
31	CA	1045	C
31	CA	1046	A
31	CA	1061	U
31	CA	1069	A
31	CA	1070	A
31	CA	1088	A
31	CA	1089	A
31	CA	1128	G
31	CA	1141	U
31	CA	1253	A
31	CA	1286	A
31	CA	1300	G
31	CA	1320	C
31	CA	1329	U
31	CA	1379	U
31	CA	1452	G
31	CA	1490	A
31	CA	1497	U
31	CA	1509	A
31	CA	1535	A
31	CA	1536	C
31	CA	1607	C

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Mol	Chain	Res	Type
31	CA	1647	U
31	CA	1730	C
31	CA	1786	A
31	CA	1870	C
31	CA	1871	A
31	CA	2035	G
31	CA	2095	A
31	CA	2119	A
31	CA	2126	A
31	CA	2146	C
31	CA	2157	G
31	CA	2164	C
31	CA	2225	A
31	CA	2282	G
31	CA	2286	G
31	CA	2326	C
31	CA	2423	U
31	CA	2425	A
31	CA	2430	A
31	CA	2680	U
31	CA	2681	C
31	CA	2778	A
31	CA	2779	U
31	CA	2797	U
31	CA	2849	U
31	CA	2873	A
54	DA	138	U
54	DA	141	G
54	DA	199	A
54	DA	271	G
54	DA	278	A
54	DA	370	G
54	DA	403	U
54	DA	503	A
54	DA	620	G
54	DA	764	A
54	DA	784	G
54	DA	859	G
54	DA	961	C
54	DA	984	A
54	DA	1061	U
54	DA	1069	A

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Mol	Chain	Res	Type
54	DA	1070	A
54	DA	1087	G
54	DA	1088	A
54	DA	1089	A
54	DA	1128	G
54	DA	1141	U
54	DA	1142	A
54	DA	1175	A
54	DA	1253	A
54	DA	1286	A
54	DA	1300	G
54	DA	1320	C
54	DA	1490	A
54	DA	1497	U
54	DA	1509	A
54	DA	1535	A
54	DA	1607	C
54	DA	1647	U
54	DA	1730	C
54	DA	1870	C
54	DA	1871	A
54	DA	1936	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	2501	C
54	DA	2585	U
54	DA	2681	C
54	DA	2797	U
54	DA	2798	U
54	DA	2873	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	2MG	AA	1207	1	18,26,27	1.11	2 (11%)	21,38,41	2.58	4 (19%)
1	4OC	AA	1402	1	15,23,24	0.81	0	21,32,35	1.32	2 (9%)
1	5MC	AA	1407	1	14,22,23	0.87	1 (7%)	17,32,35	0.71	1 (5%)
1	UR3	AA	1498	1	13,22,23	0.84	0	18,32,35	0.63	0
1	2MG	AA	1516	1	18,26,27	1.30	2 (11%)	21,38,41	2.51	4 (19%)
1	MA6	AA	1518	1	18,26,27	0.67	0	15,38,41	0.65	0
1	MA6	AA	1519	1	18,26,27	0.62	0	15,38,41	0.55	0
1	PSU	AA	516	1,55	15,21,22	1.14	2 (13%)	16,30,33	3.47	2 (12%)
1	G7M	AA	527	1	18,26,27	1.11	1 (5%)	21,39,42	3.31	5 (23%)
1	2MG	AA	966	1	18,26,27	1.17	2 (11%)	21,38,41	2.52	3 (14%)
1	5MC	AA	967	1	14,22,23	0.85	1 (7%)	17,32,35	0.66	1 (5%)
12	D2T	AL	89	12	4,9,10	0.46	0	4,11,13	1.43	1 (25%)
1	2MG	BA	1207	1	18,26,27	1.17	2 (11%)	21,38,41	2.55	4 (19%)
1	4OC	BA	1402	1	15,23,24	0.87	0	21,32,35	1.30	2 (9%)
1	5MC	BA	1407	1	14,22,23	0.85	1 (7%)	17,32,35	0.71	1 (5%)
1	UR3	BA	1498	1	13,22,23	1.14	2 (15%)	18,32,35	0.53	0
1	2MG	BA	1516	1	18,26,27	1.22	2 (11%)	21,38,41	2.55	4 (19%)
1	MA6	BA	1518	1	18,26,27	0.68	0	15,38,41	0.62	0
1	MA6	BA	1519	1	18,26,27	0.58	0	15,38,41	0.58	0
1	PSU	BA	516	1	15,21,22	1.16	2 (13%)	16,30,33	3.49	2 (12%)
1	G7M	BA	527	1	18,26,27	1.10	1 (5%)	21,39,42	3.45	5 (23%)
1	2MG	BA	966	1,55	18,26,27	1.09	2 (11%)	21,38,41	2.52	4 (19%)
1	5MC	BA	967	1	14,22,23	0.83	1 (7%)	17,32,35	0.65	1 (5%)
12	D2T	BL	89	12	4,9,10	0.54	0	4,11,13	1.60	1 (25%)
31	6MZ	CA	1618	31	17,25,26	0.73	0	15,36,39	0.90	1 (6%)
31	2MG	CA	1835	31	18,26,27	1.14	1 (5%)	21,38,41	2.47	4 (19%)
31	PSU	CA	1911	31	15,21,22	1.14	1 (6%)	16,30,33	3.46	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	3TD	CA	1915	31	15,22,23	0.98	2 (13%)	17,32,35	0.99	1 (5%)
31	PSU	CA	1917	31	15,21,22	1.16	1 (6%)	16,30,33	3.53	1 (6%)
31	5MU	CA	1939	31	13,22,23	1.17	1 (7%)	16,32,35	4.79	3 (18%)
31	5MC	CA	1962	31	14,22,23	0.82	1 (7%)	17,32,35	0.60	1 (5%)
31	6MZ	CA	2030	31	17,25,26	0.79	0	15,36,39	0.94	1 (6%)
31	G7M	CA	2069	31	18,26,27	0.91	1 (5%)	21,39,42	3.08	5 (23%)
31	OMG	CA	2251	31	18,26,27	1.16	2 (11%)	21,38,41	2.76	4 (19%)
31	2MG	CA	2445	31	18,26,27	1.27	2 (11%)	21,38,41	2.54	4 (19%)
31	PSU	CA	2457	31	15,21,22	1.13	2 (13%)	16,30,33	3.45	1 (6%)
31	OMC	CA	2498	55,31	15,22,23	0.89	1 (6%)	20,31,34	0.57	0
31	2MA	CA	2503	31	17,25,26	0.89	0	18,37,40	1.02	1 (5%)
31	PSU	CA	2504	31	15,21,22	1.09	2 (13%)	16,30,33	3.46	1 (6%)
31	OMU	CA	2552	31	14,22,23	1.20	2 (14%)	19,31,34	2.91	2 (10%)
31	PSU	CA	2580	31	15,21,22	1.22	2 (13%)	16,30,33	3.55	2 (12%)
31	PSU	CA	2605	31	15,21,22	1.11	2 (13%)	16,30,33	3.53	2 (12%)
31	1MG	CA	745	31	17,26,27	1.24	1 (5%)	19,39,42	1.09	2 (10%)
31	PSU	CA	746	55,31	15,21,22	1.34	2 (13%)	16,30,33	3.49	1 (6%)
31	5MU	CA	747	31	13,22,23	1.09	1 (7%)	16,32,35	4.78	3 (18%)
31	PSU	CA	955	31	15,21,22	1.15	2 (13%)	16,30,33	3.52	1 (6%)
30	MEQ	CD	150	30	6,8,10	0.39	0	7,9,12	0.99	1 (14%)
40	4D4	CN	81	40	7,11,12	1.02	1 (14%)	5,13,15	0.80	0
54	6MZ	DA	1618	54	17,25,26	0.78	0	15,36,39	0.88	1 (6%)
54	2MG	DA	1835	54	18,26,27	1.06	1 (5%)	21,38,41	2.51	4 (19%)
54	PSU	DA	1911	54	15,21,22	1.11	2 (13%)	16,30,33	3.45	1 (6%)
54	3TD	DA	1915	54	15,22,23	0.95	2 (13%)	17,32,35	1.03	1 (5%)
54	PSU	DA	1917	54	15,21,22	1.22	1 (6%)	16,30,33	3.52	1 (6%)
54	5MU	DA	1939	54	13,22,23	1.14	1 (7%)	16,32,35	4.77	3 (18%)
54	5MC	DA	1962	54	14,22,23	0.90	1 (7%)	17,32,35	0.68	0
54	6MZ	DA	2030	54	17,25,26	0.72	0	15,36,39	0.88	1 (6%)
54	G7M	DA	2069	54	18,26,27	1.00	1 (5%)	21,39,42	3.05	5 (23%)
54	OMG	DA	2251	54	18,26,27	1.00	1 (5%)	21,38,41	2.66	4 (19%)
54	2MG	DA	2445	54	18,26,27	1.18	3 (16%)	21,38,41	2.74	4 (19%)
54	H2U	DA	2449	54	17,21,22	0.56	0	23,30,33	0.64	0
54	PSU	DA	2457	54	15,21,22	1.05	2 (13%)	16,30,33	3.47	1 (6%)
54	OMC	DA	2498	55,54	15,22,23	0.85	0	20,31,34	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	2MA	DA	2503	55,54	17,25,26	0.79	0	18,37,40	1.15	2 (11%)
54	PSU	DA	2504	54	15,21,22	1.21	2 (13%)	16,30,33	3.48	1 (6%)
54	OMU	DA	2552	54	14,22,23	1.13	2 (14%)	19,31,34	2.94	2 (10%)
54	PSU	DA	2580	54	15,21,22	1.43	4 (26%)	16,30,33	3.57	2 (12%)
54	PSU	DA	2604	54	15,21,22	1.26	2 (13%)	16,30,33	3.54	2 (12%)
54	PSU	DA	2605	54	15,21,22	1.11	2 (13%)	16,30,33	3.53	2 (12%)
54	1MG	DA	745	54	17,26,27	1.37	3 (17%)	19,39,42	1.18	3 (15%)
54	PSU	DA	746	55,54	15,21,22	1.70	4 (26%)	16,30,33	3.48	1 (6%)
54	5MU	DA	747	54	13,22,23	1.14	1 (7%)	16,32,35	4.71	3 (18%)
54	PSU	DA	955	54	15,21,22	1.47	4 (26%)	16,30,33	3.52	1 (6%)
30	MEQ	DD	150[A]	30	7,9,10	0.46	0	8,10,12	1.30	2 (25%)
30	MEQ	DD	150[B]	30	7,9,10	2.24	1 (14%)	8,10,12	2.20	3 (37%)
40	4D4	DN	81[A]	-	7,11,12	1.03	1 (14%)	5,13,15	0.91	0
40	4D4	DN	81[B]	-	7,11,12	0.87	0	5,13,15	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	AA	1407	1	-	0/3/25/26	0/2/2/2
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,55	-	0/5/27/28	0/3/3/3
1	5MC	BA	967	1	-	0/3/25/26	0/2/2/2
12	D2T	BL	89	12	-	0/2/12/14	0/0/0/0
31	6MZ	CA	1618	31	-	0/5/27/28	0/3/3/3
31	2MG	CA	1835	31	-	0/5/27/28	0/3/3/3
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
31	5MU	CA	1939	31	-	0/3/25/26	0/2/2/2
31	5MC	CA	1962	31	-	0/3/25/26	0/2/2/2
31	6MZ	CA	2030	31	-	0/5/27/28	0/3/3/3
31	G7M	CA	2069	31	-	0/3/25/26	0/3/3/3
31	OMG	CA	2251	31	-	0/5/27/28	0/3/3/3
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
31	OMC	CA	2498	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	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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 (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	DA	746	PSU	C2'-C1'	-3.77	1.50	1.53
54	DA	955	PSU	C2'-C1'	-3.05	1.50	1.53
54	DA	746	PSU	O4'-C1'	-2.85	1.40	1.44
54	DA	2580	PSU	O4'-C1'	-2.61	1.40	1.44
31	CA	746	PSU	O4'-C1'	-2.49	1.40	1.44
54	DA	2580	PSU	C6-C5	-2.37	1.35	1.38
54	DA	2580	PSU	C5-C1'	-2.28	1.50	1.52
54	DA	745	1MG	C8-N7	-2.28	1.30	1.34
54	DA	2457	PSU	C6-C5	-2.18	1.35	1.38
54	DA	2604	PSU	C6-C5	-2.17	1.35	1.38
31	CA	1915	3TD	C6-C5	-2.13	1.35	1.38
54	DA	1915	3TD	C6-C5	-2.11	1.35	1.38
54	DA	746	PSU	C6-C5	-2.09	1.35	1.38
54	DA	2504	PSU	C6-C5	-2.09	1.35	1.38
1	BA	516	PSU	C6-C5	-2.09	1.35	1.38
31	CA	2580	PSU	C6-C5	-2.09	1.35	1.38
54	DA	1911	PSU	C6-C5	-2.08	1.35	1.38
54	DA	2445	2MG	O3'-C3'	-2.08	1.38	1.43
1	BA	967	5MC	C6-C5	-2.06	1.34	1.40
31	CA	2457	PSU	C6-C5	-2.05	1.35	1.38
31	CA	1962	5MC	C6-C5	-2.05	1.34	1.40
1	AA	1407	5MC	C6-C5	-2.05	1.34	1.40
31	CA	2504	PSU	C6-C5	-2.05	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	955	PSU	C6-C5	-2.04	1.35	1.38
54	DA	2605	PSU	C6-C5	-2.04	1.35	1.38
1	BA	1407	5MC	C6-C5	-2.03	1.34	1.40
1	AA	967	5MC	C6-C5	-2.03	1.34	1.40
54	DA	1962	5MC	C6-C5	-2.02	1.34	1.40
54	DA	955	PSU	C6-C5	-2.02	1.35	1.38
1	AA	516	PSU	C6-C5	-2.02	1.35	1.38
31	CA	2605	PSU	C6-C5	-2.01	1.35	1.38
54	DA	955	PSU	C5-C1'	-2.01	1.50	1.52
54	DA	2552	OMU	C6-N1	2.13	1.38	1.35
54	DA	1915	3TD	C4-N3	2.15	1.41	1.38
1	BA	1498	UR3	C6-N1	2.19	1.38	1.35
31	CA	2251	OMG	C6-C5	2.22	1.45	1.41
31	CA	2498	OMC	C6-N1	2.22	1.38	1.35
1	AA	1207	2MG	C6-C5	2.24	1.45	1.41
1	BA	966	2MG	C6-C5	2.25	1.45	1.41
31	CA	1915	3TD	C4-N3	2.26	1.41	1.38
54	DA	745	1MG	C6-N1	2.36	1.41	1.38
40	CN	81	4D4	CB-CA	2.39	1.58	1.54
31	CA	2552	OMU	C6-N1	2.44	1.38	1.35
40	DN	81[A]	4D4	CB-CA	2.48	1.58	1.54
54	DA	2445	2MG	C6-C5	2.50	1.46	1.41
1	BA	1207	2MG	C6-C5	2.62	1.46	1.41
54	DA	2580	PSU	C4-N3	2.66	1.37	1.33
1	BA	1498	UR3	C4-N3	2.68	1.42	1.38
1	BA	1516	2MG	C6-C5	2.72	1.46	1.41
1	AA	966	2MG	C6-C5	2.72	1.46	1.41
54	DA	2457	PSU	C4-N3	2.77	1.38	1.33
54	DA	2604	PSU	C4-N3	2.86	1.38	1.33
54	DA	2445	2MG	C6-N1	2.99	1.38	1.33
1	BA	527	G7M	C6-N1	3.00	1.38	1.33
54	DA	746	PSU	C4-N3	3.04	1.38	1.33
54	DA	1835	2MG	C6-N1	3.06	1.38	1.33
31	CA	2445	2MG	C6-C5	3.07	1.47	1.41
1	AA	527	G7M	C6-N1	3.08	1.38	1.33
54	DA	1939	5MU	C4-N3	3.09	1.38	1.33
31	CA	2069	G7M	C6-N1	3.13	1.38	1.33
54	DA	747	5MU	C4-N3	3.13	1.38	1.33
31	CA	2552	OMU	C4-N3	3.13	1.38	1.33
31	CA	2504	PSU	C4-N3	3.14	1.38	1.33
54	DA	2605	PSU	C4-N3	3.16	1.38	1.33
54	DA	2552	OMU	C4-N3	3.17	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1516	2MG	C6-C5	3.19	1.47	1.41
54	DA	1917	PSU	C4-N3	3.20	1.38	1.33
1	BA	516	PSU	C4-N3	3.21	1.38	1.33
31	CA	2605	PSU	C4-N3	3.22	1.38	1.33
54	DA	1911	PSU	C4-N3	3.23	1.38	1.33
54	DA	2504	PSU	C4-N3	3.27	1.38	1.33
31	CA	747	5MU	C4-N3	3.28	1.38	1.33
1	BA	966	2MG	C6-N1	3.28	1.38	1.33
31	CA	2457	PSU	C4-N3	3.28	1.39	1.33
31	CA	1917	PSU	C4-N3	3.29	1.39	1.33
54	DA	2069	G7M	C6-N1	3.29	1.39	1.33
31	CA	2580	PSU	C4-N3	3.31	1.39	1.33
54	DA	955	PSU	C4-N3	3.32	1.39	1.33
31	CA	955	PSU	C4-N3	3.32	1.39	1.33
31	CA	746	PSU	C4-N3	3.33	1.39	1.33
1	AA	516	PSU	C4-N3	3.33	1.39	1.33
1	AA	1207	2MG	C6-N1	3.33	1.39	1.33
31	CA	1835	2MG	C6-N1	3.33	1.39	1.33
54	DA	745	1MG	C6-C5	3.38	1.47	1.40
54	DA	2251	OMG	C6-N1	3.39	1.39	1.33
31	CA	1911	PSU	C4-N3	3.39	1.39	1.33
1	BA	1207	2MG	C6-N1	3.40	1.39	1.33
1	BA	1516	2MG	C6-N1	3.40	1.39	1.33
31	CA	1939	5MU	C4-N3	3.42	1.39	1.33
31	CA	2251	OMG	C6-N1	3.42	1.39	1.33
1	AA	966	2MG	C6-N1	3.43	1.39	1.33
31	CA	2445	2MG	C6-N1	3.43	1.39	1.33
1	AA	1516	2MG	C6-N1	3.43	1.39	1.33
31	CA	745	1MG	C6-C5	3.92	1.48	1.40
30	DD	150[B]	MEQ	CB-CA	5.83	1.61	1.53

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	747	5MU	C5-C4-N3	-12.09	115.20	125.35
31	CA	1939	5MU	C5-C4-N3	-12.08	115.21	125.35
54	DA	1939	5MU	C5-C4-N3	-12.02	115.26	125.35
54	DA	747	5MU	C5-C4-N3	-11.94	115.33	125.35
31	CA	2069	G7M	C5-C6-N1	-9.95	110.52	123.52
1	AA	527	G7M	C5-C6-N1	-9.95	110.52	123.52
54	DA	2069	G7M	C5-C6-N1	-9.84	110.66	123.52
1	BA	527	G7M	C5-C6-N1	-9.79	110.72	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DA	2445	2MG	C5-C6-N1	-9.07	111.67	123.52
31	CA	2445	2MG	C5-C6-N1	-8.71	112.14	123.52
1	AA	1207	2MG	C5-C6-N1	-8.69	112.16	123.52
1	AA	966	2MG	C5-C6-N1	-8.61	112.26	123.52
31	CA	2251	OMG	C5-C6-N1	-8.51	112.40	123.52
1	BA	966	2MG	C5-C6-N1	-8.48	112.44	123.52
1	BA	1207	2MG	C5-C6-N1	-8.38	112.56	123.52
31	CA	1835	2MG	C5-C6-N1	-8.27	112.70	123.52
54	DA	1835	2MG	C5-C6-N1	-8.25	112.74	123.52
1	BA	1516	2MG	C5-C6-N1	-8.24	112.75	123.52
1	AA	1516	2MG	C5-C6-N1	-8.09	112.95	123.52
54	DA	2251	OMG	C5-C6-N1	-8.06	112.98	123.52
1	BA	527	G7M	C6-C5-C4	-6.32	113.64	120.86
1	AA	527	G7M	C6-C5-C4	-5.68	114.37	120.86
31	CA	2069	G7M	C6-C5-C4	-4.43	115.79	120.86
54	DA	2069	G7M	C6-C5-C4	-4.26	115.99	120.86
54	DA	2069	G7M	N3-C2-N1	-3.89	122.27	127.56
1	AA	527	G7M	N3-C2-N1	-3.73	122.49	127.56
1	BA	527	G7M	N3-C2-N1	-3.60	122.65	127.56
31	CA	2069	G7M	N3-C2-N1	-3.56	122.71	127.56
54	DA	2552	OMU	C5-C4-N3	-3.43	114.85	123.28
31	CA	745	1MG	C6-C5-C4	-3.43	117.48	119.93
31	CA	2552	OMU	C5-C4-N3	-3.42	114.88	123.28
1	AA	1516	2MG	C6-C5-C4	-3.27	117.12	120.86
54	DA	2251	OMG	N3-C2-N1	-3.24	123.14	127.56
1	BA	1516	2MG	C6-C5-C4	-3.15	117.26	120.86
54	DA	1915	3TD	C5-C4-N3	-3.09	116.13	118.65
31	CA	1915	3TD	C5-C4-N3	-3.03	116.18	118.65
31	CA	2251	OMG	N3-C2-N1	-3.00	123.47	127.56
54	DA	745	1MG	C6-C5-C4	-2.99	117.80	119.93
1	BA	1207	2MG	C6-C5-C4	-2.98	117.45	120.86
54	DA	2445	2MG	C6-C5-C4	-2.94	117.50	120.86
31	CA	2445	2MG	C6-C5-C4	-2.86	117.58	120.86
1	AA	966	2MG	C6-C5-C4	-2.80	117.66	120.86
54	DA	1835	2MG	C6-C5-C4	-2.79	117.67	120.86
31	CA	2251	OMG	C6-C5-C4	-2.69	117.78	120.86
1	BA	966	2MG	C6-C5-C4	-2.68	117.80	120.86
1	AA	1207	2MG	C6-C5-C4	-2.68	117.80	120.86
54	DA	745	1MG	C5-C6-N1	-2.65	114.88	118.35
30	DD	150[A]	MEQ	O-C-CA	-2.59	118.78	125.72
31	CA	1835	2MG	C6-C5-C4	-2.53	117.97	120.86
31	CA	745	1MG	C5-C6-N1	-2.52	115.05	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2605	PSU	C4-C5-C1'	-2.51	117.00	121.22
30	CD	150	MEQ	O-C-CA	-2.43	119.22	125.72
54	DA	2251	OMG	C6-C5-C4	-2.41	118.10	120.86
30	DD	150[A]	MEQ	CG-CB-CA	-2.39	108.60	114.03
54	DA	2605	PSU	C4-C5-C1'	-2.33	117.30	121.22
54	DA	745	1MG	O4'-C4'-C3'	-2.05	100.99	105.16
54	DA	2604	PSU	C4-C5-C1'	-2.01	117.83	121.22
54	DA	2503	2MA	CM2-C2-N3	2.02	120.66	117.22
1	AA	516	PSU	O4'-C1'-C2'	2.02	106.88	104.69
1	BA	516	PSU	O4'-C1'-C2'	2.03	106.89	104.69
31	CA	2445	2MG	N2-C2-N3	2.05	119.32	116.94
54	DA	2445	2MG	N2-C2-N3	2.06	119.33	116.94
31	CA	1962	5MC	CM5-C5-C6	2.08	122.84	118.63
54	DA	1939	5MU	C5M-C5-C6	2.09	122.87	118.63
54	DA	747	5MU	C5M-C5-C6	2.13	122.95	118.63
31	CA	1939	5MU	C5M-C5-C6	2.16	123.01	118.63
1	AA	1407	5MC	CM5-C5-C6	2.17	123.02	118.63
1	BA	967	5MC	CM5-C5-C6	2.17	123.03	118.63
12	AL	89	D2T	C-CA-N	2.19	114.78	109.95
1	BA	1407	5MC	CM5-C5-C6	2.19	123.08	118.63
31	CA	747	5MU	C5M-C5-C6	2.20	123.09	118.63
1	AA	967	5MC	CM5-C5-C6	2.22	123.12	118.63
1	BA	1516	2MG	N2-C2-N3	2.22	119.52	116.94
1	AA	1516	2MG	N2-C2-N3	2.28	119.59	116.94
1	AA	1207	2MG	N2-C2-N3	2.32	119.63	116.94
31	CA	1835	2MG	N2-C2-N3	2.37	119.69	116.94
54	DA	1835	2MG	N2-C2-N3	2.40	119.73	116.94
1	BA	966	2MG	N2-C2-N3	2.45	119.78	116.94
1	BA	1207	2MG	N2-C2-N3	2.47	119.80	116.94
12	BL	89	D2T	C-CA-N	2.53	115.54	109.95
54	DA	2069	G7M	O4'-C1'-N9	2.61	113.03	108.11
31	CA	2503	2MA	C2-N3-C4	2.80	116.64	115.29
54	DA	1618	6MZ	C2-N1-C6	2.82	118.50	116.47
54	DA	2580	PSU	O4'-C1'-C2'	2.84	107.77	104.69
54	DA	2030	6MZ	C2-N1-C6	2.85	118.52	116.47
31	CA	2069	G7M	O4'-C1'-N9	2.91	113.59	108.11
31	CA	2030	6MZ	C2-N1-C6	2.94	118.58	116.47
31	CA	1618	6MZ	C2-N1-C6	3.02	118.64	116.47
31	CA	2580	PSU	O4'-C1'-C2'	3.10	108.04	104.69
54	DA	2503	2MA	C2-N3-C4	3.20	116.83	115.29
30	DD	150[B]	MEQ	CB-CA-N	3.23	119.62	110.54
1	BA	1402	4OC	CM4-N4-C4	3.24	125.60	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	DD	150[B]	MEQ	CG-CB-CA	3.36	121.66	114.03
1	AA	1402	4OC	CM4-N4-C4	3.37	125.71	122.87
30	DD	150[B]	MEQ	CB-CG-CD	3.63	121.55	113.26
1	AA	1402	4OC	C2-N3-C4	4.15	120.71	115.43
1	BA	1402	4OC	C2-N3-C4	4.18	120.75	115.43
1	AA	527	G7M	O4'-C1'-N9	5.13	117.80	108.11
1	BA	527	G7M	O4'-C1'-N9	5.91	119.28	108.11
1	AA	1516	2MG	C6-N1-C2	6.26	124.20	115.24
31	CA	1835	2MG	C6-N1-C2	6.32	124.30	115.24
1	BA	1516	2MG	C6-N1-C2	6.45	124.47	115.24
1	AA	966	2MG	C6-N1-C2	6.47	124.51	115.24
31	CA	2445	2MG	C6-N1-C2	6.49	124.54	115.24
1	BA	966	2MG	C6-N1-C2	6.50	124.54	115.24
54	DA	1835	2MG	C6-N1-C2	6.51	124.56	115.24
1	BA	1207	2MG	C6-N1-C2	6.55	124.63	115.24
1	AA	1207	2MG	C6-N1-C2	6.67	124.79	115.24
1	AA	527	G7M	C6-N1-C2	7.08	124.18	115.88
54	DA	2069	G7M	C6-N1-C2	7.22	124.34	115.88
31	CA	2069	G7M	C6-N1-C2	7.41	124.57	115.88
54	DA	2445	2MG	C6-N1-C2	7.44	125.89	115.24
1	BA	527	G7M	C6-N1-C2	7.45	124.61	115.88
54	DA	2251	OMG	C6-N1-C2	7.70	124.90	115.88
31	CA	2251	OMG	C6-N1-C2	8.06	125.33	115.88
31	CA	2552	OMU	C4-N3-C2	12.05	126.91	114.21
54	DA	2552	OMU	C4-N3-C2	12.12	126.98	114.21
54	DA	955	PSU	C4-N3-C2	13.48	126.41	115.16
54	DA	1911	PSU	C4-N3-C2	13.50	126.42	115.16
31	CA	2580	PSU	C4-N3-C2	13.52	126.44	115.16
31	CA	1911	PSU	C4-N3-C2	13.53	126.45	115.16
54	DA	2604	PSU	C4-N3-C2	13.54	126.46	115.16
31	CA	2504	PSU	C4-N3-C2	13.54	126.46	115.16
31	CA	2457	PSU	C4-N3-C2	13.54	126.46	115.16
31	CA	2605	PSU	C4-N3-C2	13.55	126.46	115.16
31	CA	746	PSU	C4-N3-C2	13.57	126.48	115.16
31	CA	955	PSU	C4-N3-C2	13.58	126.48	115.16
54	DA	2605	PSU	C4-N3-C2	13.58	126.49	115.16
54	DA	2580	PSU	C4-N3-C2	13.60	126.50	115.16
1	AA	516	PSU	C4-N3-C2	13.60	126.50	115.16
54	DA	1917	PSU	C4-N3-C2	13.62	126.52	115.16
54	DA	2457	PSU	C4-N3-C2	13.64	126.54	115.16
54	DA	746	PSU	C4-N3-C2	13.64	126.54	115.16
1	BA	516	PSU	C4-N3-C2	13.66	126.56	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
54	DA	2504	PSU	C4-N3-C2	13.66	126.56	115.16
31	CA	1917	PSU	C4-N3-C2	13.76	126.64	115.16
54	DA	747	5MU	C4-N3-C2	14.23	127.03	115.16
54	DA	1939	5MU	C4-N3-C2	14.45	127.22	115.16
31	CA	747	5MU	C4-N3-C2	14.50	127.26	115.16
31	CA	1939	5MU	C4-N3-C2	14.55	127.30	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1518	MA6	1	0
1	AA	1519	MA6	1	0
1	BA	1518	MA6	1	0
1	BA	1519	MA6	1	0
31	CA	2030	6MZ	2	0
31	CA	2445	2MG	1	0
31	CA	2503	2MA	1	0
31	CA	747	5MU	1	0
54	DA	2030	6MZ	1	0
54	DA	2445	2MG	1	0
54	DA	2449	H2U	1	0
54	DA	2498	OMC	1	0
54	DA	747	5MU	1	0
30	DD	150[B]	MEQ	1	0
40	DN	81[B]	4D4	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	PG4	AA	1670	-	12,12,12	0.28	0	11,11,11	0.42	0
57	MPD	AA	1671	-	6,7,7	0.42	0	6,10,10	0.38	0
58	PUT	AA	1672	-	5,5,5	0.27	0	4,4,4	0.20	0
58	PUT	AA	1673	-	5,5,5	0.20	0	4,4,4	0.20	0
58	PUT	AA	1674	-	5,5,5	0.20	0	4,4,4	0.21	0
58	PUT	AA	1675	-	5,5,5	0.25	0	4,4,4	0.24	0
57	MPD	AA	1676	-	6,7,7	0.40	0	6,10,10	0.36	0
59	TAC	AA	1678	55	33,35,35	0.48	0	42,58,58	0.60	0
61	PEG	AL	201	-	6,6,6	0.27	0	5,5,5	0.09	0
56	PG4	BA	1601	-	12,12,12	0.22	0	11,11,11	0.22	0
59	TAC	BA	1602	55	33,35,35	0.42	0	42,58,58	0.65	0
62	EDO	D1	101	-	3,3,3	0.64	0	2,2,2	0.19	0
63	PGE	D1	102	-	9,9,9	0.31	0	8,8,8	0.28	0
61	PEG	D1	103	-	6,6,6	0.44	0	5,5,5	0.13	0
63	PGE	D3	101	-	9,9,9	0.31	0	8,8,8	0.22	0
61	PEG	D3	102	-	6,6,6	0.34	0	5,5,5	0.23	0
62	EDO	DA	3001	-	3,3,3	0.81	0	2,2,2	0.15	0
58	PUT	DA	3002	-	5,5,5	0.20	0	4,4,4	0.14	0
62	EDO	DA	3003	-	3,3,3	0.73	0	2,2,2	0.16	0
62	EDO	DA	3004	-	3,3,3	0.70	0	2,2,2	0.18	0
64	SPD	DA	3183	-	9,9,9	0.14	0	8,8,8	0.21	0
58	PUT	DA	3184	-	5,5,5	0.28	0	4,4,4	0.20	0
65	1PE	DA	3185	-	15,15,15	0.17	0	14,14,14	0.17	0
63	PGE	DA	3186	-	9,9,9	0.36	0	8,8,8	0.56	0
64	SPD	DA	3187	-	9,9,9	0.18	0	8,8,8	0.42	0
58	PUT	DA	3188	-	5,5,5	0.45	0	4,4,4	0.29	0
58	PUT	DA	3189	-	5,5,5	0.49	0	4,4,4	0.43	0
57	MPD	DA	3190	-	6,7,7	0.38	0	6,10,10	0.44	0
66	ACY	DA	3191	-	0,3,3	0.00	-	0,3,3	0.00	-
57	MPD	DA	3192	-	6,7,7	0.42	0	6,10,10	0.57	0
56	PG4	DA	3193	-	12,12,12	0.32	0	11,11,11	0.43	0
62	EDO	DA	3194	-	3,3,3	0.62	0	2,2,2	0.11	0
58	PUT	DA	3195	-	5,5,5	0.34	0	4,4,4	0.48	0
66	ACY	DA	3196	-	0,3,3	0.00	-	0,3,3	0.00	-
62	EDO	DA	3197	-	3,3,3	0.61	0	2,2,2	0.28	0
62	EDO	DA	3198	-	3,3,3	0.65	0	2,2,2	0.42	0
61	PEG	DA	3199	-	6,6,6	0.31	0	5,5,5	0.20	0
61	PEG	DA	3200	-	6,6,6	0.53	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	0.39	0
57	MPD	DA	3203	-	6,7,7	0.61	0	6,10,10	0.59	0
58	PUT	DA	3204	-	5,5,5	0.38	0	4,4,4	0.28	0
64	SPD	DA	3205	-	9,9,9	0.26	0	8,8,8	0.18	0
57	MPD	DA	3206	-	6,7,7	0.60	0	6,10,10	0.51	0
62	EDO	DA	3207	-	3,3,3	0.68	0	2,2,2	0.21	0
62	EDO	DA	3208	-	3,3,3	0.58	0	2,2,2	0.36	0
57	MPD	DA	3209	-	6,7,7	0.39	0	6,10,10	0.27	0
67	GUN	DA	3210	-	9,12,12	2.07	2 (22%)	7,17,17	4.82	5 (71%)
58	PUT	DA	3211	-	5,5,5	0.35	0	4,4,4	0.16	0
58	PUT	DA	3212	-	5,5,5	0.40	0	4,4,4	0.30	0
63	PGE	DA	3213	-	9,9,9	0.18	0	8,8,8	0.18	0
62	EDO	DA	3214	-	3,3,3	0.64	0	2,2,2	0.28	0
56	PG4	DA	3215	-	12,12,12	0.18	0	11,11,11	0.14	0
63	PGE	DA	3216	-	9,9,9	0.16	0	8,8,8	0.25	0
61	PEG	DA	3217	-	6,6,6	0.32	0	5,5,5	0.07	0
58	PUT	DA	3218	-	5,5,5	0.17	0	4,4,4	0.20	0
68	TRS	DA	3219	-	7,7,7	0.54	0	9,9,9	0.41	0
58	PUT	DA	3220	-	5,5,5	0.23	0	4,4,4	0.15	0
58	PUT	DA	3221	-	5,5,5	0.48	0	4,4,4	0.58	0
58	PUT	DA	3222	-	5,5,5	0.28	0	4,4,4	0.36	0
64	SPD	DA	3223	-	9,9,9	0.20	0	8,8,8	0.63	0
63	PGE	DA	3224	-	9,9,9	0.26	0	8,8,8	0.16	0
61	PEG	DA	3225	-	6,6,6	0.51	0	5,5,5	0.23	0
61	PEG	DA	3226	-	6,6,6	0.44	0	5,5,5	0.24	0
62	EDO	DB	210	-	3,3,3	0.58	0	2,2,2	0.27	0
62	EDO	DB	211	-	3,3,3	0.58	0	2,2,2	0.22	0
63	PGE	DD	301	-	9,9,9	0.31	0	8,8,8	0.32	0
57	MPD	DE	301	-	6,7,7	0.54	0	6,10,10	0.68	0
57	MPD	DE	302	-	6,7,7	0.49	0	6,10,10	0.34	0
57	MPD	DK	201	-	6,7,7	0.46	0	6,10,10	0.25	0
61	PEG	DL	201	-	6,6,6	0.15	0	5,5,5	0.13	0
57	MPD	DN	201	-	6,7,7	0.64	0	6,10,10	0.32	0
61	PEG	DP	201	-	6,6,6	0.32	0	5,5,5	0.13	0
61	PEG	DQ	201	-	6,6,6	0.23	0	5,5,5	0.14	0
56	PG4	DQ	202	-	12,12,12	0.17	0	11,11,11	0.16	0
56	PG4	DR	202	-	12,12,12	0.44	0	11,11,11	0.55	0
63	PGE	DS	201	-	9,9,9	0.50	0	8,8,8	0.48	0
56	PG4	DS	202	-	12,12,12	0.48	0	11,11,11	0.42	0
57	MPD	DS	203	-	6,7,7	0.37	0	6,10,10	0.51	0
57	MPD	DT	201	-	6,7,7	0.48	0	6,10,10	0.13	0
57	MPD	DT	202	-	6,7,7	0.42	0	6,10,10	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	PGE	DU	101	-	9,9,9	0.27	0	8,8,8	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1678	55	-	0/8/74/74	0/4/4/4
61	PEG	AL	201	-	-	0/4/4/4	0/0/0/0
56	PG4	BA	1601	-	-	0/10/10/10	0/0/0/0
59	TAC	BA	1602	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
63	PGE	D3	101	-	-	0/7/7/7	0/0/0/0
61	PEG	D3	102	-	-	0/4/4/4	0/0/0/0
62	EDO	DA	3001	-	-	0/1/1/1	0/0/0/0
58	PUT	DA	3002	-	-	0/3/3/3	0/0/0/0
62	EDO	DA	3003	-	-	0/1/1/1	0/0/0/0
62	EDO	DA	3004	-	-	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
57	MPD	DA	3203	-	-	0/5/5/5	0/0/0/0
58	PUT	DA	3204	-	-	0/3/3/3	0/0/0/0
64	SPD	DA	3205	-	-	0/7/7/7	0/0/0/0
57	MPD	DA	3206	-	-	0/5/5/5	0/0/0/0
62	EDO	DA	3207	-	-	0/1/1/1	0/0/0/0
62	EDO	DA	3208	-	-	0/1/1/1	0/0/0/0
57	MPD	DA	3209	-	-	0/5/5/5	0/0/0/0
67	GUN	DA	3210	-	-	0/0/0/0	0/2/2/2
58	PUT	DA	3211	-	-	0/3/3/3	0/0/0/0
58	PUT	DA	3212	-	-	0/3/3/3	0/0/0/0
63	PGE	DA	3213	-	-	0/7/7/7	0/0/0/0
62	EDO	DA	3214	-	-	0/1/1/1	0/0/0/0
56	PG4	DA	3215	-	-	0/10/10/10	0/0/0/0
63	PGE	DA	3216	-	-	0/7/7/7	0/0/0/0
61	PEG	DA	3217	-	-	0/4/4/4	0/0/0/0
58	PUT	DA	3218	-	-	0/3/3/3	0/0/0/0
68	TRS	DA	3219	-	-	0/9/9/9	0/0/0/0
58	PUT	DA	3220	-	-	0/3/3/3	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
64	SPD	DA	3223	-	-	0/7/7/7	0/0/0/0
63	PGE	DA	3224	-	-	0/7/7/7	0/0/0/0
61	PEG	DA	3225	-	-	0/4/4/4	0/0/0/0
61	PEG	DA	3226	-	-	0/4/4/4	0/0/0/0
62	EDO	DB	210	-	-	0/1/1/1	0/0/0/0
62	EDO	DB	211	-	-	0/1/1/1	0/0/0/0
63	PGE	DD	301	-	-	0/7/7/7	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	3210	GUN	C6-N1	3.30	1.39	1.33
67	DA	3210	GUN	C6-C5	4.53	1.50	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	DA	3210	GUN	C5-C6-N1	-8.80	112.02	123.52
67	DA	3210	GUN	C6-C5-C4	-3.01	117.42	120.86
67	DA	3210	GUN	N3-C2-N1	-2.62	123.99	127.56
67	DA	3210	GUN	C5-C4-N9	-2.53	106.64	111.12
67	DA	3210	GUN	C6-N1-C2	7.90	125.14	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

32 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	AA	1670	PG4	1	0
59	AA	1678	TAC	1	0
59	BA	1602	TAC	1	0
63	D1	102	PGE	2	0
61	D1	103	PEG	1	0
61	D3	102	PEG	2	0
58	DA	3189	PUT	1	0
57	DA	3190	MPD	1	0
57	DA	3192	MPD	2	0
56	DA	3193	PG4	1	0
62	DA	3194	EDO	1	0
58	DA	3195	PUT	3	0
62	DA	3197	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	DA	3200	PEG	1	0
57	DA	3203	MPD	2	0
58	DA	3212	PUT	1	0
63	DA	3213	PGE	1	0
56	DA	3215	PG4	1	0
63	DA	3216	PGE	1	0
58	DA	3218	PUT	1	0
68	DA	3219	TRS	1	0
58	DA	3221	PUT	3	0
58	DA	3222	PUT	1	0
64	DA	3223	SPD	4	0
63	DA	3224	PGE	3	0
62	DB	211	EDO	1	0
63	DD	301	PGE	2	0
57	DN	201	MPD	1	0
61	DP	201	PEG	1	0
56	DR	202	PG4	5	0
56	DS	202	PG4	1	0
63	DU	101	PGE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.42	52 (3%) 49 36	43, 97, 239, 285	0
1	BA	1522/1534 (99%)	1.36	391 (25%) 1 0	52, 139, 267, 278	0
2	AB	224/224 (100%)	1.57	78 (34%) 0 0	78, 123, 207, 275	0
2	BB	224/224 (100%)	1.90	84 (37%) 0 0	93, 139, 208, 261	0
3	AC	206/206 (100%)	0.57	19 (9%) 11 5	73, 101, 135, 157	0
3	BC	206/206 (100%)	1.95	83 (40%) 0 0	103, 141, 180, 219	0
4	AD	205/205 (100%)	0.29	6 (2%) 55 43	53, 96, 127, 158	0
4	BD	205/205 (100%)	0.09	2 (0%) 84 77	53, 77, 106, 135	0
5	AE	155/155 (100%)	0.45	6 (3%) 43 31	60, 87, 139, 174	0
5	BE	150/155 (96%)	0.73	18 (12%) 6 3	71, 91, 142, 229	0
6	AF	106/106 (100%)	0.55	13 (12%) 5 3	72, 97, 120, 134	0
6	BF	100/106 (94%)	0.86	9 (9%) 12 6	79, 112, 139, 147	0
7	AG	151/151 (100%)	1.46	42 (27%) 1 0	99, 128, 157, 169	0
7	BG	151/151 (100%)	3.74	108 (71%) 0 0	139, 193, 209, 220	0
8	AH	129/129 (100%)	0.41	6 (4%) 35 24	66, 85, 113, 128	0
8	BH	129/129 (100%)	0.83	19 (14%) 3 2	86, 110, 145, 164	0
9	AI	127/127 (100%)	1.83	45 (35%) 0 0	85, 123, 161, 188	0
9	BI	127/127 (100%)	3.74	77 (60%) 0 0	130, 168, 201, 223	0
10	AJ	99/99 (100%)	1.38	21 (21%) 1 1	85, 111, 142, 157	0
10	BJ	98/99 (98%)	4.86	73 (74%) 0 0	132, 163, 188, 200	0
11	AK	117/117 (100%)	1.24	28 (23%) 1 1	52, 102, 138, 153	0
11	BK	117/117 (100%)	1.04	24 (20%) 1 1	73, 109, 139, 160	0
12	AL	122/123 (99%)	0.32	2 (1%) 74 66	48, 66, 99, 126	0
12	BL	122/123 (99%)	1.21	30 (24%) 1 0	75, 91, 112, 133	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	1.92	47 (41%) 0 0	90, 118, 167, 184	0
13	BM	114/114 (100%)	5.81	106 (92%) 0 0	195, 228, 237, 241	0
14	AN	100/100 (100%)	1.39	21 (21%) 1 1	82, 108, 198, 210	0
14	BN	100/100 (100%)	4.08	73 (73%) 0 0	125, 173, 232, 242	0
15	AO	88/88 (100%)	0.55	7 (7%) 15 7	63, 87, 108, 128	0
15	BO	88/88 (100%)	1.08	17 (19%) 2 1	75, 105, 125, 144	0
16	AP	82/82 (100%)	1.17	16 (19%) 1 1	60, 79, 114, 133	0
16	BP	82/82 (100%)	2.48	44 (53%) 0 0	89, 105, 151, 161	0
17	AQ	80/80 (100%)	0.61	6 (7%) 17 9	63, 79, 114, 136	0
17	BQ	80/80 (100%)	1.98	30 (37%) 0 0	94, 119, 143, 147	0
18	AR	55/55 (100%)	1.09	13 (23%) 1 1	68, 91, 126, 154	0
18	BR	55/55 (100%)	0.80	5 (9%) 11 6	71, 89, 123, 150	0
19	AS	79/79 (100%)	1.37	22 (27%) 1 0	94, 109, 146, 153	0
19	BS	79/79 (100%)	5.37	71 (89%) 0 0	206, 223, 234, 242	0
20	AT	86/86 (100%)	0.67	5 (5%) 26 16	67, 79, 116, 132	0
20	BT	85/86 (98%)	2.92	55 (64%) 0 0	101, 121, 164, 175	0
21	AU	56/56 (100%)	1.50	15 (26%) 1 0	80, 118, 156, 170	0
21	BU	56/56 (100%)	0.77	8 (14%) 4 2	75, 100, 143, 156	0
22	C1	56/56 (100%)	2.89	36 (64%) 0 0	94, 138, 164, 182	0
22	D1	56/56 (100%)	0.32	0 100 100	20, 41, 64, 95	0
23	C2	50/51 (98%)	4.05	40 (80%) 0 0	126, 141, 153, 175	0
23	D2	51/51 (100%)	0.32	2 (3%) 43 31	49, 63, 89, 104	0
24	C3	46/46 (100%)	3.68	36 (78%) 0 0	99, 109, 119, 131	0
24	D3	46/46 (100%)	0.37	2 (4%) 39 27	30, 42, 56, 99	0
25	C4	64/64 (100%)	2.51	33 (51%) 0 0	105, 121, 134, 140	0
25	D4	64/64 (100%)	0.36	0 100 100	34, 41, 52, 63	0
26	C5	38/38 (100%)	2.72	23 (60%) 0 0	100, 114, 124, 134	0
26	D5	38/38 (100%)	0.38	0 100 100	31, 46, 62, 82	0
27	C0	58/58 (100%)	2.44	30 (51%) 0 0	98, 113, 132, 135	0
27	D0	58/58 (100%)	0.25	0 100 100	28, 35, 54, 72	0
28	CB	118/120 (98%)	1.78	40 (33%) 0 0	132, 189, 251, 254	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	120/120 (100%)	0.14	0 100 100	29, 56, 101, 148	0
29	CC	271/271 (100%)	1.36	78 (28%) 1 0	80, 112, 146, 165	0
29	DC	271/271 (100%)	0.09	1 (0%) 93 90	28, 56, 84, 100	0
30	CD	208/209 (99%)	2.21	103 (49%) 0 0	86, 121, 156, 181	0
30	DD	208/209 (99%)	0.01	0 100 100	18, 39, 67, 88	0
31	CA	2876/2904 (99%)	1.74	893 (31%) 1 0	71, 170, 260, 285	0
32	CE	201/201 (100%)	2.99	124 (61%) 0 0	112, 159, 194, 210	0
32	DE	201/201 (100%)	0.15	6 (2%) 54 41	24, 55, 100, 139	0
33	CF	177/177 (100%)	4.98	153 (86%) 0 0	198, 211, 219, 226	0
33	DF	177/177 (100%)	0.48	7 (3%) 42 30	50, 79, 125, 137	0
34	CG	176/176 (100%)	3.79	134 (76%) 0 0	130, 170, 205, 215	0
34	DG	176/176 (100%)	0.24	5 (2%) 56 44	42, 70, 97, 139	0
35	CH	149/149 (100%)	2.24	74 (49%) 0 0	84, 151, 170, 180	0
35	DH	149/149 (100%)	1.87	63 (42%) 0 0	74, 150, 187, 199	0
36	CJ	134/134 (100%)	8.41	130 (97%) 0 0	227, 245, 255, 263	0
36	DJ	134/134 (100%)	5.70	111 (82%) 0 0	196, 220, 229, 237	0
37	CK	142/142 (100%)	1.66	52 (36%) 0 0	95, 117, 152, 194	0
37	DK	142/142 (100%)	-0.03	0 100 100	19, 34, 58, 72	0
38	CL	122/123 (99%)	1.14	23 (18%) 2 1	90, 109, 141, 158	0
38	DL	123/123 (100%)	-0.07	0 100 100	28, 43, 70, 106	0
39	CM	144/144 (100%)	3.63	106 (73%) 0 0	104, 151, 201, 235	0
39	DM	144/144 (100%)	0.18	2 (1%) 78 69	18, 55, 84, 116	0
40	CN	135/136 (99%)	1.35	38 (28%) 1 0	92, 112, 142, 180	0
40	DN	135/136 (99%)	-0.19	0 100 100	25, 39, 67, 86	0
41	CO	120/125 (96%)	2.25	55 (45%) 0 0	101, 123, 143, 177	0
41	DO	125/125 (100%)	0.01	0 100 100	24, 36, 65, 108	0
42	CP	116/117 (99%)	3.69	93 (80%) 0 0	139, 162, 177, 181	0
42	DP	117/117 (100%)	0.17	0 100 100	36, 56, 84, 93	0
43	CQ	114/114 (100%)	2.11	47 (41%) 0 0	100, 117, 149, 164	0
43	DQ	114/114 (100%)	-0.01	3 (2%) 59 47	30, 49, 77, 109	0
44	CR	117/117 (100%)	2.33	57 (48%) 0 0	89, 122, 157, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DR	117/117 (100%)	0.13	1 (0%) 85 79	18, 29, 48, 72	0
45	CS	103/103 (100%)	3.82	79 (76%) 0 0	107, 133, 172, 185	0
45	DS	103/103 (100%)	-0.16	0 100 100	19, 41, 69, 91	0
46	CT	110/110 (100%)	2.28	55 (50%) 0 0	99, 127, 167, 182	0
46	DT	110/110 (100%)	-0.05	0 100 100	19, 33, 60, 116	0
47	CU	93/93 (100%)	3.54	67 (72%) 0 0	123, 147, 176, 185	0
47	DU	93/93 (100%)	0.57	5 (5%) 29 19	31, 53, 109, 124	0
48	CV	102/102 (100%)	4.69	85 (83%) 0 0	113, 161, 198, 209	0
48	DV	102/102 (100%)	0.44	10 (9%) 10 5	42, 60, 121, 157	0
49	CW	94/94 (100%)	2.41	49 (52%) 0 0	116, 137, 156, 161	0
49	DW	94/94 (100%)	-0.23	0 100 100	31, 51, 76, 86	0
50	CX	75/76 (98%)	3.19	41 (54%) 0 0	103, 126, 140, 170	0
50	DX	76/76 (100%)	-0.05	1 (1%) 79 71	25, 39, 64, 104	0
51	CY	77/77 (100%)	1.85	31 (40%) 0 0	97, 117, 142, 161	0
51	DY	77/77 (100%)	0.09	1 (1%) 79 71	38, 54, 88, 103	0
52	CZ	62/62 (100%)	4.12	49 (79%) 0 0	127, 163, 175, 186	0
52	DZ	62/62 (100%)	0.59	6 (9%) 10 5	48, 70, 103, 126	0
53	DI	135/135 (100%)	2.50	69 (51%) 0 0	78, 150, 197, 207	1 (0%)
54	DA	2873/2904 (98%)	0.46	123 (4%) 39 27	17, 44, 217, 299	0
All	All	20633/20745 (99%)	1.39	5069 (24%) 1 0	17, 108, 239, 299	1 (0%)

All (5069) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	DJ	54	PRO	28.0
36	CJ	69	PHE	27.5
36	CJ	76	ALA	25.4
36	DJ	53	LEU	23.7
36	CJ	14	ALA	23.3
36	CJ	13	VAL	23.2
36	CJ	54	PRO	21.1
36	CJ	55	ILE	20.3
9	BI	128	SER	19.5
36	CJ	57	VAL	18.2
45	CS	50	GLY	17.9

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Mol	Chain	Res	Type	RSRZ
36	CJ	59	ILE	17.9
10	BJ	74	VAL	17.6
33	CF	85	ILE	17.5
9	BI	31	ASN	17.0
33	CF	128	TYR	17.0
36	CJ	11	LEU	17.0
33	CF	40	VAL	16.6
54	DA	2120	G	16.2
13	BM	10	PRO	16.0
39	CM	101	ILE	16.0
36	CJ	12	GLN	15.9
36	CJ	23	PRO	15.8
31	CA	1067	A	15.7
39	CM	80	SER	15.6
36	DJ	76	ALA	15.3
36	DJ	80	LEU	15.3
1	BA	211	G	15.2
19	BS	48	THR	15.1
36	DJ	96	ASP	15.0
36	DJ	67	PHE	14.9
36	DJ	23	PRO	14.8
36	CJ	17	MET	14.8
13	BM	5	ALA	14.5
33	CF	76	GLY	14.5
36	DJ	94	ASN	14.5
20	BT	4	ILE	14.4
36	CJ	56	PRO	14.4
36	CJ	126	THR	14.3
31	CA	1068	G	14.2
33	CF	156	ILE	14.1
31	CA	2172	U	14.0
36	CJ	51	LYS	13.8
39	CM	81	ASP	13.7
48	CV	20	GLY	13.6
10	BJ	8	ILE	13.6
1	BA	209	U	13.5
36	CJ	68	THR	13.4
48	CV	13	VAL	13.3
53	DI	131	THR	13.2
36	CJ	80	LEU	13.2
36	CJ	21	SER	13.2
36	CJ	87	LYS	13.1

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Mol	Chain	Res	Type	RSRZ
52	CZ	45	GLN	13.1
36	CJ	38	PHE	13.1
36	DJ	135	SER	13.1
36	DJ	88	SER	13.0
36	DJ	55	ILE	12.9
36	CJ	61	VAL	12.8
36	CJ	22	PRO	12.7
36	CJ	71	THR	12.7
36	DJ	79	LEU	12.7
54	DA	2110	G	12.7
36	CJ	82	LYS	12.6
9	BI	44	ALA	12.6
36	DJ	78	VAL	12.6
19	BS	14	HIS	12.6
36	CJ	8	TYR	12.6
9	BI	67	VAL	12.5
36	CJ	20	PRO	12.5
50	CX	54	GLY	12.4
34	CG	40	ALA	12.4
19	BS	38	SER	12.3
45	CS	27	ILE	12.3
39	CM	92	LEU	12.2
31	CA	1066	U	12.1
39	CM	114	GLY	12.1
53	DI	128	THR	12.0
36	CJ	60	THR	12.0
36	CJ	28	LEU	12.0
54	DA	2163	A	12.0
36	DJ	114	ALA	12.0
29	CC	27	GLY	11.9
36	CJ	42	PHE	11.9
13	BM	23	TYR	11.8
1	BA	1302	C	11.8
13	BM	45	ILE	11.8
36	CJ	138	LEU	11.7
36	CJ	99	GLY	11.7
10	BJ	73	LEU	11.7
36	DJ	52	GLY	11.7
34	CG	32	GLU	11.7
9	AI	130	ARG	11.6
54	DA	2111	U	11.6
47	CU	43	ILE	11.6

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Mol	Chain	Res	Type	RSRZ
48	CV	80	ALA	11.6
36	CJ	9	VAL	11.5
13	BM	22	ILE	11.5
36	DJ	137	GLY	11.4
9	BI	40	GLY	11.4
36	DJ	20	PRO	11.4
33	CF	157	THR	11.4
39	CM	100	ILE	11.3
19	BS	12	ASP	11.3
1	BA	983	A	11.3
10	BJ	76	ILE	11.3
48	CV	19	LYS	11.3
33	CF	154	ILE	11.3
48	CV	36	VAL	11.2
14	BN	60	GLN	11.2
36	CJ	121	ASP	11.2
10	BJ	101	SER	11.1
31	CA	1537	G	11.1
36	DJ	13	VAL	11.1
33	CF	106	ILE	11.1
1	BA	1242	G	11.1
33	CF	155	THR	11.1
9	BI	126	GLN	11.0
36	DJ	138	LEU	11.0
43	CQ	85	SER	11.0
53	DI	96	PHE	10.9
36	CJ	98	VAL	10.9
48	CV	78	GLY	10.9
36	CJ	47	ASP	10.9
33	CF	129	SER	10.9
14	BN	33	ASP	10.9
10	BJ	87	LEU	10.8
9	BI	16	ALA	10.8
36	CJ	62	TYR	10.8
7	BG	8	GLY	10.8
48	CV	89	ASP	10.8
36	CJ	83	ALA	10.7
33	CF	117	LEU	10.6
45	CS	96	VAL	10.6
19	BS	5	LEU	10.6
14	AN	21	PHE	10.5
52	CZ	32	ALA	10.5

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Mol	Chain	Res	Type	RSRZ
34	CG	62	TRP	10.5
7	BG	43	VAL	10.5
36	CJ	85	GLY	10.4
13	BM	2	ALA	10.4
1	BA	1030	U	10.4
9	BI	127	PHE	10.3
19	BS	29	LYS	10.3
10	BJ	26	VAL	10.3
1	AA	1030	U	10.3
33	CF	35	THR	10.3
33	CF	86	GLY	10.3
36	CJ	75	PRO	10.3
36	DJ	12	GLN	10.2
36	CJ	33	VAL	10.2
36	CJ	132	THR	10.2
42	CP	63	LYS	10.2
10	BJ	77	VAL	10.2
1	BA	1016	A	10.1
34	CG	43	VAL	10.1
7	BG	116	MET	10.1
19	BS	24	GLU	10.1
30	CD	26	VAL	10.1
42	CP	64	TYR	10.1
14	BN	49	GLN	10.1
36	CJ	139	VAL	10.1
9	BI	130	ARG	10.1
13	BM	95	LEU	10.0
36	CJ	53	LEU	10.0
23	C2	21	TYR	10.0
7	BG	42	ILE	10.0
19	BS	39	THR	9.9
36	CJ	130	GLU	9.9
13	BM	32	ALA	9.9
36	CJ	74	PRO	9.9
31	CA	2110	G	9.9
7	BG	62	PHE	9.9
54	DA	2124	G	9.9
23	C2	47	VAL	9.9
36	CJ	67	PHE	9.8
34	CG	105	LEU	9.8
54	DA	2118	U	9.8
36	CJ	129	ILE	9.8

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Mol	Chain	Res	Type	RSRZ
7	BG	4	ARG	9.8
52	CZ	31	GLN	9.8
54	DA	2125	G	9.8
19	BS	66	MET	9.8
24	C3	1	MET	9.8
36	DJ	133	ALA	9.7
45	CS	63	VAL	9.7
23	C2	24	THR	9.7
13	BM	55	THR	9.7
1	AA	86	G	9.6
33	CF	144	ASP	9.6
48	CV	87	PHE	9.6
34	CG	103	ILE	9.6
33	CF	153	ASP	9.6
3	BC	193	TYR	9.6
1	BA	1032	G	9.6
31	CA	1065	U	9.6
36	DJ	24	VAL	9.5
36	CJ	120	ALA	9.5
49	CW	94	ALA	9.4
54	DA	2174	C	9.4
19	BS	63	THR	9.4
32	CE	128	ALA	9.4
19	BS	37	ARG	9.3
13	BM	19	LEU	9.3
33	CF	151	GLY	9.3
14	BN	36	ALA	9.3
1	BA	1026	G	9.3
48	CV	31	SER	9.3
31	CA	1095	A	9.3
13	BM	33	ILE	9.2
32	CE	119	ILE	9.2
34	CG	52	PHE	9.2
36	DJ	22	PRO	9.2
13	BM	46	SER	9.2
19	BS	31	LEU	9.2
34	CG	33	LEU	9.2
10	BJ	41	PRO	9.2
13	BM	56	LEU	9.2
14	BN	27	LEU	9.1
36	CJ	77	ALA	9.1
45	CS	32	THR	9.1

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Mol	Chain	Res	Type	RSRZ
33	CF	147	ASP	9.1
36	CJ	94	ASN	9.1
13	BM	39	ILE	9.1
19	BS	49	ILE	9.1
10	BJ	22	THR	9.0
13	BM	48	LEU	9.0
1	BA	1024	G	9.0
24	C3	42	LEU	9.0
36	CJ	24	VAL	9.0
24	C3	35	ARG	9.0
52	CZ	15	ASN	9.0
9	BI	39	PHE	9.0
36	CJ	89	GLY	9.0
19	BS	32	ARG	8.9
36	DJ	84	ALA	8.9
36	DJ	131	GLY	8.9
50	CX	53	CYS	8.9
10	BJ	98	VAL	8.9
10	BJ	42	LEU	8.9
7	BG	106	GLU	8.9
36	DJ	59	ILE	8.8
36	DJ	85	GLY	8.8
2	BB	135	LEU	8.8
36	CJ	96	ASP	8.8
7	AG	4	ARG	8.8
36	CJ	78	VAL	8.8
36	CJ	122	ILE	8.8
14	BN	43	ASN	8.8
31	CA	2402	U	8.8
13	BM	30	SER	8.8
52	CZ	40	SER	8.8
31	CA	75	G	8.8
36	CJ	43	ASN	8.8
9	BI	17	ALA	8.8
13	BM	94	GLY	8.8
33	CF	113	ASP	8.8
9	BI	38	TYR	8.8
36	DJ	134	ARG	8.7
10	BJ	6	ILE	8.7
45	CS	35	PHE	8.7
45	CS	103	ALA	8.7
31	CA	2126	A	8.7

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Mol	Chain	Res	Type	RSRZ
47	CU	55	VAL	8.7
14	BN	54	ASP	8.7
48	CV	26	LYS	8.7
48	CV	88	GLU	8.7
13	BM	29	ARG	8.7
52	CZ	42	LEU	8.7
19	BS	13	LEU	8.7
13	BM	96	PRO	8.6
54	DA	1172	C	8.6
2	BB	34	ALA	8.6
9	BI	68	LYS	8.6
33	CF	105	THR	8.6
36	CJ	90	SER	8.6
47	CU	60	THR	8.6
32	CE	33	VAL	8.6
12	AL	124	ALA	8.6
47	CU	75	GLY	8.6
14	BN	22	ALA	8.6
14	BN	35	ASN	8.5
33	CF	65	PRO	8.5
47	CU	57	VAL	8.5
10	BJ	75	ASP	8.5
20	BT	3	ASN	8.5
31	CA	2125	G	8.5
34	CG	157	TYR	8.5
1	BA	1222	G	8.5
1	BA	942	G	8.5
7	BG	133	THR	8.5
14	BN	52	PRO	8.5
18	BR	20	GLU	8.5
1	BA	1017	U	8.5
13	BM	105	ASN	8.5
26	C5	38	GLY	8.4
36	CJ	86	ILE	8.4
39	CM	82	LEU	8.4
45	CS	49	ILE	8.4
48	CV	79	LYS	8.4
13	BM	63	PHE	8.4
36	DJ	36	MET	8.4
23	C2	45	GLN	8.4
39	CM	79	LEU	8.3
9	BI	4	ASN	8.3

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Mol	Chain	Res	Type	RSRZ
34	CG	26	ILE	8.3
52	CZ	41	HIS	8.3
14	BN	31	ILE	8.3
36	DJ	66	SER	8.3
54	DA	2127	G	8.3
31	CA	1094	U	8.3
22	C1	3	VAL	8.2
33	CF	165	GLU	8.2
33	CF	97	TRP	8.2
9	BI	5	GLN	8.2
50	CX	56	ASP	8.2
42	CP	103	VAL	8.2
1	BA	1307	U	8.2
53	DI	130	PRO	8.2
36	CJ	84	ALA	8.2
33	CF	173	PHE	8.2
36	CJ	45	LYS	8.2
43	CQ	115	ASN	8.1
39	CM	85	VAL	8.1
7	BG	49	THR	8.1
22	C1	5	GLN	8.1
24	C3	33	ARG	8.1
33	CF	131	GLY	8.1
39	CM	10	GLU	8.1
13	BM	31	LYS	8.1
31	CA	613	A	8.1
48	DV	56	GLY	8.1
19	BS	60	VAL	8.1
21	AU	2	PRO	8.1
7	BG	52	GLN	8.1
36	CJ	31	GLN	8.1
42	CP	29	HIS	8.1
1	BA	1020	G	8.1
22	C1	2	ALA	8.0
1	BA	1028	C	8.0
30	CD	8	LYS	8.0
19	BS	11	ILE	8.0
42	CP	40	ILE	8.0
1	BA	1218	C	8.0
34	CG	57	GLY	8.0
14	BN	21	PHE	8.0
10	BJ	72	ARG	8.0

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Mol	Chain	Res	Type	RSRZ
1	BA	204	G	8.0
1	BA	958	A	8.0
36	CJ	50	GLU	8.0
48	CV	12	ILE	8.0
33	CF	152	LEU	7.9
48	CV	25	VAL	7.9
13	BM	4	ILE	7.9
50	CX	33	ALA	7.9
1	BA	1243	C	7.9
9	AI	21	ILE	7.9
13	BM	40	ALA	7.9
33	CF	176	PRO	7.9
36	DJ	69	PHE	7.9
10	BJ	90	LEU	7.9
14	BN	47	LYS	7.9
10	BJ	38	GLY	7.9
2	BB	67	ILE	7.9
14	BN	4	GLN	7.8
32	CE	104	ALA	7.8
33	CF	143	TYR	7.8
31	CA	1211	C	7.8
36	CJ	46	THR	7.8
31	CA	1175	A	7.8
1	BA	1296	C	7.8
36	CJ	123	GLU	7.8
39	CM	7	SER	7.8
10	BJ	7	ARG	7.8
34	CG	2	SER	7.8
36	CJ	88	SER	7.8
50	CX	63	ALA	7.8
54	DA	2121	G	7.8
13	BM	64	VAL	7.8
48	CV	75	ALA	7.8
19	BS	41	PHE	7.8
23	C2	36	LEU	7.7
31	CA	1535	A	7.7
42	CP	24	THR	7.7
34	CG	171	THR	7.7
48	CV	50	PRO	7.7
31	CA	329	G	7.7
54	DA	138	U	7.7
16	BP	52	LEU	7.7

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Mol	Chain	Res	Type	RSRZ
10	BJ	19	ASP	7.7
1	BA	1025	U	7.7
48	CV	51	ALA	7.7
33	CF	69	LYS	7.7
36	CJ	58	VAL	7.6
13	BM	103	LYS	7.6
27	C0	56	LYS	7.6
19	BS	52	HIS	7.6
33	CF	31	VAL	7.6
31	CA	1069	A	7.6
48	CV	33	LYS	7.6
14	BN	50	THR	7.6
23	C2	37	LYS	7.6
10	BJ	80	THR	7.6
33	CF	110	ARG	7.6
9	BI	58	VAL	7.6
1	BA	984	C	7.6
32	CE	150	THR	7.6
47	CU	87	LEU	7.5
1	BA	985	C	7.5
1	BA	1274	A	7.5
13	BM	6	GLY	7.5
48	CV	14	LEU	7.5
36	DJ	19	ASN	7.5
29	CC	239	ASN	7.5
13	BM	13	LYS	7.5
32	CE	47	LYS	7.5
36	DJ	87	LYS	7.5
1	AA	1031	C	7.5
7	BG	17	LYS	7.5
33	CF	130	MET	7.5
19	BS	76	PRO	7.5
39	CM	78	ARG	7.5
25	C4	61	CYS	7.5
16	BP	17	TYR	7.4
7	BG	16	PRO	7.4
31	CA	1103	A	7.4
33	CF	107	ALA	7.4
36	DJ	98	VAL	7.4
53	DI	121	SER	7.4
34	CG	111	HIS	7.4
10	BJ	102	LEU	7.4

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Mol	Chain	Res	Type	RSRZ
34	CG	172	LYS	7.4
50	CX	26	PHE	7.4
1	AA	1032	G	7.4
3	BC	192	THR	7.4
45	CS	59	ILE	7.4
53	DI	132	TYR	7.4
39	CM	102	GLY	7.3
1	AA	844	G	7.3
9	BI	66	THR	7.3
40	CN	136	MET	7.3
42	CP	54	VAL	7.3
54	DA	896	A	7.3
1	BA	1031	C	7.3
11	BK	47	ALA	7.3
13	BM	93	ARG	7.3
24	C3	36	ALA	7.3
52	CZ	29	ARG	7.3
13	BM	41	GLU	7.3
36	CJ	18	ALA	7.3
54	DA	2172	U	7.3
32	CE	143	LEU	7.3
33	CF	83	TYR	7.3
26	C5	10	LEU	7.3
36	CJ	136	MET	7.3
16	AP	47	GLU	7.3
1	BA	208	U	7.2
13	BM	24	GLY	7.2
36	DJ	89	GLY	7.2
54	DA	2175	C	7.2
48	CV	48	PRO	7.2
36	CJ	44	ALA	7.2
36	DJ	99	GLY	7.2
33	CF	39	GLY	7.2
33	CF	132	VAL	7.2
32	CE	12	LEU	7.2
33	CF	75	ALA	7.2
36	CJ	27	ALA	7.2
25	C4	28	ASN	7.2
24	C3	37	LYS	7.2
19	BS	61	PHE	7.2
7	BG	41	SER	7.2
45	CS	37	GLU	7.2

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Mol	Chain	Res	Type	RSRZ
33	CF	93	GLY	7.2
48	CV	29	LEU	7.2
43	CQ	84	ILE	7.2
34	CG	80	THR	7.1
52	CZ	37	LEU	7.1
31	CA	2666	C	7.1
48	CV	43	LYS	7.1
2	BB	82	ASP	7.1
13	BM	83	LEU	7.1
1	BA	1221	G	7.1
54	DA	2116	G	7.1
13	BM	86	TYR	7.1
2	AB	123	ASP	7.1
10	BJ	100	ILE	7.1
7	BG	111	ARG	7.1
31	CA	2174	C	7.1
47	CU	72	GLN	7.1
14	BN	34	VAL	7.1
42	CP	51	ALA	7.1
10	BJ	91	ASP	7.1
10	BJ	95	GLY	7.1
13	BM	99	GLY	7.1
31	CA	2163	A	7.1
35	CH	132	PHE	7.1
53	DI	129	LEU	7.1
36	CJ	113	LYS	7.1
19	BS	74	PHE	7.1
34	CG	8	PRO	7.1
34	CG	102	VAL	7.1
39	CM	8	PRO	7.1
1	BA	94	G	7.1
13	BM	47	GLU	7.1
30	CD	25	THR	7.1
7	BG	137	LYS	7.1
46	CT	43	ALA	7.1
13	BM	80	LEU	7.0
36	CJ	79	LEU	7.0
1	BA	1245	C	7.0
54	DA	1077	A	7.0
23	C2	53	LYS	7.0
2	BB	12	ALA	7.0
31	CA	549	G	7.0

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Mol	Chain	Res	Type	RSRZ
50	CX	60	PHE	7.0
47	CU	15	HIS	7.0
36	CJ	73	THR	7.0
52	CZ	33	ALA	7.0
31	CA	2127	G	7.0
9	AI	20	PHE	7.0
14	BN	30	ILE	7.0
33	CF	136	ILE	7.0
47	CU	47	VAL	7.0
47	CU	85	VAL	7.0
9	BI	71	GLY	7.0
48	CV	77	THR	7.0
30	CD	10	GLY	7.0
33	CF	28	VAL	6.9
1	BA	213	G	6.9
39	CM	20	GLY	6.9
24	C3	30	VAL	6.9
31	CA	1049	C	6.9
36	CJ	97	LYS	6.9
9	BI	32	GLN	6.9
19	BS	69	HIS	6.9
10	BJ	10	LEU	6.9
1	BA	80	A	6.9
13	BM	79	ARG	6.9
19	BS	6	LYS	6.9
10	BJ	35	GLN	6.9
1	BA	203	G	6.9
7	BG	5	ARG	6.9
42	CP	62	LEU	6.9
7	BG	75	VAL	6.9
51	CY	78	TYR	6.9
36	CJ	70	VAL	6.9
39	CM	89	VAL	6.9
1	BA	1271	A	6.9
13	BM	54	ASP	6.9
33	CF	121	SER	6.9
1	BA	1241	G	6.9
14	AN	31	ILE	6.9
43	CQ	110	ILE	6.9
36	DJ	103	ARG	6.8
35	DH	137	GLU	6.8
1	BA	1021	A	6.8

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Mol	Chain	Res	Type	RSRZ
9	BI	125	PRO	6.8
31	CA	331	C	6.8
52	CZ	49	ASP	6.8
33	CF	112	ARG	6.8
36	DJ	117	MET	6.8
34	CG	174	ALA	6.8
34	CG	148	LEU	6.8
31	CA	103	A	6.8
36	CJ	41	ALA	6.8
53	DI	134	GLU	6.8
50	CX	52	GLY	6.8
14	BN	32	SER	6.8
32	CE	55	SER	6.8
23	C2	15	ALA	6.8
44	CR	118	ALA	6.8
31	CA	355	U	6.8
10	BJ	25	ILE	6.8
31	CA	1046	A	6.8
35	CH	11	ASN	6.8
1	BA	989	U	6.8
7	BG	151	PHE	6.8
33	CF	135	GLN	6.8
35	CH	74	ALA	6.8
14	BN	20	TYR	6.8
47	CU	59	ASN	6.8
52	CZ	17	GLU	6.8
45	CS	28	ALA	6.8
36	DJ	116	ASP	6.8
13	BM	109	ARG	6.7
19	BS	21	LYS	6.7
1	BA	1022	A	6.7
45	CS	36	ALA	6.7
23	C2	44	ARG	6.7
43	CQ	111	LYS	6.7
31	CA	878	A	6.7
9	AI	129	LYS	6.7
19	BS	30	PRO	6.7
13	BM	85	CYS	6.7
41	CO	119	SER	6.7
33	CF	80	ARG	6.7
30	CD	4	LEU	6.7
32	CE	164	LEU	6.7

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Mol	Chain	Res	Type	RSRZ
33	CF	60	ILE	6.7
2	BB	187	VAL	6.7
9	AI	19	VAL	6.7
13	BM	65	VAL	6.7
34	CG	169	VAL	6.7
16	BP	41	PRO	6.6
32	CE	172	ALA	6.6
46	CT	84	ARG	6.6
1	BA	959	A	6.6
1	BA	82	G	6.6
14	BN	2	ALA	6.6
31	CA	267	C	6.6
17	BQ	70	THR	6.6
52	CZ	47	ARG	6.6
7	BG	54	SER	6.6
1	BA	1219	A	6.6
9	AI	88	MET	6.6
1	BA	202	G	6.6
33	CF	102	ARG	6.6
7	BG	15	ASP	6.6
13	BM	77	ILE	6.6
10	BJ	11	LYS	6.6
32	CE	131	THR	6.6
43	CQ	12	GLN	6.6
13	BM	35	ALA	6.6
16	BP	57	ILE	6.6
14	BN	37	SER	6.6
33	CF	34	ILE	6.6
13	BM	61	ALA	6.6
34	CG	104	ASN	6.6
48	CV	81	ASP	6.6
45	CS	20	VAL	6.6
34	CG	45	HIS	6.6
9	BI	41	ARG	6.6
29	CC	233	GLY	6.5
48	CV	32	GLY	6.5
7	BG	129	GLU	6.5
27	C0	2	ALA	6.5
31	CA	1077	A	6.5
35	CH	136	SER	6.5
32	CE	140	ASP	6.5
9	BI	129	LYS	6.5

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Mol	Chain	Res	Type	RSRZ
14	BN	45	VAL	6.5
36	DJ	33	VAL	6.5
31	CA	318	C	6.5
36	CJ	81	LYS	6.5
7	BG	144	MET	6.5
31	CA	1084	A	6.5
39	CM	120	VAL	6.5
50	CX	25	ARG	6.5
1	BA	1275	A	6.5
19	BS	71	LEU	6.5
23	C2	49	TYR	6.5
24	C3	32	ALA	6.5
10	BJ	99	GLN	6.5
31	CA	1064	C	6.5
48	CV	39	ILE	6.5
7	BG	73	VAL	6.5
54	DA	2176	A	6.5
7	BG	65	ALA	6.5
23	C2	52	ALA	6.5
27	C0	43	ALA	6.5
36	DJ	97	LYS	6.5
31	CA	2797	U	6.5
1	BA	844	G	6.5
7	BG	134	ALA	6.5
10	BJ	27	GLU	6.5
31	CA	877	A	6.4
31	CA	1048	A	6.4
31	CA	183	C	6.4
32	CE	127	GLU	6.4
34	CG	167	GLU	6.4
48	CV	35	ILE	6.4
10	BJ	39	PRO	6.4
31	CA	1536	C	6.4
7	BG	71	PRO	6.4
13	BM	25	VAL	6.4
46	CT	82	MET	6.4
47	CU	37	ASP	6.4
1	BA	1314	C	6.4
10	AJ	35	GLN	6.4
33	CF	116	GLY	6.4
35	CH	72	ILE	6.4
54	DA	2132	U	6.4

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Mol	Chain	Res	Type	RSRZ
31	CA	1087	G	6.4
33	CF	23	ASN	6.4
43	CQ	91	ALA	6.4
9	BI	14	SER	6.4
35	CH	107	GLY	6.4
36	DJ	95	LYS	6.4
33	CF	95	ARG	6.4
12	BL	124	ALA	6.4
22	C1	35	GLY	6.4
31	CA	1202	G	6.4
9	BI	90	TYR	6.4
33	CF	25	VAL	6.4
36	DJ	106	LEU	6.4
31	CA	931	U	6.4
31	CA	356	G	6.4
36	DJ	68	THR	6.4
2	BB	37	LYS	6.4
3	BC	197	GLY	6.4
44	CR	106	PHE	6.4
8	BH	2	SER	6.4
14	BN	28	LYS	6.4
54	DA	2109	U	6.4
31	CA	892	A	6.3
31	CA	12	U	6.3
31	CA	289	G	6.3
36	CJ	52	GLY	6.3
2	BB	131	LYS	6.3
32	CE	142	ALA	6.3
30	CD	97	SER	6.3
45	CS	58	VAL	6.3
7	BG	48	GLU	6.3
42	CP	104	GLN	6.3
31	CA	1238	G	6.3
31	CA	1407	G	6.3
48	CV	52	LEU	6.3
25	C4	43	HIS	6.3
31	CA	1086	A	6.3
33	CF	175	PHE	6.3
54	DA	2126	A	6.3
48	CV	42	VAL	6.3
10	BJ	21	ALA	6.3
47	CU	83	ALA	6.3

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Mol	Chain	Res	Type	RSRZ
13	AM	33	ILE	6.3
23	C2	43	VAL	6.3
50	CX	34	GLY	6.3
9	BI	37	GLN	6.3
42	CP	38	GLN	6.3
1	AA	87	C	6.3
37	CK	97	PRO	6.3
34	CG	30	ASN	6.3
31	CA	1093	G	6.3
32	CE	11	ALA	6.3
14	BN	53	ARG	6.2
42	CP	30	ARG	6.2
32	CE	138	LEU	6.2
9	BI	43	THR	6.2
31	CA	2128	G	6.2
45	CS	61	ALA	6.2
9	BI	18	ARG	6.2
54	DA	2141	G	6.2
32	CE	124	PHE	6.2
13	AM	30	SER	6.2
41	CO	28	LEU	6.2
47	CU	10	VAL	6.2
26	C5	32	LYS	6.2
31	CA	1075	C	6.2
32	CE	24	ASN	6.2
10	BJ	37	ARG	6.2
13	BM	62	LYS	6.2
54	DA	2123	G	6.2
54	DA	2147	A	6.2
7	BG	39	ALA	6.2
9	AI	17	ALA	6.2
13	BM	9	ILE	6.2
33	CF	67	ILE	6.2
49	CW	29	ILE	6.2
42	CP	32	PRO	6.2
1	BA	1050	G	6.2
3	BC	71	ALA	6.2
31	CA	846	U	6.2
53	DI	136	ILE	6.2
10	BJ	89	ARG	6.1
44	CR	29	SER	6.1
30	CD	74	GLU	6.1

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Mol	Chain	Res	Type	RSRZ
41	CO	120	GLU	6.1
32	CE	8	ALA	6.1
45	CS	22	LEU	6.1
3	BC	79	LYS	6.1
36	CJ	30	GLN	6.1
8	AH	2	SER	6.1
1	BA	85	U	6.1
31	CA	546	U	6.1
31	CA	1870	C	6.1
49	CW	27	PRO	6.1
45	CS	31	GLU	6.1
10	BJ	9	ARG	6.1
25	C4	41	LYS	6.1
14	BN	24	ARG	6.1
23	C2	18	GLY	6.1
1	BA	1321	U	6.1
53	DI	104	ALA	6.1
31	CA	101	A	6.1
31	CA	1083	U	6.1
31	CA	896	A	6.1
31	CA	180	G	6.1
31	CA	1105	U	6.1
13	BM	17	ILE	6.1
32	CE	193	VAL	6.1
1	BA	987	G	6.1
7	BG	66	LEU	6.1
41	CO	63	ARG	6.1
34	CG	175	LYS	6.1
36	DJ	100	LYS	6.1
1	BA	1049	U	6.1
35	DH	63	ALA	6.1
47	CU	58	VAL	6.1
10	BJ	82	LYS	6.0
20	BT	46	ALA	6.0
36	DJ	11	LEU	6.0
36	CJ	135	SER	6.0
36	DJ	21	SER	6.0
48	CV	98	SER	6.0
31	CA	548	G	6.0
13	BM	28	THR	6.0
14	BN	16	LEU	6.0
31	CA	885	C	6.0

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Mol	Chain	Res	Type	RSRZ
53	DI	38	MET	6.0
2	BB	32	PHE	6.0
36	CJ	29	GLY	6.0
48	CV	95	PHE	6.0
31	CA	330	A	6.0
1	BA	1305	G	6.0
54	DA	2115	G	6.0
14	BN	46	LEU	6.0
31	CA	228	C	6.0
34	CG	82	GLY	6.0
9	BI	122	ARG	6.0
33	CF	32	GLU	6.0
31	CA	1872	A	6.0
47	CU	8	LEU	6.0
32	CE	23	PHE	6.0
36	CJ	32	GLY	6.0
10	AJ	74	VAL	6.0
34	CG	86	LYS	6.0
36	DJ	27	ALA	6.0
2	BB	40	ILE	6.0
22	C1	57	LYS	6.0
49	CW	57	TYR	6.0
34	CG	27	LYS	6.0
13	BM	11	ASP	6.0
52	CZ	14	LEU	6.0
31	CA	74	A	6.0
20	BT	79	LEU	6.0
30	CD	201	LEU	6.0
42	CP	107	ALA	6.0
43	CQ	9	GLU	6.0
19	BS	28	LYS	5.9
1	BA	210	C	5.9
42	CP	117	PHE	5.9
32	CE	88	ARG	5.9
13	BM	104	THR	5.9
2	AB	135	LEU	5.9
31	CA	1547	C	5.9
34	CG	83	PHE	5.9
10	BJ	71	LEU	5.9
48	CV	76	ALA	5.9
16	BP	20	VAL	5.9
3	BC	43	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
48	CV	3	ALA	5.9
48	CV	6	ARG	5.9
2	BB	201	PRO	5.9
2	AB	42	ASN	5.9
42	CP	99	TYR	5.9
38	CL	110	GLU	5.9
31	CA	2108	A	5.9
7	BG	132	GLY	5.9
1	BA	79	G	5.9
31	CA	1107	G	5.9
2	AB	136	MET	5.9
13	BM	58	ASP	5.9
19	BS	72	GLY	5.9
50	CX	57	HIS	5.9
50	CX	59	LEU	5.9
31	CA	1174	U	5.9
36	DJ	127	ARG	5.9
7	BG	112	GLY	5.9
33	CF	92	ARG	5.8
16	BP	60	TRP	5.8
14	AN	23	LYS	5.8
35	DH	66	ASN	5.8
54	DA	2146	C	5.8
28	CB	24	G	5.8
3	BC	195	VAL	5.8
31	CA	2118	U	5.8
45	CS	14	VAL	5.8
11	AK	82	LEU	5.8
13	BM	81	MET	5.8
10	BJ	94	ALA	5.8
13	BM	36	ALA	5.8
39	CM	77	ILE	5.8
34	CG	17	VAL	5.8
19	BS	68	GLY	5.8
34	CG	108	GLY	5.8
14	BN	61	ARG	5.8
42	CP	65	THR	5.8
31	CA	1076	C	5.8
31	CA	1213	A	5.8
44	CR	37	GLN	5.8
3	BC	156	ARG	5.8
36	CJ	95	LYS	5.8

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Mol	Chain	Res	Type	RSRZ
35	CH	110	VAL	5.8
32	CE	89	PRO	5.8
31	CA	2665	A	5.8
54	DA	1067	A	5.8
1	BA	1244	G	5.8
10	BJ	12	ALA	5.8
22	C1	6	ASN	5.8
9	BI	124	ARG	5.8
10	BJ	33	GLY	5.8
24	C3	18	PHE	5.8
31	CA	268	C	5.8
50	CX	83	GLU	5.7
19	BS	80	TYR	5.7
36	CJ	34	ASN	5.7
7	BG	69	VAL	5.7
31	CA	2168	G	5.7
32	CE	28	VAL	5.7
42	CP	61	GLN	5.7
1	BA	948	C	5.7
35	CH	140	ALA	5.7
25	C4	64	TYR	5.7
54	DA	2165	C	5.7
2	AB	6	MET	5.7
42	CP	106	LEU	5.7
53	DI	124	ASP	5.7
33	CF	126	GLY	5.7
36	CJ	133	ALA	5.7
2	AB	14	VAL	5.7
9	BI	81	HIS	5.7
42	CP	67	ASN	5.7
31	CA	2891	U	5.7
52	CZ	24	GLU	5.7
42	CP	115	LEU	5.7
7	BG	45	SER	5.7
34	CG	121	ILE	5.7
31	CA	1047	G	5.7
31	CA	1215	G	5.7
22	C1	27	SER	5.7
36	DJ	132	THR	5.7
7	BG	109	ARG	5.7
9	BI	48	VAL	5.7
13	BM	34	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
31	CA	2802	G	5.7
36	DJ	92	LYS	5.7
33	CF	41	GLY	5.7
36	DJ	93	PRO	5.7
2	BB	35	ARG	5.7
24	C3	34	ARG	5.7
31	CA	2161	C	5.7
45	CS	54	VAL	5.7
48	CV	21	LYS	5.7
10	BJ	92	LEU	5.7
3	BC	196	ILE	5.6
34	CG	54	PRO	5.7
49	CW	6	ALA	5.6
33	CF	12	VAL	5.6
19	BS	3	ARG	5.6
42	CP	66	GLY	5.6
52	CZ	59	GLU	5.6
14	BN	9	ARG	5.6
52	CZ	22	LEU	5.6
53	DI	84	TYR	5.6
10	AJ	6	ILE	5.6
31	CA	214	G	5.6
31	CA	2693	G	5.6
31	CA	2119	A	5.6
32	CE	54	GLY	5.6
36	DJ	15	ALA	5.6
1	BA	1240	U	5.6
31	CA	81	G	5.6
20	BT	47	ALA	5.6
47	CU	24	MET	5.6
23	C2	23	THR	5.6
47	CU	71	GLY	5.6
22	C1	55	ILE	5.6
42	CP	87	ILE	5.6
10	BJ	34	ALA	5.6
35	DH	87	GLU	5.6
13	AM	43	VAL	5.6
34	CG	31	GLY	5.6
49	CW	67	GLY	5.6
35	DH	70	GLU	5.6
47	CU	16	VAL	5.6
45	CS	55	ASP	5.6

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Mol	Chain	Res	Type	RSRZ
48	CV	5	ILE	5.6
42	CP	41	ALA	5.6
31	CA	2116	G	5.6
1	BA	81	A	5.6
45	CS	88	GLY	5.6
17	BQ	21	ILE	5.6
33	CF	141	ILE	5.6
37	CK	93	ILE	5.6
17	BQ	78	VAL	5.5
33	CF	26	MET	5.5
1	BA	1029	U	5.5
54	DA	1065	U	5.5
9	BI	64	TYR	5.5
34	CG	112	PRO	5.5
36	DJ	38	PHE	5.5
36	CJ	119	GLY	5.5
48	CV	28	VAL	5.5
47	CU	42	GLU	5.5
3	BC	126	ARG	5.5
50	CX	61	ALA	5.5
50	CX	68	LYS	5.5
7	BG	46	ALA	5.5
23	C2	31	PRO	5.5
26	C5	1	MET	5.5
13	BM	51	GLY	5.5
33	CF	43	ALA	5.5
31	CA	312	G	5.5
1	BA	207	C	5.5
34	CG	106	SER	5.5
19	BS	27	ASP	5.5
7	BG	150	ALA	5.5
17	BQ	63	GLU	5.5
31	CA	2170	A	5.5
1	BA	1276	G	5.5
13	BM	3	ARG	5.5
17	BQ	50	ASN	5.5
31	CA	1106	G	5.5
42	CP	52	SER	5.5
1	BA	1217	C	5.5
3	BC	103	ILE	5.5
50	CX	38	VAL	5.5
1	BA	1247	U	5.5

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Mol	Chain	Res	Type	RSRZ
16	BP	42	ILE	5.5
54	DA	2167	U	5.5
14	BN	10	GLU	5.5
46	CT	94	ASP	5.5
47	CU	61	LEU	5.5
36	CJ	125	MET	5.5
36	DJ	17	MET	5.5
50	CX	62	LYS	5.5
10	BJ	81	GLU	5.5
31	CA	895	U	5.5
13	BM	67	GLY	5.5
33	CF	99	PHE	5.5
29	CC	234	GLY	5.4
44	CR	90	ILE	5.4
32	CE	183	PHE	5.4
36	DJ	77	ALA	5.4
34	CG	151	TYR	5.4
34	CG	92	VAL	5.4
31	CA	85	G	5.4
29	CC	241	GLY	5.4
34	CG	25	THR	5.4
16	BP	16	PHE	5.4
39	CM	142	ILE	5.4
39	CM	115	GLU	5.4
1	BA	1004	A	5.4
13	BM	70	ARG	5.4
15	BO	89	ARG	5.4
44	CR	33	ARG	5.4
11	AK	19	GLY	5.4
24	C3	43	THR	5.4
34	CG	81	GLU	5.4
36	CJ	124	ALA	5.4
42	CP	33	ARG	5.4
44	CR	26	GLY	5.4
44	CR	73	GLY	5.4
50	CX	42	GLY	5.4
34	CG	7	ALA	5.4
41	CO	118	ARG	5.4
31	CA	1444	G	5.4
48	CV	49	VAL	5.4
9	BI	117	GLY	5.4
27	C0	7	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
31	CA	501	A	5.4
45	CS	101	ILE	5.4
54	DA	2166	U	5.4
7	BG	53	ARG	5.4
9	AI	55	VAL	5.4
50	CX	23	VAL	5.4
31	CA	88	G	5.4
9	BI	21	ILE	5.4
9	AI	90	TYR	5.4
20	BT	72	ALA	5.4
36	DJ	43	ASN	5.4
32	CE	147	LEU	5.3
34	CG	56	ASP	5.3
19	BS	75	ALA	5.3
19	BS	77	THR	5.3
33	CF	55	ALA	5.3
13	BM	74	SER	5.3
49	CW	1	MET	5.3
32	CE	43	THR	5.3
47	CU	56	GLU	5.3
17	BQ	17	MET	5.3
25	C4	2	PRO	5.3
31	CA	1061	U	5.3
52	CZ	44	LYS	5.3
1	BA	1027	C	5.3
3	BC	198	VAL	5.3
36	CJ	19	ASN	5.3
9	BI	30	ILE	5.3
14	BN	55	SER	5.3
49	CW	89	ILE	5.3
33	CF	36	LEU	5.3
54	DA	2178	C	5.3
31	CA	2123	G	5.3
33	CF	68	THR	5.3
2	AB	49	MET	5.3
31	CA	1085	A	5.3
41	CO	24	MET	5.3
14	BN	40	ASP	5.3
7	BG	103	TRP	5.3
1	BA	1018	G	5.3
1	BA	1270	G	5.3
47	CU	1	MET	5.3

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Mol	Chain	Res	Type	RSRZ
42	CP	25	ARG	5.3
50	CX	55	ARG	5.3
34	CG	166	ASP	5.3
46	CT	97	LEU	5.3
7	BG	91	VAL	5.3
33	CF	74	VAL	5.3
31	CA	316	C	5.3
13	BM	98	ARG	5.3
31	CA	1078	U	5.3
48	CV	60	GLU	5.3
1	AA	81	A	5.3
39	CM	28	GLY	5.3
42	CP	108	ASP	5.3
50	CX	32	LEU	5.3
9	BI	11	ARG	5.2
20	BT	36	TYR	5.2
47	DU	1	MET	5.2
24	C3	7	PRO	5.2
32	CE	118	LEU	5.2
32	CE	37	ALA	5.2
9	BI	7	TYR	5.2
31	CA	2162	G	5.2
33	CF	114	PHE	5.2
9	AI	5	GLN	5.2
34	CG	161	GLY	5.2
10	BJ	86	ALA	5.2
36	DJ	40	LYS	5.2
31	CA	308	G	5.2
31	CA	2120	G	5.2
52	CZ	35	GLY	5.2
39	CM	107	PHE	5.2
16	BP	9	HIS	5.2
37	CK	136	GLN	5.2
2	BB	33	GLY	5.2
13	BM	66	GLU	5.2
19	AS	49	ILE	5.2
2	BB	14	VAL	5.2
13	BM	60	VAL	5.2
31	CA	2803	G	5.2
36	DJ	81	LYS	5.2
32	CE	90	GLN	5.2
42	CP	26	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
14	BN	18	ASP	5.2
53	DI	135	ALA	5.2
54	DA	884	U	5.2
31	CA	1044	C	5.2
31	CA	1873	G	5.2
30	CD	186	LEU	5.2
1	BA	982	U	5.2
41	CO	29	VAL	5.2
42	CP	105	ALA	5.2
46	CT	98	LYS	5.2
31	CA	1045	C	5.2
31	CA	1104	C	5.2
30	CD	1	MET	5.2
41	CO	62	ASN	5.2
13	BM	90	ARG	5.2
14	BN	41	ARG	5.2
36	DJ	83	ALA	5.2
40	CN	72	PRO	5.2
7	BG	38	THR	5.1
31	CA	44	A	5.1
33	CF	137	ILE	5.1
9	BI	92	GLU	5.1
34	CG	117	LEU	5.1
40	CN	41	LEU	5.1
29	CC	30	PHE	5.1
31	CA	1406	U	5.1
36	DJ	14	ALA	5.1
42	CP	59	ALA	5.1
7	BG	82	GLY	5.1
37	CK	22	GLY	5.1
10	BJ	40	ILE	5.1
36	CJ	92	LYS	5.1
37	CK	142	ILE	5.1
28	CB	37	C	5.1
31	CA	2173	A	5.1
1	AA	85	U	5.1
31	CA	879	G	5.1
31	CA	2305	U	5.1
36	CJ	101	ILE	5.1
44	CR	98	ILE	5.1
51	CY	35	SER	5.1
9	AI	6	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
54	DA	1847	A	5.1
7	BG	148	ASN	5.1
17	BQ	73	TRP	5.1
30	CD	43	ASP	5.1
33	CF	77	PHE	5.1
34	CG	75	MET	5.1
37	CK	119	PHE	5.1
1	AA	1026	G	5.1
1	BA	1034	G	5.1
43	DQ	2	SER	5.1
34	CG	44	LYS	5.1
39	CM	45	GLY	5.1
15	AO	17	ARG	5.1
31	CA	45	G	5.1
49	CW	34	LYS	5.1
1	BA	90	C	5.1
23	C2	39	PHE	5.1
20	BT	60	ARG	5.1
31	CA	476	G	5.1
34	CG	51	THR	5.1
52	CZ	36	GLN	5.1
13	BM	69	LEU	5.1
51	CY	3	ARG	5.1
7	BG	141	VAL	5.1
20	BT	64	LYS	5.1
13	AM	115	PRO	5.1
13	AM	48	LEU	5.1
31	CA	344	A	5.1
39	CM	3	LEU	5.1
25	C4	40	ARG	5.1
32	CE	64	GLY	5.1
39	CM	84	LYS	5.1
9	AI	128	SER	5.1
13	BM	21	SER	5.1
31	CA	2300	C	5.1
13	AM	56	LEU	5.0
13	BM	50	GLU	5.0
29	CC	48	ARG	5.0
44	CR	6	ARG	5.0
44	CR	30	ARG	5.0
1	BA	1019	A	5.0
31	CA	626	A	5.0

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Mol	Chain	Res	Type	RSRZ
10	BJ	23	ALA	5.0
46	CT	101	SER	5.0
1	BA	1303	C	5.0
1	BA	1304	G	5.0
7	AG	53	ARG	5.0
31	CA	2107	G	5.0
31	CA	2121	G	5.0
47	CU	36	LYS	5.0
19	BS	34	TRP	5.0
31	CA	2171	A	5.0
33	CF	149	VAL	5.0
34	CG	63	ALA	5.0
42	CP	109	ALA	5.0
34	CG	58	TYR	5.0
10	AJ	76	ILE	5.0
7	AG	50	LEU	5.0
42	CP	49	VAL	5.0
1	BA	1201	A	5.0
39	CM	117	THR	5.0
10	BJ	93	ALA	5.0
34	CG	24	ILE	5.0
33	CF	56	ASP	5.0
36	CJ	35	ILE	5.0
13	AM	19	LEU	5.0
14	BN	51	LEU	5.0
20	BT	76	LYS	5.0
33	CF	122	PHE	5.0
17	BQ	53	CYS	5.0
6	AF	61	LEU	5.0
52	CZ	6	LEU	5.0
35	CH	130	VAL	5.0
45	CS	38	VAL	5.0
2	BB	213	TYR	5.0
7	BG	18	PHE	5.0
7	BG	58	GLU	5.0
1	BA	78	A	5.0
31	CA	1100	C	5.0
47	CU	46	ALA	5.0
33	DF	80	ARG	5.0
13	BM	84	GLY	4.9
36	DJ	42	PHE	4.9
13	BM	43	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
31	CA	309	A	4.9
41	CO	116	VAL	4.9
1	BA	63	C	4.9
24	C3	27	GLY	4.9
19	BS	43	ASN	4.9
13	BM	75	MET	4.9
31	CA	2667	C	4.9
33	CF	91	LEU	4.9
32	CE	4	VAL	4.9
33	CF	37	ASN	4.9
33	CF	172	ALA	4.9
31	CA	1169	A	4.9
33	CF	170	LEU	4.9
1	BA	68	G	4.9
7	BG	9	GLN	4.9
9	BI	91	ASP	4.9
14	BN	42	TRP	4.9
42	CP	69	ASP	4.9
3	BC	155	GLY	4.9
31	CA	280	U	4.9
31	CA	2860	A	4.9
34	CG	162	VAL	4.9
48	CV	30	SER	4.9
34	CG	78	GLY	4.9
30	CD	154	LYS	4.9
30	CD	132	ALA	4.9
2	BB	21	ARG	4.9
2	AB	9	MET	4.9
9	BI	20	PHE	4.9
19	BS	10	PHE	4.9
3	BC	206	GLU	4.9
14	BN	39	GLU	4.9
32	CE	122	GLU	4.9
20	BT	24	ARG	4.9
16	AP	4	ILE	4.9
31	CA	1534	U	4.9
39	CM	70	LYS	4.9
2	AB	46	THR	4.9
27	C0	8	THR	4.9
7	BG	87	VAL	4.9
10	BJ	96	VAL	4.9
31	CA	876	C	4.9

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Mol	Chain	Res	Type	RSRZ
35	CH	108	VAL	4.9
47	CU	34	VAL	4.9
31	CA	2169	A	4.9
36	CJ	25	GLY	4.9
36	CJ	116	ASP	4.9
47	CU	21	SER	4.9
1	BA	954	G	4.9
1	BA	1253	G	4.9
3	BC	107	ARG	4.8
19	BS	55	ARG	4.8
33	CF	71	ARG	4.8
20	BT	38	ALA	4.8
39	CM	108	ALA	4.8
32	CE	157	LEU	4.8
10	BJ	24	GLU	4.8
23	C2	29	THR	4.8
30	CD	38	LYS	4.8
35	CH	77	THR	4.8
34	CG	9	VAL	4.8
2	BB	123	ASP	4.8
22	C1	36	GLU	4.8
44	CR	74	ILE	4.8
13	BM	108	THR	4.8
31	CA	2124	G	4.8
36	CJ	91	GLY	4.8
2	BB	39	HIS	4.8
13	BM	68	ASP	4.8
35	DH	56	ALA	4.8
40	CN	79	ALA	4.8
41	CO	79	LEU	4.8
2	AB	37	LYS	4.8
38	CL	111	LYS	4.8
26	C5	25	VAL	4.8
6	BF	39	LEU	4.8
10	AJ	73	LEU	4.8
18	AR	23	TYR	4.8
27	C0	34	HIS	4.8
36	CJ	100	LYS	4.8
30	CD	9	VAL	4.8
32	CE	186	VAL	4.8
48	CV	83	VAL	4.8
33	CF	174	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
39	CM	113	ALA	4.8
39	CM	138	ALA	4.8
7	BG	79	ARG	4.8
51	CY	49	LEU	4.8
1	BA	1033	G	4.8
3	BC	106	VAL	4.8
9	AI	104	VAL	4.8
16	BP	80	LYS	4.8
25	C4	35	LYS	4.8
38	CL	48	PRO	4.8
13	BM	14	HIS	4.8
27	C0	9	GLN	4.8
39	CM	35	HIS	4.8
31	CA	475	C	4.8
31	CA	893	C	4.8
36	CJ	16	GLY	4.8
34	CG	10	VAL	4.8
53	DI	27	VAL	4.8
33	CF	111	ILE	4.8
45	CS	98	ILE	4.8
1	BA	4	U	4.8
31	CA	369	U	4.8
51	CY	34	HIS	4.8
13	AM	44	LYS	4.8
22	C1	15	MET	4.8
32	CE	10	SER	4.8
54	DA	1062	G	4.8
20	BT	63	ALA	4.8
27	C0	53	PHE	4.8
35	CH	15	LEU	4.8
53	DI	72	LEU	4.8
1	BA	325	A	4.8
14	BN	68	GLY	4.7
31	CA	1167	C	4.7
46	CT	47	VAL	4.7
16	BP	53	ASP	4.7
30	CD	56	LYS	4.7
37	CK	55	ILE	4.7
39	CM	4	ASN	4.7
22	C1	18	SER	4.7
7	AG	7	ILE	4.7
42	CP	46	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
43	CQ	27	GLU	4.7
33	CF	158	THR	4.7
34	CG	132	VAL	4.7
45	CS	33	VAL	4.7
19	BS	22	ALA	4.7
35	DH	105	ALA	4.7
31	CA	882	G	4.7
34	CG	6	LYS	4.7
3	BC	91	VAL	4.7
45	CS	25	LEU	4.7
45	CS	62	GLU	4.7
34	CG	160	LYS	4.7
23	C2	12	VAL	4.7
31	CA	117	G	4.7
31	CA	1214	A	4.7
9	AI	22	LYS	4.7
10	BJ	97	ASP	4.7
2	BB	80	VAL	4.7
33	CF	177	PHE	4.7
14	BN	48	LEU	4.7
20	BT	34	LYS	4.7
35	DH	67	ALA	4.7
36	CJ	15	ALA	4.7
31	CA	213	A	4.7
45	CS	26	ASP	4.7
53	DI	133	GLU	4.7
53	DI	106	PHE	4.7
36	DJ	73	THR	4.7
35	DH	86	ASP	4.7
36	DJ	86	ILE	4.7
3	BC	159	GLY	4.7
46	CT	99	ARG	4.7
7	BG	47	LEU	4.7
36	CJ	131	GLY	4.7
19	BS	81	ARG	4.7
33	CF	38	MET	4.6
3	BC	124	LEU	4.6
36	CJ	118	THR	4.6
36	CJ	26	PRO	4.6
31	CA	1606	C	4.6
32	DE	7	ASP	4.6
35	DH	77	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	AA	88	U	4.6
3	BC	119	SER	4.6
9	BI	123	ARG	4.6
39	CM	126	ARG	4.6
29	CC	47	GLY	4.6
31	CA	345	A	4.6
31	CA	1074	G	4.6
31	CA	596	U	4.6
30	CD	6	GLY	4.6
13	AM	5	ALA	4.6
32	CE	36	ALA	4.6
36	DJ	110	ALA	4.6
44	DR	118	ALA	4.6
48	CV	63	ALA	4.6
36	CJ	64	ASP	4.6
31	CA	317	G	4.6
30	CD	55	LYS	4.6
36	DJ	113	LYS	4.6
7	BG	37	SER	4.6
39	CM	90	VAL	4.6
22	C1	21	ALA	4.6
1	BA	1441	A	4.6
31	CA	1090	A	4.6
2	AB	221	VAL	4.6
7	AG	6	VAL	4.6
13	BM	16	VAL	4.6
32	CE	144	GLU	4.6
33	CF	42	GLU	4.6
42	CP	20	GLU	4.6
13	AM	39	ILE	4.6
13	BM	37	ALA	4.6
20	BT	45	ALA	4.6
20	BT	85	LYS	4.6
25	C4	37	ALA	4.6
27	C0	48	ILE	4.6
31	CA	2164	C	4.6
35	CH	143	ILE	4.6
7	AG	5	ARG	4.6
35	CH	109	GLU	4.6
43	CQ	3	ASN	4.6
50	CX	85	GLU	4.6
27	C0	29	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
54	DA	1068	G	4.6
7	BG	35	LYS	4.6
47	CU	74	ILE	4.6
1	BA	962	C	4.6
30	CD	59	ARG	4.6
31	CA	2150	C	4.6
29	CC	245	VAL	4.6
33	CF	4	LEU	4.6
20	BT	73	ALA	4.6
22	C1	11	SER	4.6
30	CD	41	ALA	4.6
35	DH	74	ALA	4.6
32	CE	7	ASP	4.6
31	CA	281	C	4.6
7	AG	58	GLU	4.6
7	AG	62	PHE	4.6
49	CW	69	GLU	4.6
20	BT	82	GLN	4.6
10	AJ	42	LEU	4.5
45	CS	51	VAL	4.5
9	AI	127	PHE	4.5
46	CT	6	LYS	4.5
13	BM	38	GLY	4.5
10	BJ	36	VAL	4.5
33	CF	133	ARG	4.5
41	CO	83	LEU	4.5
43	CQ	86	VAL	4.5
10	BJ	28	THR	4.5
54	DA	2117	A	4.5
10	BJ	85	ASP	4.5
32	CE	154	ASP	4.5
1	BA	1023	U	4.5
13	BM	57	ARG	4.5
24	C3	17	GLY	4.5
31	CA	1216	G	4.5
31	CA	1868	C	4.5
31	CA	2801	G	4.5
34	CG	69	ARG	4.5
14	AN	25	ALA	4.5
43	CQ	95	ALA	4.5
1	BA	196	A	4.5
9	AI	32	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
19	AS	56	GLN	4.5
31	CA	2106	U	4.5
1	AA	1020	G	4.5
26	C5	2	LYS	4.5
9	BI	57	MET	4.5
19	BS	40	ILE	4.5
34	CG	59	ALA	4.5
16	BP	39	PHE	4.5
30	CD	19	GLY	4.5
31	CA	2180	U	4.5
2	BB	164	ILE	4.5
31	CA	291	G	4.5
46	CT	5	ALA	4.5
54	DA	1063	G	4.5
7	AG	109	ARG	4.5
42	CP	92	PHE	4.5
14	BN	23	LYS	4.5
36	DJ	51	LYS	4.5
45	CS	60	LYS	4.5
1	BA	949	A	4.5
34	CG	76	VAL	4.5
35	CH	58	LEU	4.5
54	DA	885	C	4.5
43	CQ	31	TRP	4.5
31	CA	880	G	4.5
31	CA	1171	G	4.5
34	CG	127	THR	4.5
9	BI	15	SER	4.5
36	CJ	66	SER	4.5
33	CF	79	ILE	4.5
36	CJ	93	PRO	4.5
53	DI	118	ILE	4.5
54	DA	1064	C	4.5
30	CD	126	ASN	4.5
49	CW	43	ASP	4.5
41	CO	84	GLY	4.5
39	CM	74	THR	4.5
48	DV	52	LEU	4.5
1	BA	1306	A	4.5
33	CF	84	PRO	4.5
35	CH	133	GLN	4.5
36	CJ	137	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
48	CV	62	GLU	4.5
3	BC	76	VAL	4.5
17	BQ	83	VAL	4.5
31	CA	1530	G	4.5
2	BB	84	ALA	4.4
1	BA	1209	C	4.4
2	BB	6	MET	4.4
35	CH	47	PHE	4.4
47	CU	28	ASN	4.4
32	CE	132	LYS	4.4
40	CN	84	LYS	4.4
45	CS	78	ARG	4.4
7	BG	89	VAL	4.4
31	CA	138	U	4.4
49	CW	65	VAL	4.4
50	CX	35	SER	4.4
31	CA	1210	G	4.4
1	BA	330	C	4.4
1	BA	1317	C	4.4
31	CA	1548	A	4.4
42	CP	78	VAL	4.4
54	DA	2131	U	4.4
45	CS	18	GLN	4.4
1	BA	1005	A	4.4
1	BA	1035	A	4.4
31	CA	1043	C	4.4
49	CW	42	LEU	4.4
19	BS	42	PRO	4.4
9	BI	94	LEU	4.4
31	CA	259	G	4.4
1	BA	1236	A	4.4
26	C5	8	LYS	4.4
3	BC	53	SER	4.4
17	BQ	72	SER	4.4
48	CV	38	GLY	4.4
36	DJ	26	PRO	4.4
1	BA	842	U	4.4
1	BA	953	G	4.4
1	BA	988	G	4.4
31	CA	1052	C	4.4
36	DJ	50	GLU	4.4
1	BA	1340	A	4.4

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Mol	Chain	Res	Type	RSRZ
30	CD	166	GLY	4.4
11	BK	21	ALA	4.4
41	CO	56	LYS	4.4
18	AR	55	LEU	4.4
36	DJ	28	LEU	4.4
48	CV	27	ASN	4.4
1	BA	83	C	4.4
1	BA	981	U	4.4
54	DA	2128	G	4.4
54	DA	2119	A	4.4
10	BJ	32	THR	4.4
34	CG	99	LYS	4.4
37	CK	1	MET	4.4
7	AG	59	LEU	4.4
13	BM	101	ARG	4.4
7	AG	8	GLY	4.4
13	BM	26	GLY	4.4
31	CA	2833	U	4.4
25	C4	14	PHE	4.4
1	BA	1312	G	4.4
7	BG	77	SER	4.4
19	AS	55	ARG	4.4
31	CA	1205	A	4.4
42	CP	93	ASP	4.4
53	DI	94	ARG	4.4
7	BG	50	LEU	4.4
42	CP	27	VAL	4.4
36	DJ	49	ILE	4.4
43	CQ	34	GLU	4.3
49	CW	58	SER	4.3
50	CX	64	ASP	4.3
52	CZ	5	GLU	4.3
31	CA	2892	G	4.3
54	DA	1175	A	4.3
34	CG	41	VAL	4.3
45	CS	24	LYS	4.3
45	CS	48	LYS	4.3
47	CU	67	VAL	4.3
53	DI	101	LYS	4.3
23	C2	16	GLY	4.3
41	CO	52	ILE	4.3
7	BG	107	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
41	CO	25	ALA	4.3
2	AB	15	HIS	4.3
14	BN	6	MET	4.3
2	BB	20	THR	4.3
39	CM	30	THR	4.3
45	CS	94	THR	4.3
1	BA	212	G	4.3
32	CE	126	VAL	4.3
39	CM	130	GLY	4.3
54	DA	883	G	4.3
34	CG	48	ASN	4.3
39	CM	21	ARG	4.3
33	CF	94	GLU	4.3
41	CO	66	ALA	4.3
3	BC	111	LEU	4.3
24	C3	31	LEU	4.3
43	CQ	8	LEU	4.3
2	AB	5	SER	4.3
7	BG	57	SER	4.3
36	DJ	139	VAL	4.3
41	CO	76	VAL	4.3
1	BA	1333	A	4.3
31	CA	505	A	4.3
31	CA	2309	A	4.3
1	BA	216	U	4.3
3	BC	102	ASN	4.3
45	CS	45	GLU	4.3
13	BM	12	HIS	4.3
31	CA	1874	C	4.3
2	AB	210	VAL	4.3
40	CN	80	VAL	4.3
35	DH	94	ILE	4.3
31	CA	126	A	4.3
31	CA	1073	A	4.3
54	DA	654	A	4.3
28	CB	19	C	4.3
48	CV	86	ARG	4.3
34	CG	110	SER	4.3
47	CU	33	LYS	4.3
31	CA	1015	U	4.3
16	BP	81	ALA	4.3
31	CA	1057	A	4.3

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Mol	Chain	Res	Type	RSRZ
7	BG	55	GLY	4.3
1	BA	1273	C	4.3
32	CE	129	PRO	4.3
32	CE	178	VAL	4.3
33	CF	11	GLU	4.3
32	CE	175	ILE	4.3
33	CF	27	GLN	4.3
1	BA	121	U	4.3
1	BA	955	U	4.3
7	BG	72	THR	4.3
14	BN	7	LYS	4.3
46	CT	49	LYS	4.3
54	DA	2171	A	4.3
35	CH	13	GLY	4.3
44	CR	25	TYR	4.3
13	BM	97	VAL	4.3
15	BO	75	VAL	4.3
35	CH	142	VAL	4.3
31	CA	343	C	4.3
31	CA	1233	C	4.3
33	CF	81	GLN	4.3
13	AM	4	ILE	4.3
26	C5	12	ARG	4.3
32	CE	134	LEU	4.3
2	AB	213	TYR	4.3
31	CA	1111	A	4.3
52	CZ	11	VAL	4.3
9	BI	33	ARG	4.3
20	BT	49	LYS	4.3
14	AN	22	ALA	4.2
30	CD	188	LEU	4.2
1	BA	1363	A	4.2
36	CJ	10	LYS	4.2
13	BM	49	SER	4.2
31	CA	545	U	4.2
32	CE	190	ALA	4.2
46	CT	44	ALA	4.2
2	BB	10	LEU	4.2
35	DH	11	ASN	4.2
36	DJ	34	ASN	4.2
33	CF	138	PHE	4.2
43	CQ	13	MET	4.2

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Mol	Chain	Res	Type	RSRZ
1	BA	1281	C	4.2
19	BS	35	SER	4.2
27	C0	39	GLU	4.2
31	CA	2175	C	4.2
40	CN	116	ALA	4.2
19	BS	47	LEU	4.2
2	AB	201	PRO	4.2
3	BC	60	PRO	4.2
12	BL	70	GLU	4.2
28	CB	22	U	4.2
1	BA	174	A	4.2
1	BA	153	C	4.2
39	CM	19	LEU	4.2
13	BM	42	ASP	4.2
26	C5	20	ASP	4.2
1	BA	1331	G	4.2
31	CA	1168	G	4.2
34	CG	79	VAL	4.2
7	BG	60	GLU	4.2
3	BC	62	LYS	4.2
39	CM	75	ALA	4.2
23	C2	40	ASP	4.2
47	DU	92	ASN	4.2
19	BS	23	VAL	4.2
32	CE	32	VAL	4.2
50	CX	51	VAL	4.2
7	BG	90	GLU	4.2
31	CA	327	G	4.2
14	BN	44	ALA	4.2
1	AA	1027	C	4.2
13	AM	11	ASP	4.2
33	CF	142	ASP	4.2
44	CR	102	ASP	4.2
45	CS	7	SER	4.2
25	C4	36	LYS	4.2
48	CV	40	ASN	4.2
34	CG	35	ARG	4.2
7	BG	120	LEU	4.2
31	CA	638	G	4.2
36	CJ	115	ALA	4.2
9	BI	103	PHE	4.2
38	CL	89	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
14	BN	8	ALA	4.2
33	CF	14	LYS	4.2
52	CZ	56	LEU	4.2
14	AN	100	SER	4.2
36	CJ	39	CYS	4.2
31	CA	2165	C	4.2
47	CU	76	ARG	4.2
31	CA	241	A	4.2
27	C0	24	LEU	4.1
37	CK	94	ALA	4.1
23	C2	35	GLU	4.1
33	CF	30	ARG	4.1
31	CA	930	G	4.1
35	CH	9	VAL	4.1
42	CP	39	VAL	4.1
1	BA	1214	C	4.1
50	CX	37	ILE	4.1
31	CA	603	A	4.1
3	BC	42	TYR	4.1
7	BG	99	LEU	4.1
32	CE	200	LEU	4.1
39	CM	131	ALA	4.1
53	DI	40	GLU	4.1
21	AU	3	VAL	4.1
2	BB	186	ILE	4.1
23	C2	13	SER	4.1
53	DI	123	ILE	4.1
1	BA	108	G	4.1
31	CA	1271	G	4.1
31	CA	1875	G	4.1
3	BC	177	THR	4.1
36	CJ	110	ALA	4.1
54	DA	2106	U	4.1
48	CV	22	ARG	4.1
19	BS	70	LYS	4.1
36	CJ	128	SER	4.1
46	CT	85	ILE	4.1
11	AK	81	ASN	4.1
19	BS	36	ARG	4.1
1	BA	976	G	4.1
2	BB	129	LEU	4.1
7	BG	152	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
52	CZ	48	ARG	4.1
31	CA	1538	G	4.1
31	CA	2799	A	4.1
48	CV	11	VAL	4.1
41	CO	26	GLY	4.1
33	CF	96	MET	4.1
53	DI	88	HIS	4.1
1	BA	134	G	4.1
31	CA	2412	A	4.1
15	BO	17	ARG	4.1
32	CE	148	ILE	4.1
43	CQ	5	ILE	4.1
52	CZ	8	GLU	4.1
11	BK	55	SER	4.1
7	BG	68	ASN	4.1
30	CD	58	ASN	4.1
31	CA	884	U	4.1
32	CE	161	ALA	4.1
2	AB	16	PHE	4.1
39	CM	5	THR	4.1
48	CV	18	ASP	4.1
34	CG	113	VAL	4.1
39	CM	135	ILE	4.1
36	DJ	48	SER	4.1
42	CP	110	ALA	4.1
34	CG	129	THR	4.1
25	C4	47	LYS	4.1
35	CH	127	GLU	4.1
29	CC	249	GLY	4.1
46	CT	92	ARG	4.1
46	CT	19	LEU	4.1
2	AB	30	PHE	4.1
31	CA	2181	U	4.1
36	DJ	107	GLN	4.1
44	CR	38	ALA	4.1
53	DI	127	ALA	4.1
7	BG	102	ARG	4.1
23	C2	46	HIS	4.1
46	CT	83	LYS	4.1
31	CA	2628	C	4.1
2	BB	199	VAL	4.1
33	DF	74	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
52	CZ	21	LEU	4.1
3	BC	51	SER	4.1
31	CA	2800	A	4.1
13	BM	113	ARG	4.0
32	CE	21	ARG	4.0
42	CP	88	LYS	4.1
54	DA	1093	G	4.1
1	BA	1210	C	4.0
34	CG	109	PHE	4.0
37	CK	35	ARG	4.0
42	CP	6	ALA	4.0
7	BG	88	PRO	4.0
45	CS	52	PRO	4.0
1	BA	165	G	4.0
31	CA	1235	G	4.0
31	CA	2410	G	4.0
31	CA	1518	C	4.0
34	CG	131	ILE	4.0
36	CJ	49	ILE	4.0
50	CX	58	THR	4.0
54	DA	2161	C	4.0
3	BC	80	LYS	4.0
48	CV	47	LYS	4.0
46	CT	36	LEU	4.0
13	AM	36	ALA	4.0
36	CJ	104	ALA	4.0
13	AM	46	SER	4.0
22	C1	34	SER	4.0
33	CF	29	PRO	4.0
33	CF	22	TYR	4.0
34	CG	77	ILE	4.0
42	CP	36	TYR	4.0
49	CW	70	ILE	4.0
54	DA	2144	G	4.0
11	AK	111	THR	4.0
31	CA	1533	C	4.0
36	DJ	60	THR	4.0
34	CG	133	LEU	4.0
3	BC	50	ALA	4.0
22	C1	46	ASP	4.0
2	AB	4	VAL	4.0
24	C3	12	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
31	CA	1322	A	4.0
32	CE	101	TYR	4.0
28	CB	56	G	4.0
13	BM	52	GLN	4.0
16	BP	54	LEU	4.0
31	CA	2000	C	4.0
54	DA	277	G	4.0
11	AK	47	ALA	4.0
13	BM	15	ALA	4.0
14	BN	25	ALA	4.0
30	CD	31	ALA	4.0
46	CT	32	ALA	4.0
7	BG	110	LYS	4.0
13	AM	13	LYS	4.0
32	CE	98	LYS	4.0
16	BP	56	ARG	4.0
32	CE	67	ARG	4.0
33	CF	10	ASP	4.0
36	CJ	127	ARG	4.0
36	DJ	90	SER	4.0
48	DV	53	ASN	4.0
30	CD	180	VAL	4.0
42	CP	35	ILE	4.0
32	CE	41	GLN	4.0
35	DH	12	LEU	4.0
2	AB	32	PHE	4.0
31	CA	61	C	4.0
31	CA	1245	G	4.0
1	BA	843	U	4.0
1	BA	1224	U	4.0
45	CS	79	ARG	4.0
32	CE	75	SER	4.0
39	CM	106	GLU	4.0
42	CP	60	GLU	4.0
42	CP	97	PHE	4.0
1	BA	222	C	4.0
14	BN	72	GLY	4.0
36	DJ	124	ALA	4.0
31	CA	2877	G	4.0
39	CM	119	PRO	4.0
23	C2	30	LYS	4.0
34	CG	94	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
16	BP	58	ALA	4.0
31	CA	89	A	4.0
31	CA	357	C	4.0
54	DA	2164	C	4.0
37	CK	139	VAL	4.0
50	CX	24	LYS	4.0
31	CA	1179	G	4.0
11	AK	21	ALA	4.0
1	BA	957	U	3.9
35	CH	70	GLU	4.0
31	CA	256	A	3.9
31	CA	623	C	3.9
35	CH	134	VAL	3.9
1	BA	102	G	3.9
2	BB	89	GLN	3.9
31	CA	315	G	3.9
49	CW	91	PHE	3.9
49	CW	33	GLY	3.9
7	BG	131	LYS	3.9
7	BG	80	VAL	3.9
15	BO	12	VAL	3.9
29	CC	244	PRO	3.9
31	CA	31	C	3.9
31	CA	1098	A	3.9
7	AG	54	SER	3.9
44	CR	113	ALA	3.9
2	AB	225	ARG	3.9
5	AE	164	ILE	3.9
31	CA	2691	C	3.9
1	BA	1534	A	3.9
31	CA	1551	A	3.9
54	DA	1089	A	3.9
7	AG	18	PHE	3.9
20	BT	75	HIS	3.9
1	BA	89	U	3.9
35	CH	144	VAL	3.9
35	DH	138	VAL	3.9
44	CR	34	VAL	3.9
10	BJ	20	GLN	3.9
34	CG	67	THR	3.9
31	CA	550	C	3.9
54	DA	2145	C	3.9

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Mol	Chain	Res	Type	RSRZ
1	BA	1368	A	3.9
13	AM	8	ASN	3.9
39	CM	139	GLY	3.9
44	CR	81	ASN	3.9
10	BJ	15	HIS	3.9
3	BC	172	ARG	3.9
32	CE	201	ALA	3.9
44	CR	96	ALA	3.9
46	CT	54	ALA	3.9
31	CA	150	U	3.9
31	CA	1217	U	3.9
49	CW	46	LYS	3.9
8	BH	110	VAL	3.9
31	CA	1863	G	3.9
33	CF	139	PRO	3.9
2	BB	90	PHE	3.9
5	BE	109	GLY	3.9
17	BQ	44	LEU	3.9
25	C4	29	LEU	3.9
35	DH	96	THR	3.9
48	CV	90	GLY	3.9
52	CZ	28	LEU	3.9
3	BC	61	ALA	3.9
7	BG	108	ALA	3.9
10	BJ	16	ARG	3.9
52	CZ	25	GLN	3.9
1	AA	82	G	3.9
30	CD	46	ARG	3.9
51	CY	45	ARG	3.9
52	CZ	4	LYS	3.9
36	DJ	128	SER	3.9
39	CM	137	ALA	3.9
31	CA	1328	A	3.9
31	CA	2287	A	3.9
54	DA	892	A	3.9
9	AI	89	GLU	3.9
31	CA	1018	U	3.9
20	BT	51	PHE	3.9
27	C0	41	THR	3.9
1	BA	215	C	3.9
1	BA	1320	C	3.9
28	CB	23	G	3.9

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Mol	Chain	Res	Type	RSRZ
31	CA	307	G	3.9
31	CA	2045	C	3.9
36	DJ	104	ALA	3.9
54	DA	2122	U	3.9
1	BA	1248	A	3.9
17	BQ	46	VAL	3.9
31	CA	513	A	3.9
7	AG	79	ARG	3.9
42	CP	102	ARG	3.9
46	CT	87	PRO	3.9
29	CC	37	ASN	3.9
32	CE	87	ALA	3.9
31	CA	474	G	3.9
31	CA	2525	G	3.9
54	DA	2140	G	3.9
14	BN	63	ARG	3.8
29	CC	12	GLY	3.8
2	AB	214	LEU	3.8
21	AU	16	LEU	3.8
31	CA	1321	A	3.8
20	BT	80	THR	3.8
12	BL	108	LYS	3.8
44	CR	35	ALA	3.8
48	DV	51	ALA	3.8
31	CA	32	C	3.8
31	CA	139	U	3.8
31	CA	1203	U	3.8
34	CG	74	SER	3.8
31	CA	1056	G	3.8
2	AB	10	LEU	3.8
2	BB	182	PRO	3.8
31	CA	477	A	3.8
7	AG	56	LYS	3.8
9	BI	9	THR	3.8
35	CH	67	ALA	3.8
10	AJ	75	ASP	3.8
12	BL	117	TYR	3.8
16	AP	17	TYR	3.8
17	BQ	54	GLY	3.8
31	CA	1108	U	3.8
43	CQ	35	GLY	3.8
45	CS	87	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
33	DF	83	TYR	3.8
48	CV	93	VAL	3.8
16	BP	38	PHE	3.8
17	BQ	8	LEU	3.8
31	CA	551	G	3.8
31	CA	805	G	3.8
42	CP	76	LYS	3.8
1	BA	977	A	3.8
13	AM	32	ALA	3.8
39	CM	71	ALA	3.8
3	BC	2	GLY	3.8
31	CA	1172	C	3.8
32	CE	165	HIS	3.8
38	CL	15	GLY	3.8
47	CU	80	TRP	3.8
47	CU	91	GLN	3.8
18	BR	51	TYR	3.8
32	CE	179	SER	3.8
40	CN	73	ILE	3.8
1	BA	941	G	3.8
54	DA	882	G	3.8
1	BA	974	A	3.8
33	CF	54	ALA	3.8
16	BP	40	ASN	3.8
46	CT	86	MET	3.8
53	DI	122	GLN	3.8
31	CA	1082	U	3.8
35	CH	61	VAL	3.8
35	DH	89	LYS	3.8
36	CJ	72	LYS	3.8
39	CM	103	ILE	3.8
46	CT	105	VAL	3.8
54	DA	546	U	3.8
27	C0	52	SER	3.8
33	CF	164	GLU	3.8
33	CF	169	LEU	3.8
45	CS	34	GLU	3.8
36	DJ	115	ALA	3.8
38	CL	33	ALA	3.8
39	CM	83	ALA	3.8
1	BA	107	G	3.8
28	CB	20	G	3.8

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Mol	Chain	Res	Type	RSRZ
31	CA	1212	G	3.8
31	CA	2502	G	3.8
26	C5	3	VAL	3.8
31	CA	2111	U	3.8
31	CA	2167	U	3.8
32	CE	121	VAL	3.8
34	CG	38	ASN	3.8
34	CG	141	ILE	3.8
36	DJ	58	VAL	3.8
7	BG	59	LEU	3.8
30	CD	86	GLU	3.8
39	CM	27	LEU	3.8
53	DI	114	GLU	3.8
1	BA	1322	C	3.8
1	BA	1336	C	3.8
7	BG	119	ARG	3.8
31	CA	264	C	3.8
33	CF	150	ARG	3.8
41	CO	94	TYR	3.8
16	AP	82	ALA	3.8
33	CF	119	ALA	3.8
34	DG	177	LYS	3.8
17	BQ	5	ILE	3.8
31	CA	431	U	3.8
1	BA	460	A	3.8
11	AK	18	ASP	3.8
31	CA	1201	U	3.8
33	DF	77	PHE	3.8
31	CA	412	A	3.8
31	CA	2115	G	3.8
37	CK	128	ASN	3.8
31	CA	76	C	3.8
49	CW	37	PRO	3.8
34	CG	5	ALA	3.8
44	CR	71	GLN	3.8
48	CV	66	GLN	3.8
13	AM	42	ASP	3.8
21	AU	4	ILE	3.8
31	CA	1460	U	3.8
43	CQ	33	VAL	3.8
39	CM	95	LEU	3.8
1	BA	250	A	3.8

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Mol	Chain	Res	Type	RSRZ
1	BA	1000	A	3.8
1	BA	1323	G	3.8
7	BG	44	TYR	3.8
31	CA	597	G	3.8
33	CF	64	LYS	3.8
47	CU	84	TYR	3.8
1	BA	979	C	3.8
1	BA	1208	C	3.8
31	CA	1531	C	3.8
41	CO	93	GLY	3.8
42	CP	101	GLY	3.8
30	CD	24	VAL	3.8
13	BM	44	LYS	3.7
54	DA	1094	U	3.7
7	BG	130	ASN	3.7
8	BH	55	THR	3.7
31	CA	311	A	3.7
16	BP	11	ALA	3.7
19	BS	65	GLU	3.7
23	C2	6	ARG	3.7
31	CA	1017	G	3.7
41	CO	114	GLU	3.7
3	BC	77	ILE	3.7
11	AK	110	ILE	3.7
2	BB	57	LEU	3.7
1	BA	205	A	3.7
22	C1	4	GLN	3.7
32	CE	177	PRO	3.7
33	DF	176	PRO	3.7
31	CA	1207	C	3.7
31	CA	1320	C	3.7
14	BN	11	VAL	3.7
27	C0	17	LEU	3.7
31	CA	646	U	3.7
16	BP	10	GLY	3.7
20	BT	5	LYS	3.7
30	CD	151	THR	3.7
33	CF	7	TYR	3.7
7	BG	115	SER	3.7
13	AM	35	ALA	3.7
31	CA	1228	G	3.7
33	CF	6	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
46	CT	40	ASN	3.7
49	CW	71	LYS	3.7
35	CH	102	ALA	3.7
48	CV	15	THR	3.7
43	CQ	4	ILE	3.7
1	BA	1126	U	3.7
2	BB	88	ASP	3.7
16	BP	77	GLU	3.7
39	CM	144	GLU	3.7
31	CA	1862	G	3.7
31	CA	2383	G	3.7
49	CW	32	GLY	3.7
25	C4	48	ALA	3.7
5	BE	120	VAL	3.7
19	BS	62	VAL	3.7
45	CS	39	LEU	3.7
48	CV	72	ILE	3.7
1	BA	218	U	3.7
31	CA	257	C	3.7
38	CL	56	ASP	3.7
28	CB	51	G	3.7
31	CA	1483	G	3.7
13	BM	112	PRO	3.7
53	DI	120	ALA	3.7
7	AG	48	GLU	3.7
30	CD	73	VAL	3.7
1	BA	956	U	3.7
44	CR	91	ASP	3.7
54	DA	1066	U	3.7
48	CV	84	GLY	3.7
1	AA	78	A	3.7
42	CP	34	HIS	3.7
1	BA	378	G	3.7
2	AB	40	ILE	3.7
14	BN	58	SER	3.7
19	BS	25	SER	3.7
30	CD	35	THR	3.7
47	CU	31	VAL	3.7
31	CA	328	U	3.7
28	CB	118	C	3.7
13	AM	31	LYS	3.7
41	CO	46	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	BA	935	A	3.7
1	BA	1375	A	3.7
24	C3	26	ASN	3.7
31	CA	502	A	3.7
31	CA	1385	A	3.7
1	BA	1015	G	3.7
25	C4	57	LEU	3.7
3	BC	26	THR	3.7
54	DA	2162	G	3.7
1	BA	1235	U	3.6
7	AG	112	GLY	3.6
29	CC	242	LYS	3.6
31	CA	1173	U	3.6
50	CX	78	LYS	3.6
1	BA	135	C	3.6
34	CG	152	ARG	3.6
27	C0	20	HIS	3.6
31	CA	2117	A	3.6
46	CT	10	ALA	3.6
53	DI	100	ALA	3.6
54	DA	2114	A	3.6
2	BB	212	LEU	3.6
39	CM	127	VAL	3.6
5	BE	91	GLY	3.6
40	CN	29	GLY	3.6
49	CW	45	ASP	3.6
1	BA	1220	G	3.6
31	CA	2405	G	3.6
45	CS	6	GLN	3.6
16	BP	45	GLU	3.6
28	CB	63	C	3.6
39	CM	64	PHE	3.6
33	CF	45	ALA	3.6
39	CM	133	ALA	3.6
1	BA	1252	A	3.6
31	CA	53	A	3.6
35	DH	99	ILE	3.6
3	BC	179	ARG	3.6
8	AH	54	ASP	3.6
1	BA	1356	G	3.6
1	BA	1442	G	3.6
31	CA	353	C	3.6

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Mol	Chain	Res	Type	RSRZ
52	CZ	63	ALA	3.6
35	CH	44	ILE	3.6
31	CA	767	U	3.6
19	BS	44	MET	3.6
23	C2	20	PHE	3.6
3	AC	189	ALA	3.6
7	BG	145	ALA	3.6
31	CA	367	G	3.6
31	CA	1869	G	3.6
31	CA	2862	G	3.6
53	DI	90	GLY	3.6
9	AI	59	GLU	3.6
33	CF	51	ASP	3.6
1	BA	1280	A	3.6
26	C5	35	GLN	3.6
31	CA	405	U	3.6
31	CA	1234	U	3.6
31	CA	1325	U	3.6
35	CH	60	GLU	3.6
36	DJ	10	LYS	3.6
48	CV	73	PHE	3.6
8	BH	130	ALA	3.6
36	CJ	63	ALA	3.6
1	BA	175	C	3.6
3	BC	39	VAL	3.6
35	DH	107	GLY	3.6
44	CR	117	LEU	3.6
34	CG	18	LYS	3.6
54	DA	2180	U	3.6
36	CJ	117	MET	3.6
13	BM	76	SER	3.6
30	CD	101	PHE	3.6
31	CA	1285	A	3.6
43	CQ	59	PHE	3.6
11	AK	66	ALA	3.6
14	BN	17	ALA	3.6
9	AI	54	LEU	3.6
13	AM	16	VAL	3.6
13	AM	25	VAL	3.6
13	AM	34	LEU	3.6
27	C0	44	ILE	3.6
33	CF	47	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
3	BC	109	PRO	3.6
28	CB	27	C	3.6
28	CB	49	C	3.6
31	CA	413	C	3.6
35	DH	127	GLU	3.6
36	DJ	61	VAL	3.6
49	CW	64	VAL	3.6
31	CA	266	G	3.6
2	BB	9	MET	3.6
24	C3	5	PHE	3.6
32	CE	125	SER	3.6
14	AN	36	ALA	3.6
20	BT	87	ALA	3.6
25	C4	27	ALA	3.6
34	CG	73	ASN	3.6
51	CY	20	HIS	3.6
37	CK	141	ASP	3.6
48	CV	94	ARG	3.6
7	AG	116	MET	3.6
49	CW	48	MET	3.6
1	BA	1048	G	3.6
31	CA	1112	G	3.6
31	CA	1239	G	3.6
48	CV	91	LYS	3.6
48	CV	101	GLU	3.6
49	CW	28	ALA	3.6
30	CD	48	ILE	3.6
32	CE	73	ILE	3.6
3	BC	127	ARG	3.6
32	CE	9	GLN	3.6
36	CJ	134	ARG	3.6
37	CK	95	ARG	3.6
45	CS	80	ARG	3.6
1	BA	206	C	3.5
1	BA	219	U	3.5
1	BA	986	U	3.5
38	CL	35	VAL	3.5
31	CA	332	A	3.5
31	CA	478	A	3.5
46	CT	7	HIS	3.5
51	CY	77	LYS	3.5
1	AA	1037	C	3.5

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Mol	Chain	Res	Type	RSRZ
1	BA	1341	U	3.5
31	CA	1251	C	3.5
31	CA	1289	C	3.5
35	DH	139	PHE	3.5
11	AK	43	GLY	3.5
11	BK	67	ALA	3.5
27	C0	33	GLY	3.5
33	CF	49	LEU	3.5
33	CF	103	LEU	3.5
33	CF	171	ALA	3.5
44	CR	82	GLY	3.5
13	BM	71	ARG	3.5
18	BR	48	ARG	3.5
43	CQ	97	LEU	3.5
51	CY	18	ARG	3.5
48	DV	49	VAL	3.5
5	BE	140	THR	3.5
10	BJ	50	THR	3.5
54	DA	2168	G	3.5
31	CA	514	A	3.5
54	DA	1098	A	3.5
23	C2	7	GLU	3.5
43	CQ	11	GLU	3.5
22	C1	16	ARG	3.5
3	BC	104	ALA	3.5
9	BI	63	LEU	3.5
13	AM	7	ILE	3.5
14	BN	19	LYS	3.5
20	BT	50	ALA	3.5
44	CR	99	ALA	3.5
42	CP	58	ILE	3.5
49	CW	68	LYS	3.5
16	AP	71	VAL	3.5
45	CS	29	THR	3.5
1	BA	201	G	3.5
2	AB	82	ASP	3.5
9	BI	59	GLU	3.5
28	CB	117	G	3.5
1	BA	389	A	3.5
33	CF	87	CYS	3.5
35	CH	75	LEU	3.5
3	BC	120	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
7	AG	42	ILE	3.5
20	BT	67	ILE	3.5
9	BI	75	GLN	3.5
2	AB	44	GLU	3.5
36	DJ	46	THR	3.5
16	AP	39	PHE	3.5
2	BB	11	LYS	3.5
17	BQ	45	HIS	3.5
22	C1	8	PRO	3.5
34	CG	126	PRO	3.5
35	CH	68	ARG	3.5
36	DJ	82	LYS	3.5
40	CN	88	ASN	3.5
45	CS	82	HIS	3.5
30	CD	3	GLY	3.5
39	CM	88	GLY	3.5
54	DA	2108	A	3.5
2	BB	206	ALA	3.5
31	CA	2306	C	3.5
7	AG	69	VAL	3.5
13	BM	53	ILE	3.5
17	BQ	61	ILE	3.5
47	CU	2	ILE	3.5
30	CD	39	ASP	3.5
45	CS	93	PHE	3.5
50	CX	41	ARG	3.5
13	AM	24	GLY	3.5
32	CE	199	MET	3.5
30	CD	206	ALA	3.5
31	CA	93	G	3.5
31	CA	1143	A	3.5
42	CP	85	LYS	3.5
35	CH	14	SER	3.5
47	CU	69	ARG	3.5
8	BH	120	GLY	3.5
22	C1	26	THR	3.5
31	CA	2796	U	3.5
44	CR	45	TYR	3.5
7	AG	43	VAL	3.5
7	BG	63	GLU	3.5
16	BP	47	GLU	3.5
30	CD	189	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
42	CP	98	GLN	3.5
44	CR	65	ILE	3.5
1	BA	933	G	3.5
1	BA	1013	G	3.5
1	BA	1369	C	3.5
5	BE	108	GLY	3.5
48	DV	55	PRO	3.5
33	CF	101	GLU	3.5
41	CO	1	MET	3.5
49	CW	35	GLU	3.5
53	DI	126	LEU	3.5
47	CU	6	ARG	3.5
28	CB	97	C	3.5
2	BB	16	PHE	3.5
31	CA	361	G	3.5
54	DA	2105	U	3.4
30	CD	84	LEU	3.4
36	CJ	105	GLN	3.4
47	CU	62	VAL	3.4
31	CA	2078	C	3.4
3	BC	108	LYS	3.4
28	CB	52	A	3.4
30	CD	44	GLY	3.4
42	CP	86	GLY	3.4
1	AA	1015	G	3.4
31	CA	409	G	3.4
54	DA	1060	U	3.4
41	CO	96	ARG	3.4
2	AB	27	MET	3.4
2	BB	93	ASN	3.4
2	BB	130	THR	3.4
35	DH	125	THR	3.4
53	DI	67	THR	3.4
44	CR	39	VAL	3.4
46	CT	15	GLN	3.4
31	CA	314	C	3.4
26	C5	6	SER	3.4
28	CB	98	G	3.4
3	BC	56	VAL	3.4
32	CE	173	THR	3.4
20	BT	8	LYS	3.4
16	AP	16	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
25	C4	22	PHE	3.4
7	BG	140	ASP	3.4
31	CA	288	U	3.4
31	CA	544	C	3.4
1	BA	195	A	3.4
2	BB	31	ILE	3.4
22	C1	37	LYS	3.4
25	C4	4	ILE	3.4
35	CH	56	ALA	3.4
44	CR	21	ALA	3.4
46	CT	9	HIS	3.4
29	CC	46	ASN	3.4
33	CF	13	VAL	3.4
1	BA	1272	G	3.4
31	CA	1332	G	3.4
34	CG	49	THR	3.4
36	DJ	8	TYR	3.4
54	DA	879	G	3.4
30	CD	90	PHE	3.4
36	DJ	25	GLY	3.4
43	CQ	74	PHE	3.4
1	BA	632	U	3.4
32	CE	30	GLN	3.4
34	CG	116	GLN	3.4
36	CJ	48	SER	3.4
45	CS	15	SER	3.4
46	CT	69	LEU	3.4
20	BT	48	GLN	3.4
1	BA	151	A	3.4
1	BA	1014	A	3.4
18	BR	74	HIS	3.4
13	AM	57	ARG	3.4
29	CC	43	ARG	3.4
39	CM	24	GLY	3.4
45	CS	19	THR	3.4
46	CT	100	THR	3.4
14	AN	54	ASP	3.4
31	CA	1042	G	3.4
31	CA	1309	G	3.4
52	CZ	54	LYS	3.4
1	BA	1286	U	3.4
31	CA	2904	U	3.4

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Mol	Chain	Res	Type	RSRZ
14	AN	99	ALA	3.4
19	BS	50	ALA	3.4
29	CC	2	ALA	3.4
39	CM	42	SER	3.4
44	CR	116	ALA	3.4
3	BC	194	GLY	3.4
35	CH	16	GLY	3.4
1	BA	198	G	3.4
31	CA	2112	G	3.4
35	DH	6	LEU	3.4
25	C4	46	PRO	3.4
49	CW	54	ALA	3.4
13	AM	60	VAL	3.4
42	CP	28	VAL	3.4
51	CY	46	PHE	3.4
1	AA	1016	A	3.4
1	BA	1319	A	3.4
23	C2	22	THR	3.4
41	CO	36	THR	3.4
1	BA	1212	U	3.4
31	CA	598	U	3.4
53	DI	5	LEU	3.4
20	BT	56	PRO	3.4
31	CA	30	G	3.4
31	CA	1653	G	3.4
31	CA	1984	G	3.4
3	BC	78	GLY	3.4
9	BI	47	VAL	3.4
10	BJ	88	MET	3.4
13	AM	26	GLY	3.4
2	BB	36	ASN	3.4
10	AJ	91	ASP	3.4
13	BM	20	THR	3.4
24	C3	41	ARG	3.3
31	CA	2660	A	3.3
31	CA	2872	A	3.3
2	AB	131	LYS	3.3
31	CA	2861	U	3.3
35	CH	141	LYS	3.3
48	DV	54	GLN	3.3
43	CQ	22	PRO	3.3
35	CH	78	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
52	DZ	63	ALA	3.3
16	BP	30	GLY	3.3
42	CP	96	GLY	3.3
1	BA	100	G	3.3
1	BA	1355	G	3.3
7	AG	57	SER	3.3
9	AI	7	TYR	3.3
52	CZ	58	ASN	3.3
3	BC	144	LEU	3.3
44	CR	95	LEU	3.3
47	DU	91	GLN	3.3
31	CA	270	A	3.3
31	CA	1244	A	3.3
3	AC	195	VAL	3.3
27	C0	42	PRO	3.3
32	CE	196	VAL	3.3
35	DH	95	GLY	3.3
50	CX	36	ILE	3.3
35	DH	103	VAL	3.3
50	CX	65	GLY	3.3
24	C3	16	HIS	3.3
31	CA	1041	G	3.3
19	BS	79	THR	3.3
36	DJ	71	THR	3.3
52	CZ	18	LEU	3.3
29	CC	213	TRP	3.3
1	BA	946	A	3.3
12	BL	71	GLY	3.3
6	AF	62	MET	3.3
25	C4	58	VAL	3.3
31	CA	1253	A	3.3
35	DH	100	ALA	3.3
36	CJ	140	VAL	3.3
31	CA	611	C	3.3
32	CE	168	ASP	3.3
1	BA	1297	G	3.3
31	CA	446	G	3.3
35	DH	5	LEU	3.3
31	CA	2786	U	3.3
7	AG	134	ALA	3.3
37	CK	42	ALA	3.3
44	CR	17	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
45	CS	1	MET	3.3
47	CU	81	LYS	3.3
36	DJ	37	GLU	3.3
52	CZ	13	GLU	3.3
1	BA	1237	C	3.3
31	CA	2313	C	3.3
48	CV	69	ASN	3.3
2	AB	117	LEU	3.3
1	BA	1125	U	3.3
31	CA	290	U	3.3
1	BA	963	G	3.3
16	BP	51	ARG	3.3
24	C3	11	LYS	3.3
29	CC	5	LYS	3.3
31	CA	2677	G	3.3
6	BF	8	PHE	3.3
20	BT	81	ALA	3.3
45	CS	75	VAL	3.3
53	DI	2	ALA	3.3
14	AN	101	TRP	3.3
19	BS	59	PRO	3.3
49	CW	7	GLU	3.3
1	BA	306	A	3.3
1	BA	980	C	3.3
27	C0	27	LEU	3.3
30	CD	187	LEU	3.3
6	BF	79	ARG	3.3
17	BQ	6	ARG	3.3
31	CA	1599	U	3.3
31	CA	1729	U	3.3
16	AP	43	ALA	3.3
21	AU	19	PHE	3.3
29	CC	228	VAL	3.3
32	CE	135	ALA	3.3
42	CP	50	ALA	3.3
1	BA	1006	G	3.3
9	AI	51	PRO	3.3
31	CA	1341	G	3.3
45	CS	46	GLU	3.3
1	BA	845	A	3.3
1	BA	1362	A	3.3
20	BT	59	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
41	CO	59	SER	3.3
42	CP	56	LYS	3.3
34	CG	20	ASN	3.3
53	DI	3	LEU	3.3
32	CE	188	MET	3.3
1	BA	354	G	3.3
28	CB	54	G	3.3
31	CA	1138	G	3.3
54	DA	141	G	3.3
14	BN	13	ARG	3.3
47	CU	73	ARG	3.3
20	BT	78	ASN	3.3
31	CA	1596	A	3.3
31	CA	2632	A	3.3
34	CG	21	GLY	3.3
1	BA	110	C	3.3
1	BA	1262	C	3.3
9	AI	92	GLU	3.3
31	CA	47	C	3.3
31	CA	1539	U	3.3
33	CF	98	GLU	3.3
41	CO	85	PRO	3.3
53	DI	105	LYS	3.3
15	AO	69	TYR	3.2
31	CA	224	U	3.2
31	CA	894	U	3.2
35	CH	76	GLU	3.2
1	BA	101	A	3.2
14	BN	3	LYS	3.2
21	AU	26	ALA	3.2
24	D3	46	LYS	3.2
31	CA	262	A	3.2
31	CA	1089	A	3.2
31	CA	1958	C	3.2
31	CA	2158	A	3.2
33	CF	33	LYS	3.2
35	DH	64	ALA	3.2
40	CN	7	THR	3.2
36	CJ	37	GLU	3.2
39	CM	140	GLY	3.2
1	BA	260	G	3.2
1	BA	950	U	3.2

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Mol	Chain	Res	Type	RSRZ
1	BA	1364	U	3.2
13	BM	73	ILE	3.2
18	AR	51	TYR	3.2
31	CA	1546	G	3.2
2	AB	134	ALA	3.2
1	BA	54	C	3.2
2	AB	139	ARG	3.2
6	BF	10	VAL	3.2
17	AQ	83	VAL	3.2
31	CA	1330	C	3.2
31	CA	2651	C	3.2
32	CE	187	VAL	3.2
33	CF	148	ARG	3.2
47	CU	35	ALA	3.2
31	CA	279	A	3.2
23	C2	41	PRO	3.2
37	CK	21	THR	3.2
3	BC	204	LYS	3.2
13	BM	59	GLU	3.2
14	BN	12	LYS	3.2
30	CD	103	ASP	3.2
39	CM	13	LYS	3.2
47	CU	40	LYS	3.2
45	CS	5	PHE	3.2
45	CS	92	TRP	3.2
3	BC	154	SER	3.2
11	AK	97	ILE	3.2
51	CY	47	VAL	3.2
31	CA	128	C	3.2
31	CA	184	C	3.2
31	CA	619	G	3.2
31	CA	1319	C	3.2
31	CA	2844	G	3.2
54	DA	2143	C	3.2
1	BA	109	A	3.2
29	CC	251	GLN	3.2
31	CA	1614	A	3.2
7	AG	23	LEU	3.2
7	BG	13	LEU	3.2
9	AI	24	GLY	3.2
9	BI	61	LEU	3.2
16	BP	50	THR	3.2

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Mol	Chain	Res	Type	RSRZ
44	CR	23	GLY	3.2
21	AU	17	ARG	3.2
1	BA	96	U	3.2
34	CG	165	ALA	3.2
43	CQ	2	SER	3.2
39	CM	141	LYS	3.2
1	BA	106	C	3.2
1	BA	186	C	3.2
1	BA	470	C	3.2
7	AG	52	GLN	3.2
22	C1	51	GLY	3.2
31	CA	124	G	3.2
31	CA	624	C	3.2
31	CA	1643	G	3.2
31	CA	1237	A	3.2
5	BE	103	THR	3.2
5	BE	112	ARG	3.2
13	BM	102	THR	3.2
30	CD	121	THR	3.2
1	BA	1121	U	3.2
30	CD	14	ILE	3.2
31	CA	2122	U	3.2
45	CS	47	VAL	3.2
53	DI	35	VAL	3.2
33	CF	127	ASN	3.2
32	CE	197	GLU	3.2
1	BA	1037	C	3.2
7	AG	47	LEU	3.2
9	BI	45	ARG	3.2
9	BI	52	LEU	3.2
11	AK	100	LEU	3.2
41	CO	103	ARG	3.2
1	BA	1041	G	3.2
1	BA	1357	A	3.2
31	CA	43	G	3.2
31	CA	389	G	3.2
31	CA	1279	G	3.2
14	BN	73	PHE	3.2
31	CA	1395	A	3.2
46	CT	3	THR	3.2
30	CD	96	ILE	3.2
48	CV	92	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
39	CM	15	ALA	3.2
33	CF	19	GLU	3.2
33	CF	24	SER	3.2
7	BG	2	PRO	3.2
12	BL	81	LEU	3.2
31	CA	1600	C	3.2
32	CE	184	ASP	3.2
47	CU	49	LYS	3.2
23	D2	5	ILE	3.2
31	CA	881	G	3.2
31	CA	1734	G	3.2
31	CA	2895	G	3.2
32	CE	77	ILE	3.2
9	BI	42	GLU	3.2
25	C4	65	ALA	3.2
48	CV	64	ALA	3.2
54	DA	1078	U	3.2
54	DA	2130	U	3.2
7	BG	85	TYR	3.2
16	BP	18	GLN	3.2
32	CE	35	TYR	3.2
39	DM	104	GLN	3.2
8	AH	121	LEU	3.2
46	CT	48	LYS	3.2
52	CZ	30	MET	3.2
48	CV	9	ASP	3.2
31	CA	236	C	3.2
1	BA	223	A	3.2
13	BM	92	ARG	3.2
20	BT	77	ALA	3.2
31	CA	2245	U	3.2
37	CK	6	ALA	3.2
39	CM	118	THR	3.2
42	CP	53	THR	3.2
37	CK	40	HIS	3.2
45	CS	66	HIS	3.2
46	CT	11	ARG	3.2
47	CU	45	ALA	3.2
31	CA	406	G	3.2
31	CA	1185	G	3.2
31	CA	1334	G	3.2
31	CA	2627	G	3.2

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Mol	Chain	Res	Type	RSRZ
7	BG	149	LYS	3.2
44	CR	101	PHE	3.2
3	BC	85	GLU	3.2
3	BC	105	GLU	3.2
31	CA	33	C	3.2
31	CA	1615	C	3.2
41	CO	113	ILE	3.1
44	CR	89	GLU	3.2
2	AB	47	VAL	3.1
2	AB	53	ALA	3.1
31	CA	1176	U	3.1
42	CP	70	ALA	3.1
30	CD	191	GLY	3.1
30	CD	198	GLY	3.1
53	DI	32	GLY	3.1
31	CA	2819	G	3.1
25	C4	49	MET	3.1
36	DJ	47	ASP	3.1
1	AA	1025	U	3.1
31	CA	1060	U	3.1
40	CN	56	ALA	3.1
15	AO	16	GLY	3.1
33	CF	62	GLY	3.1
1	BA	86	G	3.1
13	BM	87	ARG	3.1
14	BN	69	ARG	3.1
15	AO	21	ASP	3.1
21	BU	2	PRO	3.1
31	CA	70	G	3.1
19	BS	18	LYS	3.1
24	C3	14	ARG	3.1
31	CA	1252	G	3.1
31	CA	2808	G	3.1
35	CH	139	PHE	3.1
43	CQ	93	ARG	3.1
53	DI	119	PRO	3.1
12	BL	37	VAL	3.1
45	CS	100	GLY	3.1
6	AF	63	ASN	3.1
7	BG	70	ARG	3.1
9	BI	6	TYR	3.1
10	BJ	17	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
7	BG	101	MET	3.1
9	AI	62	ASP	3.1
14	BN	38	ASP	3.1
29	DC	272	SER	3.1
36	CJ	65	ARG	3.1
31	CA	368	A	3.1
1	BA	1064	G	3.1
3	AC	103	ILE	3.1
31	CA	2159	G	3.1
22	C1	30	VAL	3.1
31	CA	1224	U	3.1
35	CH	21	VAL	3.1
35	DH	16	GLY	3.1
1	BA	1263	C	3.1
31	CA	11	C	3.1
26	C5	19	ARG	3.1
34	CG	42	GLU	3.1
2	BB	62	SER	3.1
14	AN	18	ASP	3.1
1	BA	172	A	3.1
31	CA	423	A	3.1
31	CA	443	A	3.1
31	CA	849	A	3.1
31	CA	1133	A	3.1
16	AP	78	VAL	3.1
1	BA	187	G	3.1
1	BA	326	G	3.1
1	BA	1002	G	3.1
17	BQ	82	ALA	3.1
31	CA	2334	U	3.1
32	CE	34	ALA	3.1
40	CN	89	VAL	3.1
41	CO	7	GLY	3.1
45	CS	30	GLY	3.1
54	DA	2113	U	3.1
54	DA	2133	G	3.1
1	BA	379	C	3.1
2	BB	145	GLU	3.1
3	AC	82	GLU	3.1
31	CA	151	C	3.1
15	BO	87	LEU	3.1
27	C0	23	THR	3.1

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Mol	Chain	Res	Type	RSRZ
32	CE	22	ASP	3.1
14	BN	57	PRO	3.1
2	BB	45	LYS	3.1
31	CA	104	A	3.1
1	BA	1211	U	3.1
13	AM	15	ALA	3.1
31	CA	1387	A	3.1
31	CA	2725	A	3.1
30	CD	89	GLU	3.1
1	BA	1366	C	3.1
31	CA	1059	G	3.1
31	CA	1471	G	3.1
33	DF	117	LEU	3.1
35	CH	6	LEU	3.1
7	AG	151	PHE	3.1
29	CC	50	THR	3.1
36	DJ	136	MET	3.1
36	DJ	75	PRO	3.1
9	AI	85	ARG	3.1
12	BL	50	ARG	3.1
32	CE	103	GLY	3.1
13	AM	64	VAL	3.1
48	CV	37	GLU	3.1
49	CW	23	ALA	3.1
31	CA	508	A	3.1
2	AB	157	LEU	3.1
1	BA	214	C	3.1
1	BA	1001	C	3.1
1	BA	191	G	3.1
25	C4	39	LYS	3.1
30	CD	176	ASP	3.1
31	CA	215	G	3.1
11	BK	110	ILE	3.1
29	CC	49	ILE	3.1
19	BS	51	VAL	3.1
39	CM	86	GLU	3.1
26	C5	29	ALA	3.1
31	CA	1864	U	3.1
31	CA	233	A	3.1
31	CA	2749	A	3.1
33	CF	57	LEU	3.1
43	CQ	6	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
45	CS	12	HIS	3.1
1	BA	1327	C	3.1
2	AB	35	ARG	3.1
10	BJ	45	ARG	3.1
29	CC	225	MET	3.1
30	CD	179	ARG	3.1
36	CJ	36	MET	3.1
1	BA	1310	G	3.1
27	C0	18	PRO	3.1
31	CA	313	G	3.1
31	CA	625	G	3.1
31	CA	1099	G	3.1
32	CE	156	ASN	3.1
54	DA	2148	G	3.1
12	BL	48	ALA	3.0
19	AS	50	ALA	3.0
31	CA	100	U	3.0
35	DH	65	ALA	3.0
47	CU	23	ALA	3.0
22	C1	53	LYS	3.0
47	CU	93	LEU	3.0
49	CW	2	PHE	3.0
51	CY	30	LEU	3.0
19	AS	32	ARG	3.0
31	CA	1275	A	3.0
1	BA	1038	C	3.0
19	AS	46	GLY	3.0
32	CE	56	GLY	3.0
35	DH	126	GLY	3.0
37	CK	137	PRO	3.0
41	CO	18	GLN	3.0
49	CW	24	ASN	3.0
7	BG	105	VAL	3.0
32	CE	15	SER	3.0
33	CF	162	SER	3.0
36	DJ	57	VAL	3.0
45	CS	64	VAL	3.0
31	CA	494	G	3.0
52	CZ	34	SER	3.0
22	C1	52	ARG	3.0
53	DI	47	GLU	3.0
31	CA	1204	A	3.0

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Mol	Chain	Res	Type	RSRZ
32	CE	141	MET	3.0
43	CQ	16	ASP	3.0
45	CS	56	GLY	3.0
54	DA	2309	A	3.0
19	BS	56	GLN	3.0
3	BC	200	VAL	3.0
7	BG	64	VAL	3.0
7	BG	122	ASN	3.0
27	C0	55	VAL	3.0
31	CA	1468	U	3.0
39	CM	134	ALA	3.0
1	BA	847	G	3.0
28	CB	102	G	3.0
31	CA	1016	G	3.0
36	CJ	108	GLU	3.0
26	C5	33	HIS	3.0
29	CC	235	GLY	3.0
44	CR	59	GLN	3.0
1	AA	1441	A	3.0
1	BA	1239	A	3.0
2	AB	36	ASN	3.0
30	CD	29	VAL	3.0
50	CX	67	VAL	3.0
1	BA	473	U	3.0
8	AH	55	THR	3.0
10	BJ	83	THR	3.0
19	BS	15	LEU	3.0
32	CE	5	LEU	3.0
35	CH	5	LEU	3.0
20	BT	9	LYS	3.0
34	CG	125	CYS	3.0
19	BS	26	GLY	3.0
29	CC	98	ASP	3.0
30	CD	18	ASP	3.0
31	CA	518	G	3.0
31	CA	1324	G	3.0
51	CY	55	GLY	3.0
30	CD	83	ARG	3.0
32	CE	69	ARG	3.0
33	CF	8	TYR	3.0
35	DH	25	TYR	3.0
1	BA	975	A	3.0

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Mol	Chain	Res	Type	RSRZ
31	CA	504	A	3.0
54	DA	2153	C	3.0
30	CD	91	THR	3.0
31	CA	1396	U	3.0
7	BG	76	LYS	3.0
7	BG	118	LEU	3.0
35	DH	124	THR	3.0
39	CM	94	THR	3.0
34	CG	158	LYS	3.0
52	CZ	10	SER	3.0
3	BC	31	ASP	3.0
34	CG	16	ASP	3.0
9	BI	119	ARG	3.0
31	CA	86	G	3.0
41	CO	97	ILE	3.0
46	CT	95	ARG	3.0
35	CH	22	LYS	3.0
2	AB	69	PHE	3.0
2	BB	162	PHE	3.0
31	CA	1229	C	3.0
31	CA	2406	A	3.0
32	CE	65	THR	3.0
34	CG	50	LEU	3.0
2	AB	156	GLY	3.0
2	BB	13	GLY	3.0
42	CP	100	HIS	3.0
11	BK	86	VAL	3.0
30	CD	60	VAL	3.0
1	BA	105	G	3.0
35	CH	36	ALA	3.0
1	AA	4	U	3.0
12	BL	24	LEU	3.0
16	BP	6	LEU	3.0
31	CA	2166	U	3.0
31	CA	2820	A	3.0
33	CF	159	THR	3.0
36	DJ	119	GLY	3.0
30	CD	77	ARG	3.0
12	BL	82	ILE	3.0
25	C4	15	LYS	3.0
37	CK	138	GLN	3.0
43	CQ	38	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
30	CD	30	GLU	3.0
2	BB	29	PRO	3.0
21	AU	11	PRO	3.0
39	CM	98	ALA	3.0
1	BA	324	G	3.0
17	AQ	53	CYS	3.0
31	CA	1542	U	3.0
2	AB	74	ARG	3.0
31	CA	2668	G	3.0
31	CA	16	C	3.0
31	CA	1383	A	3.0
13	AM	17	ILE	3.0
32	CE	191	ASP	3.0
29	CC	236	GLU	3.0
51	CY	56	MET	3.0
30	CD	98	VAL	3.0
42	CP	90	VAL	3.0
33	CF	109	PRO	2.9
43	CQ	42	ALA	2.9
1	BA	1313	U	2.9
54	DA	1729	U	2.9
30	CD	42	ASN	2.9
44	CR	7	GLY	2.9
51	CY	61	LYS	2.9
1	BA	380	G	2.9
31	CA	1092	C	2.9
31	CA	1277	G	2.9
54	DA	1731	G	2.9
54	DA	2177	C	2.9
9	AI	28	ILE	2.9
13	AM	45	ILE	2.9
15	BO	26	GLU	2.9
31	CA	272	A	2.9
20	AT	20	HIS	2.9
1	BA	1065	U	2.9
5	AE	115	LEU	2.9
14	BN	97	LYS	2.9
35	DH	132	PHE	2.9
38	CL	49	ARG	2.9
39	CM	60	ARG	2.9
9	BI	10	GLY	2.9
31	CA	850	U	2.9

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Mol	Chain	Res	Type	RSRZ
7	AG	68	ASN	2.9
11	BK	68	GLU	2.9
34	DG	173	GLU	2.9
2	BB	189	THR	2.9
14	AN	32	SER	2.9
28	CB	110	C	2.9
35	DH	136	SER	2.9
54	DA	1087	G	2.9
1	AA	1019	A	2.9
1	BA	1246	A	2.9
15	AO	27	VAL	2.9
40	CN	36	VAL	2.9
46	CT	90	LYS	2.9
35	CH	106	ALA	2.9
48	CV	2	ALA	2.9
10	AJ	39	PRO	2.9
30	CD	185	ASN	2.9
42	CP	80	GLU	2.9
1	BA	95	C	2.9
31	CA	2364	C	2.9
46	CT	55	ILE	2.9
19	BS	58	VAL	2.9
1	BA	1347	G	2.9
31	CA	1236	G	2.9
31	CA	1622	G	2.9
36	DJ	44	ALA	2.9
1	BA	167	A	2.9
31	CA	1088	A	2.9
34	CG	28	GLY	2.9
54	DA	1090	A	2.9
1	BA	1330	U	2.9
16	AP	45	GLU	2.9
17	BQ	60	GLU	2.9
2	BB	42	ASN	2.9
3	AC	80	LYS	2.9
46	CT	16	LYS	2.9
16	BP	35	ARG	2.9
39	CM	73	ILE	2.9
42	CP	89	ASP	2.9
44	CR	13	ARG	2.9
46	CT	103	ILE	2.9
6	AF	97	THR	2.9

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Mol	Chain	Res	Type	RSRZ
11	BK	65	VAL	2.9
14	AN	55	SER	2.9
19	AS	39	THR	2.9
30	CD	5	VAL	2.9
31	CA	115	C	2.9
31	CA	2129	C	2.9
38	CL	69	VAL	2.9
29	CC	240	PHE	2.9
40	CN	78	LEU	2.9
1	BA	133	U	2.9
3	BC	73	PRO	2.9
31	CA	2783	U	2.9
50	CX	70	GLU	2.9
31	CA	271	G	2.9
6	BF	59	TYR	2.9
9	BI	22	LYS	2.9
31	CA	1590	A	2.9
47	CU	68	LYS	2.9
2	BB	208	ARG	2.9
7	BG	143	ARG	2.9
18	AR	48	ARG	2.9
38	CL	38	ILE	2.9
47	CU	30	ILE	2.9
10	AJ	36	VAL	2.9
31	CA	1454	C	2.9
43	CQ	17	VAL	2.9
2	AB	12	ALA	2.9
2	AB	85	LEU	2.9
2	BB	134	ALA	2.9
7	BG	127	ALA	2.9
17	BQ	75	LEU	2.9
20	BT	65	GLY	2.9
54	DA	897	C	2.9
24	C3	23	ALA	2.9
34	CG	107	LEU	2.9
36	DJ	120	ALA	2.9
29	CC	26	LYS	2.9
29	CC	59	LYS	2.9
30	CD	134	HIS	2.9
31	CA	1326	U	2.9
33	CF	72	LYS	2.9
11	BK	98	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	BA	104	G	2.9
31	CA	2742	G	2.9
20	BT	32	ILE	2.9
3	BC	125	GLU	2.9
23	C2	32	GLU	2.9
29	CC	100	GLU	2.9
1	BA	67	C	2.9
3	AC	43	LEU	2.9
4	AD	117	LEU	2.9
9	BI	69	GLY	2.9
34	CG	61	GLY	2.9
34	CG	173	GLU	2.9
19	BS	33	THR	2.9
31	CA	198	C	2.9
35	DH	15	LEU	2.9
37	CK	15	TRP	2.9
1	BA	1315	U	2.9
39	CM	38	GLN	2.9
1	BA	1046	A	2.9
28	CB	119	A	2.9
33	CF	104	ILE	2.9
2	BB	217	VAL	2.9
13	BM	78	LYS	2.9
31	CA	776	G	2.9
31	CA	2414	G	2.9
33	CF	140	GLU	2.9
38	CL	21	CYS	2.9
38	CL	112	PHE	2.9
43	CQ	32	VAL	2.9
20	BT	41	ALA	2.9
36	DJ	118	THR	2.9
44	CR	92	ARG	2.9
1	AA	1277	C	2.9
1	BA	1136	C	2.9
31	CA	335	C	2.9
31	CA	816	C	2.9
31	CA	2863	C	2.9
1	BA	943	U	2.9
31	CA	34	U	2.9
31	CA	102	U	2.9
33	CF	5	HIS	2.9
51	CY	31	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
7	AG	110	LYS	2.9
42	CP	68	LYS	2.9
46	CT	4	ILE	2.9
29	CC	44	ASN	2.9
1	BA	969	A	2.9
30	CD	153	GLY	2.9
31	CA	1871	A	2.9
31	CA	2147	A	2.9
37	CK	56	VAL	2.9
39	CM	52	GLY	2.9
46	CT	20	VAL	2.9
54	DA	613	A	2.9
1	BA	377	G	2.9
1	BA	993	G	2.9
2	AB	34	ALA	2.9
24	C3	22	MET	2.9
31	CA	411	G	2.9
31	CA	1166	G	2.9
31	CA	2838	G	2.9
31	CA	2890	G	2.9
27	C0	12	SER	2.8
1	BA	194	C	2.8
1	BA	972	C	2.8
20	BT	55	GLN	2.8
31	CA	114	U	2.8
37	CK	3	THR	2.8
40	CN	60	GLN	2.8
47	CU	29	THR	2.8
17	AQ	4	LYS	2.8
22	C1	32	LYS	2.8
29	CC	248	TRP	2.8
32	CE	16	GLU	2.8
37	CK	98	GLU	2.8
37	CK	125	TYR	2.8
29	CC	238	ARG	2.8
36	DJ	140	VAL	2.8
39	CM	122	VAL	2.8
46	CT	8	ARG	2.8
53	DI	42	ARG	2.8
13	AM	40	ALA	2.8
31	CA	866	A	2.8
1	BA	951	G	2.8

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Mol	Chain	Res	Type	RSRZ
31	CA	583	G	2.8
31	CA	1037	G	2.8
33	CF	61	SER	2.8
1	BA	999	C	2.8
1	BA	1230	C	2.8
5	BE	80	THR	2.8
31	CA	1764	C	2.8
14	BN	26	GLU	2.8
9	AI	18	ARG	2.8
29	CC	101	ARG	2.8
35	CH	27	ARG	2.8
2	AB	17	GLY	2.8
19	BS	67	VAL	2.8
32	CE	158	PHE	2.8
33	CF	100	PHE	2.8
43	CQ	30	VAL	2.8
29	CC	202	LEU	2.8
18	AR	24	LYS	2.8
1	AA	412	A	2.8
1	AA	1492	A	2.8
1	BA	1227	A	2.8
31	CA	182	A	2.8
31	CA	1439	A	2.8
49	CW	75	GLN	2.8
31	CA	906	U	2.8
31	CA	1443	U	2.8
31	CA	1880	U	2.8
47	CU	27	SER	2.8
34	CG	122	THR	2.8
35	CH	137	GLU	2.8
1	BA	1277	C	2.8
1	BA	1370	G	2.8
28	CB	21	G	2.8
30	CD	184	ARG	2.8
31	CA	242	G	2.8
31	CA	261	G	2.8
2	AB	151	ILE	2.8
31	CA	838	C	2.8
31	CA	1026	G	2.8
31	CA	1206	G	2.8
31	CA	2896	C	2.8
44	CR	14	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
47	CU	12	ARG	2.8
47	CU	70	HIS	2.8
53	DI	125	ARG	2.8
15	BO	15	PHE	2.8
32	CE	171	ASP	2.8
34	CG	66	GLY	2.8
29	CC	19	VAL	2.8
33	CF	89	VAL	2.8
51	CY	54	LYS	2.8
52	CZ	2	LYS	2.8
32	DE	11	ALA	2.8
50	CX	84	ALA	2.8
1	BA	1264	U	2.8
31	CA	810	U	2.8
1	AA	1022	A	2.8
14	BN	70	PRO	2.8
28	CB	50	A	2.8
31	CA	1525	A	2.8
32	CE	48	THR	2.8
36	CJ	112	THR	2.8
2	AB	90	PHE	2.8
28	CB	4	C	2.8
31	CA	1708	C	2.8
31	CA	2859	G	2.8
31	CA	2876	G	2.8
35	CH	17	ASP	2.8
23	C2	42	VAL	2.8
33	CF	146	VAL	2.8
7	AG	66	LEU	2.8
9	AI	63	LEU	2.8
13	BM	8	ASN	2.8
6	AF	98	GLU	2.8
30	CD	28	GLU	2.8
34	CG	55	ARG	2.8
31	CA	29	U	2.8
1	BA	1254	A	2.8
3	AC	68	ILE	2.8
29	CC	64	ILE	2.8
31	CA	310	A	2.8
31	CA	2835	A	2.8
39	CM	11	GLY	2.8
9	BI	56	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
19	AS	27	ASP	2.8
28	CB	26	C	2.8
31	CA	179	C	2.8
9	BI	19	VAL	2.8
29	CC	33	LEU	2.8
31	CA	2046	G	2.8
39	CM	61	LEU	2.8
7	BG	139	GLU	2.8
29	CC	28	LYS	2.8
31	CA	615	U	2.8
31	CA	1742	U	2.8
52	CZ	60	LYS	2.8
7	BG	14	PRO	2.8
42	CP	45	SER	2.8
49	CW	84	PRO	2.8
1	BA	1044	A	2.8
37	CK	17	VAL	2.8
46	CT	39	THR	2.8
2	BB	133	GLU	2.8
31	CA	435	C	2.8
31	CA	1730	C	2.8
34	CG	87	LEU	2.8
54	DA	1076	C	2.8
7	AG	65	ALA	2.8
7	BG	98	ALA	2.8
9	AI	16	ALA	2.8
19	AS	22	ALA	2.8
1	BA	1231	G	2.8
31	CA	1036	G	2.8
31	CA	1651	G	2.8
31	CA	2307	G	2.8
1	AA	1286	U	2.8
1	BA	1295	U	2.8
32	CE	151	GLY	2.8
21	AU	12	PHE	2.8
34	CG	156	PRO	2.8
8	BH	59	LEU	2.8
14	AN	27	LEU	2.8
32	CE	13	THR	2.8
32	CE	17	THR	2.8
35	DH	142	VAL	2.8
45	CS	13	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
52	CZ	46	VAL	2.8
1	AA	1534	A	2.8
2	BB	64	LYS	2.8
25	C4	25	LYS	2.8
31	CA	666	A	2.8
31	CA	815	C	2.8
31	CA	1327	A	2.8
31	CA	2072	C	2.8
54	DA	2173	A	2.8
16	BP	26	ASN	2.8
16	BP	29	ASN	2.8
1	BA	103	U	2.8
1	BA	455	G	2.8
1	BA	457	G	2.8
1	BA	1334	G	2.8
30	CD	76	GLY	2.8
31	CA	230	G	2.8
31	CA	273	G	2.8
31	CA	408	G	2.8
31	CA	1529	G	2.8
31	CA	2629	U	2.8
35	DH	88	GLY	2.8
48	CV	55	PRO	2.8
48	CV	58	ILE	2.8
53	DI	76	PHE	2.8
40	CN	124	LEU	2.8
53	DI	86	THR	2.8
1	AA	205	A	2.7
1	AA	1036	A	2.7
1	BA	1287	A	2.7
31	CA	1528	A	2.7
31	CA	1532	A	2.7
54	DA	1072	C	2.8
9	AI	4	ASN	2.7
9	AI	31	ASN	2.7
9	BI	8	GLY	2.7
29	CC	127	GLY	2.7
2	BB	44	GLU	2.7
10	BJ	31	ARG	2.7
20	BT	71	LYS	2.7
35	CH	4	ILE	2.7
35	CH	41	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
35	DH	143	ILE	2.7
37	CK	129	GLU	2.7
40	CN	59	ARG	2.7
47	CU	88	LYS	2.7
29	CC	227	PRO	2.7
31	CA	7	G	2.7
31	CA	535	G	2.7
31	CA	989	G	2.7
31	CA	1731	G	2.7
31	CA	2100	G	2.7
19	BS	57	HIS	2.7
30	CD	104	VAL	2.7
34	CG	4	VAL	2.7
49	CW	60	VAL	2.7
10	AJ	29	ALA	2.7
30	CD	75	ALA	2.7
1	BA	352	C	2.7
31	CA	903	C	2.7
31	CA	71	A	2.7
31	CA	227	A	2.7
31	CA	1609	A	2.7
31	CA	2657	A	2.7
13	AM	41	GLU	2.7
31	CA	87	U	2.7
31	CA	1113	U	2.7
48	CV	82	ARG	2.7
37	CK	89	PHE	2.7
2	AB	43	LEU	2.7
3	AC	66	VAL	2.7
1	AA	1276	G	2.7
1	BA	220	G	2.7
1	BA	1266	G	2.7
1	BA	1343	G	2.7
31	CA	1543	G	2.7
45	CS	83	TYR	2.7
1	AA	1028	C	2.7
6	AF	88	MET	2.7
13	BM	111	GLY	2.7
30	CD	87	GLY	2.7
31	CA	57	C	2.7
31	CA	1467	U	2.7
31	CA	2130	U	2.7

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Mol	Chain	Res	Type	RSRZ
35	DH	76	GLU	2.7
16	BP	4	ILE	2.7
31	CA	432	A	2.7
31	CA	1608	A	2.7
31	CA	2101	A	2.7
54	DA	1088	A	2.7
2	AB	68	LEU	2.7
2	BB	114	LEU	2.7
49	CW	12	GLN	2.7
52	DZ	6	LEU	2.7
13	AM	12	HIS	2.7
32	CE	72	SER	2.7
14	BN	59	ARG	2.7
35	CH	10	ALA	2.7
44	CR	68	ALA	2.7
47	CU	77	ARG	2.7
1	BA	945	G	2.7
1	BA	1454	G	2.7
30	CD	88	GLU	2.7
31	CA	1524	G	2.7
32	CE	53	THR	2.7
34	CG	84	THR	2.7
47	CU	86	THR	2.7
3	BC	203	PHE	2.7
28	CB	25	U	2.7
31	CA	235	U	2.7
35	CH	119	ASN	2.7
53	DI	11	ILE	2.7
31	CA	216	A	2.7
31	CA	354	A	2.7
31	CA	1722	A	2.7
6	AF	96	VAL	2.7
11	AK	80	LYS	2.7
53	DI	55	VAL	2.7
20	BT	68	HIS	2.7
25	C4	60	ALA	2.7
34	DG	111	HIS	2.7
32	DE	2	GLU	2.7
37	CK	53	TYR	2.7
48	CV	56	GLY	2.7
1	AA	1127	G	2.7
1	BA	1316	G	2.7

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Mol	Chain	Res	Type	RSRZ
1	BA	1386	G	2.7
3	AC	64	ILE	2.7
3	AC	101	ILE	2.7
3	BC	14	ILE	2.7
29	CC	45	ASN	2.7
31	CA	258	G	2.7
31	CA	1250	G	2.7
31	CA	1450	G	2.7
31	CA	1861	G	2.7
31	CA	2798	U	2.7
54	DA	881	G	2.7
31	CA	1079	C	2.7
31	CA	1363	C	2.7
47	CU	44	LYS	2.7
32	CE	120	VAL	2.7
32	CE	176	ASP	2.7
36	CJ	106	LEU	2.7
42	CP	111	ARG	2.7
48	CV	41	LEU	2.7
1	BA	199	A	2.7
3	AC	190	HIS	2.7
7	BG	51	ALA	2.7
14	BN	29	ALA	2.7
16	BP	27	ALA	2.7
39	CM	143	GLU	2.7
1	AA	89	U	2.7
1	BA	952	U	2.7
12	BL	67	ILE	2.7
25	C4	6	THR	2.7
28	CB	74	U	2.7
31	CA	112	U	2.7
35	DH	29	PHE	2.7
51	CY	29	PHE	2.7
1	BA	1003	G	2.7
3	BC	181	ASP	2.7
10	AJ	77	VAL	2.7
18	AR	29	LEU	2.7
31	CA	510	C	2.7
31	CA	1311	G	2.7
31	CA	2148	G	2.7
31	CA	2365	G	2.7
43	CQ	41	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
14	BN	101	TRP	2.7
43	CQ	112	GLU	2.7
42	CP	75	GLY	2.7
24	C3	15	SER	2.7
34	CG	138	LYS	2.7
42	CP	5	SER	2.7
1	BA	157	U	2.7
7	AG	49	THR	2.7
20	BT	52	ASN	2.7
27	C0	10	THR	2.7
31	CA	1340	U	2.7
52	CZ	55	THR	2.7
3	BC	84	VAL	2.7
19	AS	60	VAL	2.7
31	CA	433	C	2.7
31	CA	565	C	2.7
35	CH	149	GLU	2.7
35	DH	18	GLN	2.7
35	DH	110	VAL	2.7
31	CA	2692	G	2.7
34	CG	145	ALA	2.7
19	AS	57	HIS	2.7
31	CA	2766	A	2.7
11	BK	85	MET	2.7
40	CN	50	ARG	2.7
52	CZ	26	PHE	2.7
31	CA	1963	U	2.7
53	DI	82	ILE	2.7
2	BB	46	THR	2.7
37	CK	50	THR	2.7
3	AC	39	VAL	2.7
11	AK	84	VAL	2.7
34	CG	90	VAL	2.7
37	CK	49	ASP	2.7
42	CP	48	LEU	2.7
44	CR	18	LEU	2.7
1	BA	87	C	2.7
15	BO	19	ALA	2.7
30	CD	182	ALA	2.7
48	CV	71	ALA	2.7
1	BA	177	G	2.7
29	CC	212	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
31	CA	326	G	2.7
31	CA	386	G	2.7
31	CA	512	G	2.7
31	CA	799	G	2.7
31	CA	855	G	2.7
31	CA	1333	G	2.7
31	CA	1867	G	2.7
1	BA	65	A	2.6
31	CA	94	A	2.6
31	CA	609	A	2.6
31	CA	1272	A	2.6
31	CA	1652	A	2.6
31	CA	2358	A	2.6
37	CK	92	MET	2.6
31	CA	1487	U	2.6
31	CA	2109	U	2.6
7	BG	30	LEU	2.6
12	AL	73	ASN	2.6
13	AM	114	LYS	2.6
35	DH	104	THR	2.6
39	CM	116	VAL	2.6
41	CO	23	ASN	2.6
53	DI	81	LEU	2.6
2	AB	65	GLY	2.6
1	BA	1342	C	2.6
17	BQ	66	PRO	2.6
2	AB	208	ARG	2.6
11	BK	63	ALA	2.6
13	BM	106	ALA	2.6
31	CA	237	C	2.6
31	CA	795	C	2.6
31	CA	1135	C	2.6
34	CG	154	PRO	2.6
33	CF	70	ALA	2.6
39	CM	132	ARG	2.6
40	CN	16	ARG	2.6
46	CT	58	ALA	2.6
53	DI	91	ALA	2.6
18	AR	74	HIS	2.6
39	CM	50	PHE	2.6
14	BN	100	SER	2.6
1	BA	1007	U	2.6

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Mol	Chain	Res	Type	RSRZ
20	BT	39	ILE	2.6
31	CA	926	G	2.6
31	CA	2583	G	2.6
33	CF	44	ILE	2.6
53	DI	98	GLU	2.6
1	BA	482	A	2.6
31	CA	2814	A	2.6
52	CZ	38	GLN	2.6
7	AG	64	VAL	2.6
7	BG	113	ASP	2.6
42	CP	47	VAL	2.6
7	BG	78	ARG	2.6
25	C4	45	ARG	2.6
1	BA	307	C	2.6
1	BA	1149	C	2.6
1	BA	1265	C	2.6
1	BA	1383	C	2.6
2	AB	186	ILE	2.6
12	BL	105	SER	2.6
23	C2	9	ILE	2.6
29	CC	272	SER	2.6
44	CR	94	ILE	2.6
53	DI	52	MET	2.6
1	BA	1475	G	2.6
5	BE	36	LEU	2.6
23	C2	34	LEU	2.6
31	CA	48	G	2.6
31	CA	2318	G	2.6
1	BA	468	A	2.6
29	CC	237	GLY	2.6
31	CA	278	A	2.6
31	CA	575	A	2.6
31	CA	1070	A	2.6
35	DH	98	ASP	2.6
51	CY	50	ARG	2.6
3	AC	191	THR	2.6
10	BJ	79	PRO	2.6
39	CM	121	THR	2.6
45	CS	81	LYS	2.6
21	AU	36	GLU	2.6
31	CA	581	C	2.6
31	CA	2177	C	2.6

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Mol	Chain	Res	Type	RSRZ
2	BB	151	ILE	2.6
39	CM	1	MET	2.6
1	BA	1301	U	2.6
11	BK	64	GLN	2.6
31	CA	390	U	2.6
10	AJ	5	ARG	2.6
42	CP	81	ARG	2.6
52	CZ	43	LEU	2.6
39	CM	91	ASP	2.6
1	BA	1215	G	2.6
31	CA	526	A	2.6
31	CA	808	G	2.6
31	CA	1024	G	2.6
31	CA	2363	G	2.6
31	CA	2526	G	2.6
49	CW	5	ASN	2.6
22	C1	33	THR	2.6
44	CR	10	ALA	2.6
44	CR	57	PHE	2.6
32	CE	136	GLN	2.6
49	CW	50	MET	2.6
3	BC	74	GLY	2.6
7	BG	83	SER	2.6
20	BT	16	LYS	2.6
36	DJ	16	GLY	2.6
12	BL	23	ALA	2.6
40	CN	69	PRO	2.6
41	CO	68	ALA	2.6
47	CU	92	ASN	2.6
1	BA	1067	A	2.6
1	BA	1339	A	2.6
1	BA	1361	G	2.6
8	BH	49	PHE	2.6
31	CA	941	A	2.6
31	CA	1091	G	2.6
31	CA	1225	G	2.6
51	CY	48	THR	2.6
1	BA	1228	C	2.6
5	BE	159	LYS	2.6
23	C2	25	LYS	2.6
29	CC	60	GLN	2.6
31	CA	2260	C	2.6

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Mol	Chain	Res	Type	RSRZ
19	BS	46	GLY	2.6
31	CA	653	U	2.6
31	CA	2244	U	2.6
31	CA	2423	U	2.6
48	CV	44	LYS	2.6
34	CG	91	GLY	2.6
42	CP	44	GLY	2.6
53	DI	59	LEU	2.6
3	AC	168	TYR	2.6
30	CD	45	TYR	2.6
34	CG	130	GLU	2.6
22	C1	45	ALA	2.6
35	CH	111	ALA	2.6
44	CR	27	ALA	2.6
44	CR	42	ALA	2.6
1	BA	139	A	2.6
2	AB	60	ILE	2.6
28	CB	116	G	2.6
31	CA	46	G	2.6
31	CA	377	G	2.6
31	CA	488	G	2.6
38	CL	3	GLN	2.6
40	CN	45	GLN	2.6
7	AG	55	GLY	2.6
9	BI	87	LEU	2.6
10	BJ	56	HIS	2.6
24	D3	1	MET	2.6
31	CA	1909	C	2.6
31	CA	2149	U	2.6
33	CF	16	LEU	2.6
39	CM	112	LEU	2.6
42	CP	83	LEU	2.6
54	DA	143	C	2.6
54	DA	893	C	2.6
11	BK	94	GLU	2.6
12	BL	16	VAL	2.6
42	CP	74	VAL	2.6
2	AB	45	LYS	2.6
12	BL	14	ARG	2.6
36	DJ	39	CYS	2.6
39	CM	29	LYS	2.6
49	CW	10	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
14	BN	66	GLN	2.6
2	AB	114	LEU	2.6
3	AC	81	GLY	2.6
9	AI	82	GLY	2.6
31	CA	633	A	2.6
1	BA	1223	C	2.6
29	CC	180	GLU	2.6
29	CC	243	HIS	2.6
31	CA	2132	U	2.6
31	CA	2157	G	2.6
31	CA	2449	U	2.6
47	CU	32	LEU	2.6
31	CA	178	G	2.6
31	CA	536	G	2.6
54	DA	1061	U	2.6
9	BI	85	ARG	2.6
41	CO	8	ARG	2.6
42	CP	82	ALA	2.6
19	AS	30	PRO	2.6
48	CV	99	ASN	2.6
40	CN	54	THR	2.5
41	CO	33	ILE	2.5
48	CV	103	ILE	2.5
2	BB	65	GLY	2.5
40	CN	90	GLU	2.5
1	BA	221	C	2.5
1	BA	848	C	2.5
16	BP	19	VAL	2.5
1	BA	1039	G	2.5
20	BT	29	ARG	2.5
29	CC	265	LYS	2.5
30	CD	20	VAL	2.5
48	CV	70	VAL	2.5
53	DI	26	VAL	2.5
53	DI	50	VAL	2.5
29	CC	62	TYR	2.5
31	CA	2186	G	2.5
54	DA	2152	G	2.5
33	CF	2	ALA	2.5
48	CV	85	PHE	2.5
2	BB	202	GLY	2.5
32	CE	108	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
38	CL	68	GLY	2.5
43	CQ	114	LEU	2.5
52	DZ	5	GLU	2.5
11	AK	96	THR	2.5
24	C3	24	THR	2.5
32	CE	100	MET	2.5
37	CK	34	ARG	2.5
53	DI	8	LYS	2.5
5	BE	46	VAL	2.5
35	DH	108	VAL	2.5
1	AA	183	C	2.5
1	BA	461	A	2.5
45	CS	95	ASP	2.5
9	AI	64	TYR	2.5
20	AT	87	ALA	2.5
22	C1	29	SER	2.5
31	CA	1430	G	2.5
31	CA	2238	G	2.5
44	CR	67	ALA	2.5
9	AI	23	PRO	2.5
10	BJ	78	GLU	2.5
47	CU	4	GLU	2.5
53	DI	107	GLU	2.5
27	C0	19	LYS	2.5
19	AS	3	ARG	2.5
24	C3	21	ARG	2.5
31	CA	1438	U	2.5
31	CA	2871	U	2.5
16	AP	21	VAL	2.5
19	AS	67	VAL	2.5
34	CG	15	VAL	2.5
35	CH	103	VAL	2.5
46	CT	45	VAL	2.5
7	BG	26	PHE	2.5
1	BA	532	A	2.5
31	CA	52	A	2.5
31	CA	222	A	2.5
31	CA	394	C	2.5
31	CA	1278	C	2.5
31	CA	2047	C	2.5
31	CA	2146	C	2.5
45	CS	53	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
31	CA	2411	A	2.5
54	DA	2179	C	2.5
45	CS	102	SER	2.5
10	AJ	43	PRO	2.5
13	AM	47	GLU	2.5
1	AA	1034	G	2.5
1	BA	61	G	2.5
2	BB	41	ILE	2.5
3	BC	54	ARG	2.5
5	BE	157	ARG	2.5
9	BI	65	ILE	2.5
28	CB	41	G	2.5
31	CA	260	G	2.5
31	CA	1910	G	2.5
33	CF	82	GLY	2.5
35	CH	80	ILE	2.5
37	CK	83	GLY	2.5
46	CT	46	LEU	2.5
2	AB	187	VAL	2.5
18	AR	47	THR	2.5
20	BT	58	VAL	2.5
22	C1	44	THR	2.5
33	CF	18	THR	2.5
51	CY	4	VAL	2.5
23	C2	19	HIS	2.5
38	CL	37	ASP	2.5
42	CP	2	ASP	2.5
53	DI	29	ASP	2.5
53	DI	80	THR	2.5
31	CA	2178	C	2.5
31	CA	2787	C	2.5
35	CH	69	ALA	2.5
38	CL	83	ALA	2.5
39	CM	76	GLU	2.5
1	BA	1145	A	2.5
9	AI	33	ARG	2.5
31	CA	118	A	2.5
31	CA	244	A	2.5
31	CA	1302	A	2.5
32	DE	9	GLN	2.5
35	CH	123	ARG	2.5
39	CM	65	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
52	CZ	39	GLN	2.5
5	BE	115	LEU	2.5
19	BS	16	LEU	2.5
1	BA	88	U	2.5
1	BA	1290	G	2.5
31	CA	1248	G	2.5
31	CA	1455	G	2.5
31	CA	1647	U	2.5
31	CA	1719	G	2.5
20	BT	19	LYS	2.5
22	C1	12	LYS	2.5
23	C2	17	THR	2.5
30	CD	133	THR	2.5
32	DE	6	LYS	2.5
33	CF	145	LYS	2.5
35	CH	128	HIS	2.5
35	CH	135	HIS	2.5
43	CQ	25	THR	2.5
10	BJ	66	GLU	2.5
37	CK	9	GLU	2.5
11	AK	98	ARG	2.5
1	BA	1226	C	2.5
31	CA	240	C	2.5
31	CA	1726	C	2.5
31	CA	1986	C	2.5
39	CM	34	GLY	2.5
1	BA	1269	A	2.5
1	BA	1324	A	2.5
11	AK	42	LEU	2.5
17	BQ	64	CYS	2.5
18	AR	68	LEU	2.5
29	CC	93	LEU	2.5
31	CA	631	A	2.5
31	CA	1254	A	2.5
31	CA	1635	A	2.5
44	CR	66	ASN	2.5
1	BA	1148	U	2.5
12	BL	119	VAL	2.5
13	BM	27	LYS	2.5
14	AN	47	LYS	2.5
30	CD	204	LYS	2.5
28	CB	64	G	2.5

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Mol	Chain	Res	Type	RSRZ
31	CA	277	G	2.5
31	CA	1355	G	2.5
31	CA	1361	G	2.5
31	CA	1521	G	2.5
31	CA	2242	G	2.5
32	CE	50	ALA	2.5
34	CG	13	ALA	2.5
2	AB	124	GLY	2.5
7	AG	82	GLY	2.5
41	CO	105	GLY	2.5
7	BG	124	LEU	2.5
31	CA	385	C	2.5
43	CQ	19	SER	2.5
50	CX	74	PRO	2.5
1	BA	197	A	2.5
20	BT	84	ASN	2.5
31	CA	1847	A	2.5
54	DA	1073	A	2.5
54	DA	1084	A	2.5
1	BA	1205	U	2.5
28	CB	32	U	2.5
54	DA	1176	U	2.5
2	BB	30	PHE	2.5
8	BH	90	ASP	2.5
3	BC	123	GLN	2.5
13	AM	38	GLY	2.5
31	CA	15	G	2.5
31	CA	54	G	2.5
31	CA	604	G	2.5
31	CA	1633	G	2.5
31	CA	2732	G	2.5
29	CC	74	ILE	2.5
48	CV	17	LYS	2.5
1	BA	469	C	2.5
1	AA	121	U	2.5
17	BQ	13	VAL	2.5
17	BQ	23	VAL	2.5
35	CH	45	GLU	2.5
54	DA	1058	U	2.5
2	AB	64	LYS	2.5
13	BM	91	HIS	2.5
15	BO	7	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
33	CF	78	LYS	2.5
34	CG	123	ALA	2.5
41	CO	111	ALA	2.5
50	CX	66	LYS	2.5
1	BA	1365	G	2.5
28	CB	96	G	2.5
31	CA	333	G	2.5
31	CA	883	G	2.5
31	CA	2816	G	2.5
37	CK	140	LEU	2.5
43	DQ	114	LEU	2.5
48	DV	48	PRO	2.4
49	CW	20	LEU	2.5
31	CA	420	C	2.4
31	CA	817	C	2.4
31	CA	2066	C	2.4
2	AB	50	PHE	2.4
31	CA	306	U	2.4
34	CG	101	ASN	2.4
41	CO	107	ASN	2.4
44	CR	110	VAL	2.4
3	BC	112	ASP	2.4
31	CA	1598	A	2.4
10	BJ	70	HIS	2.4
29	CC	15	HIS	2.4
30	CD	102	ALA	2.4
33	CF	168	ALA	2.4
35	CH	59	ALA	2.4
7	BG	123	GLU	2.4
14	AN	26	GLU	2.4
15	BO	67	LEU	2.4
29	CC	259	SER	2.4
31	CA	690	G	2.4
54	DA	1059	G	2.4
54	DA	2107	G	2.4
1	AA	1148	U	2.4
28	CB	28	C	2.4
31	CA	67	U	2.4
31	CA	897	C	2.4
31	CA	1732	C	2.4
31	CA	2275	C	2.4
5	AE	82	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
10	BJ	29	ALA	2.4
35	DH	148	ALA	2.4
39	CM	72	ALA	2.4
1	BA	152	A	2.4
1	BA	1213	A	2.4
31	CA	255	A	2.4
12	BL	86	ARG	2.4
32	CE	44	ARG	2.4
46	CT	110	ARG	2.4
2	BB	214	LEU	2.4
7	AG	120	LEU	2.4
2	BB	193	PRO	2.4
33	CF	120	LYS	2.4
43	CQ	14	LYS	2.4
2	BB	191	SER	2.4
2	BB	226	SER	2.4
3	BC	122	SER	2.4
14	BN	14	VAL	2.4
16	AP	38	PHE	2.4
21	AU	37	PHE	2.4
1	AA	1033	G	2.4
26	C5	13	ASN	2.4
31	CA	27	G	2.4
31	CA	366	C	2.4
31	CA	1466	U	2.4
31	CA	1507	C	2.4
31	CA	2522	U	2.4
54	DA	1083	U	2.4
31	CA	2152	G	2.4
13	BM	100	GLN	2.4
39	CM	53	GLY	2.4
11	AK	56	ARG	2.4
14	BN	15	ALA	2.4
21	BU	17	ARG	2.4
34	CG	68	ALA	2.4
35	CH	65	ALA	2.4
2	AB	31	ILE	2.4
2	BB	15	HIS	2.4
14	BN	71	HIS	2.4
33	CF	134	GLU	2.4
30	CD	2	ILE	2.4
31	CA	6	A	2.4

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Mol	Chain	Res	Type	RSRZ
31	CA	547	A	2.4
31	CA	1260	A	2.4
31	CA	2059	A	2.4
36	DJ	122	ILE	2.4
25	C4	38	THR	2.4
40	CN	74	THR	2.4
50	CX	43	THR	2.4
16	BP	15	PRO	2.4
29	CC	231	PRO	2.4
45	CS	77	PHE	2.4
9	BI	34	SER	2.4
14	BN	5	SER	2.4
8	BH	122	GLY	2.4
11	BK	43	GLY	2.4
21	BU	9	ASN	2.4
1	BA	990	C	2.4
11	BK	13	ARG	2.4
24	C3	39	ARG	2.4
39	CM	33	ARG	2.4
54	DA	1727	C	2.4
1	BA	351	G	2.4
1	BA	944	G	2.4
16	BP	7	ALA	2.4
19	BS	20	GLU	2.4
26	C5	30	GLU	2.4
37	CK	20	ALA	2.4
33	CF	9	LYS	2.4
8	BH	121	LEU	2.4
11	BK	97	ILE	2.4
35	CH	12	LEU	2.4
6	BF	92	THR	2.4
31	CA	1096	A	2.4
31	CA	1142	A	2.4
31	CA	2322	A	2.4
43	CQ	92	VAL	2.4
53	DI	33	VAL	2.4
1	BA	992	U	2.4
2	BB	153	ASP	2.4
26	C5	24	ARG	2.4
35	DH	123	ARG	2.4
41	CO	101	GLY	2.4
35	CH	20	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
51	CY	16	ASN	2.4
2	AB	83	ALA	2.4
29	CC	210	ALA	2.4
31	CA	509	C	2.4
31	CA	2310	C	2.4
53	DI	83	ALA	2.4
12	BL	49	LEU	2.4
31	CA	1186	G	2.4
31	CA	2409	G	2.4
2	BB	156	GLY	2.4
11	AK	16	VAL	2.4
15	BO	79	THR	2.4
29	CC	29	PRO	2.4
29	CC	204	VAL	2.4
31	CA	149	A	2.4
31	CA	2060	A	2.4
31	CA	2154	A	2.4
31	CA	2346	A	2.4
31	CA	2639	A	2.4
31	CA	2758	A	2.4
31	CA	2778	A	2.4
33	CF	108	VAL	2.4
31	CA	2079	U	2.4
34	CG	135	GLY	2.4
35	DH	92	GLY	2.4
39	CM	69	ARG	2.4
43	CQ	101	ARG	2.4
39	CM	36	LYS	2.4
50	CX	27	GLY	2.4
5	BE	75	ALA	2.4
8	BH	116	ALA	2.4
34	CG	65	ALA	2.4
31	CA	540	C	2.4
31	CA	854	C	2.4
2	AB	41	ILE	2.4
15	BO	3	LEU	2.4
30	CD	138	LEU	2.4
22	C1	42	HIS	2.4
1	AA	1024	G	2.4
31	CA	205	G	2.4
31	CA	489	G	2.4
31	CA	539	G	2.4

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Mol	Chain	Res	Type	RSRZ
31	CA	875	G	2.4
2	BB	107	VAL	2.4
3	AC	105	GLU	2.4
10	BJ	51	VAL	2.4
13	AM	62	LYS	2.4
34	CG	29	LYS	2.4
41	CO	99	LYS	2.4
33	CF	166	GLY	2.4
31	CA	392	U	2.4
1	BA	1036	A	2.4
11	AK	38	GLN	2.4
31	CA	1097	U	2.4
31	CA	1486	U	2.4
28	CB	29	A	2.4
31	CA	677	A	2.4
31	CA	1354	A	2.4
31	CA	1522	A	2.4
11	BK	25	ALA	2.4
24	C3	13	ASN	2.4
35	CH	39	ALA	2.4
31	CA	680	C	2.4
50	CX	80	ILE	2.4
53	DI	95	LEU	2.4
21	AU	34	ARG	2.4
24	C3	2	LYS	2.4
41	CO	45	ARG	2.4
45	CS	71	LYS	2.4
49	CW	79	ARG	2.4
18	AR	32	TYR	2.4
1	AA	1029	U	2.4
1	BA	69	G	2.4
3	BC	70	THR	2.4
20	BT	13	GLN	2.4
34	CG	164	TYR	2.4
31	CA	543	G	2.4
31	CA	1865	U	2.4
31	CA	2061	G	2.4
31	CA	2633	G	2.4
36	DJ	64	ASP	2.4
1	AA	80	A	2.4
1	BA	66	A	2.4
12	BL	113	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
28	CB	15	A	2.4
31	CA	1508	A	2.4
35	CH	105	ALA	2.4
49	CW	74	ALA	2.4
51	CY	39	TRP	2.4
53	DI	22	ALA	2.4
54	DA	1080	A	2.4
16	AP	74	LEU	2.4
36	CJ	103	ARG	2.4
36	CJ	109	ILE	2.4
31	CA	351	C	2.4
31	CA	672	C	2.4
31	CA	1306	C	2.4
31	CA	2888	C	2.4
2	AB	39	HIS	2.3
40	CN	9	PHE	2.3
3	BC	15	VAL	2.3
9	AI	47	VAL	2.3
11	AK	32	VAL	2.3
51	CY	15	GLY	2.3
43	CQ	18	PRO	2.3
2	BB	159	ASP	2.3
46	CT	68	ASP	2.3
32	CE	84	THR	2.3
1	BA	846	G	2.3
7	AG	39	ALA	2.3
31	CA	26	G	2.3
31	CA	248	G	2.3
31	CA	620	G	2.3
31	CA	1116	G	2.3
31	CA	1983	G	2.3
41	CO	91	ALA	2.3
42	CP	71	ALA	2.3
47	CU	78	SER	2.3
1	AA	1	A	2.3
31	CA	1496	A	2.3
31	CA	1866	A	2.3
31	CA	2071	A	2.3
31	CA	2654	A	2.3
54	DA	2311	A	2.3
31	CA	517	C	2.3
5	BE	123	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
7	BG	27	VAL	2.3
45	CS	4	VAL	2.3
45	CS	76	LYS	2.3
2	AB	21	ARG	2.3
13	AM	37	ALA	2.3
34	CG	34	THR	2.3
9	BI	72	ILE	2.3
17	BQ	67	LEU	2.3
23	C2	48	ILE	2.3
37	CK	36	LEU	2.3
31	CA	185	G	2.3
31	CA	1137	G	2.3
1	BA	55	A	2.3
1	BA	1042	A	2.3
1	BA	1150	A	2.3
30	CD	82	PHE	2.3
31	CA	515	A	2.3
31	CA	2753	A	2.3
1	BA	381	C	2.3
1	BA	1066	C	2.3
14	AN	98	LYS	2.3
21	BU	6	VAL	2.3
30	CD	49	GLN	2.3
30	CD	203	VAL	2.3
31	CA	2248	C	2.3
34	CG	22	GLN	2.3
42	CP	19	GLN	2.3
21	AU	13	ASP	2.3
31	CA	2296	U	2.3
31	CA	2312	U	2.3
31	CA	2818	U	2.3
39	CM	56	PRO	2.3
40	CN	77	PRO	2.3
42	CP	77	ALA	2.3
2	AB	211	THR	2.3
29	CC	257	THR	2.3
30	CD	95	SER	2.3
40	CN	17	ASN	2.3
48	CV	74	ASN	2.3
6	AF	42	TRP	2.3
9	BI	13	LYS	2.3
11	AK	75	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
14	AN	3	LYS	2.3
23	C2	38	LYS	2.3
31	CA	622	G	2.3
31	CA	971	G	2.3
32	CE	63	LYS	2.3
31	CA	1616	A	2.3
31	CA	2311	A	2.3
31	CA	2367	G	2.3
20	AT	61	GLN	2.3
1	BA	1132	C	2.3
24	C3	28	ARG	2.3
25	C4	26	HIS	2.3
29	CC	65	VAL	2.3
29	CC	232	HIS	2.3
37	CK	47	HIS	2.3
41	CO	64	ARG	2.3
54	DA	278	A	2.3
31	CA	393	C	2.3
31	CA	584	C	2.3
31	CA	898	C	2.3
31	CA	1117	C	2.3
31	CA	1728	C	2.3
31	CA	2527	C	2.3
31	CA	2830	C	2.3
6	AF	66	ALA	2.3
9	BI	78	ALA	2.3
45	CS	42	ALA	2.3
19	AS	47	LEU	2.3
8	BH	89	LYS	2.3
40	CN	126	ILE	2.3
46	CT	96	ILE	2.3
50	DX	10	THR	2.3
14	BN	62	ASN	2.3
13	AM	113	ARG	2.3
1	AA	1001	C	2.3
31	CA	132	G	2.3
31	CA	381	G	2.3
31	CA	1208	C	2.3
31	CA	1456	G	2.3
31	CA	1642	G	2.3
31	CA	1922	G	2.3
31	CA	2325	G	2.3

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Mol	Chain	Res	Type	RSRZ
31	CA	2435	A	2.3
13	AM	10	PRO	2.3
13	BM	82	ASP	2.3
19	BS	64	ASP	2.3
31	CA	2321	U	2.3
31	CA	2815	C	2.3
31	CA	2903	U	2.3
35	DH	141	LYS	2.3
40	CN	103	TYR	2.3
42	CP	72	ALA	2.3
2	AB	162	PHE	2.3
2	AB	202	GLY	2.3
2	BB	74	ARG	2.3
6	BF	91	ARG	2.3
10	AJ	37	ARG	2.3
17	AQ	10	GLY	2.3
18	AR	73	ARG	2.3
21	BU	19	PHE	2.3
26	C5	36	ARG	2.3
29	CC	41	GLY	2.3
35	CH	34	GLY	2.3
19	BS	4	SER	2.3
17	BQ	29	VAL	2.3
8	BH	54	ASP	2.3
21	BU	8	GLU	2.3
32	CE	29	HIS	2.3
31	CA	25	U	2.3
1	BA	973	G	2.3
1	BA	1367	C	2.3
11	BK	66	ALA	2.3
31	CA	175	G	2.3
31	CA	254	G	2.3
31	CA	640	C	2.3
31	CA	1021	A	2.3
31	CA	1323	C	2.3
31	CA	1353	A	2.3
31	CA	1358	G	2.3
31	CA	2153	C	2.3
31	CA	2793	C	2.3
31	CA	2795	C	2.3
36	CJ	40	LYS	2.3
54	DA	1075	C	2.3

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Mol	Chain	Res	Type	RSRZ
54	DA	1870	C	2.3
14	BN	96	LEU	2.3
29	CC	112	ALA	2.3
34	CG	37	LEU	2.3
37	CK	118	MET	2.3
26	C5	23	ILE	2.3
42	CP	15	ARG	2.3
29	CC	266	PHE	2.3
32	CE	70	SER	2.3
37	CK	131	ASN	2.3
7	AG	105	VAL	2.3
32	DE	14	VAL	2.3
13	AM	50	GLU	2.3
35	DH	8	LYS	2.3
49	CW	14	LYS	2.3
1	AA	84	U	2.3
1	AA	1125	U	2.3
1	BA	960	U	2.3
3	BC	190	HIS	2.3
31	CA	1621	U	2.3
31	CA	2491	U	2.3
31	CA	2845	U	2.3
33	CF	46	ASP	2.3
35	DH	7	ASP	2.3
35	DH	128	HIS	2.3
1	BA	1384	C	2.3
1	BA	994	A	2.3
7	BG	10	ARG	2.3
27	C0	38	ARG	2.3
30	CD	71	ALA	2.3
31	CA	2104	C	2.3
31	CA	1469	A	2.3
34	CG	3	ARG	2.3
7	BG	7	ILE	2.3
7	BG	29	ILE	2.3
6	AF	8	PHE	2.3
28	CB	18	G	2.3
31	CA	1555	G	2.3
31	CA	2630	G	2.3
34	CG	53	GLY	2.3
12	BL	34	CYS	2.3
2	AB	115	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
21	AU	5	LYS	2.3
29	CC	97	LYS	2.3
11	BK	84	VAL	2.3
25	C4	8	ARG	2.3
33	CF	115	ARG	2.3
41	CO	88	ALA	2.3
2	AB	111	ILE	2.3
31	CA	320	A	2.3
31	CA	804	A	2.3
31	CA	1134	A	2.3
44	CR	15	LYS	2.3
54	DA	2154	A	2.3
2	AB	89	GLN	2.3
31	CA	2688	G	2.3
31	CA	2852	G	2.3
16	BP	3	THR	2.2
22	C1	54	VAL	2.2
30	CD	34	VAL	2.2
35	CH	79	THR	2.2
35	DH	20	ASN	2.2
39	CM	110	VAL	2.2
3	AC	127	ARG	2.2
4	AD	154	ARG	2.2
49	CW	9	ARG	2.2
1	BA	1358	U	2.2
15	BO	18	ASP	2.2
22	C1	19	HIS	2.2
2	BB	104	TRP	2.2
5	BE	124	LEU	2.2
7	AG	61	ALA	2.2
37	CK	126	ALA	2.2
11	AK	94	GLU	2.2
30	CD	17	GLU	2.2
31	CA	105	C	2.2
31	CA	995	C	2.2
31	CA	1472	C	2.2
32	CE	51	GLU	2.2
1	BA	74	A	2.2
54	DA	1057	A	2.2
17	BQ	11	ARG	2.2
53	DI	4	ASN	2.2
1	AA	1187	G	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	58	G	2.2
31	CA	396	G	2.2
31	CA	491	G	2.2
31	CA	1401	G	2.2
31	CA	1429	G	2.2
31	CA	1445	G	2.2
36	CJ	102	SER	2.2
39	CM	40	SER	2.2
1	BA	84	U	2.2
1	BA	991	U	2.2
2	BB	87	CYS	2.2
16	AP	46	LYS	2.2
2	AB	84	ALA	2.2
3	BC	87	LEU	2.2
36	DJ	74	PRO	2.2
11	AK	107	ILE	2.2
15	BO	11	ILE	2.2
16	AP	75	ILE	2.2
29	CC	83	TYR	2.2
36	DJ	141	GLU	2.2
42	CP	84	GLU	2.2
26	C5	37	GLN	2.2
28	CB	47	C	2.2
31	CA	1488	C	2.2
9	AI	58	VAL	2.2
11	AK	129	VAL	2.2
53	DI	108	VAL	2.2
1	BA	71	A	2.2
1	BA	609	A	2.2
28	CB	53	A	2.2
54	DA	2886[A]	A	2.2
37	CK	78	THR	2.2
22	C1	28	LEU	2.2
31	CA	1	G	2.2
31	CA	801	G	2.2
31	CA	1296	G	2.2
31	CA	1382	G	2.2
31	CA	2690	U	2.2
35	DH	13	GLY	2.2
35	DH	54	LEU	2.2
3	AC	77	ILE	2.2
36	DJ	123	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
41	CO	77	ALA	2.2
42	CP	57	ALA	2.2
45	CS	23	GLU	2.2
23	D2	28	ARG	2.2
29	CC	270	ARG	2.2
1	BA	1200	C	2.2
9	BI	120	LYS	2.2
20	AT	58	VAL	2.2
30	CD	92	VAL	2.2
31	CA	1398	C	2.2
31	CA	2200	C	2.2
40	CN	71	LYS	2.2
1	BA	263	A	2.2
1	BA	478	A	2.2
1	BA	978	A	2.2
1	BA	1151	A	2.2
2	BB	68	LEU	2.2
3	BC	44	THR	2.2
26	C5	21	GLY	2.2
28	CB	73	A	2.2
31	CA	1916	A	2.2
37	CK	38	GLY	2.2
39	CM	37	GLY	2.2
51	CY	2	SER	2.2
54	DA	2169	A	2.2
4	AD	113	GLU	2.2
10	AJ	10	LEU	2.2
31	CA	1779	U	2.2
32	CE	68	ALA	2.2
39	CM	51	GLU	2.2
10	BJ	18	ILE	2.2
35	DH	44	ILE	2.2
49	CW	16	ALA	2.2
51	CY	73	ALA	2.2
2	AB	7	ARG	2.2
10	AJ	62	ARG	2.2
31	CA	768	G	2.2
31	CA	1540	G	2.2
31	CA	1860	G	2.2
46	CT	1	MET	2.2
36	DJ	105	GLN	2.2
46	CT	18	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
12	BL	51	LYS	2.2
23	C2	50	LYS	2.2
48	CV	97	LYS	2.2
1	BA	1325	C	2.2
11	AK	74	VAL	2.2
29	CC	268	VAL	2.2
31	CA	238	C	2.2
31	CA	334	C	2.2
31	CA	2681	C	2.2
3	AC	83	ASP	2.2
9	AI	91	ASP	2.2
9	BI	53	GLU	2.2
15	BO	14	GLU	2.2
20	BT	70	ASN	2.2
39	CM	49	GLY	2.2
43	DQ	115	ASN	2.2
45	CS	57	GLY	2.2
1	AA	306	A	2.2
1	BA	1318	A	2.2
2	BB	69	PHE	2.2
12	BL	114	ARG	2.2
16	AP	50	THR	2.2
19	AS	77	THR	2.2
20	AT	80	THR	2.2
31	CA	243	U	2.2
31	CA	2743	U	2.2
31	CA	2433	A	2.2
31	CA	2837	A	2.2
34	CG	149	ARG	2.2
38	CL	109	SER	2.2
40	CN	40	ARG	2.2
42	CP	91	SER	2.2
49	CW	63	ILE	2.2
53	DI	113	PHE	2.2
25	C4	3	LYS	2.2
34	DG	99	LYS	2.2
31	CA	841	G	2.2
31	CA	1300	G	2.2
31	CA	1449	G	2.2
31	CA	2029	G	2.2
54	DA	1074	G	2.2
54	DA	2156	G	2.2

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Mol	Chain	Res	Type	RSRZ
12	BL	52	VAL	2.2
36	DJ	9	VAL	2.2
40	CN	92	TRP	2.2
1	BA	1112	C	2.2
29	CC	6	CYS	2.2
31	CA	1053	C	2.2
32	CE	2	GLU	2.2
39	CM	22	GLY	2.2
9	BI	49	ARG	2.2
34	CG	170	ARG	2.2
39	CM	41	ARG	2.2
41	CO	72	ASP	2.2
43	CQ	40	LEU	2.2
44	CR	22	LYS	2.2
54	DA	2797	U	2.2
2	AB	67	ILE	2.2
35	CH	63	ALA	2.2
35	DH	4	ILE	2.2
35	DH	69	ALA	2.2
1	BA	459	A	2.2
9	BI	51	PRO	2.2
13	AM	96	PRO	2.2
31	CA	196	A	2.2
31	CA	699	A	2.2
31	CA	1156	A	2.2
31	CA	1287	A	2.2
31	CA	1876	A	2.2
43	CQ	26	VAL	2.2
51	CY	7	VAL	2.2
9	BI	89	GLU	2.2
21	AU	8	GLU	2.2
31	CA	1408	G	2.2
31	CA	1421	G	2.2
31	CA	2659	G	2.2
1	BA	1460	C	2.2
9	AI	27	LYS	2.2
24	C3	25	LYS	2.2
31	CA	1607	C	2.2
32	CE	40	ARG	2.2
36	DJ	29	GLY	2.2
40	CN	6	ARG	2.2
45	CS	90	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
9	AI	94	LEU	2.2
30	CD	200	ASP	2.2
31	CA	1409	U	2.2
39	CM	66	PHE	2.2
41	CO	11	ASN	2.2
11	BK	102	ALA	2.2
17	AQ	21	ILE	2.2
24	C3	8	SER	2.2
27	C0	14	ILE	2.2
34	CG	97	ALA	2.2
38	CL	14	SER	2.2
49	CW	40	ILE	2.2
3	BC	69	HIS	2.2
47	DU	24	MET	2.2
31	CA	1877	A	2.2
3	BC	116	VAL	2.2
7	AG	60	GLU	2.2
11	BK	20	VAL	2.2
26	C5	15	LYS	2.2
27	C0	36	VAL	2.2
29	CC	172	VAL	2.2
32	CE	102	ARG	2.2
44	CR	28	ARG	2.2
1	AA	1320	C	2.2
1	BA	64	G	2.2
1	BA	267	C	2.2
1	BA	322	C	2.2
1	BA	1051	C	2.2
31	CA	537	G	2.2
31	CA	585	G	2.2
31	CA	1071	G	2.2
31	CA	1148	U	2.2
31	CA	1645	G	2.2
43	CQ	24	ASP	2.2
11	AK	45	ALA	2.2
32	CE	39	ALA	2.2
32	CE	182	ALA	2.2
2	AB	154	MET	2.2
4	AD	178	MET	2.2
9	AI	9	THR	2.2
3	BC	72	ARG	2.2
29	CC	18	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
40	CN	135	VAL	2.2
42	CP	7	ARG	2.2
9	AI	8	GLY	2.1
30	CD	135	GLY	2.1
31	CA	637	A	2.2
31	CA	2850	A	2.2
19	AS	15	LEU	2.1
19	AS	74	PHE	2.1
31	CA	2807	U	2.1
49	CW	26	PHE	2.1
1	BA	995	C	2.1
6	AF	6	ILE	2.1
17	AQ	9	GLN	2.1
31	CA	106	C	2.1
31	CA	246	C	2.1
31	CA	445	C	2.1
34	CG	64	GLN	2.1
37	CK	67	ASN	2.1
1	AA	201	G	2.1
1	BA	112	G	2.1
30	CD	23	PRO	2.1
31	CA	914	G	2.1
31	CA	2286	G	2.1
39	CM	136	GLU	2.1
40	CN	47	GLU	2.1
41	CO	39	PRO	2.1
52	CZ	9	LYS	2.1
52	DZ	2	LYS	2.1
54	DA	1171	G	2.1
3	BC	88	ARG	2.1
16	BP	28	ARG	2.1
47	CU	18	GLU	2.1
29	CC	223	THR	2.1
8	BH	71	VAL	2.1
19	AS	51	VAL	2.1
36	DJ	70	VAL	2.1
5	AE	76	LEU	2.1
9	BI	35	LEU	2.1
13	AM	63	PHE	2.1
37	CK	60	ASP	2.1
52	DZ	49	ASP	2.1
1	BA	93	U	2.1

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Mol	Chain	Res	Type	RSRZ
1	BA	1123	U	2.1
8	BH	36	ILE	2.1
10	AJ	20	GLN	2.1
23	C2	8	LYS	2.1
30	CD	146	ILE	2.1
31	CA	667	U	2.1
36	DJ	31	GLN	2.1
42	CP	23	ALA	2.1
44	CR	84	LYS	2.1
31	CA	2712	C	2.1
1	BA	1309	G	2.1
29	CC	230	HIS	2.1
31	CA	17	G	2.1
31	CA	24	G	2.1
31	CA	1038	G	2.1
31	CA	1452	G	2.1
31	CA	1992	G	2.1
48	CV	100	SER	2.1
2	AB	224	GLY	2.1
5	BE	114	VAL	2.1
9	AI	66	THR	2.1
11	BK	30	THR	2.1
12	BL	93	VAL	2.1
32	CE	14	VAL	2.1
34	CG	14	GLY	2.1
2	AB	57	LEU	2.1
2	AB	132	LYS	2.1
18	AR	25	ASP	2.1
32	CE	99	LYS	2.1
33	DF	78	LYS	2.1
35	CH	89	LYS	2.1
31	CA	734	A	2.1
31	CA	1373	A	2.1
46	CT	109	ASP	2.1
2	BB	111	ILE	2.1
8	BH	35	ALA	2.1
9	BI	121	ALA	2.1
31	CA	2473	U	2.1
32	CE	25	GLU	2.1
31	CA	1102	C	2.1
31	CA	2362	C	2.1
8	BH	123	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
30	CD	50	VAL	2.1
37	CK	124	VAL	2.1
45	CS	67	GLY	2.1
1	BA	1144	G	2.1
28	CB	67	G	2.1
31	CA	618	G	2.1
31	CA	831	G	2.1
31	CA	1124	G	2.1
31	CA	1266	G	2.1
31	CA	1475	G	2.1
31	CA	2067	G	2.1
31	CA	2444	G	2.1
42	CP	3	LYS	2.1
48	CV	4	LYS	2.1
11	BK	100	LEU	2.1
16	BP	32	PHE	2.1
18	BR	23	TYR	2.1
20	BT	31	PHE	2.1
47	DU	87	LEU	2.1
1	BA	467	U	2.1
1	BA	1122	U	2.1
3	BC	110	GLU	2.1
3	BC	170	GLU	2.1
4	BD	35	GLU	2.1
13	AM	3	ARG	2.1
51	CY	28	ARG	2.1
13	AM	53	ILE	2.1
31	CA	422	A	2.1
31	CA	429	A	2.1
46	CT	93	ALA	2.1
10	AJ	58	ASN	2.1
2	BB	154	MET	2.1
9	AI	125	PRO	2.1
31	CA	436	C	2.1
31	CA	1462	C	2.1
35	CH	126	GLY	2.1
39	CM	87	GLY	2.1
53	DI	89	PRO	2.1
12	BL	87	VAL	2.1
30	CD	199	SER	2.1
37	CK	120	ARG	2.1
39	CM	18	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	BA	148	G	2.1
2	AB	8	ASP	2.1
10	BJ	60	ASP	2.1
31	CA	407	G	2.1
31	CA	1063	G	2.1
31	CA	2087	G	2.1
31	CA	2857	G	2.1
41	CO	43	GLU	2.1
35	CH	18	GLN	2.1
31	CA	2401	U	2.1
35	DH	39	ALA	2.1
37	CK	81	ILE	2.1
30	CD	11	MET	2.1
31	CA	10	A	2.1
31	CA	2868	A	2.1
31	CA	2873	A	2.1
45	CS	43	ASN	2.1
1	BA	1045	C	2.1
1	BA	1140	C	2.1
1	BA	1443	C	2.1
17	BQ	22	VAL	2.1
31	CA	853	C	2.1
31	CA	1295	C	2.1
52	CZ	50	VAL	2.1
2	BB	108	ARG	2.1
4	BD	47	ARG	2.1
49	CW	44	HIS	2.1
2	BB	220	THR	2.1
21	BU	16	LEU	2.1
30	CD	156	PHE	2.1
45	CS	99	THR	2.1
47	CU	51	PHE	2.1
51	CY	38	PHE	2.1
24	C3	6	GLN	2.1
1	BA	224	U	2.1
1	BA	1232	U	2.1
3	BC	55	ILE	2.1
10	AJ	8	ILE	2.1
11	BK	45	ALA	2.1
1	BA	1187	G	2.1
14	BN	76	LYS	2.1
29	CC	253	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
30	CD	209	ALA	2.1
31	CA	649	G	2.1
46	CT	42	LYS	2.1
29	CC	209	GLY	2.1
2	AB	217	VAL	2.1
6	BF	84	VAL	2.1
14	AN	13	ARG	2.1
31	CA	528	A	2.1
31	CA	972	A	2.1
31	CA	1008	A	2.1
31	CA	1286	A	2.1
31	CA	2336	A	2.1
39	CM	123	ARG	2.1
6	BF	58	HIS	2.1
7	AG	123	GLU	2.1
10	BJ	54	SER	2.1
28	CB	30	C	2.1
30	CD	100	LEU	2.1
30	CD	145	SER	2.1
31	CA	678	C	2.1
31	CA	692	C	2.1
31	CA	994	C	2.1
32	CE	107	SER	2.1
35	DH	135	HIS	2.1
2	BB	127	ASP	2.1
8	BH	48	ASP	2.1
13	BM	114	LYS	2.1
38	CL	2	ILE	2.1
41	CO	106	ASP	2.1
47	CU	39	THR	2.1
1	BA	1308	U	2.1
11	AK	79	ILE	2.1
16	BP	67	ILE	2.1
31	CA	2299	U	2.1
19	BS	8	GLY	2.1
39	DM	102	GLY	2.1
3	BC	164	ARG	2.1
24	C3	3	ARG	2.1
20	BT	21	ASN	2.1
31	CA	245	G	2.1
31	CA	370	G	2.1
31	CA	561	G	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	612	G	2.1
31	CA	859	G	2.1
31	CA	1055	G	2.1
44	CR	53	ARG	2.1
54	DA	1091	G	2.1
1	BA	1216	A	2.1
1	BA	1267	C	2.1
5	AE	81	LEU	2.1
10	AJ	102	LEU	2.1
16	BP	12	LYS	2.1
31	CA	125	A	2.1
31	CA	239	C	2.1
31	CA	1039	A	2.1
31	CA	1170	C	2.1
31	CA	1646	C	2.1
31	CA	2160	C	2.1
31	CA	2176	A	2.1
31	CA	2882	A	2.1
37	CK	23	LYS	2.1
54	DA	2142	A	2.1
17	BQ	9	GLN	2.1
12	BL	97	THR	2.1
18	AR	45	THR	2.1
20	BT	12	ILE	2.1
31	CA	2585	U	2.1
35	DH	52	ALA	2.1
45	CS	41	ILE	2.1
9	AI	117	GLY	2.1
24	C3	38	GLY	2.1
53	DI	31	ARG	2.1
53	DI	46	ARG	2.1
6	AF	90	MET	2.1
8	AH	110	VAL	2.1
46	CT	2	GLU	2.1
51	CY	44	LYS	2.1
53	DI	103	ASN	2.1
1	BA	111	G	2.1
1	BA	275	G	2.1
1	BA	1385	G	2.1
2	BB	50	PHE	2.1
31	CA	68	G	2.1
31	CA	107	G	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	1807	G	2.1
31	CA	2822	G	2.1
31	CA	2846	G	2.1
33	CF	20	PHE	2.1
35	DH	47	PHE	2.1
50	CX	45	PHE	2.1
54	DA	2885[A]	G	2.1
16	BP	74	LEU	2.0
30	CD	140	HIS	2.0
1	BA	176	C	2.0
1	BA	217	C	2.0
1	BA	316	C	2.0
1	BA	1285	A	2.0
16	BP	68	SER	2.0
31	CA	1735	A	2.0
31	CA	2179	C	2.0
3	BC	180	ALA	2.0
7	BG	84	THR	2.0
14	AN	20	TYR	2.0
15	AO	11	ILE	2.0
21	BU	15	ALA	2.0
31	CA	2259	U	2.0
32	CE	26	ALA	2.0
42	CP	113	ALA	2.0
12	BL	104	CYS	2.0
2	BB	128	LYS	2.0
19	BS	17	LYS	2.0
34	CG	124	GLU	2.0
38	CL	53	LYS	2.0
47	CU	54	GLU	2.0
48	DV	47	LYS	2.0
5	AE	74	VAL	2.0
15	BO	29	VAL	2.0
16	BP	36	VAL	2.0
37	CK	48	VAL	2.0
44	CR	104	VAL	2.0
48	CV	34	VAL	2.0
29	CC	86	ASN	2.0
51	CY	32	ASN	2.0
4	AD	21	LEU	2.0
7	BG	23	LEU	2.0
46	CT	33	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	AA	95	C	2.0
1	BA	1186	G	2.0
2	BB	63	ARG	2.0
1	AA	1188	A	2.0
1	BA	136	C	2.0
1	BA	1251	A	2.0
31	CA	440	C	2.0
31	CA	953	G	2.0
31	CA	1478	G	2.0
31	CA	1493	C	2.0
31	CA	1644	C	2.0
31	CA	1811	G	2.0
31	CA	2156	G	2.0
31	CA	2669	G	2.0
41	CO	2	ARG	2.0
48	CV	65	ILE	2.0
52	CZ	7	ARG	2.0
1	BA	92	U	2.0
1	BA	323	U	2.0
8	AH	116	ALA	2.0
22	C1	56	ALA	2.0
25	C4	21	GLY	2.0
30	CD	85	ALA	2.0
12	BL	39	THR	2.0
15	AO	22	THR	2.0
29	CC	36	LYS	2.0
42	CP	22	GLY	2.0
7	AG	141	VAL	2.0
20	BT	35	VAL	2.0
30	CD	122	VAL	2.0
38	CL	84	CYS	2.0
41	CO	100	CYS	2.0
2	AB	158	PRO	2.0
30	CD	152	PRO	2.0
34	DG	101	ASN	2.0
3	BC	65	ARG	2.0
12	BL	72	HIS	2.0
44	CR	64	ARG	2.0
3	BC	75	ILE	2.0
4	AD	31	LYS	2.0
14	AN	28	LYS	2.0
20	BT	6	SER	2.0

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Mol	Chain	Res	Type	RSRZ
34	CG	134	LYS	2.0
37	CK	71	ASP	2.0
1	BA	62	U	2.0
1	BA	91	U	2.0
1	BA	132	C	2.0
1	BA	166	U	2.0
1	BA	331	G	2.0
31	CA	275	C	2.0
31	CA	564	C	2.0
38	CL	28	SER	2.0
1	BA	1329	A	2.0
22	C1	49	TYR	2.0
31	CA	665	U	2.0
31	CA	324	A	2.0
31	CA	1517	G	2.0
31	CA	2455	G	2.0
31	CA	2722	G	2.0
31	CA	2813	A	2.0
54	DA	2159	G	2.0
3	BC	173	VAL	2.0
8	BH	111	MET	2.0
19	AS	66	MET	2.0
27	C0	57	VAL	2.0
5	BE	150	PRO	2.0
15	BO	54	ARG	2.0
41	CO	87	PHE	2.0
20	BT	61	GLN	2.0
35	CH	73	ASN	2.0
3	BC	89	LYS	2.0
40	CN	8	LYS	2.0
47	CU	9	LYS	2.0
51	DY	77	LYS	2.0
6	AF	36	ILE	2.0
32	CE	198	GLU	2.0
39	CM	26	GLY	2.0
40	CN	48	ALA	2.0
42	CP	37	ALA	2.0
48	DV	57	GLY	2.0
1	BA	464	U	2.0
1	BA	1354	U	2.0
19	AS	25	SER	2.0
31	CA	269	C	2.0

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Mol	Chain	Res	Type	RSRZ
31	CA	987	C	2.0
31	CA	1447	C	2.0
1	AA	1285	A	2.0
31	CA	469	G	2.0
31	CA	911	A	2.0
31	CA	1193	G	2.0
31	CA	2134	A	2.0
31	CA	2144	G	2.0
31	CA	2482	A	2.0
31	CA	2812	G	2.0
34	CG	11	VAL	2.0
52	DZ	53	VAL	2.0
54	DA	1733	G	2.0
41	CO	4	ARG	2.0
43	CQ	20	PHE	2.0
19	AS	31	LEU	2.0
3	BC	8	ASN	2.0
35	CH	43	ASN	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
31	OMG	CA	2251	24/25	0.88	0.23	-	85,90,93,93	0
54	5MU	DA	747	21/22	0.98	0.17	-	26,28,32,37	0
31	PSU	CA	2605	20/21	0.92	0.20	-	79,81,83,84	0
1	2MG	BA	1516	24/25	0.88	0.20	-	79,86,93,95	0
1	5MC	BA	967	21/22	0.72	0.33	-	149,158,161,161	0
31	2MG	CA	1835	24/25	0.93	0.17	-	71,73,76,77	0
31	2MA	CA	2503	23/24	0.78	0.30	-	107,109,110,110	0
54	OMG	DA	2251	24/25	0.98	0.17	-	23,27,30,30	0
54	PSU	DA	746	20/21	0.98	0.18	-	28,30,33,36	0
31	5MC	CA	1962	21/22	0.93	0.18	-	70,77,80,82	0
31	PSU	CA	1917	20/21	0.81	0.26	-	120,125,134,134	0
1	PSU	BA	516	20/21	0.90	0.16	-	80,89,91,94	0
31	5MU	CA	747	21/22	0.83	0.23	-	116,120,122,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	PSU	DA	1917	20/21	0.94	0.15	-	80,84,91,91	0
54	5MC	DA	1962	21/22	0.97	0.20	-	44,46,49,50	0
1	5MC	AA	1407	21/22	0.97	0.13	-	51,52,54,55	0
31	PSU	CA	746	20/21	0.84	0.22	-	116,118,119,120	0
54	H2U	DA	2449	20/21	0.98	0.20	-	24,27,28,32	0
54	6MZ	DA	1618	23/24	0.99	0.19	-	25,28,31,33	0
54	PSU	DA	2605	20/21	0.97	0.18	-	33,42,46,46	0
40	4D4	DN	81[B]	12/13	0.96	0.23	-	26,28,31,32	9
1	MA6	AA	1518	24/25	0.98	0.16	-	50,54,56,57	0
12	D2T	BL	89	10/11	0.88	0.28	-	83,85,93,94	0
31	2MG	CA	2445	24/25	0.86	0.34	-	97,100,102,102	0
40	4D4	DN	81[A]	12/13	0.96	0.23	-	30,36,49,50	9
31	6MZ	CA	1618	23/24	0.89	0.25	-	134,138,143,145	0
1	MA6	BA	1519	24/25	0.92	0.23	-	80,82,87,88	0
1	UR3	BA	1498	21/22	0.93	0.14	-	84,87,94,94	0
1	G7M	AA	527	24/25	0.97	0.15	-	55,58,62,63	0
1	MA6	BA	1518	24/25	0.92	0.23	-	84,86,92,93	0
1	4OC	BA	1402	22/23	0.94	0.16	-	74,77,79,80	0
54	PSU	DA	2604	20/21	0.96	0.20	-	36,42,53,53	0
1	PSU	AA	516	20/21	0.96	0.14	-	76,78,82,82	0
31	G7M	CA	2069	24/25	0.83	0.27	-	102,104,108,109	0
31	OMU	CA	2552	21/22	0.86	0.43	-	88,92,94,95	0
1	5MC	AA	967	21/22	0.93	0.16	-	74,88,90,91	0
31	OMC	CA	2498	21/22	0.91	0.26	-	91,94,95,95	0
54	2MG	DA	2445	24/25	0.98	0.20	-	14,25,28,29	0
31	6MZ	CA	2030	23/24	0.84	0.26	-	101,104,106,107	0
31	PSU	CA	1911	20/21	0.86	0.27	-	127,137,139,140	0
54	OMC	DA	2498	21/22	0.99	0.20	-	21,22,27,29	0
30	MEQ	DD	150[A]	10/11	0.96	0.24	-	17,22,27,29	10
31	3TD	CA	1915	21/22	0.80	0.30	-	149,155,157,158	0
1	2MG	AA	966	24/25	0.93	0.15	-	79,84,91,91	0
30	MEQ	CD	150	9/11	0.88	0.28	-	92,98,133,136	0
31	PSU	CA	2504	20/21	0.85	0.23	-	93,103,106,106	0
31	PSU	CA	955	20/21	0.83	0.23	-	100,105,108,108	0
1	2MG	AA	1207	24/25	0.92	0.15	-	99,103,105,108	0
54	PSU	DA	955	20/21	0.99	0.20	-	25,26,29,30	0
31	5MU	CA	1939	21/22	0.92	0.17	-	70,77,78,80	0
1	G7M	BA	527	24/25	0.94	0.14	-	70,73,78,79	0
54	PSU	DA	2504	20/21	0.98	0.18	-	45,53,56,57	0
54	6MZ	DA	2030	23/24	0.99	0.21	-	13,23,28,28	0
54	2MG	DA	1835	24/25	0.97	0.20	-	53,55,56,58	0
54	G7M	DA	2069	24/25	0.99	0.19	-	24,30,37,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	PSU	CA	2457	20/21	0.91	0.17	-	96,97,99,99	0
1	UR3	AA	1498	21/22	0.97	0.16	-	54,56,61,63	0
31	1MG	CA	745	24/25	0.91	0.25	-	103,107,111,114	0
54	2MA	DA	2503	23/24	0.98	0.19	-	26,42,46,47	0
54	PSU	DA	2457	20/21	0.99	0.18	-	20,28,30,31	0
54	3TD	DA	1915	21/22	0.91	0.21	-	105,110,116,117	0
54	OMU	DA	2552	21/22	0.98	0.22	-	35,37,44,47	0
1	2MG	BA	1207	24/25	0.87	0.27	-	150,152,156,160	0
40	4D4	CN	81	12/13	0.89	0.30	-	108,112,131,132	0
30	MEQ	DD	150[B]	10/11	0.96	0.24	-	25,29,41,41	10
31	PSU	CA	2580	20/21	0.86	0.20	-	93,99,101,101	0
1	2MG	BA	966	24/25	0.78	0.29	-	149,156,167,168	0
54	PSU	DA	2580	20/21	0.98	0.21	-	24,30,36,37	0
1	4OC	AA	1402	22/23	0.97	0.16	-	52,59,61,62	0
54	1MG	DA	745	24/25	0.99	0.20	-	19,26,31,33	0
54	5MU	DA	1939	21/22	0.98	0.19	-	31,36,38,39	0
12	D2T	AL	89	10/11	0.92	0.23	-	60,63,71,72	0
1	2MG	AA	1516	24/25	0.96	0.15	-	52,54,56,57	0
1	5MC	BA	1407	21/22	0.87	0.21	-	98,109,111,115	0
54	PSU	DA	1911	20/21	0.94	0.17	-	83,90,91,92	0
1	MA6	AA	1519	24/25	0.97	0.16	-	53,56,61,65	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(\AA^2)	Q<0.9
58	PUT	DA	3212	6/6	0.89	0.65	96.95	47,53,59,60	0
55	MG	CA	3132	1/1	0.68	0.98	43.35	129,129,129,129	0
57	MPD	DA	3203	8/8	0.74	0.60	41.42	89,92,98,99	0
61	PEG	DA	3217	7/7	0.64	0.64	32.39	92,95,99,99	0
58	PUT	AA	1674	6/6	0.77	0.57	28.82	88,90,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
63	PGE	DA	3213	10/10	0.82	0.48	26.68	83,85,89,89	0
55	MG	DA	3172	1/1	0.54	0.59	26.63	86,86,86,86	0
55	MG	DA	3182	1/1	0.45	0.43	25.45	65,65,65,65	0
61	PEG	DA	3200	7/7	0.78	0.56	25.22	56,57,59,61	0
55	MG	CA	3002	1/1	0.31	2.03	24.13	278,278,278,278	0
55	MG	AA	1661	1/1	0.51	1.15	21.20	182,182,182,182	0
58	PUT	DA	3218	6/6	0.79	0.41	21.13	73,74,75,75	0
61	PEG	D3	102	7/7	0.74	1.16	20.72	73,79,82,82	0
58	PUT	DA	3220	6/6	0.82	0.42	19.88	93,96,99,100	0
57	MPD	AA	1676	8/8	0.59	0.64	19.36	97,99,100,103	0
55	MG	AA	1607	1/1	0.95	0.56	17.62	91,91,91,91	0
64	SPD	DA	3183	10/10	0.92	0.41	17.50	48,57,60,60	0
58	PUT	DA	3221	6/6	0.78	0.40	16.87	45,46,49,51	0
62	EDO	DA	3001	4/4	0.86	0.37	16.24	74,76,76,77	0
61	PEG	DQ	201	7/7	0.47	0.95	15.91	104,105,105,106	0
63	PGE	D1	102	10/10	0.66	0.67	15.79	89,92,93,93	0
55	MG	DA	3177	1/1	0.93	0.32	15.31	84,84,84,84	0
58	PUT	AA	1673	6/6	0.81	0.35	14.24	122,122,123,123	0
63	PGE	D3	101	10/10	0.67	0.61	14.21	82,83,87,87	0
55	MG	CA	3021	1/1	0.86	0.79	12.95	182,182,182,182	0
64	SPD	DA	3205	10/10	0.79	0.34	12.82	76,83,85,85	0
56	PG4	DA	3193	13/13	0.86	0.69	12.81	59,61,70,71	0
58	PUT	AA	1672	6/6	0.67	0.72	12.50	98,98,100,101	0
58	PUT	DA	3189	6/6	0.91	0.31	12.04	38,44,47,47	0
55	MG	DA	3127	1/1	0.98	0.34	11.69	71,71,71,71	0
57	MPD	DE	302	8/8	0.77	0.60	11.63	92,94,95,96	0
58	PUT	DA	3195	6/6	0.81	0.40	11.46	49,55,59,60	0
55	MG	DA	3125	1/1	0.74	0.46	11.22	84,84,84,84	0
65	1PE	DA	3202	16/16	0.85	0.42	11.19	52,59,65,67	0
57	MPD	DE	301	8/8	0.80	0.64	11.17	98,102,104,105	0
55	MG	CA	3146	1/1	0.58	0.49	10.01	76,76,76,76	1
55	MG	DA	3065	1/1	0.89	0.37	9.93	59,59,59,59	0
55	MG	CA	3109	1/1	0.03	0.99	9.34	175,175,175,175	0
57	MPD	DA	3192	8/8	0.85	0.46	8.95	68,72,74,74	0
62	EDO	DA	3197	4/4	0.92	0.27	8.82	66,66,67,67	0
66	ACY	DA	3201	4/4	0.91	0.28	7.99	53,56,57,57	0
63	PGE	DA	3224	10/10	0.83	0.34	7.58	79,85,88,88	0
57	MPD	AA	1671	8/8	0.90	0.72	7.54	96,98,99,101	0
56	PG4	DA	3215	13/13	0.83	0.27	7.50	91,98,100,100	0
63	PGE	DD	301	10/10	0.84	0.34	7.33	63,66,69,69	0
55	MG	AA	1642	1/1	0.67	0.41	7.09	153,153,153,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
64	SPD	DA	3223	10/10	0.92	0.27	7.00	39,42,46,46	0
57	MPD	DA	3206	8/8	0.72	0.53	6.85	93,94,95,95	0
56	PG4	DS	202	13/13	0.90	0.30	6.56	49,51,61,62	0
63	PGE	DU	101	10/10	0.85	0.44	6.26	62,68,78,78	0
65	1PE	DA	3185	16/16	0.90	0.22	5.82	42,50,62,64	0
61	PEG	D1	103	7/7	0.81	0.36	5.77	57,60,61,63	0
55	MG	CA	3136	1/1	0.74	0.59	5.74	156,156,156,156	0
62	EDO	D1	101	4/4	0.84	0.29	5.22	63,64,67,70	0
58	PUT	DA	3204	6/6	0.90	0.33	5.08	63,65,68,69	0
55	MG	AA	1612	1/1	0.86	0.30	5.03	65,65,65,65	0
55	MG	DA	3038	1/1	0.96	0.23	5.00	27,27,27,27	0
55	MG	CA	3130	1/1	0.85	0.36	4.89	101,101,101,101	0
61	PEG	AL	201	7/7	0.79	0.33	4.84	78,79,82,82	0
55	MG	CA	3025	1/1	0.24	0.48	4.41	180,180,180,180	0
55	MG	DA	3163	1/1	0.56	0.19	4.36	76,76,76,76	0
55	MG	DA	3014	1/1	0.98	0.29	4.13	24,24,24,24	0
64	SPD	DA	3187	10/10	0.93	0.25	3.96	32,35,43,46	0
56	PG4	BA	1601	13/13	0.82	0.33	3.83	90,95,98,99	0
58	PUT	DA	3211	6/6	0.84	0.28	3.75	57,65,66,66	0
55	MG	DA	3027	1/1	0.93	0.25	3.61	76,76,76,76	0
63	PGE	DS	201	10/10	0.84	0.32	3.24	61,66,67,68	0
55	MG	BA	1603	1/1	0.92	0.28	3.07	95,95,95,95	0
55	MG	CA	3150	1/1	0.85	0.30	3.01	80,80,80,80	0
55	MG	DA	3133	1/1	0.82	0.22	2.72	70,70,70,70	0
67	GUN	DA	3210	11/11	0.77	0.32	2.67	66,68,71,71	0
56	PG4	AA	1670	13/13	0.85	0.22	2.23	80,86,94,94	0
62	EDO	DA	3198	4/4	0.94	0.25	2.11	53,55,55,55	0
55	MG	DA	3128	1/1	0.91	0.20	1.75	73,73,73,73	0
55	MG	DA	3148	1/1	0.83	0.21	1.70	123,123,123,123	0
55	MG	DA	3111	1/1	0.96	0.21	1.70	38,38,38,38	0
55	MG	CA	3104	1/1	0.71	0.40	1.63	252,252,252,252	0
61	PEG	DL	201	7/7	0.88	0.21	1.50	69,70,71,71	0
56	PG4	DQ	202	13/13	0.86	0.26	1.37	62,65,71,71	0
55	MG	DA	3095	1/1	0.99	0.22	1.29	38,38,38,38	0
55	MG	AA	1647	1/1	0.97	0.20	1.15	201,201,201,201	0
55	MG	DA	3024	1/1	0.99	0.23	0.93	42,42,42,42	0
55	MG	DA	3023	1/1	0.98	0.20	0.83	27,27,27,27	0
59	TAC	AA	1678	32/32	0.90	0.19	0.50	64,73,81,82	0
55	MG	BA	1628	1/1	0.90	0.22	0.40	97,97,97,97	0
55	MG	BA	1616	1/1	0.81	0.17	0.35	136,136,136,136	0
55	MG	CA	3031	1/1	0.43	0.41	0.22	257,257,257,257	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	3088	1/1	0.89	0.23	0.14	90,90,90,90	0
55	MG	DA	3091	1/1	0.92	0.23	-0.01	28,28,28,28	0
55	MG	CA	3032	1/1	0.28	0.33	-0.08	194,194,194,194	0
55	MG	CA	3030	1/1	0.79	0.33	-0.10	128,128,128,128	0
55	MG	DA	3025	1/1	0.98	0.21	-0.14	26,26,26,26	0
57	MPD	DS	203	8/8	0.97	0.23	-0.17	36,40,42,44	0
55	MG	DA	3094	1/1	0.98	0.19	-0.26	25,25,25,25	0
55	MG	CA	3152	1/1	0.84	0.23	-0.40	87,87,87,87	0
55	MG	CA	3036	1/1	0.95	0.30	-0.47	235,235,235,235	0
55	MG	CA	3101	1/1	0.68	0.24	-0.50	115,115,115,115	0
55	MG	AA	1662	1/1	0.97	0.19	-0.71	84,84,84,84	0
55	MG	AA	1611	1/1	0.78	0.18	-0.71	88,88,88,88	0
55	MG	CA	3135	1/1	0.96	0.23	-0.84	90,90,90,90	0
55	MG	CA	3098	1/1	0.54	0.27	-0.86	231,231,231,231	0
55	MG	CA	3093	1/1	0.76	0.26	-0.94	151,151,151,151	0
55	MG	AA	1679	1/1	0.86	0.19	-0.98	163,163,163,163	0
55	MG	CA	3018	1/1	0.94	0.18	-1.01	78,78,78,78	0
58	PUT	DA	3002	6/6	0.96	0.21	-1.03	39,41,44,47	0
55	MG	AA	1657	1/1	0.73	0.20	-1.07	144,144,144,144	0
55	MG	DA	3113	1/1	0.98	0.21	-1.07	25,25,25,25	0
55	MG	CA	3010	1/1	0.97	0.27	-1.08	99,99,99,99	0
55	MG	BA	1626	1/1	0.36	0.20	-1.11	264,264,264,264	0
55	MG	BA	1615	1/1	0.94	0.18	-1.19	70,70,70,70	0
55	MG	CA	3053	1/1	0.26	0.18	-1.30	134,134,134,134	0
55	MG	AA	1668	1/1	0.97	0.14	-1.31	40,40,40,40	0
55	MG	CA	3017	1/1	0.85	0.17	-1.37	124,124,124,124	0
60	ZN	C5	101	1/1	0.97	0.08	-1.40	139,139,139,139	0
55	MG	CA	3008	1/1	0.90	0.23	-1.42	244,244,244,244	0
55	MG	AA	1644	1/1	0.76	0.14	-1.47	83,83,83,83	0
55	MG	DA	3018	1/1	0.98	0.19	-1.49	29,29,29,29	0
55	MG	CA	3060	1/1	0.58	0.15	-1.51	256,256,256,256	0
55	MG	CA	3102	1/1	0.81	0.18	-1.53	115,115,115,115	0
55	MG	CA	3062	1/1	0.84	0.24	-1.62	196,196,196,196	0
55	MG	DB	201	1/1	0.96	0.14	-1.65	63,63,63,63	0
55	MG	DA	3010	1/1	0.98	0.15	-1.70	24,24,24,24	0
60	ZN	D5	101	1/1	0.98	0.15	-1.76	55,55,55,55	0
55	MG	CA	3099	1/1	0.90	0.21	-1.81	101,101,101,101	0
55	MG	CA	3078	1/1	0.88	0.20	-1.86	134,134,134,134	0
59	TAC	BA	1602	32/32	0.85	0.15	-1.91	170,172,172,172	0
55	MG	BA	1624	1/1	0.87	0.12	-1.99	97,97,97,97	0
55	MG	CA	3094	1/1	0.94	0.08	-2.19	73,73,73,73	0
55	MG	AA	1637	1/1	0.86	0.08	-2.28	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CB	202	1/1	0.78	0.08	-2.29	128,128,128,128	0
55	MG	DA	3011	1/1	0.97	0.16	-2.34	24,24,24,24	0
55	MG	DA	3047	1/1	0.99	0.20	-2.38	34,34,34,34	0
55	MG	DA	3007	1/1	0.96	0.10	-2.41	111,111,111,111	0
55	MG	DA	3015	1/1	0.98	0.18	-2.42	17,17,17,17	0
55	MG	AA	1663	1/1	0.88	0.17	-2.47	76,76,76,76	0
55	MG	DA	3136	1/1	0.77	0.15	-2.60	100,100,100,100	0
55	MG	CB	201	1/1	0.96	0.06	-2.66	157,157,157,157	0
55	MG	DA	3036	1/1	0.94	0.18	-2.66	41,41,41,41	0
55	MG	BA	1614	1/1	0.93	0.13	-2.69	123,123,123,123	0
55	MG	CA	3012	1/1	0.72	0.21	-2.69	134,134,134,134	0
55	MG	BA	1610	1/1	0.66	0.15	-2.75	119,119,119,119	0
55	MG	DA	3104	1/1	0.99	0.13	-2.78	59,59,59,59	0
55	MG	DA	3227	1/1	0.93	0.14	-2.98	52,52,52,52	0
55	MG	DA	3123	1/1	0.95	0.15	-3.00	83,83,83,83	0
55	MG	BA	1619	1/1	0.40	0.13	-3.14	122,122,122,122	0
55	MG	DA	3044	1/1	0.98	0.14	-3.15	36,36,36,36	0
55	MG	DA	3032	1/1	0.95	0.19	-3.22	34,34,34,34	0
55	MG	CA	3050	1/1	0.94	0.16	-3.23	102,102,102,102	0
55	MG	DA	3059	1/1	0.98	0.14	-3.26	32,32,32,32	0
55	MG	DA	3019	1/1	0.98	0.12	-3.27	47,47,47,47	0
55	MG	CA	3039	1/1	0.65	0.12	-3.37	124,124,124,124	0
55	MG	DA	3110	1/1	0.99	0.20	-3.39	20,20,20,20	0
55	MG	BA	1607	1/1	0.89	0.09	-3.50	118,118,118,118	0
55	MG	AA	1633	1/1	0.84	0.12	-3.51	110,110,110,110	0
55	MG	DA	3060	1/1	0.98	0.13	-3.53	29,29,29,29	0
55	MG	BA	1622	1/1	0.95	0.11	-3.53	82,82,82,82	0
55	MG	DA	3064	1/1	0.97	0.12	-3.56	63,63,63,63	0
55	MG	CA	3085	1/1	0.69	0.18	-3.63	82,82,82,82	0
55	MG	DA	3072	1/1	0.98	0.12	-3.65	49,49,49,49	0
55	MG	CA	3051	1/1	0.88	0.11	-3.73	82,82,82,82	0
55	MG	CA	3005	1/1	0.85	0.18	-3.84	224,224,224,224	0
55	MG	DA	3051	1/1	0.98	0.14	-3.88	24,24,24,24	0
55	MG	CA	3100	1/1	0.83	0.10	-3.90	135,135,135,135	0
55	MG	CA	3019	1/1	0.87	0.09	-3.91	102,102,102,102	0
55	MG	DA	3085	1/1	0.98	0.15	-3.92	45,45,45,45	0
55	MG	AA	1656	1/1	0.91	0.14	-4.05	124,124,124,124	0
55	MG	AA	1639	1/1	0.87	0.07	-4.22	120,120,120,120	0
55	MG	CA	3087	1/1	0.90	0.10	-4.44	91,91,91,91	0
55	MG	AA	1643	1/1	0.97	0.14	-4.77	64,64,64,64	0
60	ZN	AB	301	1/1	0.71	0.18	-4.80	198,198,198,198	0
55	MG	BA	1617	1/1	0.97	0.07	-5.12	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3067	1/1	0.99	0.09	-5.15	51,51,51,51	0
55	MG	CA	3023	1/1	0.92	0.13	-5.24	134,134,134,134	0
55	MG	BA	1634	1/1	0.93	0.09	-5.32	66,66,66,66	0
55	MG	AA	1659	1/1	0.92	0.04	-5.49	73,73,73,73	0
55	MG	DA	3229	1/1	0.98	0.08	-5.51	38,38,38,38	0
55	MG	BA	1604	1/1	0.91	0.07	-5.55	99,99,99,99	0
55	MG	DA	3102	1/1	0.96	0.11	-5.63	52,52,52,52	0
55	MG	DA	3093	1/1	0.95	0.16	-5.83	31,31,31,31	0
63	PGE	DA	3186	10/10	0.96	0.15	-5.84	29,33,36,37	0
55	MG	CA	3043	1/1	0.96	0.10	-5.84	73,73,73,73	0
55	MG	DA	3100	1/1	0.96	0.16	-5.91	34,34,34,34	0
55	MG	CA	3143	1/1	0.80	0.08	-6.14	85,85,85,85	0
55	MG	BA	1612	1/1	0.87	0.07	-6.29	101,101,101,101	0
55	MG	AA	1631	1/1	0.98	0.07	-6.54	60,60,60,60	0
55	MG	DA	3030	1/1	0.97	0.13	-6.66	14,14,14,14	0
55	MG	DA	3096	1/1	0.93	0.10	-6.91	51,51,51,51	0
55	MG	AA	1646	1/1	0.95	0.07	-6.93	53,53,53,53	0
55	MG	DA	3098	1/1	0.97	0.08	-6.96	39,39,39,39	0
55	MG	DA	3005	1/1	0.88	0.12	-7.00	69,69,69,69	0
55	MG	DA	3151	1/1	0.80	0.10	-7.84	54,54,54,54	0
55	MG	DD	302	1/1	0.97	0.09	-7.92	53,53,53,53	0
55	MG	DA	3028	1/1	0.98	0.16	-8.37	41,41,41,41	0
55	MG	DA	3048	1/1	0.99	0.12	-11.06	47,47,47,47	0
55	MG	DA	3103	1/1	0.93	0.10	-11.21	46,46,46,46	0
55	MG	AA	1629	1/1	0.97	0.08	-12.81	82,82,82,82	0
55	MG	AA	1648	1/1	0.98	0.09	-13.04	63,63,63,63	0
55	MG	AA	1653	1/1	0.95	0.06	-14.03	81,81,81,81	0
55	MG	DA	3008	1/1	0.97	0.07	-21.33	73,73,73,73	0
55	MG	DA	3037	1/1	0.99	0.21	-	26,26,26,26	0
58	PUT	DA	3184	6/6	0.87	0.36	-	45,45,47,48	0
55	MG	AA	1604	1/1	0.83	0.35	-	64,64,64,64	0
55	MG	DA	3086	1/1	0.97	0.16	-	41,41,41,41	0
57	MPD	DT	201	8/8	0.76	0.36	-	85,87,92,92	0
55	MG	DA	3112	1/1	0.63	0.50	-	291,291,291,291	0
55	MG	DA	3049	1/1	0.93	0.13	-	31,31,31,31	0
55	MG	DR	203	1/1	0.92	0.44	-	108,108,108,108	0
55	MG	BA	1609	1/1	0.89	0.35	-	172,172,172,172	0
57	MPD	DA	3209	8/8	0.86	0.35	-	65,68,71,72	0
55	MG	DB	209	1/1	0.74	0.81	-	87,87,87,87	0
55	MG	DA	3122	1/1	0.88	0.26	-	86,86,86,86	0
55	MG	CA	3026	1/1	0.73	0.30	-	123,123,123,123	0
55	MG	DA	3173	1/1	0.56	0.89	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	3097	1/1	0.93	0.10	-	110,110,110,110	0
55	MG	CA	3057	1/1	0.70	0.34	-	128,128,128,128	0
55	MG	AA	1625	1/1	0.81	0.35	-	63,63,63,63	0
55	MG	CA	3024	1/1	0.92	0.25	-	104,104,104,104	0
55	MG	CA	3034	1/1	0.88	0.31	-	144,144,144,144	0
55	MG	BA	1629	1/1	0.63	1.63	-	124,124,124,124	0
55	MG	AA	1609	1/1	0.76	0.28	-	96,96,96,96	0
55	MG	AA	1610	1/1	0.76	0.52	-	97,97,97,97	0
55	MG	CB	203	1/1	0.13	0.11	-	146,146,146,146	0
55	MG	DA	3156	1/1	0.92	0.27	-	74,74,74,74	0
55	MG	BA	1608	1/1	0.47	0.18	-	243,243,243,243	0
55	MG	AA	1650	1/1	0.97	0.08	-	75,75,75,75	0
62	EDO	DA	3194	4/4	0.88	0.29	-	60,61,62,63	0
55	MG	DA	3041	1/1	0.94	0.08	-	50,50,50,50	0
55	MG	AA	1638	1/1	0.96	0.22	-	94,94,94,94	0
55	MG	DA	3134	1/1	0.82	0.25	-	65,65,65,65	0
55	MG	CA	3107	1/1	0.82	0.35	-	90,90,90,90	0
55	MG	AA	1613	1/1	0.91	0.97	-	68,68,68,68	0
55	MG	CA	3149	1/1	0.92	0.63	-	73,73,73,73	0
55	MG	CA	3045	1/1	0.95	0.08	-	142,142,142,142	0
55	MG	CA	3037	1/1	-0.11	0.45	-	256,256,256,256	0
55	MG	CA	3080	1/1	0.86	0.08	-	120,120,120,120	0
62	EDO	DA	3208	4/4	0.57	0.57	-	88,90,91,91	0
55	MG	DA	3142	1/1	0.92	0.36	-	73,73,73,73	0
56	PG4	DR	202	13/13	0.79	0.47	-	55,64,74,75	0
55	MG	DA	3118	1/1	0.88	0.24	-	65,65,65,65	0
58	PUT	DA	3188	6/6	0.93	0.25	-	30,31,33,39	0
55	MG	DA	3140	1/1	0.97	0.12	-	43,43,43,43	0
55	MG	CA	3059	1/1	0.02	0.72	-	240,240,240,240	0
55	MG	DA	3021	1/1	0.98	0.09	-	55,55,55,55	0
55	MG	DA	3063	1/1	0.92	0.24	-	219,219,219,219	0
55	MG	DA	3109	1/1	0.98	0.10	-	29,29,29,29	0
55	MG	CA	3072	1/1	0.97	0.51	-	255,255,255,255	0
55	MG	DA	3082	1/1	0.93	0.08	-	57,57,57,57	0
55	MG	AA	1626	1/1	0.47	1.85	-	104,104,104,104	0
55	MG	CA	3139	1/1	-0.17	0.64	-	128,128,128,128	0
55	MG	DA	3045	1/1	0.85	0.14	-	90,90,90,90	0
55	MG	DA	3121	1/1	0.93	0.40	-	90,90,90,90	0
55	MG	DA	3076	1/1	0.98	0.12	-	25,25,25,25	0
55	MG	DA	3074	1/1	0.98	0.16	-	32,32,32,32	0
55	MG	CA	3061	1/1	0.93	0.21	-	227,227,227,227	0
55	MG	CA	3110	1/1	0.30	1.04	-	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	3124	1/1	0.85	0.49	-	127,127,127,127	0
55	MG	AA	1623	1/1	0.76	0.68	-	74,74,74,74	0
55	MG	CA	3148	1/1	0.69	0.70	-	80,80,80,80	0
55	MG	CA	3027	1/1	0.47	0.26	-	277,277,277,277	0
55	MG	BA	1631	1/1	0.84	0.67	-	151,151,151,151	0
55	MG	CA	3127	1/1	0.73	0.27	-	85,85,85,85	0
55	MG	AA	1617	1/1	0.64	0.42	-	93,93,93,93	0
55	MG	CA	3120	1/1	0.88	0.38	-	75,75,75,75	0
55	MG	CA	3129	1/1	-0.01	0.75	-	118,118,118,118	0
55	MG	DA	3012	1/1	0.97	0.14	-	39,39,39,39	0
55	MG	CA	3013	1/1	0.62	0.22	-	251,251,251,251	0
55	MG	DA	3137	1/1	0.98	0.25	-	55,55,55,55	0
55	MG	DA	3126	1/1	0.78	0.26	-	70,70,70,70	0
55	MG	AA	1654	1/1	0.23	0.35	-	241,241,241,241	0
55	MG	BA	1606	1/1	0.53	0.26	-	190,190,190,190	0
55	MG	DA	3144	1/1	0.87	0.47	-	65,65,65,65	0
58	PUT	DA	3222	6/6	0.94	0.25	-	46,49,51,52	0
55	MG	DA	3145	1/1	0.41	0.81	-	111,111,111,111	0
55	MG	CA	3090	1/1	0.88	0.11	-	106,106,106,106	0
55	MG	DA	3114	1/1	0.90	0.10	-	59,59,59,59	0
55	MG	DA	3080	1/1	0.93	0.08	-	105,105,105,105	0
55	MG	BA	1645	1/1	0.98	0.06	-	87,87,87,87	0
55	MG	DA	3046	1/1	0.98	0.05	-	47,47,47,47	0
55	MG	DA	3056	1/1	0.97	0.21	-	39,39,39,39	0
55	MG	CA	3044	1/1	0.76	0.09	-	93,93,93,93	0
55	MG	BA	1642	1/1	0.89	0.70	-	164,164,164,164	0
55	MG	DA	3147	1/1	0.72	0.37	-	98,98,98,98	0
55	MG	AA	1624	1/1	0.61	1.11	-	92,92,92,92	0
55	MG	DA	3162	1/1	0.94	0.20	-	70,70,70,70	0
55	MG	DA	3174	1/1	0.85	0.39	-	79,79,79,79	0
55	MG	DA	3101	1/1	0.98	0.19	-	30,30,30,30	0
55	MG	BA	1625	1/1	0.61	1.00	-	231,231,231,231	0
55	MG	DA	3062	1/1	0.98	0.15	-	33,33,33,33	0
55	MG	CA	3122	1/1	-0.23	1.55	-	182,182,182,182	0
55	MG	DA	3179	1/1	0.34	0.71	-	100,100,100,100	0
55	MG	DA	3135	1/1	0.91	0.40	-	73,73,73,73	0
55	MG	CA	3155	1/1	-0.02	0.24	-	240,240,240,240	0
55	MG	AA	1636	1/1	0.65	0.24	-	103,103,103,103	0
55	MG	CA	3009	1/1	0.46	0.23	-	217,217,217,217	0
55	MG	DA	3017	1/1	0.98	0.12	-	56,56,56,56	0
55	MG	AA	1641	1/1	0.89	0.08	-	81,81,81,81	0
61	PEG	DA	3199	7/7	0.83	0.41	-	62,66,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3092	1/1	0.99	0.15	-	18,18,18,18	0
55	MG	CA	3119	1/1	0.50	0.61	-	188,188,188,188	0
55	MG	CA	3091	1/1	0.77	0.35	-	202,202,202,202	0
55	MG	DA	3050	1/1	0.93	0.14	-	35,35,35,35	0
55	MG	CA	3131	1/1	0.78	0.48	-	145,145,145,145	0
55	MG	CA	3049	1/1	0.86	0.13	-	81,81,81,81	0
55	MG	CA	3069	1/1	0.81	0.06	-	95,95,95,95	0
55	MG	BA	1621	1/1	0.94	0.15	-	103,103,103,103	0
55	MG	DA	3119	1/1	0.97	0.07	-	53,53,53,53	0
62	EDO	DA	3207	4/4	0.89	0.33	-	57,58,59,59	0
55	MG	AA	1665	1/1	0.78	0.31	-	158,158,158,158	0
55	MG	CA	3046	1/1	0.70	0.45	-	228,228,228,228	0
55	MG	CA	3029	1/1	0.94	0.16	-	113,113,113,113	0
55	MG	AA	1615	1/1	0.59	0.55	-	81,81,81,81	0
55	MG	CA	3154	1/1	0.86	0.37	-	200,200,200,200	0
55	MG	DA	3159	1/1	0.43	0.62	-	74,74,74,74	0
55	MG	DA	3139	1/1	0.91	0.64	-	58,58,58,58	1
55	MG	AA	1605	1/1	0.53	0.64	-	97,97,97,97	0
55	MG	DA	3040	1/1	0.93	0.16	-	30,30,30,30	0
55	MG	DA	3115	1/1	0.96	0.16	-	35,35,35,35	0
57	MPD	DK	201	8/8	0.83	0.25	-	91,92,94,95	0
55	MG	AA	1619	1/1	0.83	0.34	-	94,94,94,94	0
55	MG	BA	1627	1/1	0.68	0.21	-	264,264,264,264	0
55	MG	CA	3123	1/1	0.78	0.24	-	199,199,199,199	0
55	MG	DA	3078	1/1	0.96	0.10	-	32,32,32,32	0
55	MG	DA	3154	1/1	0.84	0.40	-	58,58,58,58	0
55	MG	BA	1643	1/1	0.75	0.32	-	134,134,134,134	0
55	MG	DA	3043	1/1	0.94	0.13	-	34,34,34,34	0
55	MG	CA	3079	1/1	0.77	0.52	-	177,177,177,177	0
55	MG	AA	1632	1/1	0.69	0.15	-	110,110,110,110	0
55	MG	CA	3081	1/1	0.73	0.35	-	153,153,153,153	0
55	MG	DA	3129	1/1	0.72	1.15	-	69,69,69,69	0
55	MG	CA	3115	1/1	0.92	0.60	-	76,76,76,76	0
55	MG	DA	3079	1/1	0.90	0.08	-	76,76,76,76	0
55	MG	CA	3052	1/1	0.94	0.19	-	96,96,96,96	0
55	MG	CA	3011	1/1	0.60	0.27	-	120,120,120,120	0
55	MG	CA	3063	1/1	0.77	0.61	-	257,257,257,257	0
55	MG	CA	3020	1/1	0.89	0.54	-	269,269,269,269	0
55	MG	BA	1639	1/1	0.81	0.67	-	88,88,88,88	0
55	MG	CA	3055	1/1	0.27	0.58	-	94,94,94,94	0
55	MG	DA	3016	1/1	0.97	0.18	-	62,62,62,62	0
55	MG	DA	3124	1/1	0.65	0.32	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	3141	1/1	0.26	0.41	-	115,115,115,115	0
55	MG	CA	3065	1/1	0.82	0.17	-	119,119,119,119	0
55	MG	BA	1633	1/1	0.90	0.08	-	57,57,57,57	0
55	MG	DA	3034	1/1	0.98	0.15	-	29,29,29,29	0
55	MG	DA	3088	1/1	0.96	0.14	-	56,56,56,56	0
55	MG	DA	3107	1/1	1.00	0.16	-	39,39,39,39	0
55	MG	CA	3082	1/1	0.74	0.20	-	229,229,229,229	0
55	MG	DA	3171	1/1	0.37	0.55	-	83,83,83,83	0
55	MG	DA	3132	1/1	0.88	0.29	-	66,66,66,66	0
55	MG	DA	3149	1/1	0.94	0.20	-	66,66,66,66	0
55	MG	CA	3108	1/1	0.93	0.41	-	72,72,72,72	0
55	MG	AA	1655	1/1	0.85	0.07	-	100,100,100,100	0
55	MG	CA	3070	1/1	0.42	0.20	-	188,188,188,188	0
55	MG	CA	3033	1/1	0.47	0.42	-	246,246,246,246	0
55	MG	DA	3029	1/1	0.94	0.14	-	49,49,49,49	0
55	MG	CA	3022	1/1	0.89	0.16	-	142,142,142,142	0
55	MG	DA	3157	1/1	0.72	0.46	-	69,69,69,69	0
68	TRS	DA	3219	8/8	0.71	0.48	-	95,98,100,101	0
55	MG	CA	3040	1/1	0.85	0.11	-	71,71,71,71	0
55	MG	AA	1614	1/1	0.65	0.51	-	126,126,126,126	0
55	MG	DA	3083	1/1	0.95	0.07	-	60,60,60,60	0
55	MG	CA	3066	1/1	0.68	0.78	-	284,284,284,284	0
55	MG	DA	3097	1/1	0.87	0.12	-	45,45,45,45	0
55	MG	DA	3077	1/1	0.95	0.14	-	22,22,22,22	0
55	MG	CA	3103	1/1	0.80	0.47	-	260,260,260,260	0
55	MG	BA	1618	1/1	0.87	0.12	-	144,144,144,144	0
55	MG	CA	3095	1/1	0.86	0.10	-	112,112,112,112	0
55	MG	DM	201	1/1	0.94	0.04	-	55,55,55,55	0
55	MG	DA	3057	1/1	0.95	0.12	-	49,49,49,49	0
55	MG	BA	1630	1/1	0.97	0.12	-	101,101,101,101	0
55	MG	AA	1652	1/1	0.98	0.24	-	40,40,40,40	0
55	MG	DA	3120	1/1	0.97	0.33	-	48,48,48,48	0
55	MG	DB	207	1/1	0.90	0.91	-	99,99,99,99	0
55	MG	CA	3092	1/1	0.57	0.13	-	113,113,113,113	0
55	MG	DA	3090	1/1	0.92	0.20	-	21,21,21,21	0
55	MG	DA	3180	1/1	0.49	1.29	-	99,99,99,99	0
55	MG	CA	3004	1/1	0.12	1.51	-	243,243,243,243	0
55	MG	CA	3042	1/1	0.96	0.09	-	92,92,92,92	0
66	ACY	DA	3196	4/4	0.80	0.29	-	79,80,80,80	0
55	MG	CA	3134	1/1	0.67	0.58	-	99,99,99,99	0
55	MG	DB	208	1/1	0.91	0.26	-	66,66,66,66	0
55	MG	DA	3175	1/1	0.58	0.60	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3026	1/1	1.00	0.10	-	29,29,29,29	0
55	MG	AA	1621	1/1	0.74	0.43	-	88,88,88,88	0
55	MG	BA	1623	1/1	0.80	0.28	-	37,37,37,37	0
55	MG	CA	3047	1/1	0.91	0.15	-	94,94,94,94	0
55	MG	CA	3075	1/1	0.47	0.11	-	215,215,215,215	0
55	MG	CA	3016	1/1	0.77	0.08	-	106,106,106,106	0
55	MG	DA	3054	1/1	0.97	0.09	-	47,47,47,47	0
55	MG	BA	1605	1/1	0.67	0.32	-	250,250,250,250	0
66	ACY	DA	3191	4/4	0.96	0.18	-	55,55,56,57	0
55	MG	CA	3076	1/1	0.65	0.59	-	246,246,246,246	0
55	MG	CA	3073	1/1	0.93	0.28	-	197,197,197,197	0
55	MG	DA	3058	1/1	0.98	0.06	-	37,37,37,37	0
55	MG	CA	3153	1/1	0.48	0.48	-	138,138,138,138	0
55	MG	DA	3116	1/1	0.98	0.12	-	45,45,45,45	0
55	MG	AA	1651	1/1	0.92	0.14	-	68,68,68,68	0
55	MG	CA	3054	1/1	0.41	0.16	-	201,201,201,201	0
55	MG	AA	1608	1/1	0.86	0.51	-	97,97,97,97	0
55	MG	DA	3035	1/1	0.98	0.17	-	20,20,20,20	0
55	MG	DA	3020	1/1	0.96	0.31	-	11,11,11,11	0
55	MG	BA	1611	1/1	0.85	0.13	-	191,191,191,191	0
61	PEG	DA	3226	7/7	0.89	0.32	-	55,59,63,64	0
55	MG	CA	3096	1/1	0.88	0.14	-	117,117,117,117	0
55	MG	AA	1627	1/1	0.73	0.36	-	88,88,88,88	0
55	MG	DA	3164	1/1	0.85	0.40	-	75,75,75,75	0
55	MG	DA	3033	1/1	0.97	0.19	-	19,19,19,19	0
55	MG	DA	3152	1/1	0.94	0.29	-	43,43,43,43	0
55	MG	DA	3106	1/1	0.99	0.17	-	32,32,32,32	0
55	MG	DA	3170	1/1	0.71	0.45	-	80,80,80,80	0
55	MG	DR	201	1/1	0.79	0.63	-	55,55,55,55	0
62	EDO	DA	3004	4/4	0.76	0.42	-	112,113,114,114	0
55	MG	CA	3114	1/1	0.80	0.37	-	102,102,102,102	0
55	MG	AA	1645	1/1	0.91	0.07	-	48,48,48,48	0
55	MG	CA	3140	1/1	0.70	0.47	-	91,91,91,91	0
55	MG	AA	1630	1/1	0.86	0.18	-	124,124,124,124	0
55	MG	CA	3067	1/1	0.66	0.18	-	239,239,239,239	0
55	MG	BA	1640	1/1	0.48	0.77	-	101,101,101,101	0
55	MG	CA	3068	1/1	0.81	0.19	-	107,107,107,107	0
55	MG	BA	1644	1/1	0.74	0.12	-	87,87,87,87	0
55	MG	DA	3108	1/1	0.90	0.18	-	39,39,39,39	0
55	MG	DA	3052	1/1	0.97	0.12	-	33,33,33,33	0
55	MG	AA	1669	1/1	0.92	0.11	-	109,109,109,109	0
55	MG	DA	3143	1/1	0.89	0.38	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3158	1/1	0.94	0.09	-	55,55,55,55	0
55	MG	DA	3230	1/1	0.97	0.34	-	37,37,37,37	0
55	MG	DB	206	1/1	0.44	0.48	-	106,106,106,106	0
55	MG	CA	3137	1/1	0.82	0.13	-	95,95,95,95	0
55	MG	DA	3131	1/1	0.79	0.32	-	85,85,85,85	0
62	EDO	DA	3003	4/4	0.86	0.44	-	47,49,50,50	0
57	MPD	DA	3190	8/8	0.89	0.26	-	87,88,89,93	0
55	MG	DA	3166	1/1	0.79	0.96	-	92,92,92,92	0
55	MG	CA	3038	1/1	0.60	0.58	-	154,154,154,154	0
55	MG	AA	1601	1/1	0.70	1.54	-	100,100,100,100	0
55	MG	DA	3031	1/1	0.99	0.17	-	35,35,35,35	0
55	MG	DA	3176	1/1	0.69	0.46	-	91,91,91,91	0
55	MG	DA	3155	1/1	0.76	0.58	-	71,71,71,71	0
55	MG	CA	3015	1/1	0.75	0.29	-	143,143,143,143	0
62	EDO	DA	3214	4/4	0.88	0.28	-	74,74,74,75	0
55	MG	AA	1622	1/1	-0.27	1.24	-	119,119,119,119	0
55	MG	AA	1634	1/1	0.86	0.11	-	106,106,106,106	0
55	MG	AA	1649	1/1	0.92	0.10	-	58,58,58,58	0
55	MG	DA	3069	1/1	0.99	0.19	-	36,36,36,36	0
55	MG	BA	1635	1/1	0.66	0.13	-	226,226,226,226	0
55	MG	DA	3165	1/1	0.86	0.29	-	74,74,74,74	0
55	MG	DA	3075	1/1	0.98	0.06	-	39,39,39,39	0
61	PEG	DP	201	7/7	0.77	0.61	-	90,92,94,94	0
55	MG	CA	3145	1/1	0.22	0.49	-	234,234,234,234	0
55	MG	CA	3064	1/1	0.81	0.14	-	107,107,107,107	0
55	MG	DB	205	1/1	0.94	0.20	-	64,64,64,64	0
55	MG	CA	3035	1/1	0.88	0.33	-	201,201,201,201	0
55	MG	DA	3066	1/1	0.97	0.14	-	22,22,22,22	0
55	MG	DA	3146	1/1	0.94	0.13	-	73,73,73,73	0
55	MG	AA	1664	1/1	0.94	0.13	-	161,161,161,161	0
55	MG	BA	1641	1/1	0.79	0.35	-	98,98,98,98	0
55	MG	AA	1606	1/1	0.32	0.45	-	108,108,108,108	0
55	MG	CA	3077	1/1	0.92	0.23	-	189,189,189,189	0
55	MG	BA	1636	1/1	0.72	0.08	-	112,112,112,112	0
55	MG	DA	3105	1/1	0.95	0.17	-	31,31,31,31	0
55	MG	AA	1602	1/1	0.96	0.29	-	82,82,82,82	0
55	MG	AA	1635	1/1	0.81	0.09	-	96,96,96,96	0
55	MG	DA	3070	1/1	0.98	0.18	-	54,54,54,54	0
55	MG	DA	3006	1/1	0.96	0.10	-	60,60,60,60	0
62	EDO	DB	211	4/4	0.93	0.26	-	74,74,75,75	0
55	MG	CA	3112	1/1	0.81	0.48	-	77,77,77,77	0
55	MG	CA	3003	1/1	0.88	0.35	-	218,218,218,218	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	C3	101	1/1	0.48	0.48	-	299,299,299,299	0
55	MG	DA	3013	1/1	0.92	0.15	-	67,67,67,67	0
55	MG	CA	3007	1/1	0.46	0.11	-	175,175,175,175	0
55	MG	CA	3089	1/1	0.88	0.94	-	209,209,209,209	0
55	MG	CA	3084	1/1	0.96	0.06	-	75,75,75,75	0
55	MG	DD	303	1/1	0.89	0.26	-	53,53,53,53	0
55	MG	BA	1637	1/1	0.95	0.20	-	99,99,99,99	0
55	MG	CA	3001	1/1	0.43	0.28	-	258,258,258,258	0
55	MG	CA	3121	1/1	0.16	1.41	-	125,125,125,125	0
55	MG	DA	3053	1/1	0.88	0.12	-	78,78,78,78	0
55	MG	DA	3178	1/1	0.49	0.55	-	100,100,100,100	0
55	MG	DA	3084	1/1	0.97	0.10	-	44,44,44,44	0
55	MG	DB	204	1/1	0.92	0.15	-	65,65,65,65	0
55	MG	CA	3041	1/1	0.86	0.10	-	90,90,90,90	0
55	MG	DA	3160	1/1	0.88	0.16	-	56,56,56,56	0
55	MG	DA	3068	1/1	0.93	0.08	-	67,67,67,67	0
55	MG	CA	3138	1/1	0.21	0.97	-	125,125,125,125	0
55	MG	AA	1677	1/1	0.97	0.12	-	78,78,78,78	0
55	MG	BA	1632	1/1	0.37	0.07	-	219,219,219,219	0
55	MG	AA	1658	1/1	0.96	0.13	-	83,83,83,83	0
55	MG	CA	3118	1/1	0.74	0.74	-	123,123,123,123	0
55	MG	AA	1616	1/1	0.27	0.72	-	94,94,94,94	0
55	MG	CA	3126	1/1	0.94	0.15	-	78,78,78,78	0
55	MG	CA	3086	1/1	0.94	0.07	-	93,93,93,93	0
55	MG	DA	3081	1/1	0.91	0.13	-	94,94,94,94	0
57	MPD	DT	202	8/8	0.74	0.41	-	88,89,90,92	0
55	MG	AA	1618	1/1	0.86	0.71	-	81,81,81,81	0
55	MG	AA	1628	1/1	0.18	0.59	-	142,142,142,142	0
55	MG	CA	3083	1/1	0.93	0.30	-	209,209,209,209	0
55	MG	DA	3089	1/1	0.98	0.11	-	46,46,46,46	0
55	MG	CA	3048	1/1	0.75	0.12	-	92,92,92,92	0
55	MG	AA	1667	1/1	0.93	0.12	-	51,51,51,51	0
55	MG	AA	1620	1/1	0.89	0.34	-	67,67,67,67	0
55	MG	AA	1603	1/1	0.55	0.60	-	110,110,110,110	0
55	MG	AA	1666	1/1	0.98	0.04	-	54,54,54,54	0
55	MG	DA	3055	1/1	0.98	0.09	-	55,55,55,55	0
61	PEG	DA	3225	7/7	0.80	0.34	-	60,63,70,71	0
55	MG	DA	3181	1/1	0.71	0.49	-	58,58,58,58	0
55	MG	CA	3028	1/1	0.86	0.31	-	172,172,172,172	0
55	MG	CA	3113	1/1	0.94	0.38	-	57,57,57,57	0
55	MG	CA	3133	1/1	-0.20	0.62	-	194,194,194,194	0
55	MG	DA	3138	1/1	0.67	0.25	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	3106	1/1	0.68	0.52	-	83,83,83,83	0
55	MG	DB	203	1/1	0.99	0.09	-	37,37,37,37	0
58	PUT	AA	1675	6/6	0.73	0.54	-	82,83,84,84	0
55	MG	DA	3073	1/1	0.92	0.18	-	45,45,45,45	0
55	MG	CA	3144	1/1	0.78	0.29	-	62,62,62,62	0
55	MG	DA	3009	1/1	0.95	0.08	-	89,89,89,89	0
55	MG	DA	3150	1/1	0.96	0.10	-	51,51,51,51	0
55	MG	DA	3039	1/1	0.98	0.15	-	27,27,27,27	0
55	MG	DA	3042	1/1	0.93	0.21	-	28,28,28,28	0
55	MG	DA	3071	1/1	0.95	0.08	-	90,90,90,90	0
55	MG	BA	1620	1/1	0.61	0.14	-	97,97,97,97	0
55	MG	DA	3130	1/1	0.35	0.34	-	81,81,81,81	0
55	MG	AA	1660	1/1	0.86	0.28	-	275,275,275,275	0
55	MG	CA	3147	1/1	0.64	0.82	-	80,80,80,80	1
55	MG	DA	3153	1/1	0.80	0.27	-	100,100,100,100	0
55	MG	AA	1640	1/1	0.91	0.09	-	61,61,61,61	0
55	MG	CA	3125	1/1	0.76	0.39	-	120,120,120,120	0
55	MG	CA	3074	1/1	0.43	1.09	-	243,243,243,243	0
55	MG	CA	3117	1/1	0.94	0.54	-	85,85,85,85	0
55	MG	CA	3006	1/1	0.72	0.62	-	242,242,242,242	0
55	MG	CA	3071	1/1	0.82	0.84	-	257,257,257,257	0
55	MG	CA	3116	1/1	0.72	0.78	-	101,101,101,101	0
55	MG	CA	3111	1/1	0.76	0.60	-	91,91,91,91	0
55	MG	CA	3105	1/1	0.50	0.36	-	92,92,92,92	0
55	MG	DA	3228	1/1	0.97	0.07	-	44,44,44,44	0
63	PGE	DA	3216	10/10	0.84	0.44	-	57,60,68,70	0
55	MG	CA	3151	1/1	0.80	0.33	-	209,209,209,209	0
55	MG	DA	3141	1/1	0.95	0.20	-	82,82,82,82	0
55	MG	CA	3058	1/1	0.91	0.22	-	137,137,137,137	0
55	MG	DA	3168	1/1	0.19	0.75	-	109,109,109,109	0
55	MG	DA	3167	1/1	0.63	0.50	-	80,80,80,80	0
55	MG	DA	3022	1/1	0.89	0.14	-	50,50,50,50	0
55	MG	DA	3099	1/1	0.88	0.15	-	81,81,81,81	0
62	EDO	DB	210	4/4	0.84	0.34	-	76,77,77,78	0
55	MG	CA	3014	1/1	0.95	0.26	-	71,71,71,71	0
55	MG	DA	3061	1/1	0.98	0.16	-	19,19,19,19	0
55	MG	DA	3161	1/1	0.82	0.39	-	69,69,69,69	0
55	MG	CA	3128	1/1	-0.10	0.46	-	135,135,135,135	0
55	MG	DA	3087	1/1	0.93	0.18	-	45,45,45,45	0
55	MG	BA	1613	1/1	0.90	0.14	-	54,54,54,54	0
57	MPD	DN	201	8/8	0.85	0.40	-	83,88,90,91	0
55	MG	DB	202	1/1	0.99	0.14	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3169	1/1	0.97	0.20	-	72,72,72,72	0
55	MG	DA	3117	1/1	0.96	0.06	-	32,32,32,32	0
55	MG	BA	1638	1/1	0.94	0.86	-	175,175,175,175	0
55	MG	CA	3142	1/1	0.89	0.42	-	85,85,85,85	0
55	MG	CA	3056	1/1	0.72	0.20	-	119,119,119,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.