



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 27, 2016 – 03:34 AM EDT

PDB ID : 5IT8
Title : High-resolution structure of the Escherichia coli ribosome
Authors : Cocozaki, A.; Ferguson, A.
Deposited on : 2016-03-16
Resolution : 3.12 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

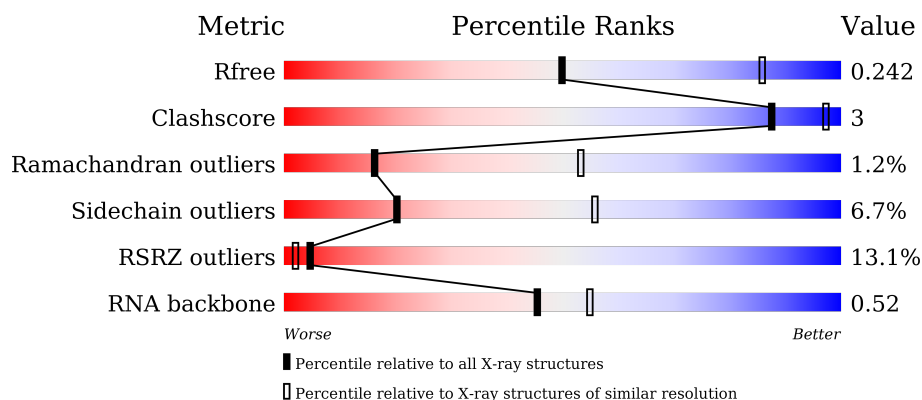
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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.



















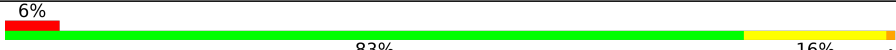
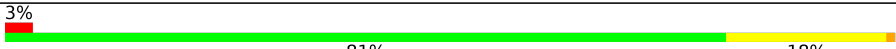

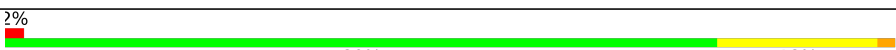





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)
RNA backbone	2183	1010 (3.54-2.70)

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>0%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>
1	BA	1534	<div> <div>9%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>.</div> </div> </div>
2	AB	224	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>16%</div> <div>.</div> </div> </div>
2	BB	224	<div> <div>8%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>.</div> </div> </div>

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

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Mol	Chain	Length	Quality of chain
15	BO	88	<div> <div>2%</div> <div>86%</div> <div>13%</div> </div>
16	AP	82	<div> <div>6%</div> <div>91%</div> <div>9%</div> </div>
16	BP	82	<div> <div>21%</div> <div>82%</div> <div>17%</div> </div>
17	AQ	80	<div> <div>6%</div> <div>83%</div> <div>18%</div> </div>
17	BQ	80	<div> <div>21%</div> <div>74%</div> <div>25%</div> </div>
18	AR	55	<div> <div>89%</div> <div>11%</div> </div>
18	BR	55	<div> <div>7%</div> <div>96%</div> </div>
19	AS	79	<div> <div>5%</div> <div>80%</div> <div>18%</div> </div>
19	BS	79	<div> <div>71%</div> <div>80%</div> <div>16%</div> </div>
20	AT	86	<div> <div>%</div> <div>88%</div> <div>9%</div> </div>
20	BT	86	<div> <div>35%</div> <div>74%</div> <div>19%</div> <div>6%</div> </div>
21	AU	56	<div> <div>18%</div> <div>80%</div> <div>20%</div> </div>
21	BU	56	<div> <div>2%</div> <div>80%</div> <div>20%</div> </div>
22	C1	56	<div> <div>45%</div> <div>80%</div> <div>16%</div> </div>
22	D1	56	<div> <div>77%</div> <div>21%</div> </div>
23	C2	51	<div> <div>67%</div> <div>76%</div> <div>22%</div> </div>
23	D2	51	<div> <div>82%</div> <div>18%</div> </div>
24	C3	46	<div> <div>46%</div> <div>83%</div> <div>15%</div> </div>
24	D3	46	<div> <div>93%</div> <div>7%</div> </div>
25	C4	64	<div> <div>27%</div> <div>92%</div> <div>8%</div> </div>
25	D4	64	<div> <div>89%</div> <div>11%</div> </div>
26	C5	38	<div> <div>42%</div> <div>89%</div> <div>11%</div> </div>
26	D5	38	<div> <div>97%</div> </div>
27	C0	58	<div> <div>29%</div> <div>78%</div> <div>21%</div> </div>
27	D0	58	<div> <div>86%</div> <div>14%</div> </div>










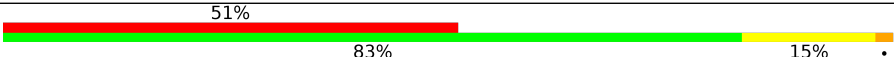









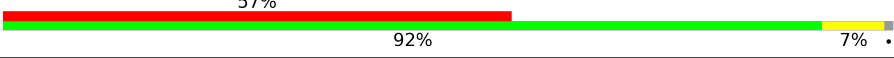




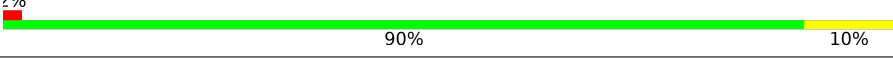
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Mol	Chain	Length	Quality of chain
28	CB	120	
28	DB	120	
29	CC	271	
29	DC	271	
30	CD	209	
31	CA	2904	
32	DD	209	
33	DA	2903	
34	CE	201	
34	DE	201	
35	CF	177	
35	DF	177	
36	CG	176	
36	DG	176	
37	CH	149	
37	DH	149	
38	CJ	134	
38	DJ	134	
39	CK	142	
39	DK	142	
40	CL	123	
40	DL	123	
41	CM	144	
41	DM	144	
42	CN	136	

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Mol	Chain	Length	Quality of chain
42	DN	136	
43	CO	125	
43	DO	125	
44	CP	117	
44	DP	117	
45	CQ	114	
45	DQ	114	
46	CR	117	
46	DR	117	
47	CS	103	
47	DS	103	
48	CT	110	
48	DT	110	
49	CU	93	
49	DU	93	
50	CV	102	
50	DV	102	
51	CW	94	
51	DW	94	
52	CX	76	
52	DX	76	
53	CY	77	
53	DY	77	
54	CZ	62	
54	DZ	62	

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Mol	Chain	Length	Quality of chain
55	DI	135	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	1608	-	-	-	X
56	MG	AA	1612	-	-	-	X
56	MG	AA	1642	-	-	-	X
56	MG	BA	1612	-	-	-	X
56	MG	BA	1624	-	-	-	X
56	MG	CA	3003	-	-	-	X
56	MG	CA	3022	-	-	-	X
56	MG	CA	3026	-	-	-	X
56	MG	CA	3032	-	-	-	X
56	MG	CA	3039	-	-	-	X
56	MG	CA	3110	-	-	-	X
56	MG	CA	3123	-	-	-	X
56	MG	CA	3133	-	-	-	X
56	MG	CA	3136	-	-	-	X
56	MG	DA	3126	-	-	-	X
56	MG	DA	3146	-	-	-	X
56	MG	DA	3171	-	-	-	X
56	MG	DA	3176	-	-	-	X
57	PG4	AA	1670	-	-	-	X
57	PG4	BA	1642	-	-	-	X
57	PG4	DA	3192	-	-	-	X
57	PG4	DA	3214	-	-	-	X
57	PG4	DS	202	-	-	-	X
58	MPD	AA	1671	-	-	-	X
58	MPD	AA	1676	-	-	-	X
58	MPD	DA	3191	-	-	-	X
58	MPD	DA	3202	-	-	-	X
58	MPD	DA	3205	-	-	-	X
58	MPD	DE	301	-	-	-	X
58	MPD	DE	302	-	-	-	X
59	PUT	AA	1672	-	-	-	X
59	PUT	AA	1673	-	-	-	X
59	PUT	AA	1674	-	-	-	X
59	PUT	DA	3183	-	-	-	X
59	PUT	DA	3188	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	PUT	DA	3194	-	-	-	X
59	PUT	DA	3203	-	-	-	X
59	PUT	DA	3210	-	-	-	X
59	PUT	DA	3211	-	-	-	X
59	PUT	DA	3217	-	-	-	X
59	PUT	DA	3219	-	-	-	X
59	PUT	DA	3220	-	-	-	X
59	PUT	DA	3221	-	-	-	X
59	PUT	DA	3227	-	-	-	X
61	PEG	AL	201	-	-	-	X
61	PEG	D1	102	-	-	-	X
61	PEG	D3	102	-	-	-	X
61	PEG	DA	3199	-	-	-	X
61	PEG	DA	3216	-	-	-	X
61	PEG	DL	201	-	-	-	X
61	PEG	DQ	201	-	-	-	X
62	EDO	D0	101	-	-	-	X
62	EDO	DA	3196	-	-	-	X
62	EDO	DA	3197	-	-	-	X
62	EDO	DA	3207	-	-	-	X
63	PGE	D3	101	-	-	-	X
63	PGE	DA	3185	-	-	-	X
63	PGE	DA	3212	-	-	-	X
63	PGE	DA	3215	-	-	-	X
63	PGE	DD	302	-	-	-	X
63	PGE	DS	201	-	-	-	X
63	PGE	DT	201	-	-	-	X
63	PGE	DU	101	-	-	-	X
64	SPD	DA	3182	-	-	-	X
64	SPD	DA	3204	-	-	-	X
64	SPD	DA	3222	-	-	-	X
65	1PE	DA	3184	-	-	-	X
65	1PE	DA	3201	-	-	-	X
66	ACY	DA	3200	-	-	-	X

2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295125 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			

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

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

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

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

- Molecule 33 is a RNA chain called 23S rRNA.

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

- Molecule 34 is a protein called 50S ribosomal protein L4.

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

- Molecule 35 is a protein called 50S ribosomal protein L5.

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

- Molecule 36 is a protein called 50S ribosomal protein L6.

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

- Molecule 37 is a protein called 50S ribosomal protein L9.

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

- Molecule 38 is a protein called 50S ribosomal protein L11.

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

- Molecule 39 is a protein called 50S ribosomal protein L13.

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

- Molecule 40 is a protein called 50S ribosomal protein L14.

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

- Molecule 41 is a protein called 50S ribosomal protein L15.

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

- Molecule 42 is a protein called 50S ribosomal protein L16.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 43 is a protein called 50S ribosomal protein L17.

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

- Molecule 44 is a protein called 50S ribosomal protein L18.

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

- Molecule 45 is a protein called 50S ribosomal protein L19.

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

- Molecule 46 is a protein called 50S ribosomal protein L20.

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

- Molecule 47 is a protein called 50S ribosomal protein L21.

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

- Molecule 48 is a protein called 50S ribosomal protein L22.

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

- Molecule 49 is a protein called 50S ribosomal protein L23.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L25.

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

- Molecule 52 is a protein called 50S ribosomal protein L27.

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

- Molecule 53 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	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
53	DY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 54 is a protein called 50S ribosomal protein L29.

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

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

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

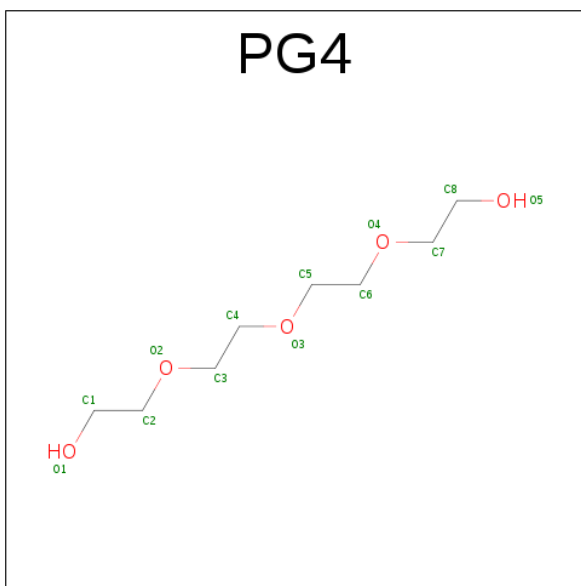
There are 2 discrepancies between the modelled and reference sequences:

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

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

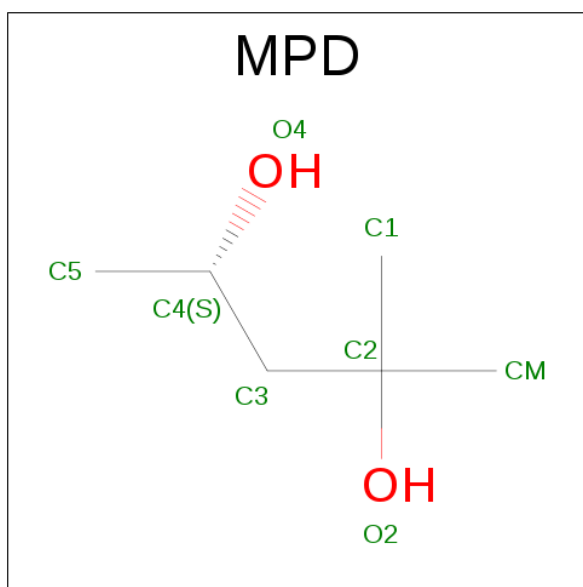
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BA	41	Total	Mg	0	0
			41	41		
56	DD	1	Total	Mg	0	0
			1	1		
56	CB	3	Total	Mg	0	0
			3	3		
56	DR	2	Total	Mg	0	0
			2	2		
56	AA	70	Total	Mg	0	0
			70	70		
56	DA	184	Total	Mg	0	0
			184	184		
56	DB	9	Total	Mg	0	0
			9	9		
56	CA	156	Total	Mg	0	0
			156	156		

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



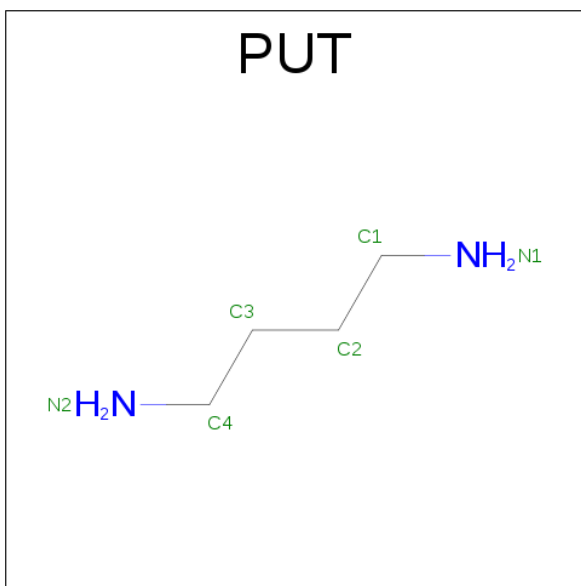
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			13	8	5		
57	BA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DQ	1	Total	C	O	0	0
			13	8	5		
57	DR	1	Total	C	O	0	0
			13	8	5		
57	DS	1	Total	C	O	0	0
			13	8	5		

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



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

- Molecule 59 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula: C₄H₁₂N₂).



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

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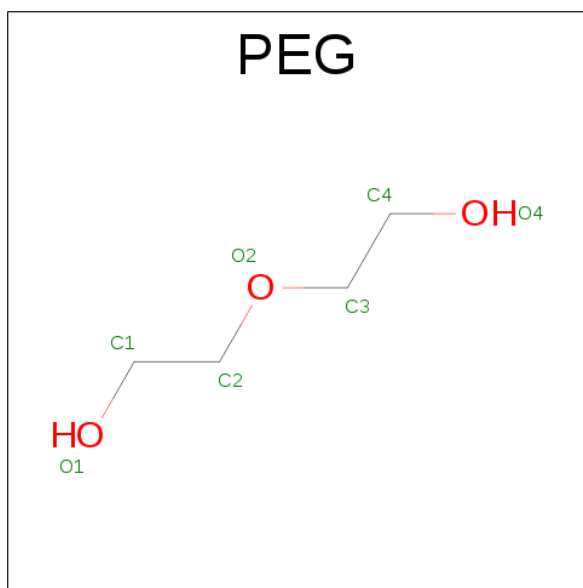
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		

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

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

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



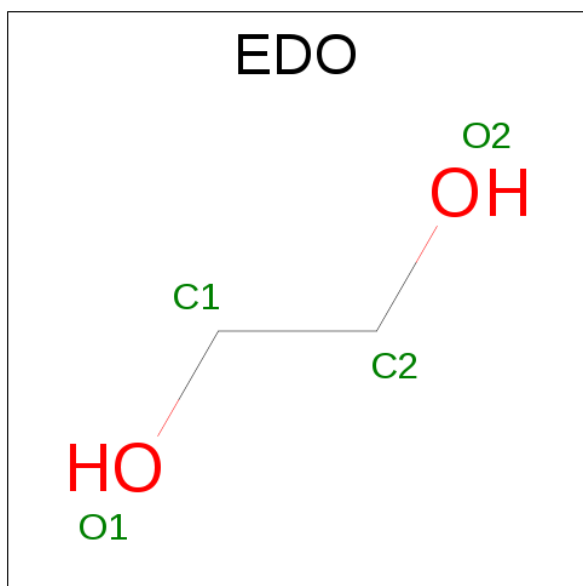
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	D1	1	Total	C	O	0	0
			7	4	3		
61	D3	1	Total	C	O	0	0
			7	4	3		

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

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



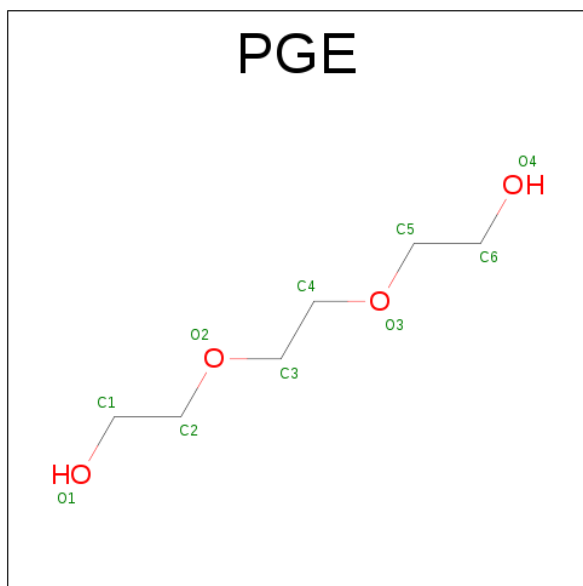
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	D1	1	Total C O 4 2 2	0	0
62	D0	1	Total C O 4 2 2	0	0
62	DB	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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).



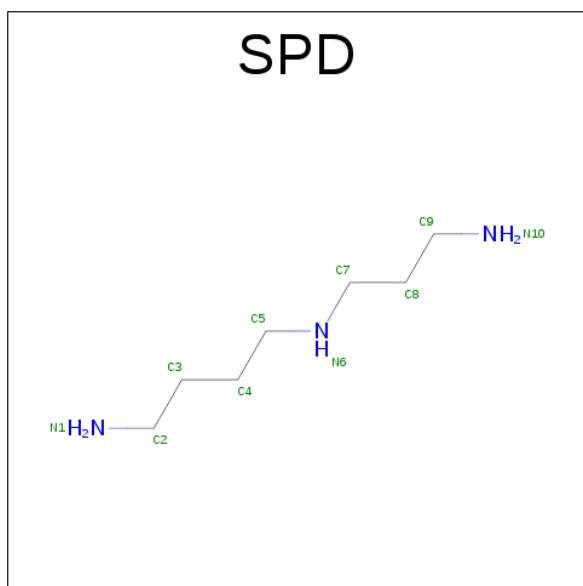
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D3	1	Total	C	O	0	0
			10	6	4		
63	DD	1	Total	C	O	0	0
			10	6	4		

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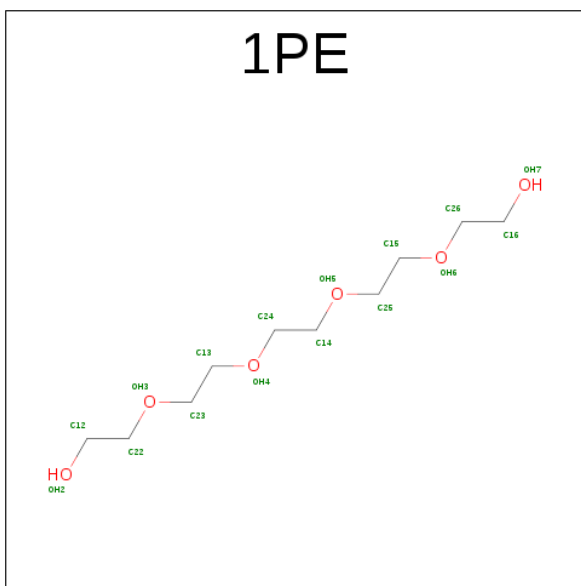
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DS	1	Total	C	O	0	0
			10	6	4		
63	DT	1	Total	C	O	0	0
			10	6	4		
63	DU	1	Total	C	O	0	0
			10	6	4		

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



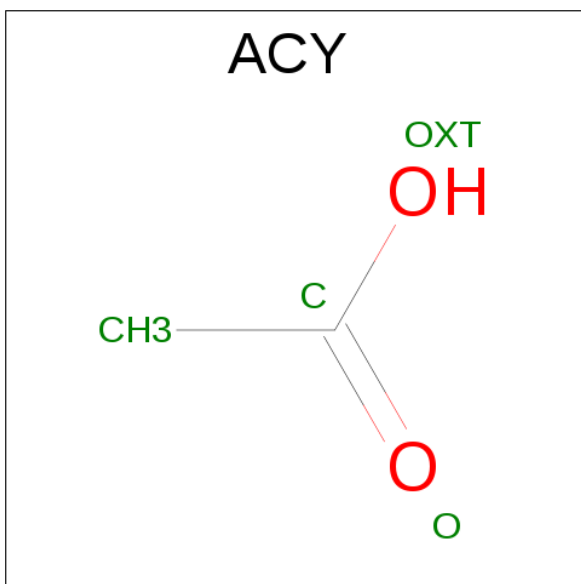
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		

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



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

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



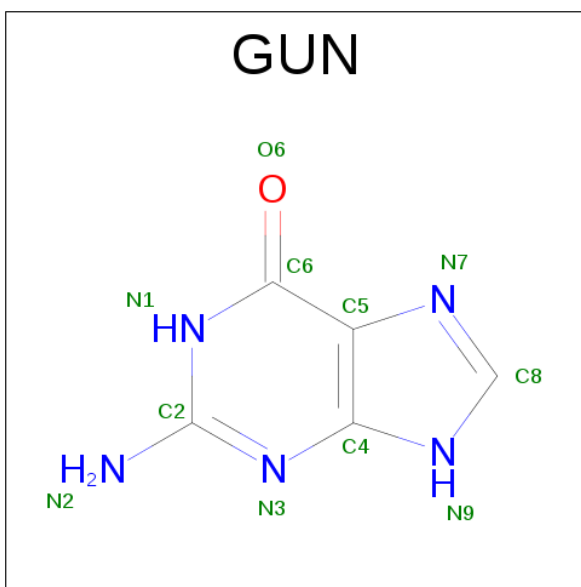
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		

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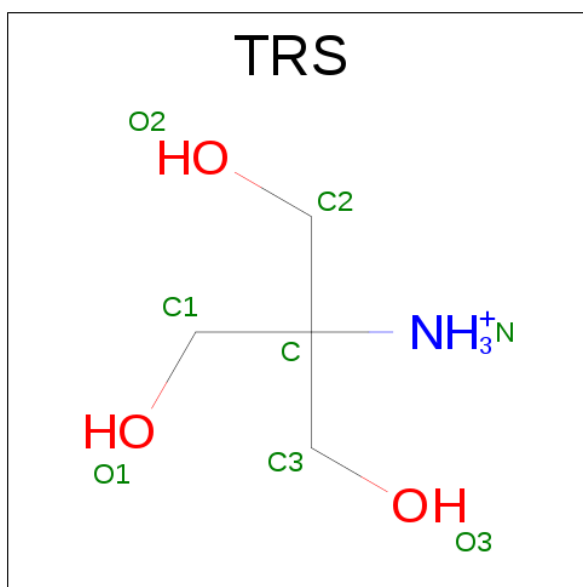
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		

- 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	O	0	0
			507	507		
69	AC	4	Total	O	0	0
			4	4		
69	AD	3	Total	O	0	0
			3	3		
69	AE	5	Total	O	0	0
			5	5		
69	AF	1	Total	O	0	0
			1	1		
69	AG	1	Total	O	0	0
			1	1		
69	AJ	2	Total	O	0	0
			2	2		
69	AK	7	Total	O	0	0
			7	7		
69	AL	10	Total	O	0	0
			10	10		
69	AM	4	Total	O	0	0
			4	4		
69	AN	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AO	2	Total	O	0	0
			2	2		
69	AP	2	Total	O	0	0
			2	2		
69	AR	1	Total	O	0	0
			1	1		
69	AS	1	Total	O	0	0
			1	1		
69	AT	3	Total	O	0	0
			3	3		
69	AU	3	Total	O	0	0
			3	3		
69	C3	3	Total	O	0	0
			3	3		
69	C4	1	Total	O	0	0
			1	1		
69	C5	1	Total	O	0	0
			1	1		
69	BA	291	Total	O	0	0
			291	291		
69	BD	11	Total	O	0	0
			11	11		
69	BE	1	Total	O	0	0
			1	1		
69	BF	1	Total	O	0	0
			1	1		
69	BK	2	Total	O	0	0
			2	2		
69	BL	2	Total	O	0	0
			2	2		
69	BN	2	Total	O	0	0
			2	2		
69	BO	1	Total	O	0	0
			1	1		
69	BP	3	Total	O	0	0
			3	3		
69	BR	1	Total	O	0	0
			1	1		
69	BT	4	Total	O	0	0
			4	4		
69	BU	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	D1	42	Total 42	O 42	0	0
69	D2	7	Total 7	O 7	0	0
69	D3	28	Total 28	O 28	0	0
69	D4	39	Total 39	O 39	0	0
69	D5	9	Total 9	O 9	0	0
69	D0	21	Total 21	O 21	0	0
69	CB	13	Total 13	O 13	0	0
69	CC	10	Total 10	O 10	0	0
69	CD	6	Total 6	O 6	0	0
69	CA	692	Total 692	O 692	0	0
69	DB	199	Total 199	O 199	0	0
69	DC	98	Total 98	O 98	0	0
69	DD	95	Total 95	O 95	0	0
69	DA	4834	Total 4834	O 4834	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	2	Total 2	O 2	0	0
69	CV	1	Total 1	O 1	0	0
69	CW	1	Total 1	O 1	0	0

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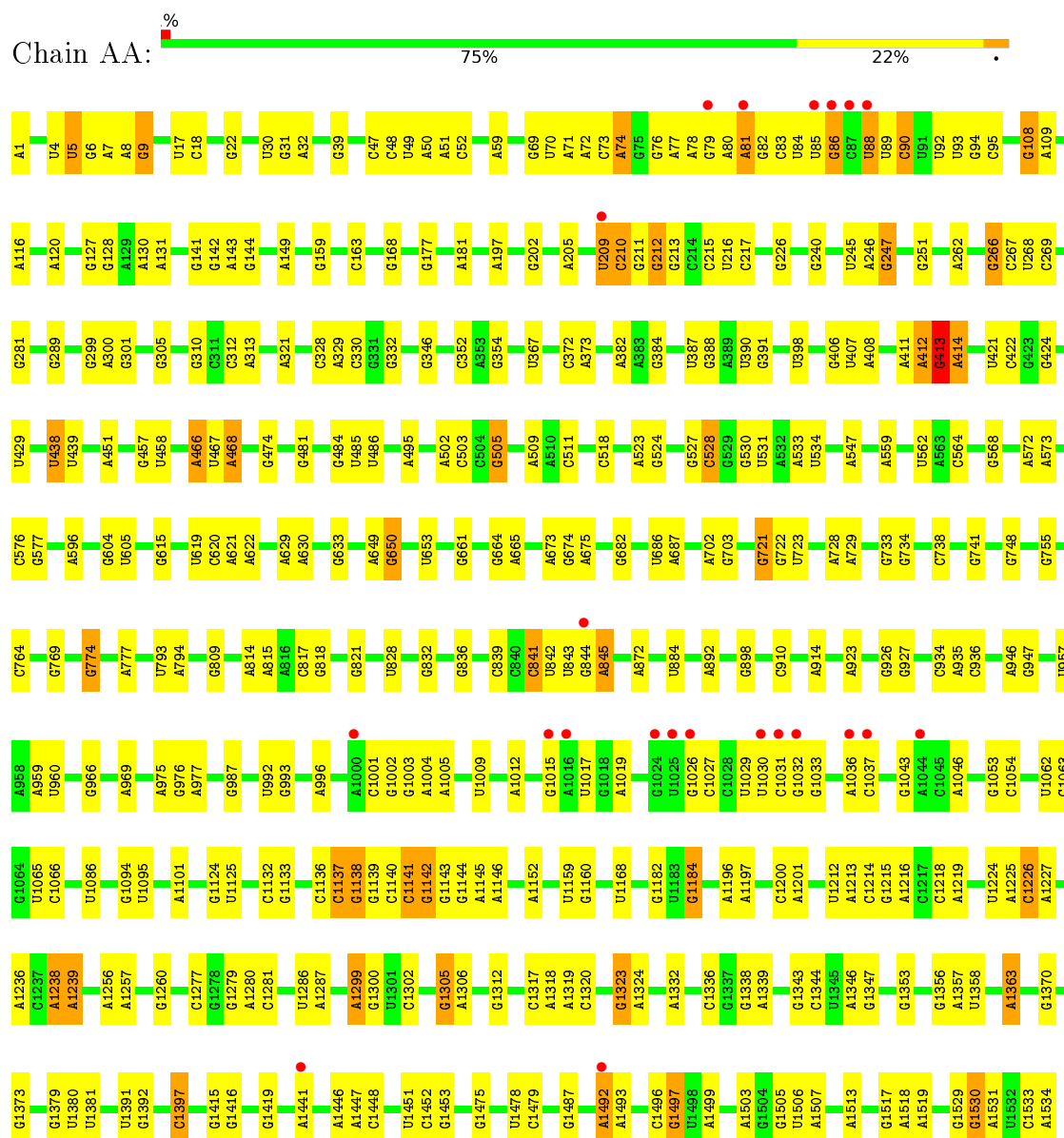
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	CY	1	Total 1	O 1	0	0
69	DE	63	Total 63	O 63	0	0
69	DF	15	Total 15	O 15	0	0
69	DG	7	Total 7	O 7	0	0
69	DH	1	Total 1	O 1	0	0
69	DK	65	Total 65	O 65	0	0
69	DL	52	Total 52	O 52	0	0
69	DM	62	Total 62	O 62	0	0
69	DN	64	Total 64	O 64	0	0
69	DO	48	Total 48	O 48	0	0
69	DP	44	Total 44	O 44	0	0
69	DQ	33	Total 33	O 33	0	0
69	DR	68	Total 68	O 68	0	0
69	DS	48	Total 48	O 48	0	0
69	DT	62	Total 62	O 62	0	0
69	DU	22	Total 22	O 22	0	0
69	DV	18	Total 18	O 18	0	0
69	DW	34	Total 34	O 34	0	0
69	DX	31	Total 31	O 31	0	0
69	DY	10	Total 10	O 10	0	0
69	DZ	5	Total 5	O 5	0	0

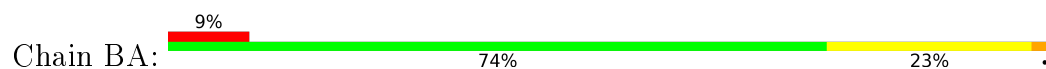
3 Residue-property plots [i](#)

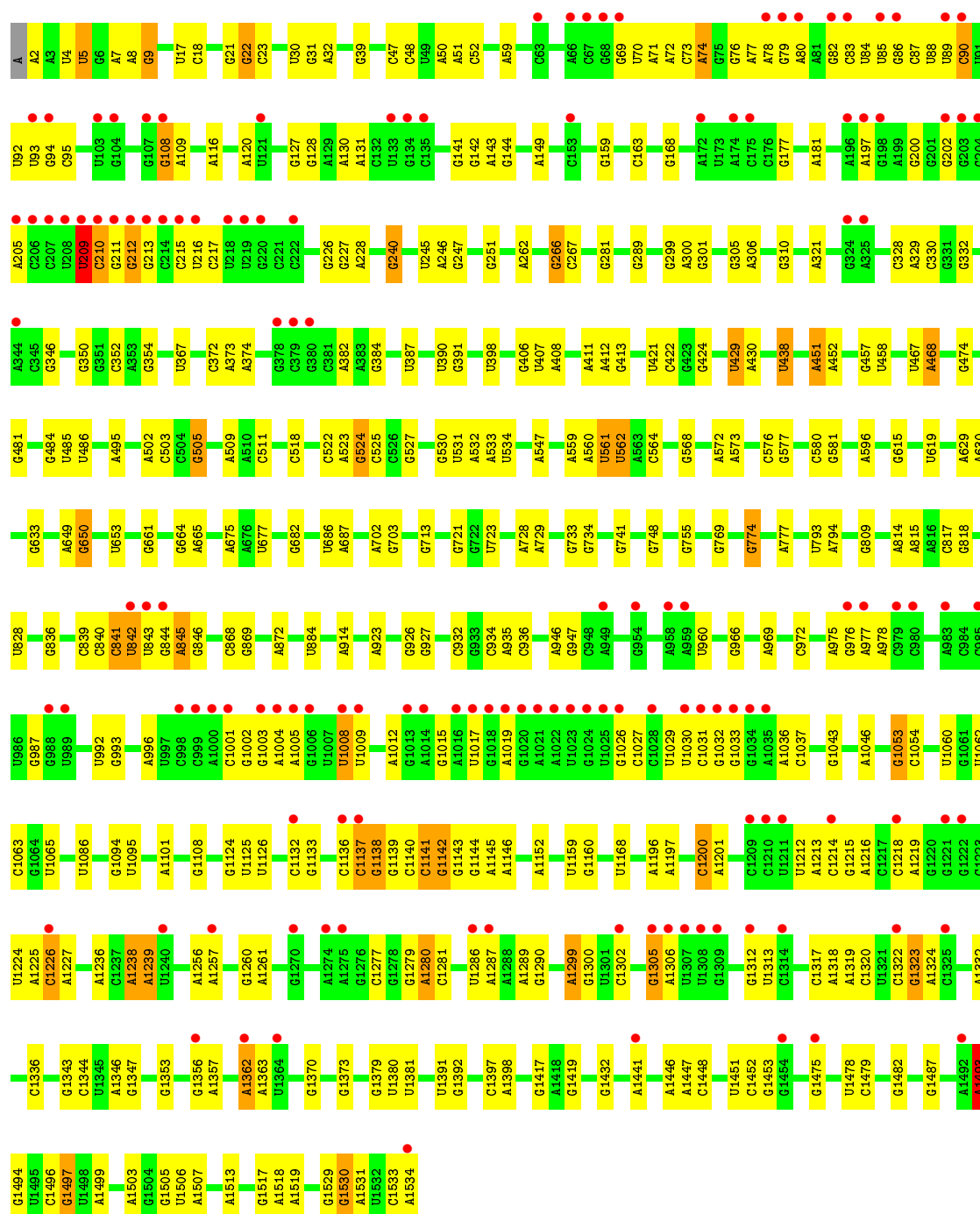
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: 16S rRNA

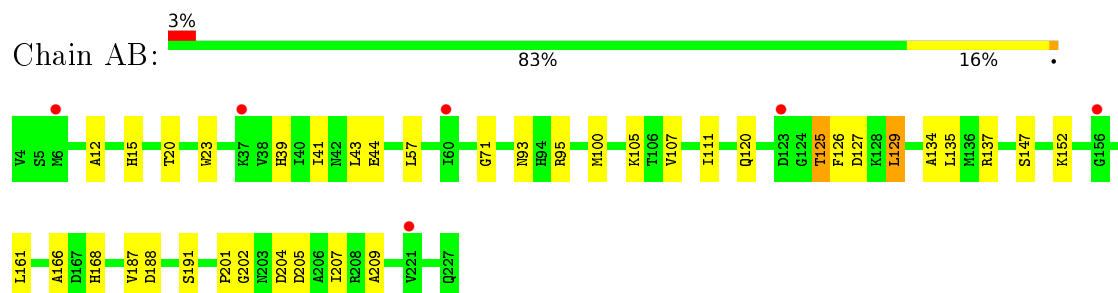


- Molecule 1: 16S rRNA

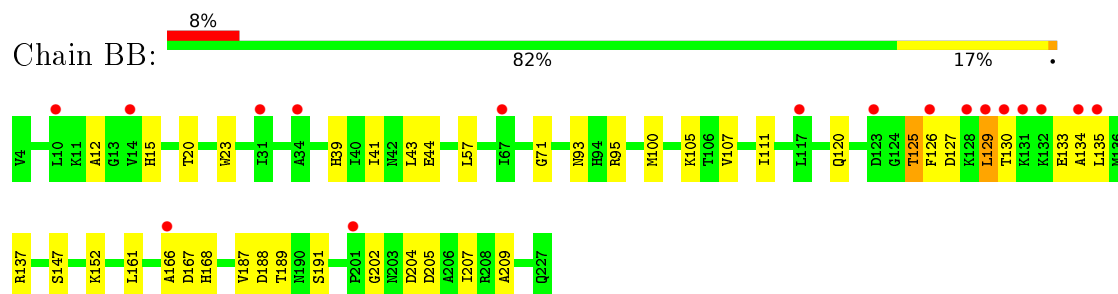




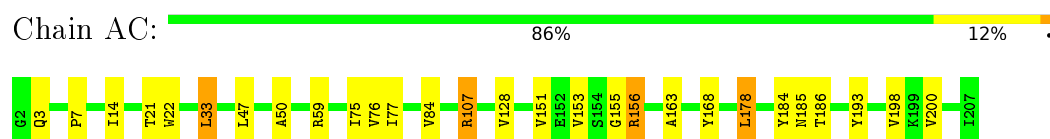
• Molecule 2: 30S ribosomal protein S2



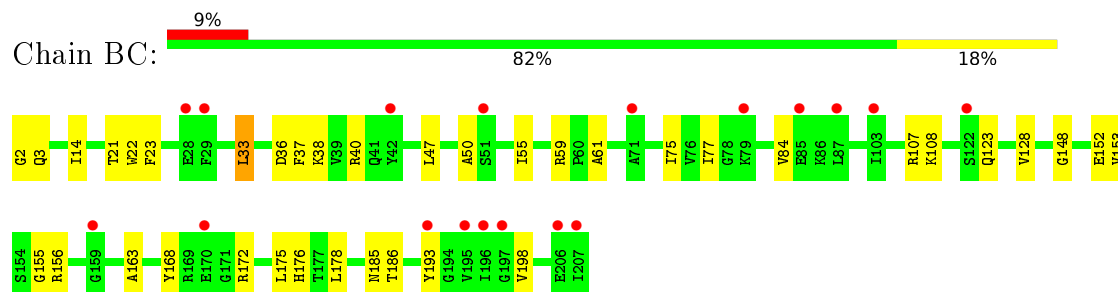
- Molecule 2: 30S ribosomal protein S2



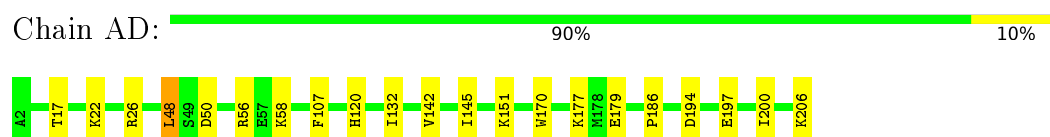
- Molecule 3: 30S ribosomal protein S3



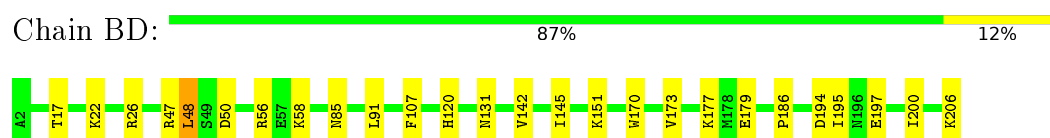
- Molecule 3: 30S ribosomal protein S3



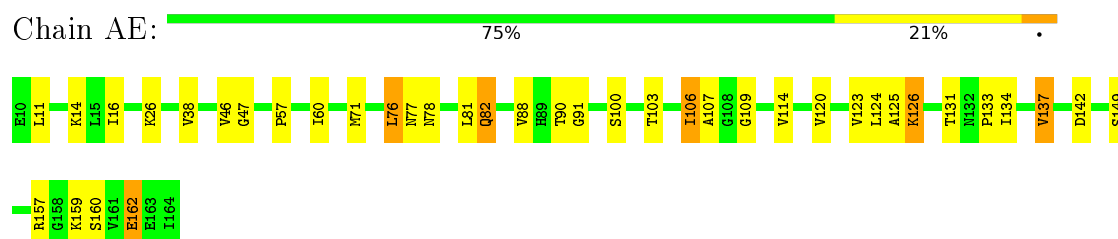
- Molecule 4: 30S ribosomal protein S4



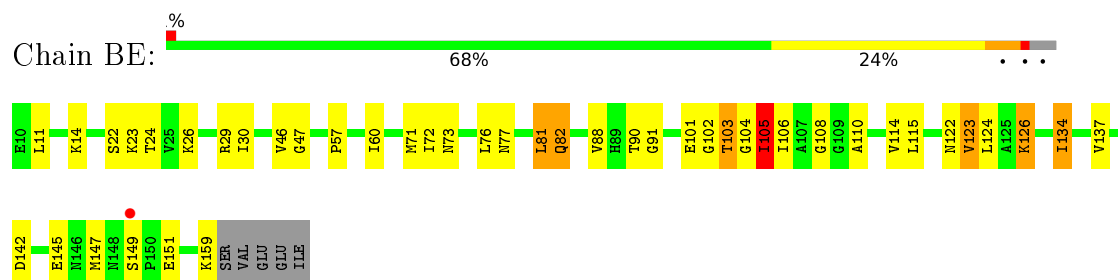
- Molecule 4: 30S ribosomal protein S4



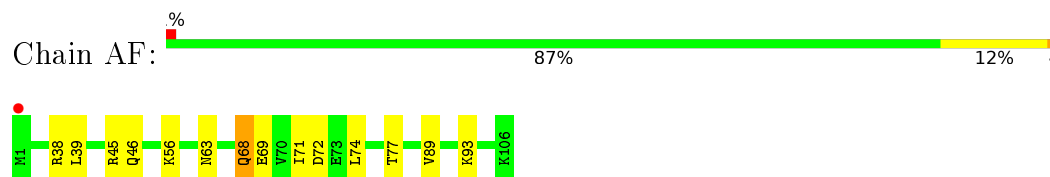
- Molecule 5: 30S ribosomal protein S5



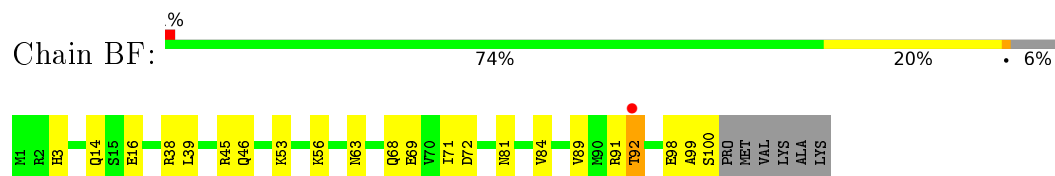
- Molecule 5: 30S ribosomal protein S5



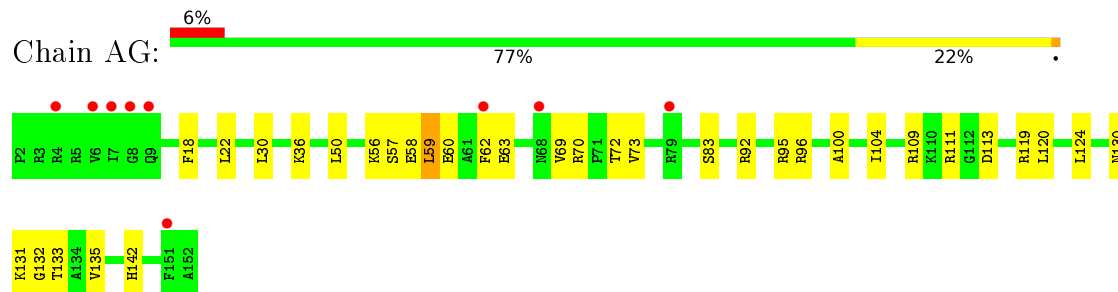
- Molecule 6: 30S ribosomal protein S6



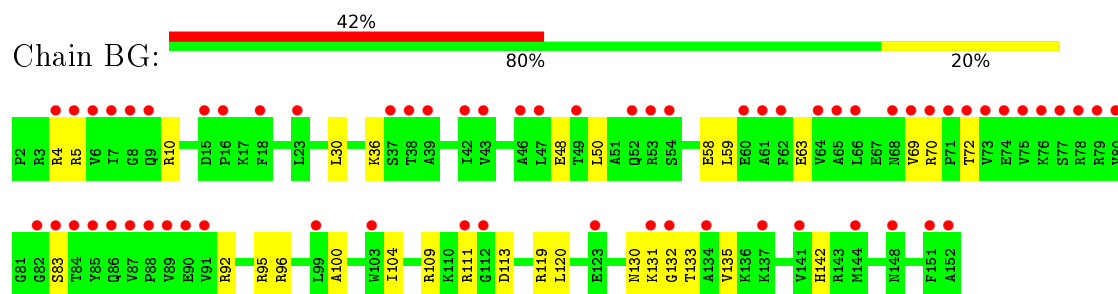
- Molecule 6: 30S ribosomal protein S6



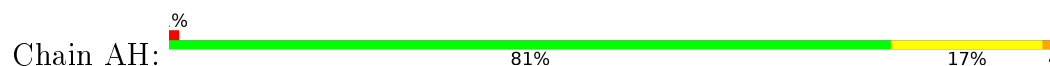
- Molecule 7: 30S ribosomal protein S7

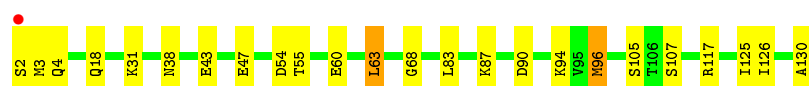


- Molecule 7: 30S ribosomal protein S7

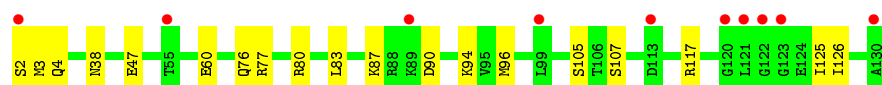
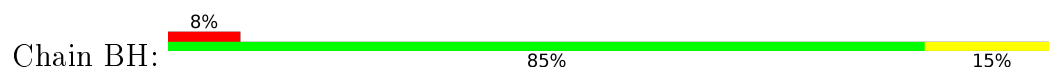


- Molecule 8: 30S ribosomal protein S8

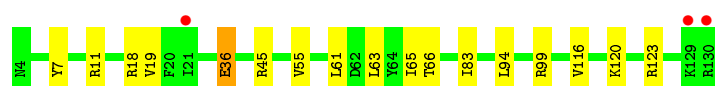
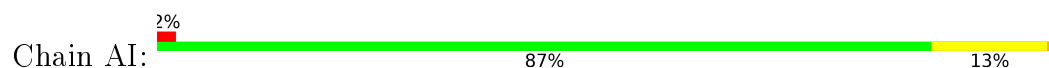




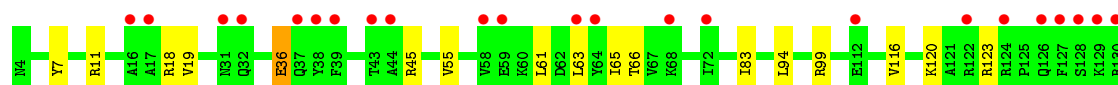
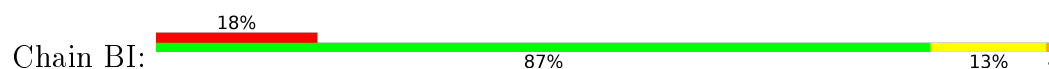
- Molecule 8: 30S ribosomal protein S8



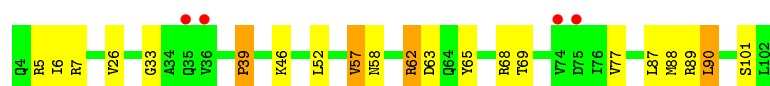
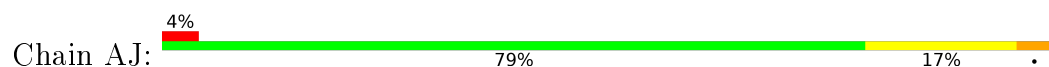
- Molecule 9: 30S ribosomal protein S9



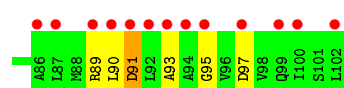
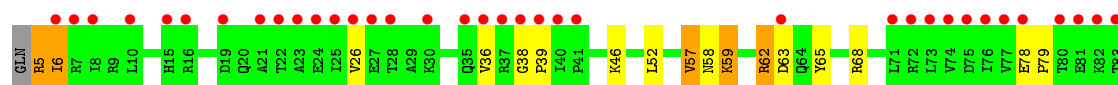
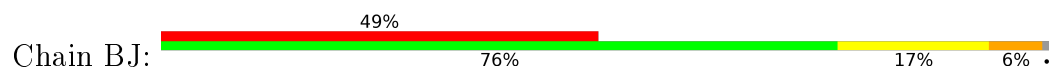
- Molecule 9: 30S ribosomal protein S9



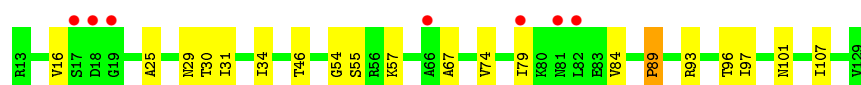
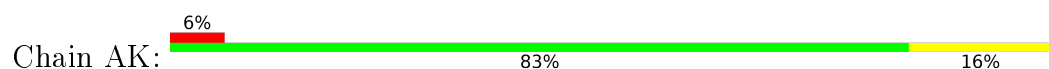
- Molecule 10: 30S ribosomal protein S10



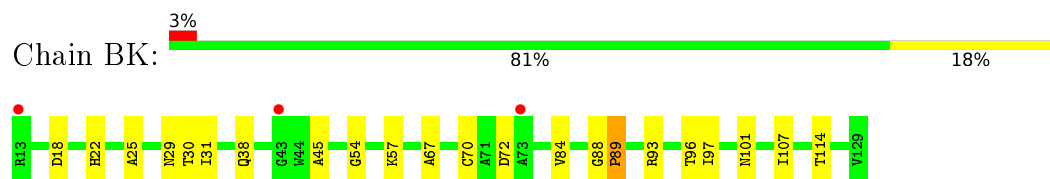
- Molecule 10: 30S ribosomal protein S10



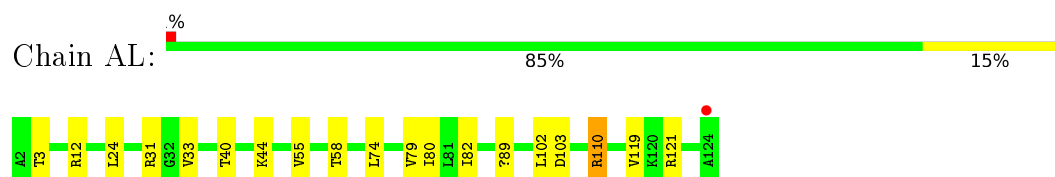
- Molecule 11: 30S ribosomal protein S11



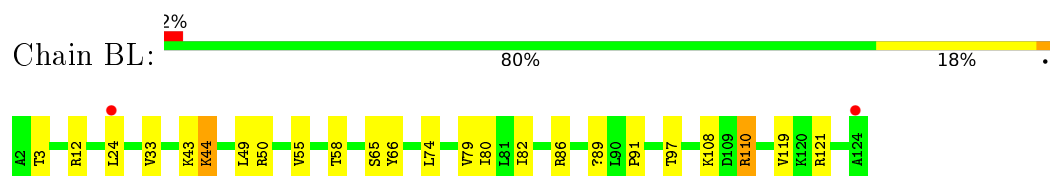
- Molecule 11: 30S ribosomal protein S11



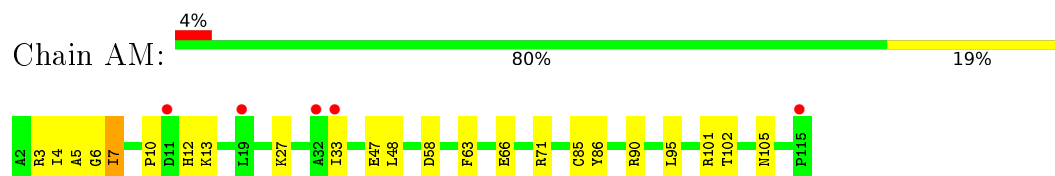
- Molecule 12: 30S ribosomal protein S12



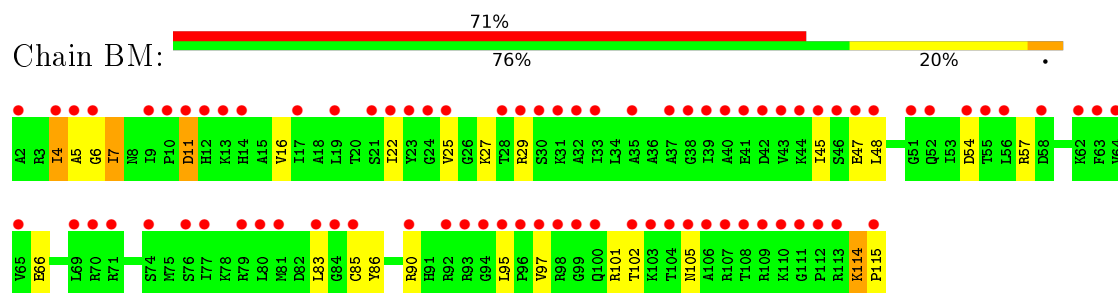
- Molecule 12: 30S ribosomal protein S12



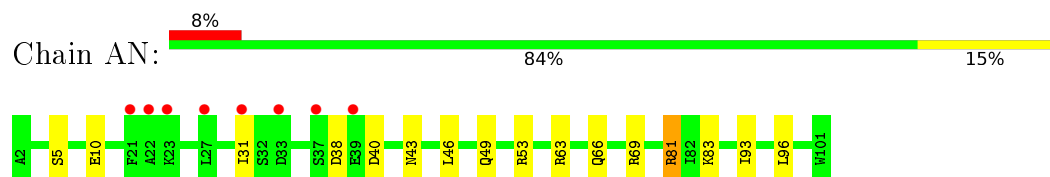
- Molecule 13: 30S ribosomal protein S13



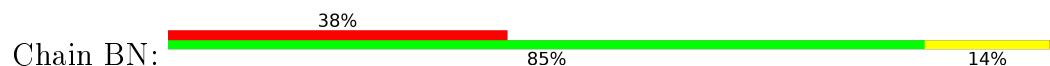
- Molecule 13: 30S ribosomal protein S13

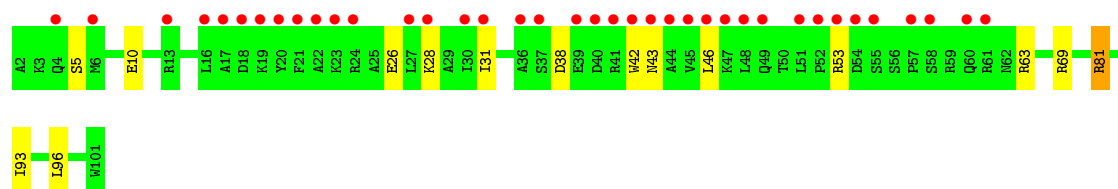


- Molecule 14: 30S ribosomal protein S14



- Molecule 14: 30S ribosomal protein S14

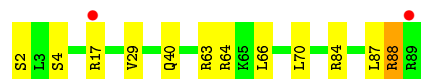
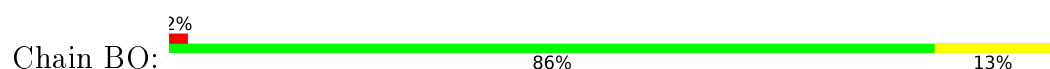




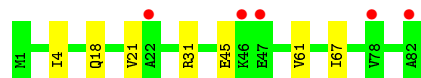
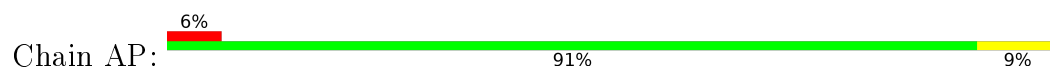
- Molecule 15: 30S ribosomal protein S15



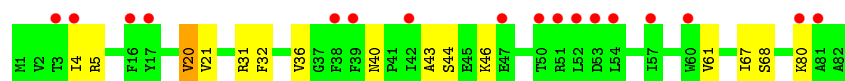
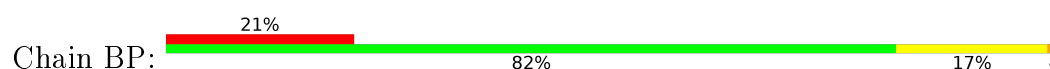
- Molecule 15: 30S ribosomal protein S15



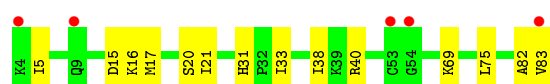
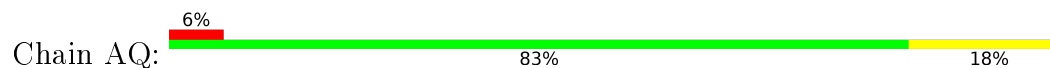
- Molecule 16: 30S ribosomal protein S16



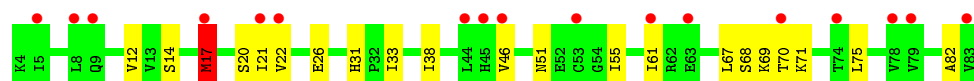
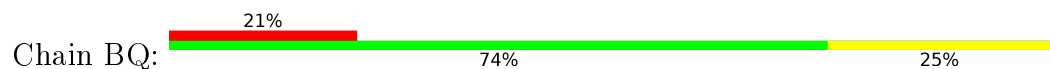
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

Chain AR:  89% 11%




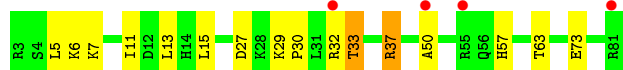
- Molecule 18: 30S ribosomal protein S18

Chain BR:  7% 96%




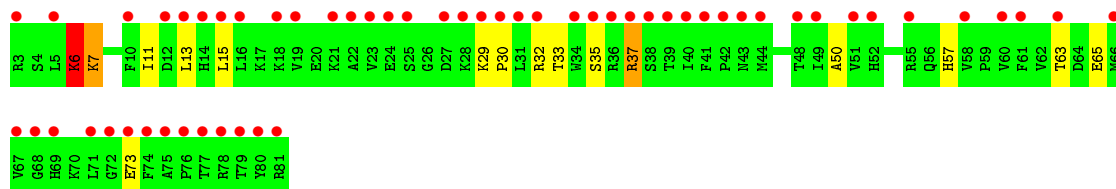
- Molecule 19: 30S ribosomal protein S19

Chain AS:  5% 80% 18%




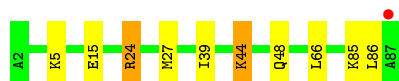
- Molecule 19: 30S ribosomal protein S19

Chain BS:  71% 80% 16%




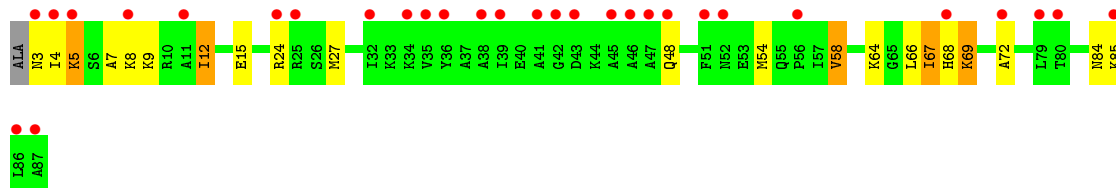
- Molecule 20: 30S ribosomal protein S20

Chain AT:  % 88% 9%




- Molecule 20: 30S ribosomal protein S20

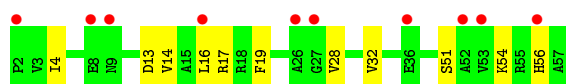
Chain BT:  35% 74% 19% 6%



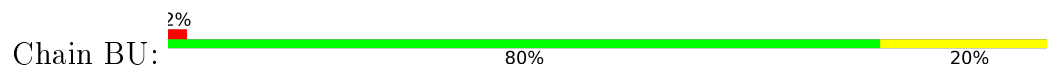
- Molecule 21: 30S ribosomal protein S21

Chain AU:  18% 80% 20%

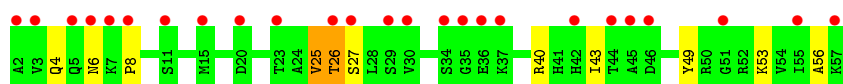
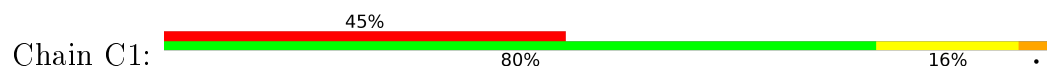




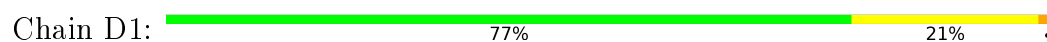
- Molecule 21: 30S ribosomal protein S21



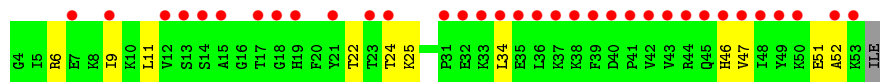
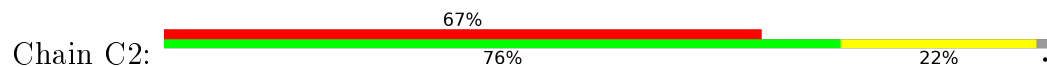
- Molecule 22: 50S ribosomal protein L32



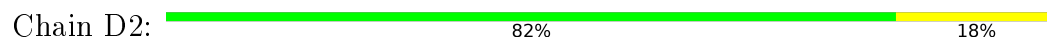
- Molecule 22: 50S ribosomal protein L32



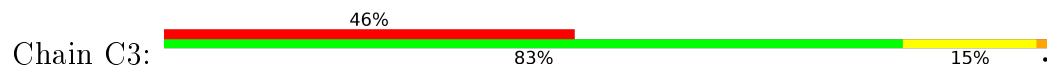
- Molecule 23: 50S ribosomal protein L33



- Molecule 23: 50S ribosomal protein L33

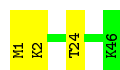


- Molecule 24: 50S ribosomal protein L34

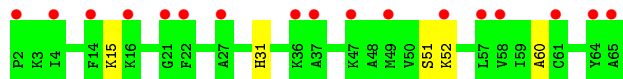
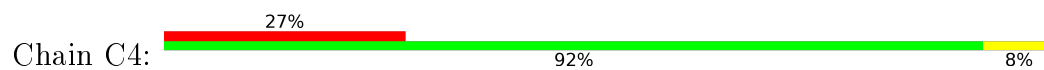


- Molecule 24: 50S ribosomal protein L34





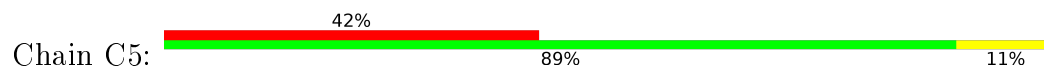
- Molecule 25: 50S ribosomal protein L35



- Molecule 25: 50S ribosomal protein L35



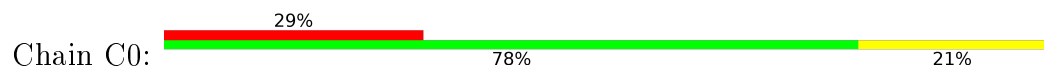
- Molecule 26: 50S ribosomal protein L36



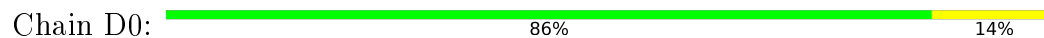
- Molecule 26: 50S ribosomal protein L36



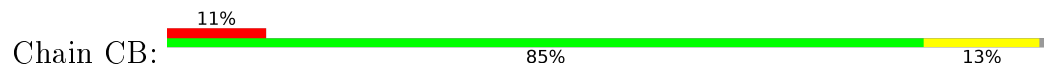
- Molecule 27: 50S ribosomal protein L30

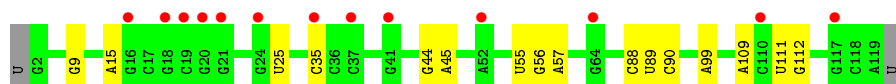


- Molecule 27: 50S ribosomal protein L30



- Molecule 28: 5S rRNA





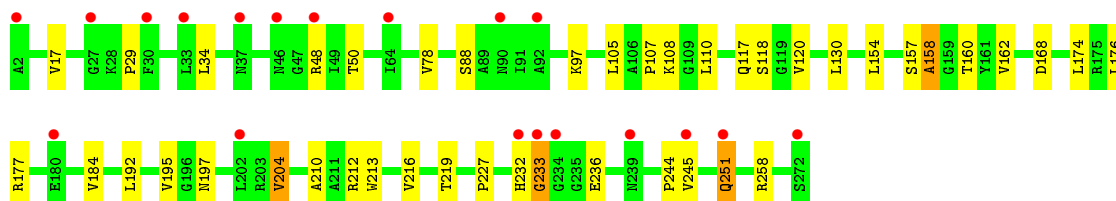
• Molecule 28: 5S rRNA

Chain DB: 85% 14%



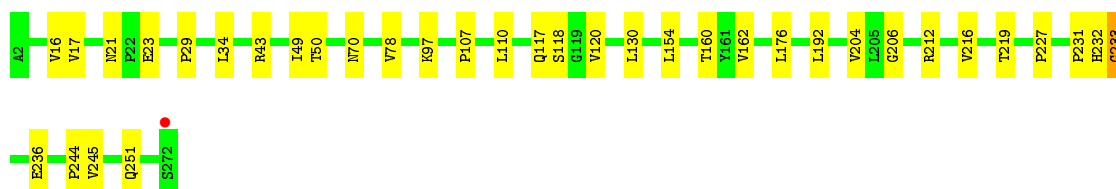
• Molecule 29: 50S ribosomal protein L2

Chain CC: 7% 84% 14%



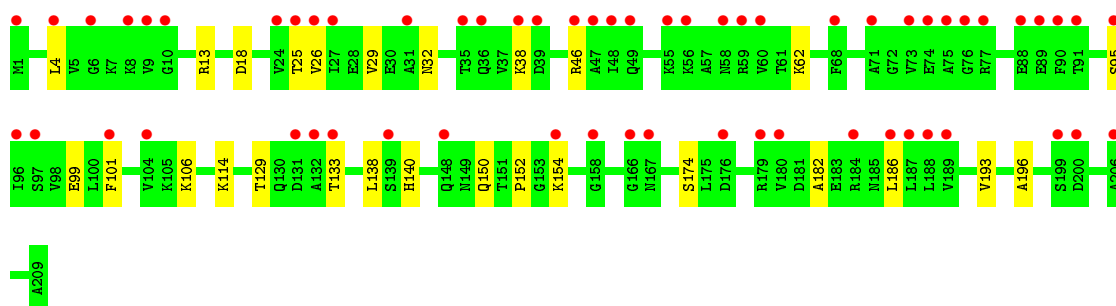
• Molecule 29: 50S ribosomal protein L2

Chain DC: 87% 13%



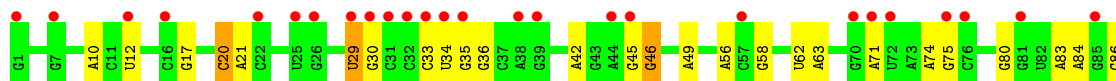
• Molecule 30: 50S ribosomal protein L3

Chain CD: 29% 87% 13%

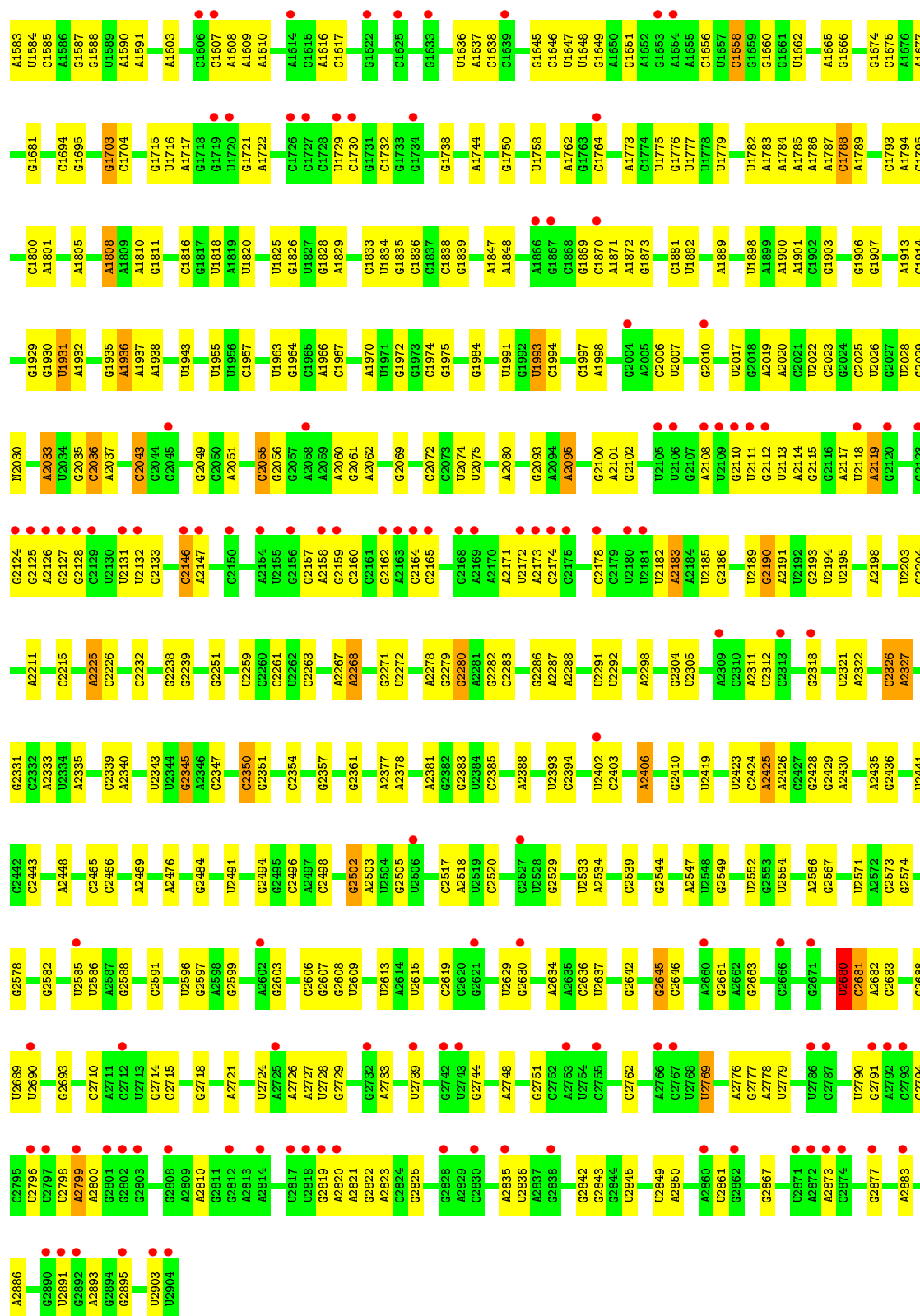


• Molecule 31: 23S rRNA

Chain CA: 15% 70% 27%



U1460	G1356	A1264	G1178	A1088	C1005	G882	C787	A685	G585	G585	A497	A404	A310	G214	U87
U1468	C1357	A1265	G1179	A1089	U1012	G883	A786	U686	A586	A586	A501	U405	A311	G215	G88
U1476	G1358	G1266	U1180	A1090	C1013	U884	A792	U688	C587	C587	A502	G406	G312	A216	A89
A1477	A1365	G1271	U1181	G1091	A1014	C885	A793	C692	U589	U589	A503	G409	G315	A221	A95
G1482	C1376	U1183	U1183	C1092	U1015	A	A794	U694	U593	U593	A504	G411	G316	A222	A101
G1482	U1273	U1184	U1184	C1093	G1016	C	C795	U694	U594	U594	A505	G412	G317	A225	U102
G1482	A1274	G1185	G1185	U1094	G1017	C	C796	U695	U594	U594	A506	G412	G318	A226	A101
U1379	U1379	G1186	G1186	A1095	U1018	C	C797	U696	U595	U595	A507	C420	G319	A227	U102
G1380	G1380	U1187	U1187	U1097	U1022	G	C798	U696	U596	U596	A508	C420	G320	A228	U113
G1381	A1276	U1188	U1188	U1098	G1026	A892	C799	U697	U597	U597	A509	G424	G321	A229	U114
G1382	C1278	A1189	A1189	C1100	A1027	U895	A800	G700	A602	A602	A512	U431	G322	A230	U115
A1383	G1278	G1190	G1190	C1101	A1028	A896	A801	G701	A603	A603	A513	U431	G323	A231	G117
U1497	A1285	G1191	G1191	U1101	A1029	A897	A802	G702	A604	A604	A514	U432	G324	A232	A118
C1507	A1286	G1192	G1192	C1102	U1033	C897	C805	U703	A605	A605	A515	A439	G325	A233	A119
G1389	A1287	G1193	G1193	A1103	U1034	G907	C806	A706	A606	A606	A516	A440	G326	A234	U120
A1508	C1289	G1194	G1194	C1104	U1035	G908	C807	A707	A607	A607	A517	U441	G327	A235	
A1509	G1297	G1195	G1195	U1105	U1036	G909	C808	A708	A608	A608	A518	U442	G328	A236	
G1510	C1297	G1196	G1196	C1106	U1037	G910	C809	A709	A609	A609	A519	U443	G329	A237	
A1515	G1300	G1197	G1197	U1107	U1038	A910	C810	A710	A610	A610	A520	U444	G330	A238	
G1516	A1301	G1198	G1198	C1108	U1039	U913	C811	A711	A611	A611	A521	U445	G331	A239	
G1517	A1302	G1199	G1199	U1109	U1040	G914	C812	A712	A612	A612	A522	U446	G332	A240	
A1522	G1303	G1200	G1200	C1110	U1041	G915	C813	A713	A613	A613	A523	U447	G333	A241	
U1523	C1306	G1201	G1201	U1111	U1042	G916	C814	A714	A614	A614	A524	U448	G334	A242	
G1524	G1310	G1202	G1202	G1112	U1043	A917	C815	A715	A615	A615	A525	U449	G335	A243	
U1529	G1311	G1203	G1203	U1113	U1044	U918	C816	A716	A616	A616	A526	U450	G336	A244	
G1530	U1312	G1204	G1204	G1114	U1045	G919	C817	A717	A617	A617	A527	U451	G337	A245	
G1531	U1313	G1205	G1205	U1115	U1046	G920	C818	A718	A618	A618	A528	U452	G338	A246	
G1532	U1314	G1206	G1206	G1116	U1047	G921	C819	A719	A619	A619	A529	U453	G339	A247	
U1533	G1315	G1207	G1207	U1117	U1048	U922	C820	A720	A620	A620	A530	U454	G340	A248	
U1534	G1316	G1208	G1208	U1118	U1049	U923	C821	A721	A621	A621	A531	U455	G341	A249	
C1535	G1317	G1209	G1209	U1119	U1050	U924	C822	A722	A622	A622	A532	U456	G342	A250	
G1536	U1318	G1210	G1210	U1120	U1051	U925	C823	A723	A623	A623	A533	U457	G343	A251	
G1537	U1319	G1211	G1211	G1121	U1052	U926	C824	A724	A624	A624	A534	U458	G344	A252	
G1538	U1320	G1212	G1212	U1122	U1053	U927	C825	A725	A625	A625	A535	U459	G345	A253	
U1539	U1321	G1213	G1213	U1123	U1054	U928	C826	A726	A626	A626	A536	U460	G346	A254	
G1540	U1322	G1214	G1214	U1124	U1055	U929	C827	A727	A627	A627	A537	U461	G347	A255	
U1541	U1323	G1215	G1215	U1125	U1056	U930	C828	A728	A628	A628	A538	U462	G348	A256	
U1542	U1324	G1216	G1216	U1126	U1057	U931	C829	A729	A629	A629	A539	U463	G349	A257	
U1543	U1325	G1217	G1217	U1127	U1058	U932	C830	A730	A630	A630	A540	U464	G350	A258	
U1544	U1326	G1218	G1218	U1128	U1059	U933	C831	A731	A631	A631	A541	U465	G351	A259	
U1545	U1327	G1219	G1219	U1129	U1060	U934	C832	A732	A632	A632	A542	U466	G352	A260	
U1546	U1328	G1220	G1220	U1130	U1061	U935	C833	A733	A633	A633	A543	U467	G353	A261	
U1547	U1329	G1221	G1221	U1131	U1062	U936	C834	A734	A634	A634	A544	U468	G354	A262	
U1548	U1330	G1222	G1222	U1132	U1063	U937	C835	A735	A635	A635	A545	U469	G355	A263	
U1549	U1331	G1223	G1223	U1133	U1064	U938	C836	A736	A636	A636	A546	U470	G356	A264	
U1550	U1332	G1224	G1224	U1134	U1065	U939	C837	A737	A637	A637	A547	U471	G357	A265	
U1551	U1333	G1225	G1225	U1135	U1066	U940	C838	A738	A638	A638	A548	U472	G358	A266	
U1552	U1334	G1226	G1226	U1136	U1067	U941	C839	A739	A639	A639	A549	U473	G359	A267	
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U1555	U1337	G1229	G1229	U1139	U1070	U944	C842	A742	A642	A642	A552	U476	G362	A270	
U1556	U1338	G1230	G1230	U1140	U1071	U945	C843	A743	A643	A643	A553	U477	G363	A271	
U1557	U1339	G1231	G1231	U1141	U1072	U946	C844	A744	A644	A644	A554	U478	G364	A272	
U1558	U1340	G1232	G1232	U1142	U1073	U947	C845	A745	A645	A645	A555	U479	G365	A273	
U1559	U1341	G1233	G1233	U1143	U1074	U948	C846	A746	A646	A646	A556	U480	G366	A274	
U1560	U1342	G1234	G1234	U1144	U1075	U949	C847	A747	A647	A647	A557	U481	G367	A275	
U1561	U1343	G1235	G1235	U1145	U1076	U950	C848	A748	A648	A648	A558	U482	G368	A276	
U1562	U1344	G1236	G1236	U1146	U1077	U951	C849	A749	A649	A649	A559	U483	G369	A277	
U1563	U1345	G1237	G1237	U1147	U1078	U952	C850	A750	A650	A650	A560	U484	G370	A278	
U1564	U1346	G1238	G1238	U1148	U1079	U953	C851	A751	A651	A651	A561	U485	G371	A279	
U1565	U1347	G1239	G1239	U1149	U1080	U954	C852	A752	A652	A652	A562	U486	G372	A280	
U1566	U1348	G1240	G1240	U1150	U1081	U955	C853	A753	A653	A653	A563	U487	G373	A281	
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U1568	U1350	G1242	G1242	U1152	U1083	U957	C855	A755	A655	A655	A565	U489	G375	A283	
U1569	U1351	G1243	G1243	U1153	U1084	U958	C856	A756	A656	A656	A566	U490	G376	A284	
U1570	U1352	G1244	G1244	U1154	U1085	U959	C857	A757	A657	A657	A567	U491	G377	A285	
U1571	U1353	G1245	G1245	U1155	U1086	U960	C858	A758	A658	A658	A568	U492	G378	A286	
U1572	U1354	G1246	G1246	U1156	U1087	U961	C859	A759	A659	A659	A569	U493	G379	A287	
U1573	U1355	G1247	G1247	U1157	U1088	U962	C860	A760	A660	A660	A570	U494	G380	A288	
U1574	U1356	G1248	G1248	U1158	U1089	U963	C861	A761	A661	A661	A571	U495	G381	A289	
U1575	U1357	G1249	G1249	U1159	U1090	U964	C862	A762	A662	A662	A572	U496	G382	A290	
U1576	U1358	G1250	G1250	U1160	U1091	U965	C863	A763	A663	A663	A573	U497	G383	A291	
U1577	U1359	G1251	G1251	U1161	U1092	U966	C864	A764	A664	A664	A574	U498	G384	A292	
U1578	U1360	G1252	G1252	U1162	U1093	U967	C865	A765	A665	A665	A575	U499	G385	A293	
U1579	U1361	G1253	G1253	U1163	U1094	U968	C866	A766	A666	A666	A576	U500	G386	A294	
U1580	U1362	G1254	G1254	U1164	U1095	U969	C867	A767	A667	A667	A577	U501	G387	A295	
U1581	U1363	G1255	G1255	U1165	U1096	U970	C868	A768	A668	A668	A578	U502	G388	A296	
U1582	U1364	G1256	G1256	U1166	U1097	U971	C869	A769	A669	A669	A579	U503	G389	A297	
U1583	U1365	G1257	G1257	U1167	U1098	U972	C870	A770	A670	A670	A580	U504	G390	A298	
U1584	U1366	G1258	G1258	U1168	U1099	U973	C871	A771	A671	A671	A581	U505	G391	A299	
U1585	U1367	G1259	G1259	U1169	U1100	U974	C872	A772	A672	A672	A582	U506	G392	A300	
U1586	U1368	G1260	G1260	U1170	U1101	U975	C873	A773	A673	A673	A583	U507	G393	A301	
U1587	U1369	G1261	G1261	U1171	U1102	U976	C874	A774	A674	A674	A584	U508	G394	A302	
U1588	U1370	G1262	G1262	U1172	U1103	U977	C875	A775	A675	A675	A585	U509	G395	A303	
U1589	U1371	G1263	G1263	U1173	U1104	U978	C876	A776	A676	A676	A586	U510	G396	A304	
U1590	U1372	G1264	G1264	U1174	U1105	U979	C877	A777	A677	A677	A587	U511	G397	A305	
U1591	U1373	G1265	G1265	U1175	U1106	U980	C878	A778	A678	A678	A588	U512	G398	A306	
U1592	U1374	G1266	G1266	U1176	U1107	U981	C879	A779	A679	A679	A589				

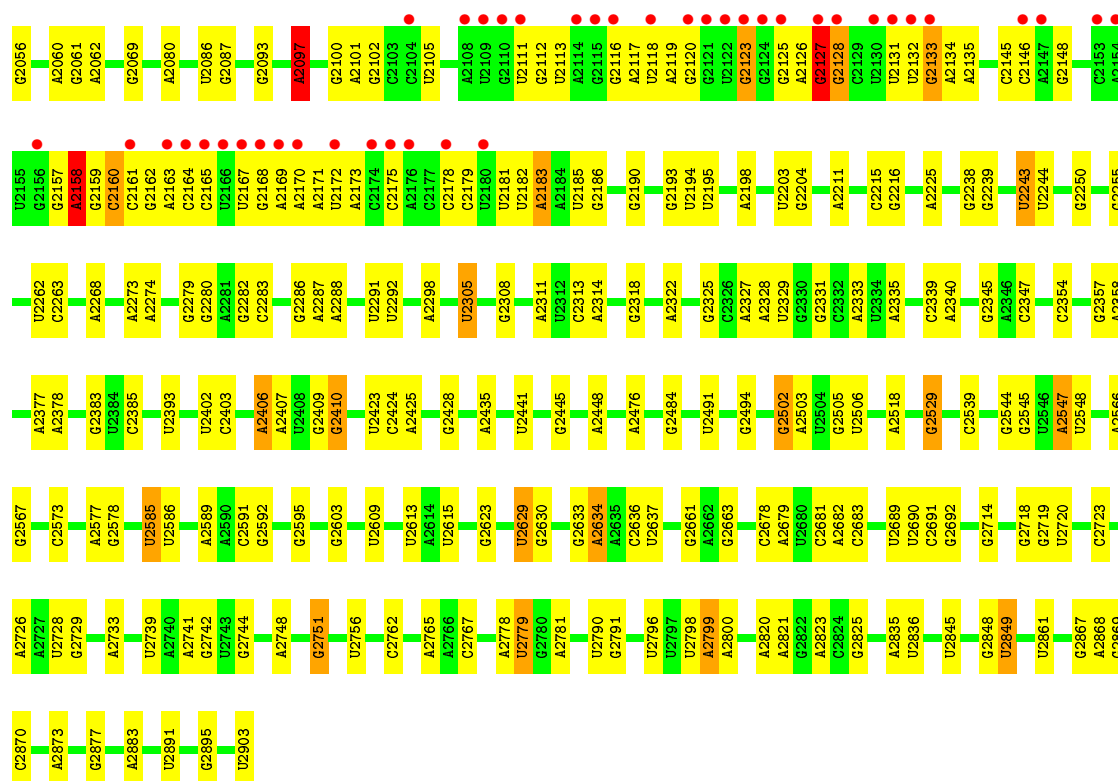


• Molecule 32: 50S ribosomal protein L3

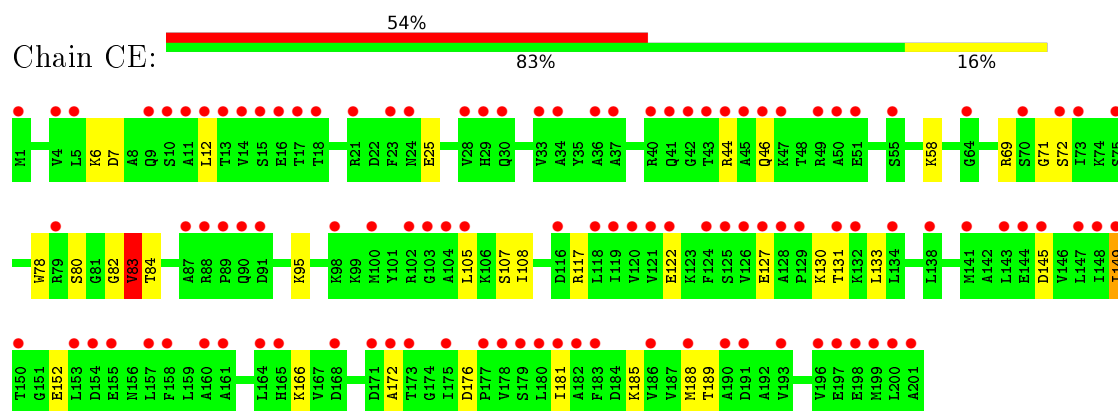
Chain DD: 88% 12%

Chain DA:

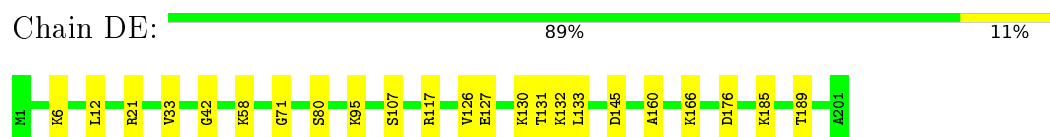




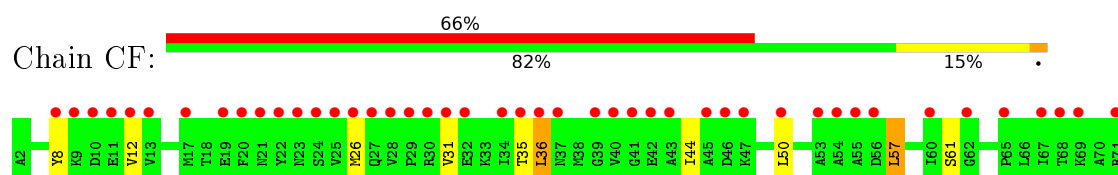
• Molecule 34: 50S ribosomal protein L4

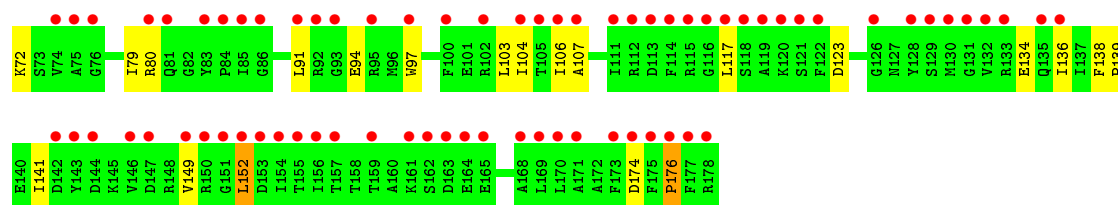


• Molecule 34: 50S ribosomal protein L4

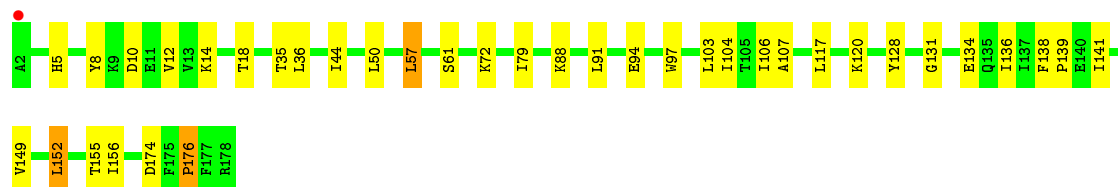
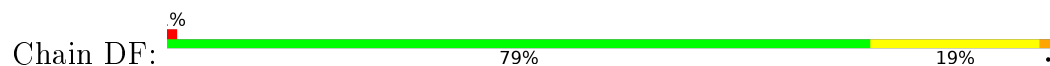


• Molecule 35: 50S ribosomal protein L5

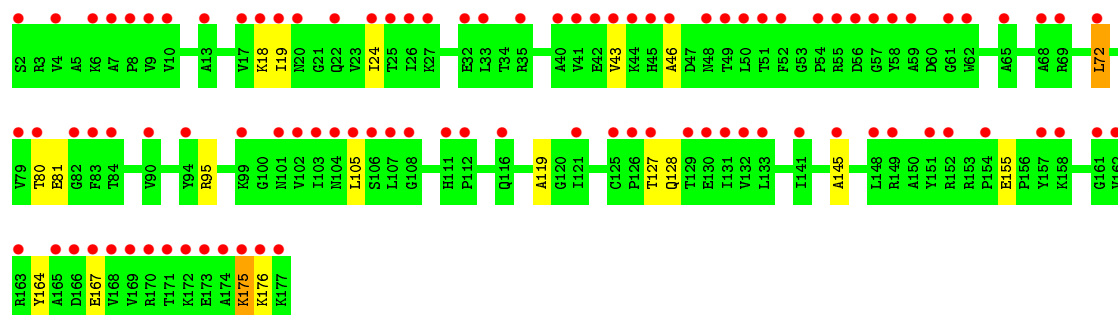
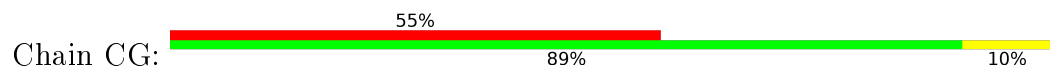




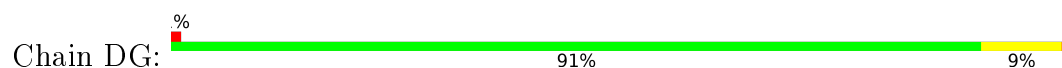
• Molecule 35: 50S ribosomal protein L5



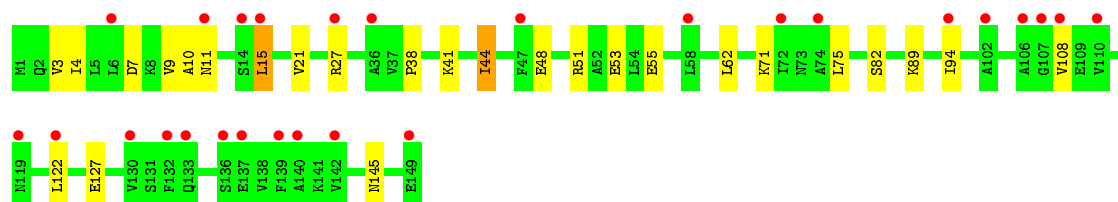
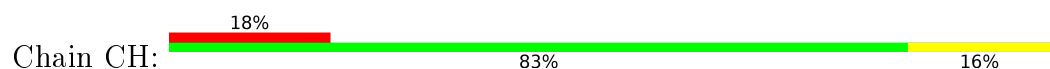
• Molecule 36: 50S ribosomal protein L6



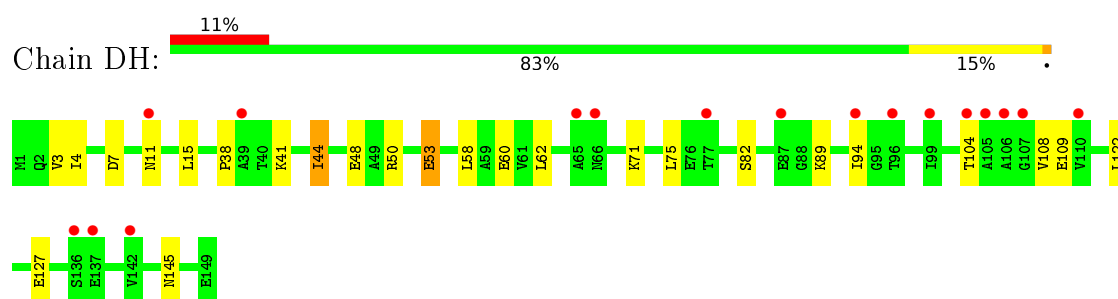
• Molecule 36: 50S ribosomal protein L6



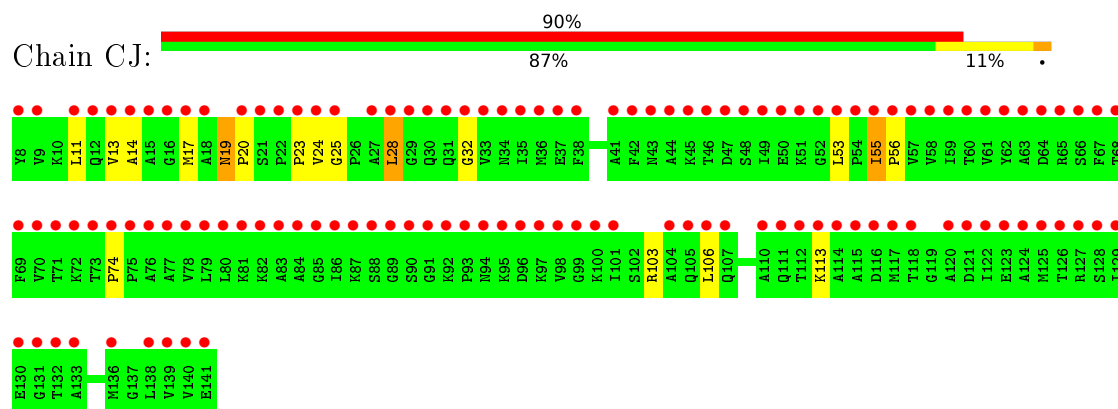
• Molecule 37: 50S ribosomal protein L9



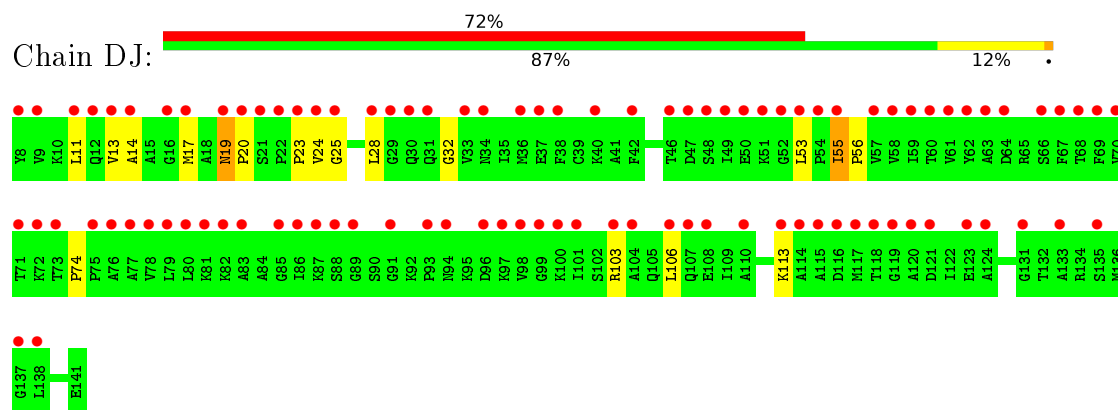
• Molecule 37: 50S ribosomal protein L9



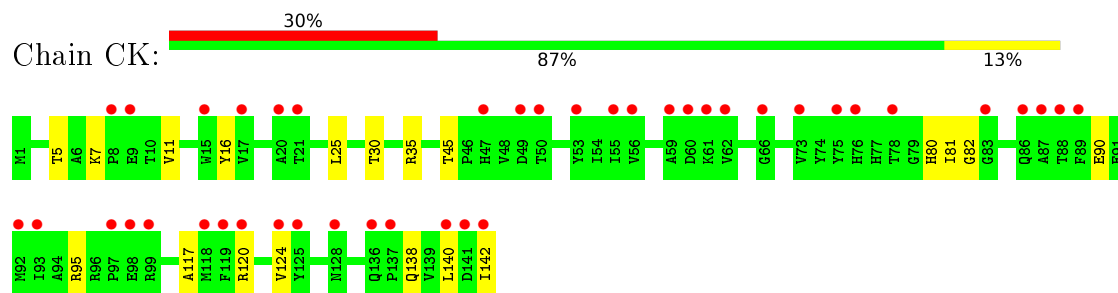
- Molecule 38: 50S ribosomal protein L11



- Molecule 38: 50S ribosomal protein L11



- Molecule 39: 50S ribosomal protein L13

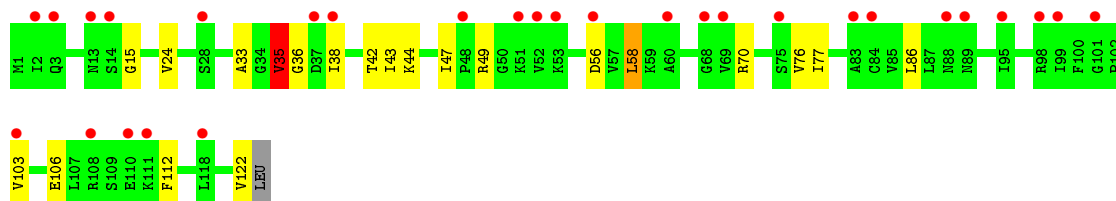
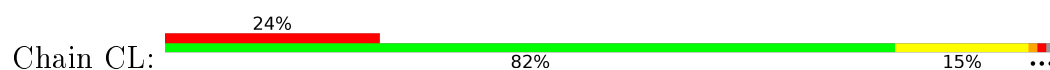


- Molecule 39: 50S ribosomal protein L13

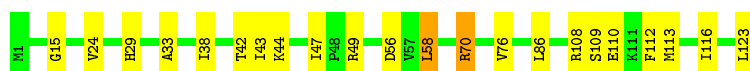
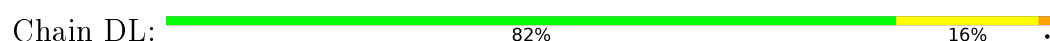




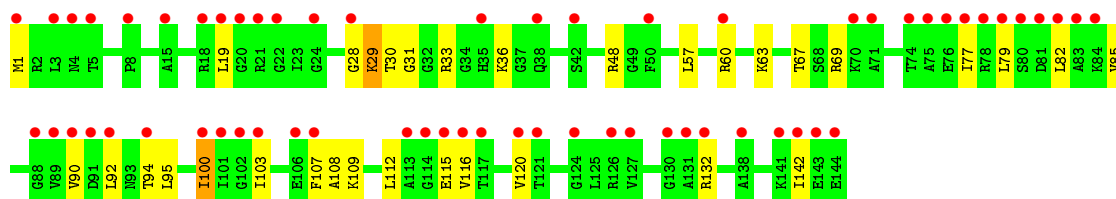
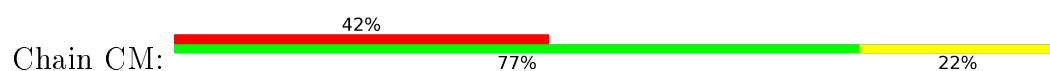
- Molecule 40: 50S ribosomal protein L14



- Molecule 40: 50S ribosomal protein L14



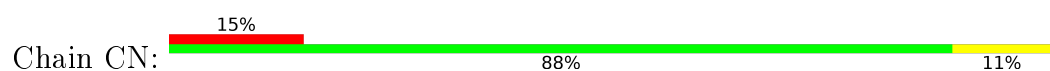
- Molecule 41: 50S ribosomal protein L15



- Molecule 41: 50S ribosomal protein L15



- Molecule 42: 50S ribosomal protein L16

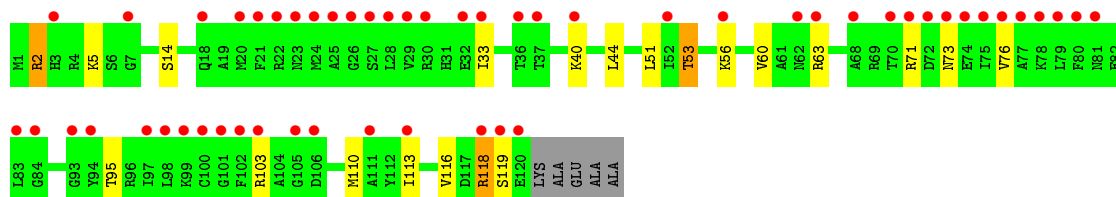
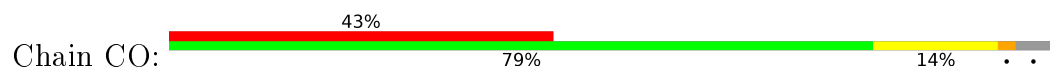


- Molecule 42: 50S ribosomal protein L16

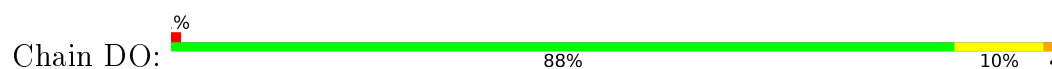




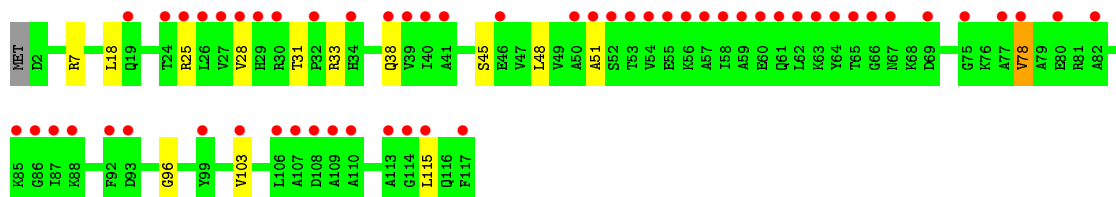
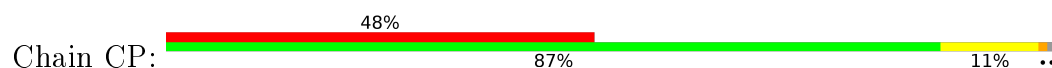
- Molecule 43: 50S ribosomal protein L17



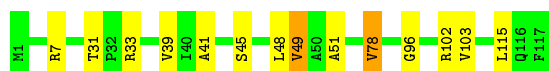
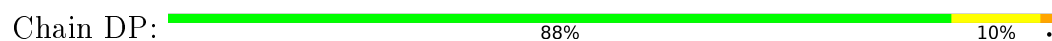
- Molecule 43: 50S ribosomal protein L17



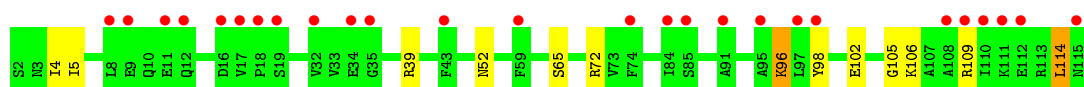
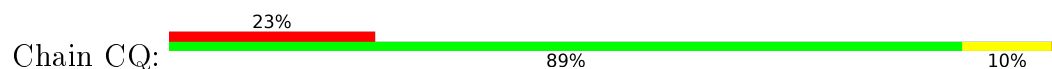
- Molecule 44: 50S ribosomal protein L18



- Molecule 44: 50S ribosomal protein L18

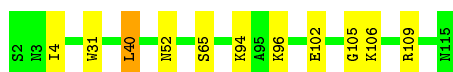


- Molecule 45: 50S ribosomal protein L19

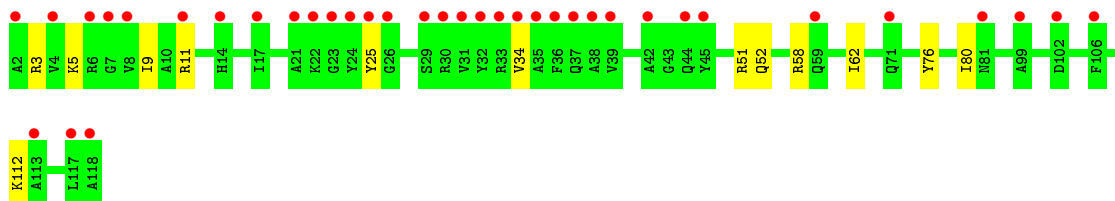
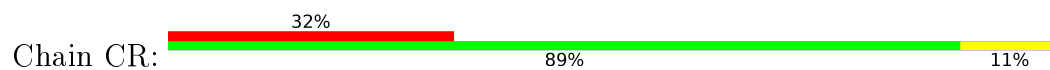


- Molecule 45: 50S ribosomal protein L19





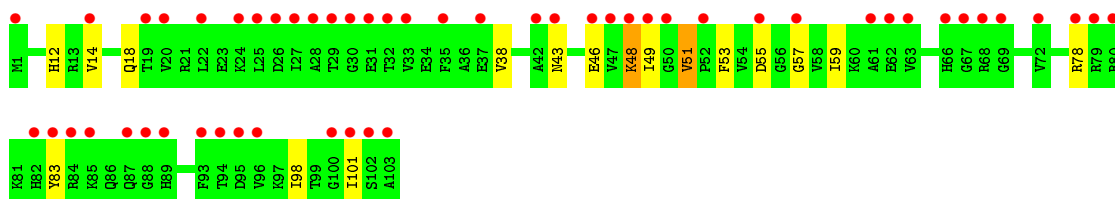
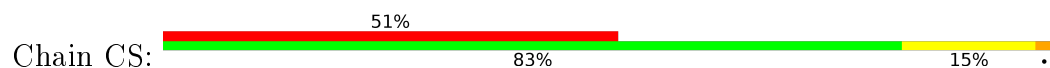
- Molecule 46: 50S ribosomal protein L20



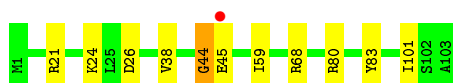
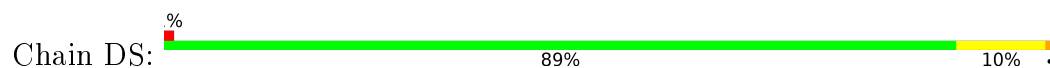
- Molecule 46: 50S ribosomal protein L20



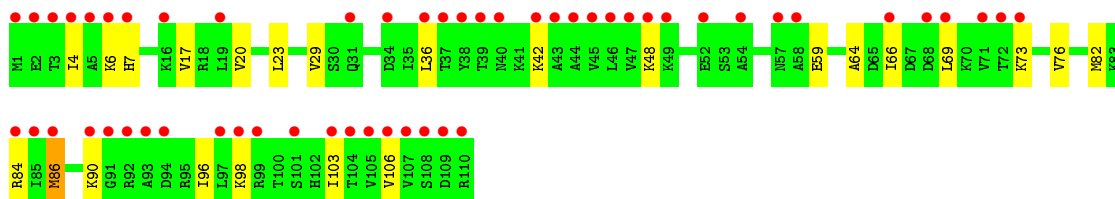
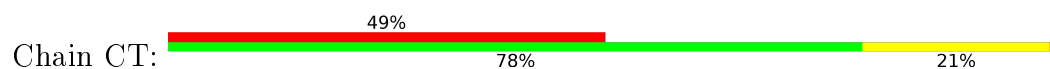
- Molecule 47: 50S ribosomal protein L21




- Molecule 47: 50S ribosomal protein L21

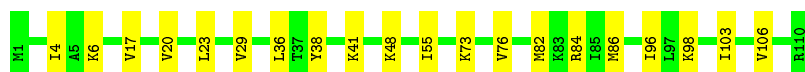


- Molecule 48: 50S ribosomal protein L22




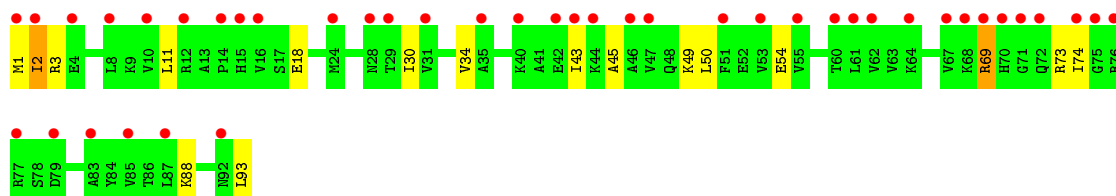
- Molecule 48: 50S ribosomal protein L22

Chain DT:  82% 18%




- Molecule 49: 50S ribosomal protein L23

Chain CU:  45% 82% 16%




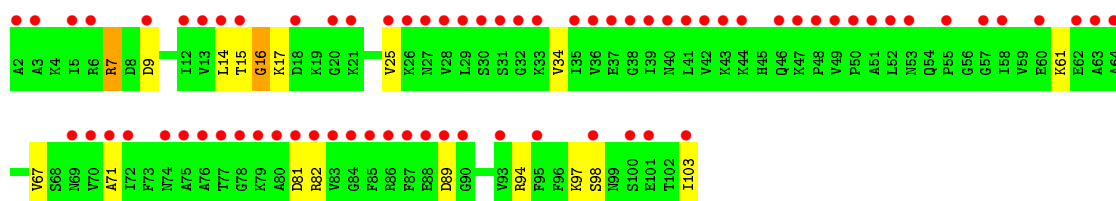
- Molecule 49: 50S ribosomal protein L23

Chain DU:  2% 88% 12%




- Molecule 50: 50S ribosomal protein L24

Chain CV:  72% 82% 16%



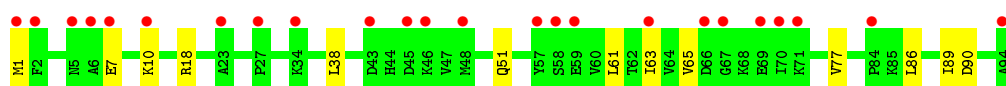
- Molecule 50: 50S ribosomal protein L24

Chain DV:  85% 14%




- Molecule 51: 50S ribosomal protein L25

Chain CW:  26% 86% 14%

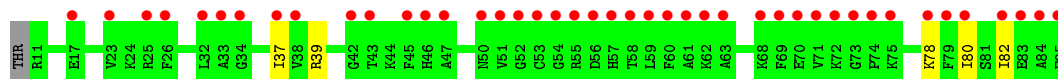
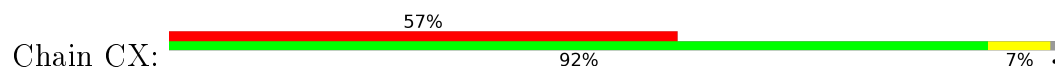


- Molecule 51: 50S ribosomal protein L25

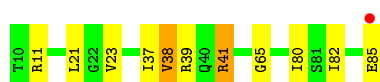
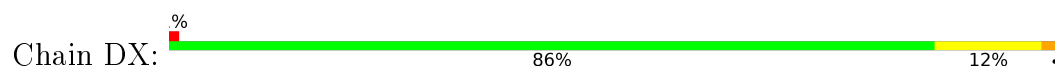
Chain DW:  87% 13%



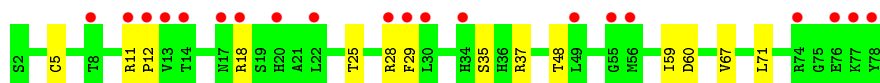
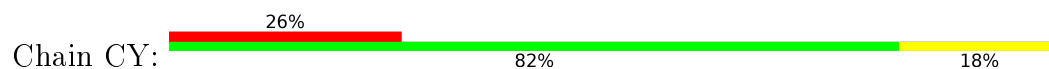
- Molecule 52: 50S ribosomal protein L27



- Molecule 52: 50S ribosomal protein L27



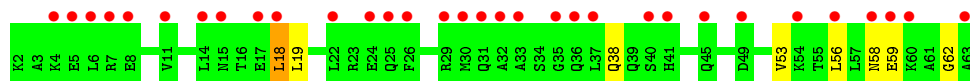
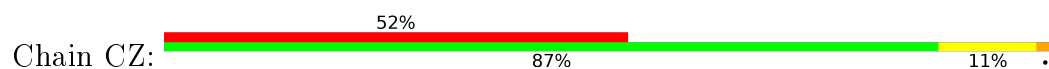
- Molecule 53: 50S ribosomal protein L28



- Molecule 53: 50S ribosomal protein L28



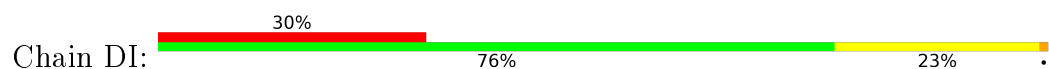
- Molecule 54: 50S ribosomal protein L29

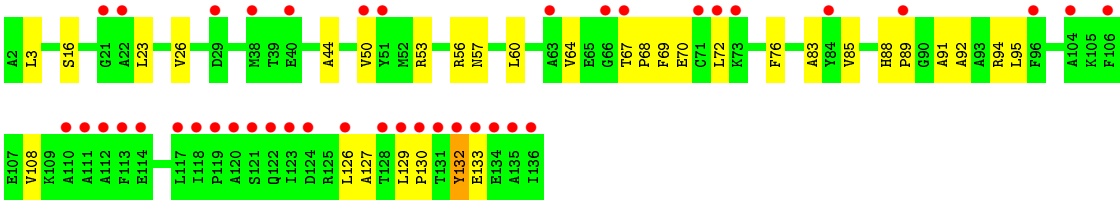


- Molecule 54: 50S ribosomal protein L29



- Molecule 55: 50S ribosomal protein L10





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.92Å 434.36Å 623.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.19 – 3.12 47.14 – 3.12	Depositor EDS
% Data completeness (in resolution range)	82.3 (47.19-3.12) 82.3 (47.14-3.12)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	22.94 (at 3.12Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.190 , 0.220 0.207 , 0.242	Depositor DCC
R_{free} test set	3321 reflections (0.40%)	DCC
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 101.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	295125	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.96	3/36593 (0.0%)	0.85	4/57081 (0.0%)
1	BA	0.96	7/36568 (0.0%)	0.84	3/57042 (0.0%)
2	AB	0.44	0/1784	0.63	0/2403
2	BB	0.43	0/1784	0.64	0/2403
3	AC	0.42	0/1652	0.64	0/2225
3	BC	0.42	0/1652	0.64	0/2225
4	AD	0.40	0/1665	0.63	0/2227
4	BD	0.40	0/1665	0.64	0/2227
5	AE	0.44	0/1157	0.72	0/1557
5	BE	0.44	0/1118	0.75	0/1504
6	AF	0.41	0/881	0.66	0/1189
6	BF	0.44	0/835	0.73	0/1128
7	AG	0.42	0/1196	0.61	0/1602
7	BG	0.43	0/1196	0.62	0/1602
8	AH	0.40	0/989	0.66	0/1326
8	BH	0.40	0/989	0.65	0/1326
9	AI	0.40	0/1034	0.65	0/1375
9	BI	0.40	0/1034	0.64	0/1375
10	AJ	0.41	0/806	0.65	0/1089
10	BJ	0.46	0/797	0.68	0/1077
11	AK	0.40	0/893	0.62	0/1205
11	BK	0.40	0/893	0.65	0/1205
12	AL	0.41	0/960	0.68	0/1286
12	BL	0.40	0/960	0.69	0/1286
13	AM	0.45	0/893	0.69	0/1193
13	BM	0.46	0/893	0.70	0/1193
14	AN	0.43	0/817	0.62	0/1088
14	BN	0.41	0/817	0.62	0/1088
15	AO	0.43	0/722	0.60	0/964
15	BO	0.40	0/722	0.62	0/964
16	AP	0.45	0/659	0.68	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	BP	0.46	0/659	0.72	0/884
17	AQ	0.45	0/658	0.69	0/881
17	BQ	0.46	0/658	0.72	0/881
18	AR	0.46	0/463	0.65	0/621
18	BR	0.47	0/463	0.63	0/621
19	AS	0.44	0/653	0.59	0/877
19	BS	0.43	0/653	0.59	0/877
20	AT	0.42	0/676	0.64	0/895
20	BT	0.45	0/671	0.66	0/888
21	AU	0.42	0/472	0.59	0/627
21	BU	0.39	0/472	0.59	0/627
22	C1	0.44	0/450	0.66	0/599
22	D1	0.48	0/450	0.72	0/599
23	C2	0.46	0/416	0.71	0/554
23	D2	0.46	0/421	0.68	0/561
24	C3	0.45	0/380	0.70	0/498
24	D3	0.53	0/380	0.74	0/498
25	C4	0.42	0/513	0.62	0/676
25	D4	0.48	0/513	0.65	0/676
26	C5	0.41	0/303	0.72	0/397
26	D5	0.47	0/303	0.74	0/397
27	C0	0.51	0/453	0.74	0/605
27	D0	0.52	0/467	0.71	0/623
28	CB	0.96	0/2828	0.86	1/4410 (0.0%)
28	DB	0.99	1/2872 (0.0%)	0.86	0/4478
29	CC	0.40	0/2122	0.69	0/2852
29	DC	0.42	0/2122	0.69	0/2852
30	CD	0.40	0/1586	0.66	0/2134
31	CA	0.99	42/69165 (0.1%)	0.86	10/107896 (0.0%)
32	DD	0.46	0/1576	0.67	0/2119
33	DA	1.03	26/69364 (0.0%)	0.89	14/108207 (0.0%)
34	CE	0.42	0/1571	0.67	0/2113
34	DE	0.44	0/1571	0.66	0/2113
35	CF	0.40	0/1435	0.65	0/1926
35	DF	0.41	0/1435	0.66	0/1926
36	CG	0.39	0/1343	0.63	1/1816 (0.1%)
36	DG	0.40	0/1343	0.60	0/1816
37	CH	0.44	0/1121	0.67	0/1515
37	DH	0.44	0/1121	0.66	0/1515
38	CJ	0.50	0/993	0.63	0/1341
38	DJ	0.50	0/993	0.63	0/1341
39	CK	0.38	0/1152	0.67	0/1551
39	DK	0.45	0/1152	0.66	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
40	CL	0.44	0/947	0.67	0/1268
40	DL	0.47	0/955	0.68	0/1279
41	CM	0.43	0/1062	0.68	0/1413
41	DM	0.42	0/1062	0.67	0/1413
42	CN	0.42	0/1081	0.71	0/1443
42	DN	0.47	0/1092	0.72	0/1457
43	CO	0.41	0/973	0.67	0/1301
43	DO	0.47	0/1006	0.70	0/1345
44	CP	0.41	0/902	0.70	0/1209
44	DP	0.42	0/910	0.69	0/1219
45	CQ	0.39	0/929	0.67	1/1242 (0.1%)
45	DQ	0.43	0/929	0.65	0/1242
46	CR	0.43	0/960	0.64	0/1278
46	DR	0.51	0/960	0.65	0/1278
47	CS	0.41	0/829	0.69	0/1107
47	DS	0.45	0/829	0.72	0/1107
48	CT	0.41	0/864	0.70	0/1156
48	DT	0.46	0/864	0.69	0/1156
49	CU	0.42	0/745	0.65	0/994
49	DU	0.43	0/745	0.66	0/994
50	CV	0.47	0/788	0.73	0/1051
50	DV	0.44	0/788	0.70	0/1051
51	CW	0.39	0/766	0.62	0/1025
51	DW	0.44	0/766	0.63	0/1025
52	CX	0.37	0/576	0.60	0/762
52	DX	0.44	0/598	0.64	0/790
53	CY	0.39	0/635	0.68	0/848
53	DY	0.42	0/635	0.69	0/848
54	CZ	0.42	0/502	0.63	0/667
54	DZ	0.42	0/502	0.61	0/667
55	DI	0.49	0/1037	0.72	1/1402 (0.1%)
All	All	0.87	79/309273 (0.0%)	0.82	35/462210 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	1
33	DA	0	15
42	CN	0	1
All	All	0	17

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	1936	A	N9-C4	-9.27	1.32	1.37
31	CA	2095	A	O5'-C5'	-8.23	1.29	1.42
31	CA	769	U	C1'-N1	7.39	1.59	1.48
1	BA	5	U	C1'-N1	7.39	1.59	1.48
31	CA	2225	A	C3'-O3'	7.31	1.52	1.42
33	DA	2097	A	O5'-C5'	-7.08	1.31	1.42
33	DA	2585	U	C1'-N1	6.99	1.59	1.48
33	DA	12	U	C1'-N1	6.87	1.59	1.48
1	BA	1493	A	C3'-O3'	6.85	1.51	1.42
31	CA	1788	C	C1'-N1	6.81	1.58	1.48
31	CA	1825	U	C1'-N1	6.58	1.58	1.48
1	AA	5	U	C1'-N1	6.46	1.58	1.48
33	DA	2585	U	N1-C2	6.44	1.44	1.38
33	DA	613	A	N9-C4	6.22	1.41	1.37
31	CA	1658	C	C1'-N1	6.19	1.58	1.48
1	BA	1008	U	O5'-C5'	-6.18	1.32	1.42
31	CA	1777	U	C1'-N1	6.17	1.57	1.48
31	CA	1656	C	C1'-N1	6.09	1.57	1.48
31	CA	2425	A	C3'-O3'	6.09	1.50	1.42
1	BA	209	U	C1'-N1	6.04	1.57	1.48
1	AA	1397	C	N1-C6	6.01	1.40	1.37
31	CA	1994	C	C1'-N1	5.99	1.57	1.48
31	CA	12	U	C1'-N1	5.95	1.57	1.48
31	CA	995	C	O5'-C5'	-5.88	1.33	1.42
33	DA	2127	G	C3'-O3'	5.83	1.50	1.42
31	CA	2586	U	C1'-N1	5.83	1.57	1.48
31	CA	253	C	C1'-N1	5.79	1.57	1.48
33	DA	2585	U	C3'-O3'	5.79	1.50	1.42
31	CA	1314	C	C1'-N1	5.78	1.57	1.48
31	CA	688	U	C1'-N1	5.77	1.57	1.48
33	DA	140	C	C1'-N1	5.74	1.57	1.48
31	CA	2619	C	C1'-N1	5.67	1.57	1.48
31	CA	2232	C	C1'-N1	5.66	1.57	1.48
33	DA	790	U	C1'-N1	5.62	1.57	1.48
31	CA	826	U	C1'-N1	5.59	1.57	1.48
31	CA	1352	U	C1'-N1	5.55	1.57	1.48
1	BA	1397	C	N1-C2	5.53	1.45	1.40
31	CA	2263	C	C1'-N1	5.51	1.57	1.48
31	CA	451	U	C1'-N1	5.49	1.56	1.48
31	CA	20	C	C1'-N1	5.45	1.56	1.48
33	DA	1170	C	C1'-N1	5.45	1.56	1.48
31	CA	692	C	C1'-N1	5.42	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2146	C	C3'-O3'	5.40	1.49	1.42
33	DA	1174	U	C1'-N1	5.40	1.56	1.48
31	CA	404	A	C3'-O3'	5.36	1.49	1.42
1	BA	932	C	C1'-N1	5.35	1.56	1.48
31	CA	546	U	C1'-N1	5.32	1.56	1.48
31	CA	2055	C	C1'-N1	5.32	1.56	1.48
33	DA	102	U	N1-C2	5.32	1.43	1.38
33	DA	653	U	C1'-N1	5.31	1.56	1.48
33	DA	2756	U	C3'-O3'	5.29	1.49	1.42
31	CA	2215	C	C1'-N1	5.26	1.56	1.48
33	DA	2767	C	C1'-N1	5.26	1.56	1.48
33	DA	1266	G	C3'-O3'	5.25	1.49	1.42
33	DA	1306	C	C1'-N1	5.25	1.56	1.48
31	CA	2591	C	C1'-N1	5.22	1.56	1.48
31	CA	2680	U	C3'-O3'	5.22	1.49	1.42
28	DB	70	C	C1'-N1	5.20	1.56	1.48
31	CA	1793	C	C1'-N1	5.17	1.56	1.48
31	CA	271	G	C3'-O3'	5.16	1.49	1.42
33	DA	2158	A	C3'-O3'	5.15	1.49	1.42
31	CA	2715	C	C1'-N1	5.14	1.56	1.48
31	CA	1306	C	C1'-N1	5.13	1.56	1.48
33	DA	271	G	C3'-O3'	5.12	1.49	1.42
33	DA	2506	U	C1'-N1	5.11	1.56	1.48
1	BA	209	U	N1-C2	5.10	1.43	1.38
31	CA	355	U	C1'-N1	5.09	1.56	1.48
33	DA	12	U	N1-C2	5.09	1.43	1.38
33	DA	12	U	P-O5'	5.08	1.64	1.59
1	AA	1397	C	C1'-N1	5.08	1.56	1.48
33	DA	1534	U	C1'-N1	5.08	1.56	1.48
33	DA	2055	C	C3'-O3'	-5.07	1.35	1.42
33	DA	1819	A	N3-C4	5.06	1.37	1.34
31	CA	29	U	C1'-N1	5.06	1.56	1.48
31	CA	2443	C	C1'-N1	5.05	1.56	1.48
31	CA	635	C	C1'-N1	5.04	1.56	1.48
31	CA	2017	U	C1'-N1	5.03	1.56	1.48
33	DA	29	U	C1'-N1	5.01	1.56	1.48
31	CA	2769	U	C1'-N1	5.01	1.56	1.48

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	CB	15	A	O4'-C1'-N9	9.17	115.54	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	DA	271	G	P-O3'-C3'	7.52	128.73	119.70
1	AA	1	A	OP1-P-OP2	-7.09	108.97	119.60
55	DI	132	TYR	C-N-CA	7.06	139.35	121.70
31	CA	892	A	OP1-P-OP2	-7.01	109.08	119.60
33	DA	892	A	OP1-P-OP2	-6.91	109.24	119.60
33	DA	1	G	OP1-P-OP2	-6.88	109.28	119.60
33	DA	1936	A	O4'-C1'-N9	6.80	113.64	108.20
1	BA	2	A	OP1-P-OP2	-6.62	109.66	119.60
1	BA	1362	A	C1'-O4'-C4'	-6.62	104.60	109.90
1	AA	413	G	C1'-O4'-C4'	-6.59	104.63	109.90
33	DA	1434	A	O4'-C1'-N9	6.59	113.47	108.20
31	CA	2406	A	C5'-C4'-O4'	6.44	116.83	109.10
31	CA	271	G	P-O3'-C3'	6.37	127.34	119.70
31	CA	2425	A	P-O3'-C3'	6.33	127.29	119.70
33	DA	784	G	P-O3'-C3'	6.21	127.15	119.70
31	CA	1128	G	C1'-O4'-C4'	-6.18	104.95	109.90
33	DA	2406	A	C5'-C4'-O4'	-6.13	101.75	109.10
31	CA	974	G	N9-C1'-C2'	5.93	121.71	114.00
33	DA	613	A	O4'-C1'-N9	5.87	112.90	108.20
33	DA	512	G	O4'-C1'-N9	5.68	112.75	108.20
45	CQ	114	LEU	CA-CB-CG	5.55	128.08	115.30
33	DA	451	U	C1'-O4'-C4'	-5.54	105.47	109.90
1	AA	841	C	P-O3'-C3'	5.51	126.31	119.70
33	DA	242	G	C3'-C2'-C1'	-5.47	97.12	101.50
31	CA	2225	A	P-O3'-C3'	5.44	126.23	119.70
31	CA	784	G	P-O3'-C3'	5.44	126.23	119.70
33	DA	1128	G	C1'-O4'-C4'	-5.44	105.55	109.90
33	DA	479	A	C3'-C2'-C1'	-5.29	97.27	101.50
1	AA	686	U	C1'-O4'-C4'	-5.28	105.68	109.90
31	CA	479	A	C3'-C2'-C1'	-5.25	97.30	101.50
1	BA	686	U	C1'-O4'-C4'	-5.21	105.73	109.90
31	CA	1379	U	P-O3'-C3'	5.08	125.80	119.70
33	DA	1395	A	C1'-O4'-C4'	-5.05	105.86	109.90
36	CG	175	LYS	C-N-CA	5.00	134.21	121.70

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	898	G	Sidechain
42	CN	69	PRO	Mainchain
33	DA	1753	G	Sidechain

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Mol	Chain	Res	Type	Group
33	DA	1954	G	Sidechain
33	DA	2250	G	Sidechain
33	DA	2358	A	Sidechain
33	DA	2589	A	Sidechain
33	DA	2595	G	Sidechain
33	DA	2692	G	Sidechain
33	DA	27	G	Sidechain
33	DA	2848	G	Sidechain
33	DA	308	G	Sidechain
33	DA	452	G	Sidechain
33	DA	512	G	Sidechain
33	DA	690	G	Sidechain
33	DA	956	G	Sidechain
33	DA	980	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	89	0
1	BA	32908	0	16580	91	0
2	AB	1753	0	1780	12	0
2	BB	1753	0	1780	16	0
3	AC	1625	0	1696	12	0
3	BC	1625	0	1696	15	0
4	AD	1643	0	1707	9	0
4	BD	1643	0	1707	12	0
5	AE	1144	0	1185	15	0
5	BE	1105	0	1148	19	0
6	AF	862	0	864	6	0
6	BF	817	0	808	9	0
7	AG	1182	0	1238	12	0
7	BG	1182	0	1238	7	0
8	AH	979	0	1031	7	0
8	BH	979	0	1031	5	0
9	AI	1022	0	1070	7	0
9	BI	1022	0	1070	7	0
10	AJ	796	0	836	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	BJ	787	0	828	10	0
11	AK	877	0	887	11	0
11	BK	877	0	887	10	0
12	AL	957	0	1017	9	0
12	BL	957	0	1017	11	0
13	AM	884	0	941	8	0
13	BM	884	0	941	13	0
14	AN	805	0	844	10	0
14	BN	805	0	844	10	0
15	AO	714	0	734	0	0
15	BO	714	0	734	1	0
16	AP	649	0	666	3	0
16	BP	649	0	666	7	0
17	AQ	649	0	691	4	0
17	BQ	649	0	691	7	0
18	AR	456	0	478	2	0
18	BR	456	0	478	1	0
19	AS	638	0	665	6	0
19	BS	638	0	665	10	0
20	AT	670	0	719	3	0
20	BT	665	0	714	8	0
21	AU	465	0	491	5	0
21	BU	465	0	491	5	0
22	C1	444	0	458	6	0
22	D1	444	0	458	9	0
23	C2	409	0	440	4	0
23	D2	414	0	442	2	0
24	C3	377	0	418	4	0
24	D3	377	0	418	1	0
25	C4	504	0	572	1	0
25	D4	504	0	572	2	0
26	C5	302	0	340	5	0
26	D5	302	0	340	1	0
27	C0	449	0	488	2	0
27	D0	463	0	504	2	0
28	CB	2529	0	1281	2	0
28	DB	2569	0	1301	5	0
29	CC	2083	0	2154	20	0
29	DC	2083	0	2154	17	0
30	CD	1565	0	1616	14	0
31	CA	62229	0	31318	254	0
32	DD	1576	0	1627	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	DA	62423	0	31410	187	0
34	CE	1552	0	1619	15	0
34	DE	1552	0	1619	11	0
35	CF	1411	0	1444	12	0
35	DF	1411	0	1444	14	0
36	CG	1323	0	1371	8	0
36	DG	1323	0	1371	9	0
37	CH	1110	0	1148	9	0
37	DH	1110	0	1148	7	0
38	CJ	979	0	1028	7	0
38	DJ	979	0	1028	6	0
39	CK	1129	0	1162	8	0
39	DK	1129	0	1162	3	0
40	CL	938	0	1012	10	0
40	DL	946	0	1023	9	0
41	CM	1053	0	1129	21	0
41	DM	1053	0	1129	11	0
42	CN	1075	0	1154	7	0
42	DN	1092	0	1177	7	0
43	CO	960	0	1000	9	0
43	DO	993	0	1034	7	0
44	CP	892	0	923	5	0
44	DP	900	0	935	8	0
45	CQ	917	0	962	8	0
45	DQ	917	0	962	5	0
46	CR	947	0	1019	10	0
46	DR	947	0	1019	13	0
47	CS	816	0	839	8	0
47	DS	816	0	839	8	0
48	CT	857	0	922	14	0
48	DT	857	0	922	13	0
49	CU	739	0	807	7	0
49	DU	739	0	807	3	0
50	CV	780	0	831	8	0
50	DV	780	0	831	5	0
51	CW	753	0	780	4	0
51	DW	753	0	780	5	0
52	CX	569	0	581	1	0
52	DX	591	0	606	7	0
53	CY	625	0	652	7	0
53	DY	625	0	652	2	0
54	CZ	501	0	531	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	DZ	501	0	531	3	0
55	DI	1023	0	1052	14	0
56	AA	70	0	0	0	0
56	BA	41	0	0	0	0
56	CA	156	0	0	0	0
56	CB	3	0	0	0	0
56	DA	184	0	0	0	0
56	DB	9	0	0	0	0
56	DD	1	0	0	0	0
56	DR	2	0	0	0	0
57	AA	13	0	18	1	0
57	BA	13	0	18	1	0
57	DA	26	0	36	1	0
57	DQ	13	0	18	0	0
57	DR	13	0	18	3	0
57	DS	13	0	18	1	0
58	AA	16	0	28	1	0
58	DA	48	0	84	1	0
58	DE	16	0	28	1	0
58	DK	8	0	14	0	0
58	DN	8	0	14	0	0
58	DS	8	0	14	0	0
58	DT	8	0	14	0	0
59	AA	24	0	48	0	0
59	DA	72	0	144	2	0
60	AB	1	0	0	0	0
60	C5	1	0	0	0	0
60	D5	1	0	0	0	0
61	AL	7	0	10	0	0
61	D1	7	0	10	2	0
61	D3	7	0	10	0	0
61	DA	35	0	50	0	0
61	DL	7	0	10	0	0
61	DP	7	0	10	0	0
61	DQ	7	0	10	0	0
62	D0	4	0	6	0	0
62	D1	4	0	6	0	0
62	DA	32	0	48	1	0
62	DB	8	0	12	0	0
63	D3	10	0	14	0	0
63	DA	40	0	56	2	0
63	DD	10	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	DS	10	0	14	2	0
63	DT	10	0	14	0	0
63	DU	10	0	14	0	0
64	DA	40	0	76	0	0
65	DA	32	0	44	1	0
66	DA	12	0	9	0	0
67	DA	11	0	5	0	0
68	DA	8	0	12	1	0
69	AA	507	0	0	1	0
69	AC	4	0	0	0	0
69	AD	3	0	0	0	0
69	AE	5	0	0	0	0
69	AF	1	0	0	0	0
69	AG	1	0	0	0	0
69	AJ	2	0	0	0	0
69	AK	7	0	0	0	0
69	AL	10	0	0	0	0
69	AM	4	0	0	1	0
69	AN	7	0	0	2	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	3	0	0	0	0
69	AU	3	0	0	0	0
69	BA	291	0	0	1	0
69	BD	11	0	0	0	0
69	BE	1	0	0	0	0
69	BF	1	0	0	0	0
69	BK	2	0	0	0	0
69	BL	2	0	0	0	0
69	BN	2	0	0	0	0
69	BO	1	0	0	0	0
69	BP	3	0	0	2	0
69	BR	1	0	0	0	0
69	BT	4	0	0	0	0
69	BU	1	0	0	0	0
69	C3	3	0	0	0	0
69	C4	1	0	0	0	0
69	C5	1	0	0	0	0
69	CA	692	0	0	5	0
69	CB	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	CC	10	0	0	0	0
69	CD	6	0	0	0	0
69	CE	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	2	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	21	0	0	0	0
69	D1	42	0	0	0	0
69	D2	7	0	0	0	0
69	D3	28	0	0	0	0
69	D4	39	0	0	0	0
69	D5	9	0	0	0	0
69	DA	4834	0	0	14	0
69	DB	199	0	0	2	0
69	DC	98	0	0	1	0
69	DD	95	0	0	0	0
69	DE	63	0	0	1	0
69	DF	15	0	0	0	0
69	DG	7	0	0	0	0
69	DH	1	0	0	0	0
69	DK	65	0	0	1	0
69	DL	52	0	0	0	0
69	DM	62	0	0	0	0
69	DN	64	0	0	0	0
69	DO	48	0	0	0	0
69	DP	44	0	0	1	0
69	DQ	33	0	0	0	0
69	DR	68	0	0	1	0
69	DS	48	0	0	0	0
69	DT	62	0	0	1	0
69	DU	22	0	0	0	0
69	DV	18	0	0	0	0
69	DW	34	0	0	2	0
69	DX	31	0	0	0	0
69	DY	10	0	0	0	0
69	DZ	5	0	0	1	0
All	All	295125	0	194409	1246	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 3.

All (1246) 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)
47:CS:14:VAL:HG21	47:CS:98:ILE:HG13	1.20	1.10
33:DA:1847:A:HO2'	33:DA:1848:A:H8	1.02	0.98
2:BB:20:THR:HA	2:BB:39:HIS:CE1	1.98	0.98
47:CS:14:VAL:CG2	47:CS:98:ILE:HG13	1.96	0.96
31:CA:1847:A:HO2'	31:CA:1848:A:H8	1.04	0.94
46:DR:20:GLN:HG3	57:DR:203:PG4:H42	1.50	0.91
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.52	0.91
26:C5:3:VAL:HG11	31:CA:2539:C:H5'	1.54	0.90
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.51	0.90
31:CA:1005:C:O2'	39:CK:30:THR:HG21	1.71	0.89
1:BA:841:C:H3'	1:BA:842:U:H5''	1.54	0.89
14:AN:66:GLN:HB2	69:AN:207:HOH:O	1.73	0.87
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.56	0.87
41:CM:77:ILE:HD11	41:CM:108:ALA:HB1	1.54	0.87
31:CA:1936:A:N6	31:CA:1963:U:H3	1.73	0.86
48:CT:86:MET:HB2	48:CT:96:ILE:HD11	1.58	0.86
31:CA:2728:U:HO2'	31:CA:2729:G:H8	1.20	0.86
1:AA:1492:A:H5''	12:AL:44:LYS:HG2	1.58	0.85
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.58	0.85
13:BM:6:GLY:HA3	13:BM:66:GLU:HG3	1.58	0.85
31:CA:1936:A:H2	31:CA:1943:U:H3	1.26	0.83
13:BM:114:LYS:HB3	13:BM:115:PRO:HD3	1.60	0.83
31:CA:2428:G:N2	41:CM:60:ARG:HH21	1.77	0.82
33:DA:2428:G:N2	41:DM:60:ARG:HH21	1.77	0.81
1:AA:664:G:H22	1:AA:741:G:H1	1.29	0.79
32:DD:4:LEU:HD12	32:DD:101:PHE:CE2	2.18	0.79
11:BK:88:GLY:H	11:BK:114:THR:HG22	1.48	0.78
1:BA:664:G:H22	1:BA:741:G:H1	1.29	0.76
29:CC:17:VAL:HB	29:CC:204:VAL:HG13	1.69	0.74
34:CE:149:ILE:HG12	34:CE:188:MET:HG2	1.68	0.74
8:BH:87:LYS:HB2	8:BH:125:ILE:HD11	1.69	0.74
1:BA:841:C:H3'	1:BA:842:U:C5'	2.16	0.74
24:C3:12:ARG:HD2	24:C3:44:VAL:HG11	1.71	0.73
48:CT:73:LYS:HB2	48:CT:106:VAL:HB	1.71	0.73
33:DA:580:U:O3'	46:DR:31:VAL:HG13	1.89	0.73
33:DA:2127:G:H4'	33:DA:2128:G:OP1	1.88	0.72
1:BA:1305:G:H21	1:BA:1332:A:H2	1.38	0.72
58:DA:3191:MPD:H12	34:DE:33:VAL:HG22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:197:GLU:HA	4:BD:200:ILE:HD12	1.71	0.72
1:AA:1305:G:H21	1:AA:1332:A:H2	1.38	0.72
31:CA:528:A:C2	31:CA:2043:C:H4'	2.25	0.72
8:AH:87:LYS:HB2	8:AH:125:ILE:HD11	1.72	0.71
4:AD:197:GLU:HA	4:AD:200:ILE:HD12	1.70	0.71
47:CS:14:VAL:HG21	47:CS:98:ILE:CG1	2.11	0.71
13:BM:22:ILE:HB	13:BM:25:VAL:CG1	2.19	0.71
31:CA:1394:U:H4'	31:CA:1603:A:H4'	1.72	0.71
31:CA:532:A:N1	31:CA:2020:A:H1'	2.05	0.71
1:AA:1358:U:H3	1:AA:1363:A:H62	1.38	0.70
31:CA:206:U:H2'	31:CA:207:A:H8	1.56	0.70
48:DT:73:LYS:HB2	48:DT:106:VAL:HB	1.72	0.70
33:DA:2262:U:H5''	52:DX:41[A]:ARG:HH12	1.57	0.69
39:DK:46:PRO:HD2	69:DK:363:HOH:O	1.91	0.69
3:BC:123:GLN:HB3	3:BC:128:VAL:HG21	1.74	0.69
36:CG:80:THR:HG23	36:CG:81:GLU:H	1.57	0.69
33:DA:135:U:H3	33:DA:144:A:H61	1.39	0.69
33:DA:2591:C:H2'	33:DA:2592:G:C8	2.27	0.69
22:C1:43:ILE:HG22	22:C1:49:TYR:HB2	1.75	0.69
30:CD:133:THR:HG22	31:CA:1993:U:H4'	1.74	0.69
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.75	0.69
19:BS:6:LYS:HD2	19:BS:7:LYS:H	1.58	0.69
33:DA:494:G:H4'	48:DT:6:LYS:HB2	1.74	0.69
33:DA:568:U:H1'	33:DA:2030:6MZ:H9C1	1.75	0.69
31:CA:1936:A:H61	31:CA:1963:U:H3	1.40	0.68
31:CA:135:U:H3	31:CA:144:A:H61	1.39	0.68
33:DA:2033:A:H5'	69:DA:3669:HOH:O	1.93	0.68
31:CA:846:U:H1'	31:CA:847:U:H5	1.58	0.68
30:CD:4:LEU:HD12	30:CD:101:PHE:CE2	2.29	0.68
48:CT:82:MET:HB2	48:CT:98:LYS:HB2	1.76	0.68
22:D1:43:ILE:HG22	22:D1:49:TYR:HB2	1.76	0.68
33:DA:1853:A:N1	33:DA:2087:G:H1'	2.09	0.68
1:AA:81:A:H61	1:AA:86:G:H1	1.42	0.67
43:CO:73:ASN:HA	43:CO:76:VAL:HG22	1.76	0.67
31:CA:17:G:H4'	46:CR:25:TYR:HE2	1.59	0.67
33:DA:2128:G:H1	33:DA:2160:C:H42	1.42	0.67
6:BF:38:ARG:HH12	6:BF:99:ALA:HB3	1.60	0.67
48:DT:82:MET:HB2	48:DT:98:LYS:HB2	1.77	0.67
3:BC:40:ARG:HH11	3:BC:55:ILE:HG23	1.59	0.66
50:CV:7:ARG:O	50:CV:25:VAL:HB	1.95	0.66
3:BC:77:ILE:HA	3:BC:84:VAL:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:DR:20:GLN:CG	57:DR:203:PG4:H42	2.26	0.66
13:BM:83:LEU:HD21	19:BS:65:GLU:HB2	1.76	0.66
41:CM:82:LEU:HD11	41:CM:116:VAL:HG23	1.78	0.66
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.77	0.66
1:BA:451:A:H2'	69:BA:1701:HOH:O	1.96	0.66
33:DA:1913:A:H4'	33:DA:1913:A:OP1	1.96	0.65
10:AJ:7:ARG:HB3	10:AJ:101:SER:HB2	1.77	0.65
31:CA:2428:G:N2	41:CM:60:ARG:NH2	2.44	0.65
31:CA:2728:U:O2'	31:CA:2729:G:H8	1.78	0.65
3:AC:77:ILE:HA	3:AC:84:VAL:HG23	1.77	0.65
43:DO:73:ASN:HA	43:DO:76:VAL:HG22	1.77	0.65
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.78	0.65
20:BT:9:LYS:O	20:BT:12:ILE:HG13	1.97	0.65
46:DR:28:ARG:HD3	69:DR:318:HOH:O	1.96	0.65
31:CA:2074:U:H2'	31:CA:2075:U:C6	2.33	0.64
31:CA:2796:U:H3	31:CA:2799:A:H61	1.45	0.64
11:AK:31:ILE:HG12	11:AK:46:THR:HG22	1.79	0.64
33:DA:2796:U:H3	33:DA:2799:A:H61	1.44	0.64
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	1.78	0.64
11:BK:88:GLY:N	11:BK:114:THR:HG22	2.13	0.64
31:CA:1105:U:H2'	31:CA:1106:G:H8	1.62	0.64
52:CX:37:ILE:HG21	52:CX:80:ILE:HG21	1.79	0.64
33:DA:1105:U:H2'	33:DA:1106:G:H8	1.63	0.64
33:DA:2428:G:H21	41:DM:60:ARG:HH21	1.44	0.64
31:CA:783:A:H4'	31:CA:1779:U:O2	1.97	0.63
2:BB:23:TRP:HB3	2:BB:39:HIS:CE1	2.33	0.63
31:CA:659:G:H4'	34:CE:95:LYS:HD3	1.81	0.63
30:CD:129:THR:HG23	30:CD:140:HIS:O	1.98	0.63
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.35	0.62
13:AM:4:ILE:HD12	13:AM:10:PRO:HG2	1.80	0.62
1:BA:1218:C:H2'	1:BA:1219:A:C8	2.35	0.62
33:DA:2428:G:N2	41:DM:60:ARG:NH2	2.47	0.62
31:CA:740:C:H5'	31:CA:1784:A:H3'	1.82	0.62
69:DA:8015:HOH:O	42:DN:55:ARG:HG3	1.97	0.62
31:CA:699:A:H2'	31:CA:700:G:O4'	2.00	0.62
55:DI:64:VAL:HG22	55:DI:69:PHE:HB2	1.82	0.62
50:DV:52:LEU:HB3	50:DV:54:GLN:HB2	1.81	0.62
44:DP:31:THR:HG22	44:DP:33:ARG:H	1.64	0.62
31:CA:674:G:H1'	34:CE:69:ARG:HH11	1.65	0.62
5:BE:106:ILE:HD11	5:BE:124:LEU:HD23	1.81	0.61
6:BF:38:ARG:NH1	6:BF:99:ALA:HB3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BT:4:ILE:HA	20:BT:8:LYS:HE2	1.81	0.61
48:CT:17:VAL:HG11	48:CT:103:ILE:HG12	1.82	0.61
19:AS:15:LEU:HD13	19:AS:33:THR:HG21	1.82	0.61
12:BL:43:LYS:HD2	12:BL:91:PRO:HG3	1.81	0.61
13:BM:22:ILE:HB	13:BM:25:VAL:HG12	1.81	0.61
40:DL:43:ILE:HD12	40:DL:56:ASP:HB2	1.83	0.61
52:DX:37:ILE:HG21	52:DX:80:ILE:HG21	1.81	0.61
17:BQ:17:MET:HB3	17:BQ:20:SER:HB3	1.82	0.61
31:CA:2469:A:H4'	42:CN:55:ARG:HD3	1.82	0.61
5:BE:104:GLY:HA3	5:BE:122:ASN:HA	1.83	0.61
31:CA:2428:G:H21	41:CM:60:ARG:HH21	1.45	0.61
4:BD:107:PHE:HB3	4:BD:145:ILE:HD11	1.83	0.60
41:CM:95:LEU:HD22	41:CM:100:ILE:HG12	1.81	0.60
36:DG:24:ILE:HD11	36:DG:43:VAL:HG11	1.82	0.60
48:DT:17:VAL:HG11	48:DT:103:ILE:HG12	1.83	0.60
1:AA:209:U:H4'	1:AA:210:C:OP2	2.01	0.60
31:CA:2845:U:H5''	45:CQ:52:ASN:O	2.00	0.60
31:CA:634:C:H2'	31:CA:635:C:C6	2.36	0.60
1:AA:1144:G:H21	1:AA:1146:A:H62	1.47	0.60
1:BA:1144:G:H21	1:BA:1146:A:H62	1.47	0.60
33:DA:1014:A:H1'	69:DA:6685:HOH:O	2.01	0.60
4:AD:107:PHE:HB3	4:AD:145:ILE:HD11	1.82	0.60
1:BA:1323:G:H2'	1:BA:1324:A:C8	2.36	0.60
36:CG:24:ILE:HD11	36:CG:43:VAL:HG11	1.82	0.60
40:CL:43:ILE:HD12	40:CL:56:ASP:HB2	1.82	0.60
31:CA:2394:C:H5''	41:CM:63:LYS:HE2	1.83	0.60
34:DE:131:THR:HG23	34:DE:160:ALA:O	2.02	0.60
1:AA:73:C:HO2'	1:AA:74:A:H8	1.50	0.60
2:AB:188:ASP:HB2	2:AB:204:ASP:OD2	2.02	0.60
1:BA:1226:C:H2'	13:BM:102:THR:HB	1.84	0.60
1:BA:73:C:HO2'	1:BA:74:A:H8	1.48	0.60
33:DA:1509:A:HO2'	33:DA:1510:G:H8	1.49	0.60
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.37	0.60
31:CA:784:G:H3'	69:CA:3484:HOH:O	2.01	0.59
31:CA:2680:U:H2'	31:CA:2681:C:C6	2.37	0.59
31:CA:1105:U:H2'	31:CA:1106:G:C8	2.37	0.59
35:CF:36:LEU:HD21	35:CF:91:LEU:CD1	2.32	0.59
48:DT:4:ILE:HG12	48:DT:106:VAL:HG22	1.84	0.59
44:CP:31:THR:HG22	44:CP:33:ARG:H	1.66	0.59
12:BL:33:VAL:HG22	12:BL:79:VAL:HG22	1.85	0.59
31:CA:2291:U:H2'	31:CA:2292:U:C6	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1447:C:H2'	31:CA:1448:G:C8	2.38	0.59
48:CT:59:GLU:HA	48:CT:64:ALA:HA	1.84	0.59
1:AA:1226:C:H2'	13:AM:102:THR:HB	1.85	0.58
46:CR:58:ARG:NH1	46:CR:62:ILE:HD11	2.19	0.58
6:BF:3:HIS:H	6:BF:92:THR:HG23	1.67	0.58
32:DD:114:LYS:HE2	33:DA:2681:C:OP2	2.03	0.58
1:BA:209:U:H4'	1:BA:210:C:OP2	2.03	0.58
1:AA:6:G:H1	5:AE:103:THR:HG21	1.68	0.58
35:CF:36:LEU:HD21	35:CF:91:LEU:HD12	1.84	0.58
2:AB:129:LEU:HD13	2:AB:134:ALA:HB2	1.86	0.58
8:AH:94:LYS:HB3	8:AH:117:ARG:HH22	1.68	0.58
31:CA:1311:G:H21	31:CA:1603:A:H62	1.50	0.58
31:CA:17:G:H4'	46:CR:25:TYR:CE2	2.37	0.58
2:BB:188:ASP:HB2	2:BB:204:ASP:OD2	2.03	0.58
33:DA:5:A:H2'	33:DA:6:A:C8	2.39	0.58
5:AE:106:ILE:HD11	5:AE:124:LEU:HD23	1.86	0.58
2:BB:129:LEU:HD13	2:BB:134:ALA:HB2	1.86	0.58
40:CL:77:ILE:HG12	45:CQ:72:ARG:HG3	1.86	0.58
22:D1:53:LYS:HE3	22:D1:56:ALA:HA	1.86	0.58
33:DA:1105:U:H2'	33:DA:1106:G:C8	2.38	0.58
35:DF:106:ILE:HD12	35:DF:139:PRO:HG2	1.85	0.58
5:AE:38:VAL:HG11	5:AE:114:VAL:HG22	1.86	0.57
12:AL:33:VAL:HG22	12:AL:79:VAL:HG22	1.85	0.57
1:BA:522:C:H5	12:BL:50:ARG:HH12	1.52	0.57
50:CV:82:ARG:HB2	50:CV:97:LYS:HG3	1.86	0.57
1:AA:774:G:H21	57:AA:1670:PG4:H51	1.69	0.57
48:CT:4:ILE:HG12	48:CT:106:VAL:HG22	1.86	0.57
20:BT:58:VAL:HG13	20:BT:72:ALA:HB1	1.85	0.57
33:DA:1645:G:H5''	33:DA:1646:C:H5'	1.86	0.57
33:DA:1182:G:H2'	33:DA:1183:U:O4'	2.05	0.57
38:CJ:14:ALA:HB3	38:CJ:17:MET:HB2	1.87	0.57
55:DI:69:PHE:HB3	55:DI:72:LEU:HD12	1.87	0.57
1:AA:202:G:HO2'	1:AA:468:A:H8	1.53	0.57
11:BK:89:PRO:HG3	21:BU:32:VAL:HG11	1.85	0.57
35:CF:106:ILE:HD12	35:CF:139:PRO:HG2	1.85	0.57
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.86	0.57
33:DA:31:C:O3'	33:DA:1238:G:H5''	2.05	0.57
44:DP:7:ARG:HG3	44:DP:96:GLY:HA3	1.86	0.57
38:DJ:14:ALA:HB3	38:DJ:17:MET:HB2	1.87	0.57
41:DM:57:LEU:HA	41:DM:60:ARG:HE	1.70	0.57
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BG:113:ASP:HB2	7:BG:119:ARG:HG3	1.87	0.56
31:CA:118:A:N3	31:CA:178:G:H1'	2.20	0.56
29:CC:219:THR:O	31:CA:1789:A:H5''	2.05	0.56
40:CL:38:ILE:HD11	40:CL:112:PHE:HZ	1.68	0.56
1:AA:1277:C:HO2'	1:AA:1279:G:H8	1.52	0.56
3:AC:151:VAL:HG12	3:AC:200:VAL:HG22	1.87	0.56
41:CM:57:LEU:HB2	41:CM:60:ARG:HH11	1.70	0.56
41:DM:57:LEU:HB2	41:DM:60:ARG:HH11	1.69	0.56
31:CA:1636:U:H2'	31:CA:1637:A:C8	2.39	0.56
6:AF:45:ARG:O	6:AF:56:LYS:HA	2.05	0.56
33:DA:2529:G:H4'	36:DG:175:LYS:HG3	1.87	0.56
55:DI:132:TYR:H	55:DI:133:GLU:HB2	1.70	0.56
33:DA:1278:C:H2'	33:DA:1279:G:H8	1.70	0.56
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.87	0.56
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.88	0.56
22:C1:53:LYS:HE3	22:C1:56:ALA:HA	1.87	0.56
51:CW:38:LEU:HD21	51:CW:65:VAL:HG11	1.87	0.56
32:DD:99:GLU:HG2	32:DD:182:ALA:HB2	1.88	0.56
31:CA:335:C:H5''	50:CV:82:ARG:HD3	1.87	0.56
6:BF:45:ARG:O	6:BF:56:LYS:HA	2.06	0.56
33:DA:1278:C:H2'	33:DA:1279:G:C8	2.40	0.56
47:DS:44:GLY:O	47:DS:45:GLU:HG2	2.06	0.55
31:CA:1509:A:HO2'	31:CA:1510:G:H8	1.52	0.55
31:CA:2036:C:H2'	31:CA:2037:A:C8	2.42	0.55
47:DS:21:ARG:HH21	57:DS:202:PG4:H71	1.70	0.55
44:CP:7:ARG:HG3	44:CP:96:GLY:HA3	1.87	0.55
8:BH:94:LYS:HB3	8:BH:117:ARG:HH22	1.71	0.55
40:DL:38:ILE:HD11	40:DL:112:PHE:HZ	1.70	0.55
1:AA:412:A:H3'	1:AA:413:G:H5'	1.87	0.55
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.89	0.55
1:BA:769:G:H4'	1:BA:1513:A:H4'	1.88	0.55
26:C5:3:VAL:HG11	31:CA:2539:C:C5'	2.34	0.55
33:DA:396:G:H1'	53:DY:29:PHE:HB3	1.87	0.55
22:D1:5:GLN:O	33:DA:2017:U:H4'	2.06	0.55
31:CA:457:A:N1	31:CA:470:A:H5''	2.22	0.55
31:CA:1974:C:H3'	69:CA:3256:HOH:O	2.07	0.55
42:CN:69:PRO:HA	42:CN:94:ALA:HB2	1.89	0.54
17:BQ:14:SER:HB3	17:BQ:22:VAL:HG12	1.88	0.54
31:CA:784:G:H5'	31:CA:785:G:OP1	2.07	0.54
1:BA:1277:C:HO2'	1:BA:1279:G:H8	1.54	0.54
2:BB:20:THR:HA	2:BB:39:HIS:HE1	1.63	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:CD:99:GLU:HG2	30:CD:182:ALA:HB2	1.88	0.54
1:BA:209:U:O2	1:BA:209:U:H2'	2.06	0.54
31:CA:1794:A:H2'	31:CA:1795:C:C6	2.43	0.54
1:BA:946:A:H2'	1:BA:947:G:C8	2.43	0.54
31:CA:2019:A:H4'	46:CR:34:VAL:HG21	1.89	0.54
53:CY:11:ARG:HG2	53:CY:12:PRO:HD2	1.90	0.54
35:DF:138:PHE:HE2	35:DF:152:LEU:HD21	1.71	0.54
36:DG:19:ILE:HG12	36:DG:24:ILE:HG12	1.89	0.54
11:AK:84:VAL:HG21	11:AK:97:ILE:HG23	1.88	0.54
11:BK:84:VAL:HG21	11:BK:97:ILE:HG23	1.90	0.54
40:CL:24:VAL:HG13	40:CL:33:ALA:HB2	1.88	0.54
33:DA:644:A:H2'	33:DA:645:C:O4'	2.08	0.54
5:AE:107:ALA:HB2	5:AE:125:ALA:HB3	1.89	0.54
5:BE:105:ILE:HA	5:BE:123:VAL:HG23	1.90	0.54
38:CJ:55:ILE:HD12	38:CJ:74:PRO:HD3	1.90	0.54
37:CH:27:ARG:HH11	53:CY:60:ASP:HA	1.71	0.54
50:DV:94:ARG:HB3	50:DV:103:ILE:HD12	1.88	0.54
31:CA:494:G:H4'	48:CT:6:LYS:HB2	1.89	0.54
21:AU:51:SER:HA	21:AU:54:LYS:HE3	1.90	0.54
1:AA:946:A:H2'	1:AA:947:G:C8	2.43	0.54
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.37	0.54
26:C5:3:VAL:CG1	31:CA:2539:C:H5'	2.35	0.54
37:CH:3:VAL:HG12	37:CH:38:PRO:HA	1.90	0.54
41:CM:57:LEU:HA	41:CM:60:ARG:HE	1.72	0.54
31:CA:244:A:H5''	41:CM:67:THR:HG21	1.90	0.54
34:DE:130:LYS:HB2	34:DE:133:LEU:HD12	1.89	0.54
1:BA:1432:G:H3'	45:CQ:106:LYS:HE2	1.89	0.53
33:DA:2327:A:H2'	33:DA:2328:A:C8	2.43	0.53
33:DA:2591:C:H2'	33:DA:2592:G:H8	1.72	0.53
51:DW:38:LEU:HD21	51:DW:65:VAL:HG11	1.88	0.53
31:CA:1645:G:H5''	31:CA:1646:C:H5'	1.89	0.53
59:DA:3211:PUT:H32	69:DA:6598:HOH:O	2.08	0.53
1:BA:202:G:H1	1:BA:215:C:H42	1.56	0.53
26:C5:36:ARG:HH22	31:CA:2539:C:H4'	1.72	0.53
2:BB:187:VAL:HG13	2:BB:191:SER:HB2	1.91	0.53
23:C2:11:LEU:HD21	23:C2:34:LEU:HD23	1.91	0.53
26:C5:4:ARG:HB2	31:CA:2466:C:OP1	2.09	0.53
22:C1:4:GLN:HA	31:CA:2615:U:C2	2.43	0.53
31:CA:373:U:H2'	31:CA:374:A:H8	1.73	0.53
36:CG:19:ILE:HG12	36:CG:24:ILE:HG12	1.89	0.53
39:CK:117:ALA:HA	39:CK:120:ARG:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DA:927:A:H2'	33:DA:928:A:C8	2.44	0.53
51:DW:63:ILE:HG22	51:DW:65:VAL:HG23	1.90	0.53
1:BA:9:G:OP2	5:BE:126:LYS:HE2	2.08	0.53
31:CA:1476:U:H2'	31:CA:1477:A:H8	1.73	0.53
43:CO:2:ARG:HA	43:CO:5:LYS:HD2	1.91	0.53
49:CU:54:GLU:HB3	49:CU:88:LYS:HD2	1.90	0.53
13:BM:90:ARG:HH21	13:BM:95:LEU:HB3	1.74	0.53
38:DJ:55:ILE:HD12	38:DJ:74:PRO:HD3	1.90	0.53
10:BJ:5:ARG:HG2	10:BJ:79:PRO:HG3	1.91	0.53
30:CD:186:LEU:HD21	45:CQ:4:ILE:HG21	1.90	0.53
54:DZ:47:ARG:HD3	69:DZ:102:HOH:O	2.07	0.53
12:BL:110:ARG:HB2	12:BL:119:VAL:HG21	1.90	0.53
16:BP:61:VAL:HG21	16:BP:67:ILE:HD11	1.91	0.53
35:DF:36:LEU:HB2	35:DF:57:LEU:HD21	1.91	0.53
42:CN:41:LEU:HD21	42:CN:124:LEU:HD22	1.90	0.53
41:DM:85:VAL:HG21	41:DM:90:VAL:HG22	1.91	0.53
5:BE:77:ASN:HB2	5:BE:82:GLN:NE2	2.25	0.52
7:BG:69:VAL:HG23	7:BG:100:ALA:HB1	1.91	0.52
16:BP:4:ILE:HG12	16:BP:21:VAL:HG22	1.90	0.52
31:CA:1779:U:C5	31:CA:1784:A:N7	2.77	0.52
40:CL:58:LEU:HD11	40:CL:86:LEU:HD13	1.91	0.52
33:DA:45:G:H5''	33:DA:46:G:H5'	1.91	0.52
32:DD:25:THR:HG21	32:DD:193:VAL:HG22	1.91	0.52
39:DK:117:ALA:HA	39:DK:120:ARG:HD2	1.91	0.52
1:BA:17:U:H2'	1:BA:18:C:C6	2.44	0.52
21:BU:14:VAL:HG22	21:BU:17:ARG:HH12	1.75	0.52
40:DL:24:VAL:HG13	40:DL:33:ALA:HB2	1.90	0.52
1:BA:9:G:H5'	5:BE:108:GLY:HA3	1.91	0.52
50:CV:94:ARG:HB3	50:CV:103:ILE:HD12	1.90	0.52
37:DH:3:VAL:HG12	37:DH:38:PRO:HA	1.92	0.52
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.38	0.52
14:BN:10:GLU:HG3	14:BN:63:ARG:HD2	1.92	0.52
1:AA:17:U:H2'	1:AA:18:C:C6	2.45	0.52
1:BA:1060:U:C5	3:BC:2:GLY:HA3	2.44	0.52
31:CA:176:A:H8	31:CA:176:A:O5'	1.93	0.52
2:AB:20:THR:HG22	2:AB:39:HIS:CE1	2.44	0.52
38:CJ:103:ARG:HA	38:CJ:106:LEU:HD12	1.91	0.52
51:CW:63:ILE:HG22	51:CW:65:VAL:HG23	1.91	0.52
33:DA:2305:U:H5''	35:DF:131:GLY:HA3	1.90	0.52
2:AB:15:HIS:HB3	2:AB:43:LEU:HD11	1.90	0.52
31:CA:1028:A:N6	31:CA:1125:G:H2'	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:9:G:OP2	5:AE:126:LYS:HE2	2.10	0.52
1:AA:1492:A:C5'	12:AL:44:LYS:HG2	2.36	0.52
27:C0:9:GLN:HB3	27:C0:32:ILE:HA	1.92	0.52
31:CA:744:U:H4'	31:CA:1658:C:H4'	1.91	0.52
33:DA:1250:G:H5''	46:DR:6:ARG:HD3	1.92	0.52
52:DX:65:GLY:HA2	52:DX:85:GLU:HG2	1.92	0.52
31:CA:1379:U:H4'	31:CA:1380:G:OP1	2.10	0.52
30:CD:25:THR:HG21	30:CD:193:VAL:HG22	1.91	0.52
34:CE:145:ASP:HA	34:CE:166:LYS:HB3	1.92	0.52
51:CW:77:VAL:HG23	51:CW:89:ILE:HG12	1.92	0.52
33:DA:839:U:H2'	33:DA:840:C:C6	2.44	0.52
45:DQ:31:TRP:CE2	45:DQ:40:LEU:HD21	2.45	0.52
48:DT:41:LYS:HD2	69:DT:344:HOH:O	2.09	0.52
31:CA:310:A:H5''	50:CV:15:THR:HG23	1.92	0.52
32:DD:150[A]:MEQ:HE3	33:DA:2032:G:C8	2.45	0.52
33:DA:2800:A:C2	33:DA:2895:G:H1'	2.45	0.52
40:DL:58:LEU:HD11	40:DL:86:LEU:HD13	1.92	0.52
33:DA:514:A:H5'	46:DR:11:ARG:HH12	1.74	0.52
7:AG:69:VAL:HG23	7:AG:100:ALA:HB1	1.91	0.51
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	1.92	0.51
31:CA:2533:U:H2'	31:CA:2534:A:O4'	2.10	0.51
33:DA:639:U:H2'	33:DA:640:C:C6	2.45	0.51
31:CA:796:C:H2'	31:CA:797:G:C8	2.45	0.51
31:CA:1651:G:OP1	43:CO:40:LYS:HE3	2.10	0.51
33:DA:1935:G:H1'	33:DA:1964:G:N2	2.25	0.51
35:DF:61:SER:HB2	35:DF:91:LEU:HD21	1.92	0.51
36:DG:95:ARG:HG2	36:DG:128:GLN:HB3	1.93	0.51
5:AE:77:ASN:HB2	5:AE:82:GLN:NE2	2.25	0.51
1:BA:1062:U:H2'	1:BA:1063:C:C6	2.46	0.51
31:CA:1936:A:N6	31:CA:1963:U:N3	2.53	0.51
33:DA:2262:U:H5''	52:DX:41[A]:ARG:NH1	2.22	0.51
44:DP:39:VAL:HB	44:DP:49:VAL:HG23	1.91	0.51
52:DX:21:LEU:HD11	52:DX:41[A]:ARG:HE	1.75	0.51
1:AA:1238:A:H5'	1:AA:1336:C:H41	1.75	0.51
2:BB:15:HIS:HB3	2:BB:43:LEU:HD11	1.92	0.51
9:BI:7:TYR:HE1	9:BI:18:ARG:HB2	1.74	0.51
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.76	0.51
23:C2:22:THR:HG21	31:CA:2419:U:H5''	1.93	0.51
31:CA:581:C:H2'	31:CA:582:A:C8	2.46	0.51
31:CA:806:C:H2'	31:CA:807:U:C6	2.46	0.51
12:AL:110:ARG:HB2	12:AL:119:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AN:10:GLU:HG3	14:AN:63:ARG:HD2	1.92	0.51
31:CA:674:G:H1'	34:CE:69:ARG:HD2	1.92	0.51
33:DA:1026:G:H2'	33:DA:1027:A:C8	2.46	0.51
54:DZ:18:LEU:HB2	54:DZ:53:VAL:HG11	1.93	0.51
2:BB:120:GLN:HE22	2:BB:137:ARG:HE	1.58	0.51
28:CB:55:U:H1'	35:CF:26:MET:HG3	1.93	0.51
41:CM:85:VAL:HG11	41:CM:90:VAL:HG22	1.92	0.51
1:AA:202:G:H1	1:AA:215:C:H42	1.58	0.51
13:AM:33:ILE:HD11	13:AM:63:PHE:HE1	1.75	0.51
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.74	0.51
21:AU:14:VAL:HG22	21:AU:17:ARG:HH12	1.76	0.51
37:CH:82:SER:HB2	37:CH:94:ILE:HD11	1.93	0.51
23:D2:11:LEU:HD21	23:D2:34:LEU:HD23	1.92	0.51
36:DG:164:TYR:HB2	36:DG:167:GLU:HB2	1.93	0.51
41:DM:85:VAL:HB	41:DM:94:THR:HG22	1.92	0.51
33:DA:1250:G:C5'	46:DR:6:ARG:HD3	2.41	0.51
1:BA:202:G:HO2'	1:BA:468:A:H8	1.57	0.51
31:CA:309:A:O3'	50:CV:16:GLY:HA2	2.10	0.51
33:DA:1101:U:H2'	33:DA:1102:C:C6	2.46	0.51
33:DA:2409:G:H2'	33:DA:2410:G:O4'	2.11	0.51
32:DD:150[A]:MEQ:HG2	69:DA:4147:HOH:O	2.11	0.51
2:AB:120:GLN:HE22	2:AB:137:ARG:HE	1.57	0.51
2:AB:187:VAL:HG13	2:AB:191:SER:HB2	1.92	0.51
31:CA:2261:C:C2	31:CA:2280:G:N2	2.79	0.51
34:CE:130:LYS:HB2	34:CE:133:LEU:HD12	1.93	0.51
37:DH:82:SER:HB2	37:DH:94:ILE:HD11	1.93	0.51
38:DJ:103:ARG:HA	38:DJ:106:LEU:HD12	1.91	0.51
49:CU:18:GLU:H	49:CU:18:GLU:CD	2.15	0.51
33:DA:2243:U:H2'	33:DA:2244:U:C6	2.47	0.51
69:DA:7302:HOH:O	46:DR:6:ARG:HG2	2.11	0.51
31:CA:1662:U:H3	31:CA:1998:A:H61	1.59	0.50
31:CA:45:G:H5''	31:CA:46:G:H5'	1.92	0.50
31:CA:571:U:H4'	31:CA:573:U:H5	1.76	0.50
29:CC:232:HIS:NE2	29:CC:244:PRO:HA	2.26	0.50
33:DA:1794:A:H2'	33:DA:1795:C:C6	2.46	0.50
33:DA:2845:U:H5''	45:DQ:52:ASN:O	2.11	0.50
34:DE:145:ASP:HA	34:DE:166:LYS:HB3	1.92	0.50
7:AG:69:VAL:HG21	7:AG:104:ILE:HD11	1.92	0.50
7:AG:70:ARG:HG2	7:AG:96:ARG:HG2	1.91	0.50
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.77	0.50
10:AJ:5:ARG:HE	10:AJ:77:VAL:HG22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1141:C:HO2'	1:BA:1142:G:H8	1.58	0.50
31:CA:2189:U:H2'	31:CA:2190:G:H8	1.75	0.50
35:CF:36:LEU:HB2	35:CF:57:LEU:HD21	1.92	0.50
38:CJ:19:ASN:H	38:CJ:20:PRO:HD2	1.77	0.50
33:DA:979:A:H2'	33:DA:982:C:H42	1.75	0.50
1:AA:845:A:O4'	1:AA:845:A:P	2.69	0.50
17:BQ:46:VAL:HG11	17:BQ:61:ILE:CG2	2.41	0.50
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.75	0.50
12:AL:55:VAL:HG21	12:AL:80:ILE:HD11	1.94	0.50
31:CA:917:A:H5''	31:CA:2268:A:H61	1.76	0.50
31:CA:608:A:H2'	31:CA:609:A:C8	2.47	0.50
35:CF:61:SER:HB2	35:CF:91:LEU:HD21	1.93	0.50
36:CG:164:TYR:HB2	36:CG:167:GLU:HB2	1.92	0.50
33:DA:1651:G:H3'	69:DA:5545:HOH:O	2.12	0.50
3:AC:156:ARG:HD3	3:AC:193:TYR:O	2.12	0.50
55:DI:50:VAL:HG11	55:DI:92:ALA:HB2	1.94	0.50
51:DW:77:VAL:HG23	51:DW:89:ILE:HG12	1.94	0.50
1:AA:79:G:H22	1:AA:90:C:H42	1.60	0.50
7:BG:70:ARG:HG2	7:BG:96:ARG:HG2	1.92	0.50
11:BK:29:ASN:HB2	11:BK:57:LYS:HE3	1.94	0.50
31:CA:1665:A:H2'	31:CA:1666:G:O4'	2.10	0.50
31:CA:1779:U:H5	31:CA:1784:A:N7	2.09	0.50
31:CA:2028:U:H2'	31:CA:2029:G:C8	2.46	0.50
31:CA:910:A:H62	42:CN:12:MET:HA	1.77	0.50
49:CU:45:ALA:O	49:CU:49:LYS:HG2	2.11	0.50
38:DJ:19:ASN:H	38:DJ:20:PRO:HD2	1.77	0.50
1:AA:1305:G:HO2'	1:AA:1306:A:H8	1.60	0.50
1:AA:1478:U:H2'	1:AA:1479:C:C6	2.46	0.50
16:AP:61:VAL:HG21	16:AP:67:ILE:HD11	1.92	0.50
31:CA:1101:U:H2'	31:CA:1102:C:C6	2.46	0.50
49:DU:54:GLU:HB3	49:DU:88:LYS:HD2	1.93	0.50
1:BA:1478:U:H2'	1:BA:1479:C:C6	2.47	0.50
5:BE:72:ILE:HG12	5:BE:145:GLU:HG3	1.94	0.50
11:BK:45:ALA:HB3	11:BK:70:CYS:HB2	1.94	0.50
19:BS:15:LEU:HD13	19:BS:33:THR:HG21	1.93	0.50
31:CA:1638:C:H5''	31:CA:2710:C:O2'	2.12	0.50
36:CG:95:ARG:HG2	36:CG:128:GLN:HB3	1.93	0.50
46:CR:76:TYR:CZ	46:CR:80:ILE:HG13	2.46	0.50
1:AA:412:A:H3'	1:AA:413:G:C5'	2.42	0.49
24:C3:2:LYS:HE2	31:CA:687:C:H5''	1.94	0.49
31:CA:1936:A:H2	31:CA:1943:U:N3	2.02	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2267:A:H5''	31:CA:2268:A:H5'	1.94	0.49
31:CA:2350:C:H2'	31:CA:2351:G:O4'	2.12	0.49
31:CA:639:U:H2'	31:CA:640:C:C6	2.46	0.49
29:CC:154:LEU:HD13	29:CC:176:LEU:HD21	1.93	0.49
33:DA:1171:G:H1'	33:DA:1179:G:N2	2.27	0.49
33:DA:1268:A:H2'	33:DA:1269:A:O4'	2.11	0.49
9:BI:19:VAL:HG22	9:BI:65:ILE:HG22	1.94	0.49
46:CR:112:LYS:HD3	47:CS:48:LYS:HG3	1.92	0.49
46:DR:76:TYR:CZ	46:DR:80:ILE:HG13	2.47	0.49
1:AA:299:G:H2'	1:AA:300:A:C8	2.46	0.49
14:AN:43:ASN:HA	14:AN:46:LEU:HD12	1.94	0.49
9:BI:120:LYS:HB2	9:BI:123:ARG:HB3	1.94	0.49
31:CA:574:A:C6	31:CA:2033:A:H5'	2.48	0.49
32:DD:186:LEU:HD21	45:DQ:4:ILE:HG21	1.93	0.49
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	1.94	0.49
16:BP:68:SER:HB3	69:BP:101:HOH:O	2.12	0.49
31:CA:727:A:H2'	31:CA:728:G:C8	2.48	0.49
29:CC:160:THR:HG22	29:CC:177:ARG:HG2	1.93	0.49
33:DA:858:G:H3'	33:DA:859:G:C8	2.47	0.49
2:AB:12:ALA:HB1	2:AB:209:ALA:HA	1.95	0.49
6:AF:46:GLN:HA	6:AF:56:LYS:HG2	1.95	0.49
9:AI:19:VAL:HG22	9:AI:65:ILE:HG22	1.94	0.49
1:BA:1496:C:H2'	1:BA:1497:G:O4'	2.12	0.49
3:BC:47:LEU:HB3	3:BC:50:ALA:HB3	1.95	0.49
17:BQ:68:SER:OG	17:BQ:71:LYS:HB3	2.11	0.49
34:CE:46:GLN:HB3	34:CE:83:VAL:HG11	1.95	0.49
33:DA:102:U:H2'	33:DA:102:U:O2	2.13	0.49
33:DA:2779:U:H5'	33:DA:2781:A:O4'	2.12	0.49
29:DC:29:PRO:HG2	29:DC:34:LEU:HD11	1.95	0.49
33:DA:585:G:N7	46:DR:6:ARG:NH1	2.60	0.49
11:AK:29:ASN:HB2	11:AK:57:LYS:HE3	1.93	0.49
12:BL:55:VAL:HG21	12:BL:80:ILE:HD11	1.95	0.49
31:CA:2190:G:H2'	31:CA:2191:A:H8	1.78	0.49
35:CF:44:ILE:HG21	35:CF:79:ILE:HG22	1.95	0.49
33:DA:1223:G:P	47:DS:68:ARG:HH22	2.35	0.49
14:BN:43:ASN:HA	14:BN:46:LEU:HD12	1.93	0.49
40:CL:103:VAL:O	40:CL:122:VAL:HB	2.12	0.49
69:DA:6392:HOH:O	43:DO:103:ARG:HA	2.13	0.49
5:AE:133:PRO:O	5:AE:137:VAL:HG13	2.11	0.49
12:AL:31:ARG:O	12:AL:58:THR:HG23	2.12	0.49
13:AM:12:HIS:HB3	69:AM:303:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:CZ:18:LEU:HB2	54:CZ:53:VAL:HG11	1.94	0.49
33:DA:1430:G:H2'	33:DA:1431:A:O4'	2.12	0.49
33:DA:2273:A:H2'	33:DA:2274:A:C8	2.47	0.49
55:DI:26:VAL:HB	55:DI:83:ALA:HB3	1.93	0.49
6:BF:46:GLN:HA	6:BF:56:LYS:HG2	1.94	0.49
50:DV:74:ASN:HD21	50:DV:99:ASN:ND2	2.11	0.49
7:BG:69:VAL:HG21	7:BG:104:ILE:HD11	1.93	0.49
33:DA:1999:C:H4'	33:DA:2723:C:O2	2.13	0.49
33:DA:2728:U:O2'	33:DA:2729:G:H5''	2.12	0.49
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	1.94	0.48
31:CA:2718:G:OP1	45:CQ:98:TYR:HD2	1.96	0.48
1:BA:1493:A:H1'	31:CA:1913:A:H61	1.78	0.48
29:CC:105:LEU:H	29:CC:105:LEU:HD12	1.78	0.48
34:CE:58:LYS:HG3	34:CE:71:GLY:HA2	1.95	0.48
33:DA:784:G:O2'	33:DA:785:G:H5''	2.13	0.48
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.94	0.48
13:AM:85:CYS:HB2	19:AS:73:GLU:HB3	1.95	0.48
1:BA:1238:A:H5'	1:BA:1336:C:H41	1.76	0.48
1:BA:299:G:H2'	1:BA:300:A:C8	2.47	0.48
23:C2:25:LYS:HD2	23:C2:52:ALA:HB1	1.94	0.48
31:CA:20:C:H2'	31:CA:21:A:H8	1.78	0.48
31:CA:833:A:H2'	31:CA:834:G:C8	2.48	0.48
29:CC:29:PRO:HG2	29:CC:34:LEU:HD11	1.94	0.48
34:CE:105:LEU:HD23	34:CE:108:ILE:HD11	1.95	0.48
33:DA:1651:G:OP1	43:DO:40:LYS:HE3	2.14	0.48
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.48	0.48
17:AQ:17:MET:HG2	17:AQ:20:SER:HB2	1.96	0.48
13:BM:85:CYS:HB2	19:BS:73:GLU:HB3	1.96	0.48
31:CA:2636:C:H2'	31:CA:2637:U:C6	2.48	0.48
47:CS:49:ILE:HB	47:CS:51:VAL:O	2.13	0.48
1:BA:212:G:H2'	1:BA:213:G:C8	2.49	0.48
32:DD:114:LYS:HD3	32:DD:196:ALA:HB2	1.95	0.48
6:BF:81:ASN:HB3	6:BF:84:VAL:HG12	1.96	0.48
31:CA:1935:G:H1'	31:CA:1964:G:N2	2.28	0.48
6:BF:99:ALA:O	6:BF:100:SER:HB3	2.14	0.48
31:CA:694:U:OP1	31:CA:1569:A:H1'	2.13	0.48
48:CT:84:ARG:HB2	48:CT:96:ILE:HB	1.96	0.48
32:DD:150[B]:MEQ:HG3	33:DA:2032:G:N3	2.28	0.48
29:DC:232:HIS:NE2	29:DC:244:PRO:HA	2.28	0.48
31:CA:1931:U:H2'	31:CA:1932:A:H8	1.79	0.48
31:CA:668:A:H2'	31:CA:670:A:H62	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1003:G:H21	1:BA:1005:A:H5'	1.79	0.48
1:BA:79:G:H22	1:BA:90:C:H42	1.61	0.48
34:CE:149:ILE:HD12	34:CE:172:ALA:HA	1.95	0.48
37:CH:15:LEU:HD22	37:CH:15:LEU:H	1.79	0.48
33:DA:1720:U:H2'	33:DA:1721:G:O4'	2.13	0.48
33:DA:2314:A:H1'	35:DF:155:THR:HG21	1.96	0.48
1:AA:1277:C:O2'	1:AA:1279:G:H8	1.97	0.48
7:AG:72:THR:HG23	7:AG:73:VAL:HG22	1.95	0.48
5:AE:157:ARG:HD2	8:AH:43:GLU:O	2.14	0.48
10:AJ:52:LEU:HB2	14:AN:81:ARG:HD2	1.96	0.48
1:BA:76:G:H1	1:BA:93:U:H3	1.62	0.48
44:CP:18:LEU:HD23	44:CP:25:ARG:HD3	1.96	0.48
31:CA:1677:A:H5''	69:CA:3685:HOH:O	2.13	0.47
31:CA:1721:G:HO2'	31:CA:1722:A:H8	1.61	0.47
31:CA:1783:A:C2	31:CA:2588:G:O4'	2.67	0.47
29:DC:231:PRO:HA	69:DC:304:HOH:O	2.14	0.47
11:AK:25:ALA:HA	11:AK:30:THR:HG22	1.96	0.47
1:BA:1277:C:O2'	1:BA:1279:G:H8	1.97	0.47
35:CF:103:LEU:HA	35:CF:107:ALA:HB3	1.96	0.47
2:BB:12:ALA:HB1	2:BB:209:ALA:HA	1.95	0.47
2:BB:166:ALA:HB3	2:BB:191:SER:HB3	1.96	0.47
22:C1:25:VAL:HG13	22:C1:26:THR:H	1.80	0.47
31:CA:1716:U:H2'	31:CA:1717:A:H8	1.78	0.47
31:CA:1775:U:H2'	31:CA:1776:G:O4'	2.14	0.47
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.49	0.47
31:CA:831:G:O5'	31:CA:831:G:H8	1.97	0.47
33:DA:2128:G:H1	33:DA:2160:C:N4	2.11	0.47
28:DB:90:C:H5'	42:DN:18[B]:ARG:HG3	1.96	0.47
1:AA:673:A:H2'	1:AA:674:G:C8	2.49	0.47
6:AF:38:ARG:HE	6:AF:63:ASN:ND2	2.13	0.47
9:AI:120:LYS:HB2	9:AI:123:ARG:HB3	1.95	0.47
12:BL:50:ARG:HB3	12:BL:66:TYR:HE1	1.80	0.47
31:CA:1447:C:H2'	31:CA:1448:G:H8	1.80	0.47
31:CA:20:C:H2'	31:CA:21:A:C8	2.48	0.47
29:CC:174:LEU:CD2	29:CC:184:VAL:HB	2.44	0.47
31:CA:2428:G:H22	41:CM:60:ARG:NH2	2.12	0.47
29:DC:154:LEU:HD13	29:DC:176:LEU:HD21	1.95	0.47
35:DF:128:TYR:HD2	35:DF:156:ILE:HD12	1.79	0.47
2:AB:166:ALA:HB3	2:AB:191:SER:HB3	1.96	0.47
31:CA:2718:G:O2'	45:CQ:96:LYS:HG3	2.15	0.47
22:D1:4:GLN:HA	33:DA:2615:U:C2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DA:2291:U:H2'	33:DA:2292:U:C6	2.49	0.47
33:DA:659:G:H4'	34:DE:95:LYS:HD3	1.95	0.47
3:BC:22:TRP:HB3	3:BC:59:ARG:H	1.79	0.47
1:BA:562:U:H1'	12:BL:12:ARG:HD2	1.97	0.47
3:BC:33:LEU:HD21	14:BN:93:ILE:HG12	1.96	0.47
35:DF:103:LEU:HA	35:DF:107:ALA:HB3	1.97	0.47
1:AA:216:U:H2'	1:AA:217:C:C6	2.49	0.47
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	1.97	0.47
3:BC:23:PHE:CD2	10:BJ:97:ASP:HB2	2.49	0.47
31:CA:1154:G:OP1	46:CR:58:ARG:HD3	2.15	0.47
40:CL:42:THR:HG23	40:CL:44:LYS:HE2	1.97	0.47
42:CN:40:ARG:HD3	42:CN:93:VAL:HG21	1.97	0.47
33:DA:2328:A:H2'	33:DA:2329:U:C6	2.49	0.47
33:DA:2636:C:H2'	33:DA:2637:U:C6	2.48	0.47
33:DA:476:G:H4'	33:DA:502:A:N1	2.30	0.47
1:AA:1003:G:H21	1:AA:1005:A:H5'	1.79	0.47
58:AA:1671:MPD:H31	20:AT:24:ARG:NH1	2.29	0.47
1:BA:216:U:H2'	1:BA:217:C:C6	2.50	0.47
31:CA:381:G:OP1	53:CY:18:ARG:HD3	2.15	0.47
33:DA:1187:G:H5''	47:DS:83:TYR:CE1	2.49	0.47
33:DA:2133:G:H21	33:DA:2158:A:N6	2.13	0.47
33:DA:2547:A:H4'	40:DL:29:HIS:NE2	2.30	0.47
34:DE:58:LYS:HG3	34:DE:71:GLY:HA2	1.95	0.47
55:DI:126:LEU:HA	55:DI:129:LEU:HD12	1.96	0.47
1:AA:1496:C:H2'	1:AA:1497:G:O4'	2.14	0.47
8:AH:2:SER:HB2	8:AH:4:GLN:HE21	1.79	0.47
10:AJ:87:LEU:HA	10:AJ:90:LEU:HD12	1.95	0.47
31:CA:1405:U:H2'	31:CA:1406:U:C6	2.49	0.47
33:DA:1716:U:H2'	33:DA:1717:A:H8	1.78	0.47
35:DF:44:ILE:HG21	35:DF:79:ILE:HG22	1.95	0.47
55:DI:23:LEU:HD13	55:DI:89:PRO:HD3	1.97	0.47
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	1.95	0.47
10:BJ:52:LEU:HB2	14:BN:81:ARG:HD2	1.97	0.47
31:CA:1703:G:H2'	31:CA:1704:C:C6	2.50	0.47
3:BC:148:GLY:HA3	3:BC:172:ARG:O	2.15	0.47
21:BU:51:SER:HA	21:BU:54:LYS:HE3	1.97	0.47
23:C2:6:ARG:HG2	23:C2:24:THR:HB	1.97	0.47
31:CA:396:G:H1'	53:CY:29:PHE:HB3	1.97	0.47
34:CE:108:ILE:HG22	41:CM:1:MET:SD	2.55	0.47
47:CS:38:VAL:HG22	47:CS:57:GLY:HA3	1.97	0.47
35:DF:104:ILE:HG23	35:DF:176:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DA:1754:A:C8	45:DQ:94:LYS:HE2	2.50	0.47
50:DV:51:ALA:O	50:DV:52:LEU:HB2	2.15	0.47
21:AU:4:ILE:HG13	21:AU:19:PHE:HA	1.97	0.46
31:CA:644:A:H2'	31:CA:645:C:O4'	2.15	0.46
35:CF:8:TYR:HA	35:CF:12:VAL:HB	1.97	0.46
39:CK:35:ARG:HH21	39:CK:140:LEU:HD11	1.79	0.46
22:D1:25:VAL:HG11	48:DT:38:TYR:HB2	1.97	0.46
32:DD:38:LYS:O	32:DD:46:ARG:HA	2.15	0.46
40:DL:15:GLY:HA2	40:DL:47:ILE:HG12	1.97	0.46
20:AT:39:ILE:HG23	20:AT:86:LEU:HD11	1.97	0.46
11:BK:25:ALA:HA	11:BK:30:THR:HG22	1.97	0.46
31:CA:139:U:H3	49:CU:2:ILE:HG21	1.80	0.46
33:DA:1794:A:H2'	33:DA:1795:C:H6	1.81	0.46
4:AD:58:LYS:HA	4:AD:200:ILE:HG12	1.97	0.46
1:BA:845:A:H8	1:BA:845:A:O5'	1.98	0.46
17:BQ:31:HIS:HE1	17:BQ:33:ILE:HD12	1.80	0.46
31:CA:320:A:H4'	31:CA:322:A:N7	2.29	0.46
31:CA:845:A:H61	31:CA:932:U:H3	1.63	0.46
23:D2:6:ARG:HG2	23:D2:24:THR:HB	1.96	0.46
32:DD:152:PRO:HB2	32:DD:154:LYS:HG2	1.97	0.46
33:DA:1190:G:H5''	41:DM:32:GLY:HA2	1.97	0.46
50:DV:14:LEU:HD11	50:DV:71:ALA:HB2	1.98	0.46
27:C0:31:ARG:HD3	31:CA:1158:C:H5''	1.97	0.46
22:C1:8:PRO:HG2	31:CA:1264:A:H5'	1.97	0.46
31:CA:2596:U:H2'	31:CA:2597:G:C8	2.51	0.46
36:DG:24:ILE:HD13	36:DG:72:LEU:HD21	1.97	0.46
31:CA:965:C:H5''	69:CA:3770:HOH:O	2.15	0.46
43:CO:103:ARG:HD3	43:CO:110:MET:SD	2.56	0.46
1:AA:202:G:H21	1:AA:466:A:H61	1.64	0.46
1:BA:1391:U:H2'	1:BA:1392:G:C8	2.51	0.46
5:BE:72:ILE:HG13	5:BE:73:ASN:N	2.30	0.46
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	1.96	0.46
31:CA:751:A:H5'	48:CT:90:LYS:HA	1.98	0.46
35:CF:104:ILE:HG23	35:CF:176:PRO:HD3	1.97	0.46
42:CN:71:LYS:HB3	42:CN:93:VAL:O	2.16	0.46
33:DA:1509:A:O2'	33:DA:1510:G:H8	1.99	0.46
33:DA:278:A:H2'	33:DA:278:A:N3	2.31	0.46
33:DA:2849:U:H4'	33:DA:2868:A:C2	2.51	0.46
9:AI:55:VAL:HG22	9:AI:94:LEU:HD22	1.96	0.46
1:BA:390:U:H2'	1:BA:391:G:C8	2.50	0.46
21:BU:4:ILE:HG13	21:BU:19:PHE:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1838:C:N4	31:CA:1898:U:H2'	2.30	0.46
31:CA:2185:U:H2'	31:CA:2186:G:C8	2.51	0.46
29:CC:88:SER:HB2	29:CC:158:ALA:HB2	1.96	0.46
30:CD:114:LYS:HD3	30:CD:196:ALA:HB2	1.97	0.46
31:CA:2642:G:H5'	39:CK:80:HIS:CG	2.51	0.46
49:CU:69:ARG:HB2	49:CU:74:ILE:HG22	1.97	0.46
40:DL:42:THR:HG23	40:DL:44:LYS:HE2	1.98	0.46
1:AA:108:G:H5'	1:AA:109:A:H5''	1.98	0.46
8:BH:2:SER:HB2	8:BH:4:GLN:HE21	1.81	0.46
10:BJ:26:VAL:HG21	10:BJ:39:PRO:HD3	1.97	0.46
33:DA:1532:A:H8	33:DA:1532:A:H5''	1.81	0.46
4:AD:177:LYS:HB3	4:AD:179:GLU:HG2	1.98	0.46
3:AC:33:LEU:HD21	14:AN:93:ILE:HG12	1.97	0.46
9:BI:116:VAL:HG21	10:BJ:62:ARG:HB2	1.98	0.46
31:CA:2025:C:H2'	31:CA:2026:U:C6	2.50	0.46
33:DA:2629:U:C5	59:DA:3194:PUT:H12	2.51	0.46
29:DC:17:VAL:HB	29:DC:204:VAL:HB	1.97	0.46
1:AA:1141:C:HO2'	1:AA:1142:G:H8	1.64	0.46
1:AA:505:G:H5'	1:AA:534:U:C2	2.51	0.46
2:AB:129:LEU:H	2:AB:129:LEU:HG	1.56	0.46
4:BD:177:LYS:HB3	4:BD:179:GLU:HG2	1.96	0.46
4:BD:48:LEU:HD21	4:BD:56:ARG:HG3	1.97	0.46
31:CA:278:A:N3	31:CA:278:A:H2'	2.31	0.46
37:CH:27:ARG:HH12	37:CH:38:PRO:HG3	1.81	0.46
33:DA:250:G:H2'	33:DA:251:A:C8	2.51	0.46
55:DI:44:ALA:HB1	55:DI:95:LEU:HD11	1.98	0.46
1:AA:1343:G:H2'	1:AA:1344:C:C6	2.51	0.45
1:AA:562:U:H1'	12:AL:12:ARG:HD2	1.96	0.45
4:BD:85:ASN:HA	5:BE:102:GLY:CA	2.35	0.45
31:CA:1380:G:H2'	31:CA:1381:G:H8	1.81	0.45
31:CA:2010:G:H5''	48:CT:42:LYS:HB2	1.98	0.45
35:DF:8:TYR:HA	35:DF:12:VAL:HB	1.97	0.45
47:DS:24:LYS:HD2	63:DS:201:PGE:H22	1.97	0.45
17:AQ:31:HIS:HE1	17:AQ:33:ILE:HD12	1.81	0.45
31:CA:1794:A:H2'	31:CA:1795:C:H6	1.81	0.45
40:CL:15:GLY:HA2	40:CL:47:ILE:HG12	1.97	0.45
31:CA:1454:C:H1'	43:CO:60:VAL:HG13	1.97	0.45
33:DA:1028:A:N6	33:DA:1125:G:H2'	2.31	0.45
28:DB:49:C:H3'	69:DB:353:HOH:O	2.17	0.45
49:DU:34:VAL:HG11	49:DU:43:ILE:HG12	1.99	0.45
1:BA:407:U:H2'	1:BA:408:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DA:1756:G:H1'	69:DA:6693:HOH:O	2.16	0.45
33:DA:2751:G:H2'	69:DA:5074:HOH:O	2.15	0.45
33:DA:388:G:N7	33:DA:390:U:H2'	2.31	0.45
33:DA:624:C:O2'	33:DA:657:U:H5''	2.16	0.45
33:DA:783:A:N3	33:DA:783:A:H2'	2.30	0.45
33:DA:811:U:H2'	41:DM:21:ARG:HA	1.97	0.45
55:DI:3:LEU:HD12	55:DI:56:ARG:CZ	2.46	0.45
1:AA:6:G:H22	5:AE:103:THR:CG2	2.30	0.45
5:AE:57:PRO:O	5:AE:60:ILE:HG13	2.16	0.45
1:BA:1012:A:H61	1:BA:1017:U:H3	1.64	0.45
1:BA:310:G:H5''	16:BP:31:ARG:HB2	1.97	0.45
31:CA:1357:C:H2'	31:CA:1358:G:O4'	2.15	0.45
37:CH:4:ILE:HD11	37:CH:44:ILE:HG22	1.99	0.45
39:CK:16:TYR:HE1	39:CK:138:GLN:HE21	1.63	0.45
2:AB:41:ILE:HD13	2:AB:202:GLY:HA2	1.98	0.45
1:BA:73:C:O2'	1:BA:74:A:H8	1.98	0.45
2:BB:41:ILE:HD13	2:BB:202:GLY:HA2	1.98	0.45
31:CA:2251:OMG:H1'	31:CA:2251:OMG:HM23	1.84	0.45
31:CA:309:A:H4'	50:CV:16:GLY:HA2	1.99	0.45
27:D0:9:GLN:HB2	27:D0:29:LEU:HD22	1.98	0.45
31:CA:136:G:H1	31:CA:143:C:H42	1.65	0.45
31:CA:2842:G:H2'	31:CA:2843:G:O4'	2.16	0.45
30:CD:26:VAL:HG21	45:CQ:5:ILE:HG12	1.99	0.45
33:DA:2262:U:H2'	33:DA:2263:C:H6	1.81	0.45
28:DB:111:U:H2'	28:DB:112:G:H8	1.82	0.45
1:AA:1012:A:H61	1:AA:1017:U:H3	1.64	0.45
9:AI:116:VAL:HG21	10:AJ:62:ARG:HB2	1.99	0.45
25:C4:60:ALA:O	41:CM:48:ARG:HD2	2.17	0.45
31:CA:2339:C:H2'	31:CA:2340:A:C8	2.52	0.45
31:CA:1783:A:H5'	31:CA:2608:G:H4'	1.99	0.45
33:DA:2313:C:H5''	35:DF:88:LYS:HD3	1.99	0.45
48:DT:84:ARG:HB2	48:DT:96:ILE:HB	1.99	0.45
1:BA:1347:G:N2	1:BA:1373:G:H2'	2.32	0.45
1:BA:518:C:H2'	1:BA:530:G:C8	2.51	0.45
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	1.99	0.45
4:BD:58:LYS:HA	4:BD:200:ILE:HG12	1.97	0.45
7:BG:111:ARG:HB3	7:BG:119:ARG:HG2	1.99	0.45
33:DA:136:G:H1	33:DA:143:C:H42	1.65	0.45
1:AA:73:C:O2'	1:AA:74:A:H8	1.98	0.45
1:BA:649:A:H2'	1:BA:650:G:O4'	2.17	0.45
31:CA:706:A:H2'	31:CA:707:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:863:A:H2'	31:CA:864:G:C8	2.52	0.45
29:CC:162:VAL:HG22	29:CC:176:LEU:HA	1.99	0.45
33:DA:1141:U:H4'	33:DA:1142:A:O4'	2.17	0.45
33:DA:833:A:H2'	33:DA:834:G:C8	2.52	0.45
44:DP:41:ALA:HB2	44:DP:48:LEU:HD21	1.99	0.45
1:AA:1347:G:N2	1:AA:1373:G:H2'	2.32	0.45
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.52	0.45
7:AG:111:ARG:HB3	7:AG:119:ARG:HG2	1.99	0.45
5:BE:57:PRO:O	5:BE:60:ILE:HG13	2.17	0.45
31:CA:1788:C:O5'	31:CA:1788:C:H6	2.00	0.45
29:CC:212:ARG:HD2	29:CC:216:VAL:O	2.17	0.45
22:D1:9:THR:CG2	33:DA:2020:A:H5'	2.46	0.45
47:DS:26:ASP:HA	63:DS:201:PGE:H52	1.99	0.45
1:AA:523:A:H61	12:AL:89:D2T:CG	2.31	0.44
1:BA:350:G:H5''	20:BT:3:ASN:HD22	1.82	0.44
1:BA:505:G:H5'	1:BA:534:U:C2	2.51	0.44
1:BA:523:A:H61	12:BL:89:D2T:CG	2.30	0.44
5:BE:90:THR:HG22	5:BE:91:GLY:H	1.82	0.44
16:BP:20:VAL:HG13	16:BP:32:PHE:HB2	1.99	0.44
31:CA:822:G:O6	31:CA:943:A:H2	1.99	0.44
42:CN:30:SER:H	42:CN:106:ASP:HB3	1.82	0.44
33:DA:2086:U:H2'	33:DA:2087:G:C8	2.52	0.44
1:AA:619:U:C2	4:AD:132:ILE:HD11	2.52	0.44
1:BA:774:G:H21	57:BA:1642:PG4:H62	1.82	0.44
1:BA:8:A:C6	4:BD:206:LYS:HB3	2.52	0.44
31:CA:1121:C:H2'	31:CA:1122:G:O4'	2.17	0.44
31:CA:1532:A:H8	31:CA:1532:A:H5''	1.83	0.44
31:CA:193:U:H5	69:CA:3405:HOH:O	2.01	0.44
33:DA:1357:C:H2'	33:DA:1358:G:O4'	2.17	0.44
36:DG:52:PHE:N	36:DG:52:PHE:CD1	2.85	0.44
1:AA:212:G:H2'	1:AA:213:G:C8	2.52	0.44
1:AA:390:U:H2'	1:AA:391:G:C8	2.53	0.44
16:BP:5:ARG:HB3	69:BP:101:HOH:O	2.16	0.44
30:CD:62:LYS:HE2	31:CA:2810:A:H5''	1.99	0.44
31:CA:247:G:H4'	31:CA:386:G:C5	2.52	0.44
44:CP:51:ALA:HB3	44:CP:78:VAL:HG13	2.00	0.44
33:DA:2339:C:H2'	33:DA:2340:A:C8	2.52	0.44
33:DA:2502:G:H5''	33:DA:2503:2MA:H5''	1.99	0.44
1:AA:77:A:H2'	1:AA:78:A:C8	2.53	0.44
8:AH:105:SER:HB2	8:AH:126:ILE:HD11	1.99	0.44
18:AR:36:SER:HA	18:AR:72:ASP:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BF:91:ARG:HD2	18:BR:61:ARG:HH22	1.83	0.44
31:CA:1182:G:H2'	31:CA:1183:U:O4'	2.17	0.44
31:CA:1681:G:O2'	31:CA:1762:A:H2'	2.18	0.44
31:CA:729:G:H2'	31:CA:1775:U:H1'	2.00	0.44
29:CC:50:THR:O	31:CA:1805:A:H1'	2.18	0.44
36:CG:24:ILE:HG21	36:CG:72:LEU:HD21	1.99	0.44
33:DA:634:C:H2'	33:DA:635:C:C6	2.53	0.44
29:DC:49:ILE:HD11	33:DA:779:U:H5''	1.99	0.44
36:DG:145:ALA:HB1	36:DG:164:TYR:HE1	1.82	0.44
28:DB:28:C:P	44:DP:31:THR:HG21	2.57	0.44
48:DT:20:VAL:HA	48:DT:23:LEU:HD12	1.98	0.44
1:AA:407:U:H2'	1:AA:408:A:C8	2.52	0.44
1:AA:649:A:H2'	1:AA:650:G:O4'	2.17	0.44
1:AA:76:G:H1	1:AA:93:U:H3	1.64	0.44
2:AB:111:ILE:HD12	2:AB:152:LYS:HA	1.99	0.44
3:AC:22:TRP:HB3	3:AC:59:ARG:H	1.82	0.44
11:AK:89:PRO:HA	11:AK:93:ARG:HD2	2.00	0.44
14:AN:83:LYS:HG3	69:AN:207:HOH:O	2.16	0.44
20:BT:69:LYS:HG3	20:BT:69:LYS:H	1.55	0.44
31:CA:2006:C:H2'	31:CA:2007:U:C6	2.52	0.44
31:CA:962:G:H4'	31:CA:2496:C:O2'	2.18	0.44
31:CA:2544:G:H5'	31:CA:2645:G:C2	2.53	0.44
31:CA:2800:A:C2	31:CA:2895:G:H1'	2.52	0.44
31:CA:281:C:H2'	31:CA:282:A:C8	2.53	0.44
36:CG:145:ALA:HB1	36:CG:164:TYR:HE1	1.83	0.44
29:DC:162:VAL:HG22	29:DC:176:LEU:HA	1.99	0.44
29:DC:16:VAL:HG22	29:DC:206:GLY:HA3	2.00	0.44
5:BE:105:ILE:H	5:BE:123:VAL:H	1.64	0.44
13:BM:6:GLY:O	13:BM:7:ILE:HG13	2.18	0.44
31:CA:321:U:H5''	34:CE:131:THR:HG23	1.99	0.44
30:CD:152:PRO:HB2	30:CD:154:LYS:HG2	1.99	0.44
48:CT:20:VAL:HA	48:CT:23:LEU:HD12	1.99	0.44
26:D5:36:ARG:HH22	33:DA:2539:C:H4'	1.83	0.44
33:DA:1168:G:H2'	33:DA:1169:A:O4'	2.17	0.44
33:DA:2298:A:H61	33:DA:2318:G:H1'	1.83	0.44
40:DL:70:ARG:HD3	40:DL:76:VAL:HG22	2.00	0.44
1:BA:21:G:H2'	1:BA:22:G:C8	2.52	0.44
9:BI:55:VAL:HG22	9:BI:94:LEU:HD22	1.99	0.44
14:BN:53:ARG:HH21	19:BS:37:ARG:HH22	1.65	0.44
24:C3:16:HIS:CD2	31:CA:464:U:HO2'	2.35	0.44
33:DA:1928:A:H2'	33:DA:1929:G:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DA:722:A:H2'	33:DA:723:C:O4'	2.18	0.44
29:DC:212:ARG:HD2	29:DC:216:VAL:O	2.18	0.44
57:DA:3192:PG4:H12	52:DX:11:ARG:HG2	1.99	0.44
1:AA:518:C:H2'	1:AA:530:G:C8	2.52	0.44
1:AA:738:C:H5''	6:AF:68:GLN:HG2	2.00	0.44
7:AG:50:LEU:HD22	7:AG:124:LEU:HD13	1.99	0.44
10:AJ:46:LYS:HG2	10:AJ:68:ARG:HG2	1.99	0.44
1:BA:240:G:OP1	1:BA:240:G:H4'	2.17	0.44
1:BA:972:C:H4'	10:BJ:59:LYS:HG2	2.00	0.44
8:BH:105:SER:HB2	8:BH:126:ILE:HD11	2.00	0.44
11:BK:89:PRO:HA	11:BK:93:ARG:HD2	1.99	0.44
19:BS:33:THR:HG22	19:BS:35:SER:H	1.83	0.44
20:BT:5:LYS:HB3	20:BT:7:ALA:H	1.82	0.44
31:CA:225:C:H2'	31:CA:226:A:O4'	2.18	0.44
31:CA:2607:G:H2'	31:CA:2608:G:O4'	2.17	0.44
36:CG:24:ILE:HD13	36:CG:72:LEU:HD21	1.99	0.44
65:DA:3184:1PE:H121	48:DT:73:LYS:HZ3	1.82	0.44
42:DN:42:THR:HG22	42:DN:93:VAL:HG12	2.00	0.44
5:AE:90:THR:HG22	5:AE:91:GLY:H	1.83	0.44
8:AH:96:MET:HE3	8:AH:130:ALA:HB1	2.00	0.44
14:BN:31:ILE:HG23	14:BN:42:TRP:HZ2	1.83	0.44
31:CA:1326:U:H2'	31:CA:1327:A:H8	1.83	0.44
61:D1:102:PEG:H12	33:DA:2008:C:H5''	1.99	0.44
33:DA:74:A:N3	33:DA:74:A:H5''	2.33	0.44
29:DC:78:VAL:HG21	29:DC:110:LEU:HD21	2.00	0.44
3:BC:14:ILE:HG21	3:BC:178:LEU:HB3	2.00	0.43
31:CA:2326:C:O2'	31:CA:2327:A:H8	2.02	0.43
28:CB:111:U:H2'	28:CB:112:G:H8	1.84	0.43
37:DH:71:LYS:HB3	37:DH:108:VAL:HG22	2.00	0.43
45:DQ:106:LYS:HA	45:DQ:109:ARG:HD3	2.00	0.43
52:DX:23:VAL:HA	52:DX:38:VAL:HG23	1.99	0.43
1:AA:310:G:H5''	16:AP:31:ARG:HB2	1.99	0.43
3:AC:14:ILE:HG21	3:AC:178:LEU:HB3	2.00	0.43
11:BK:67:ALA:HB2	11:BK:96:THR:HG23	1.99	0.43
31:CA:1183:U:H2'	31:CA:1184:U:C6	2.53	0.43
31:CA:2298:A:H61	31:CA:2318:G:H1'	1.83	0.43
29:CC:48:ARG:HD3	31:CA:773:U:O2'	2.18	0.43
33:DA:142:A:H2'	33:DA:143:C:C6	2.52	0.43
33:DA:2741:A:H2'	33:DA:2742:G:O4'	2.18	0.43
1:BA:1001:C:H2'	1:BA:1002:G:H8	1.83	0.43
1:BA:1343:G:H2'	1:BA:1344:C:C6	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:56:A:H61	31:CA:114:U:H3	1.66	0.43
31:CA:1434:A:H2'	31:CA:1435:G:C8	2.53	0.43
33:DA:281:C:H2'	33:DA:282:A:C8	2.53	0.43
33:DA:909:A:O2'	33:DA:910:A:H5'	2.18	0.43
11:AK:67:ALA:HB2	11:AK:96:THR:HG23	1.99	0.43
31:CA:373:U:H2'	31:CA:374:A:C8	2.53	0.43
30:CD:38:LYS:O	30:CD:46:ARG:HA	2.18	0.43
33:DA:571:U:H3'	47:DS:80:ARG:NH2	2.33	0.43
3:BC:153:VAL:HG12	3:BC:198:VAL:HG22	2.00	0.43
3:BC:40:ARG:HG2	3:BC:55:ILE:HG21	2.01	0.43
1:BA:619:U:H3	4:BD:131:ASN:HB3	1.83	0.43
31:CA:785:G:O2'	31:CA:1779:U:H5''	2.18	0.43
33:DA:1604:C:H5'	69:DA:5598:HOH:O	2.19	0.43
33:DA:1975:G:H21	63:DA:3223:PGE:C2	2.31	0.43
44:DP:102:ARG:HD2	69:DP:317:HOH:O	2.17	0.43
1:BA:108:G:H5'	1:BA:109:A:H5''	2.00	0.43
1:BA:1108:G:H5''	3:BC:176:HIS:CE1	2.54	0.43
10:BJ:46:LYS:HG2	10:BJ:68:ARG:HG2	1.99	0.43
31:CA:142:A:H2'	31:CA:143:C:C6	2.52	0.43
31:CA:787:C:H5''	31:CA:788:A:H5'	2.01	0.43
24:D3:2:LYS:HE2	33:DA:687:C:H5''	1.99	0.43
33:DA:191:A:H2'	33:DA:192:C:C6	2.54	0.43
33:DA:2028:U:H2'	33:DA:2029:G:O4'	2.19	0.43
33:DA:2255:G:H21	68:DA:3218:TRS:H12	1.84	0.43
36:DG:24:ILE:HG21	36:DG:72:LEU:HD21	1.98	0.43
55:DI:57:ASN:HD22	55:DI:76:PHE:C	2.22	0.43
44:DP:51:ALA:HB3	44:DP:78:VAL:HG13	2.00	0.43
1:BA:59:A:H5''	1:BA:387:U:H5''	1.99	0.43
2:BB:129:LEU:H	2:BB:129:LEU:HG	1.56	0.43
11:BK:101:ASN:HD22	11:BK:107:ILE:HG12	1.83	0.43
31:CA:1509:A:O2'	31:CA:1510:G:H8	2.00	0.43
31:CA:190:A:H2'	31:CA:191:A:O4'	2.18	0.43
31:CA:2043:C:C6	31:CA:2043:C:H5''	2.54	0.43
31:CA:95:A:H4'	54:CZ:38:GLN:O	2.19	0.43
40:CL:35:VAL:HB	40:CL:36:GLY:H	1.65	0.43
46:CR:58:ARG:HH11	46:CR:62:ILE:HD11	1.82	0.43
48:CT:36:LEU:HD13	48:CT:48:LYS:HA	2.00	0.43
49:CU:34:VAL:HG11	49:CU:43:ILE:HG12	2.00	0.43
51:CW:51:GLN:HG2	51:CW:86:LEU:HD11	2.00	0.43
22:D1:48:TYR:CE1	22:D1:53:LYS:HD3	2.54	0.43
33:DA:2097:A:H8	33:DA:2097:A:H5''	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DA:2547:A:H2'	33:DA:2548:U:C6	2.53	0.43
43:DO:44:LEU:HD23	43:DO:113:ILE:HD13	1.99	0.43
1:AA:923:A:OP1	5:AE:26:LYS:HG2	2.18	0.43
12:AL:102:LEU:HB3	12:AL:103:ASP:H	1.65	0.43
21:AU:28:VAL:O	21:AU:32:VAL:HG23	2.18	0.43
5:BE:134:ILE:HG13	5:BE:134:ILE:H	1.68	0.43
12:BL:80:ILE:HD12	12:BL:97:THR:HG22	2.00	0.43
31:CA:1188:U:H2'	31:CA:1189:A:H8	1.84	0.43
31:CA:1354:A:H2'	31:CA:1355:G:O4'	2.18	0.43
31:CA:593:U:H2'	31:CA:594:U:C6	2.54	0.43
39:CK:35:ARG:HE	39:CK:140:LEU:HD21	1.83	0.43
31:CA:1248:G:O2'	46:CR:3:ARG:HA	2.18	0.43
22:D1:22:LEU:HD23	61:D1:102:PEG:H31	2.01	0.43
33:DA:1881:C:H2'	33:DA:1882:U:O4'	2.19	0.43
38:DJ:11:LEU:HD22	38:DJ:24:VAL:HG23	2.01	0.43
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.84	0.43
1:AA:1416:G:H5''	69:AA:2080:HOH:O	2.18	0.43
4:AD:48:LEU:HD21	4:AD:56:ARG:HG3	2.00	0.43
1:BA:923:A:OP1	5:BE:26:LYS:HG2	2.19	0.43
31:CA:532:A:H2'	31:CA:532:A:N3	2.34	0.43
31:CA:588:U:H2'	31:CA:589:U:C6	2.53	0.43
31:CA:976:G:H2'	31:CA:977:G:H8	1.84	0.43
41:CM:77:ILE:CD1	41:CM:108:ALA:HB1	2.39	0.43
33:DA:1831:G:H1'	63:DA:3223:PGE:H22	2.01	0.43
33:DA:2869:G:H2'	33:DA:2870:C:O4'	2.19	0.43
33:DA:735:A:H5''	69:DA:3598:HOH:O	2.19	0.43
33:DA:804:A:H2'	33:DA:806:C:C4	2.54	0.43
28:DB:77:U:H4'	69:DW:110:HOH:O	2.19	0.43
51:DW:51:GLN:HG2	51:DW:86:LEU:HD11	2.01	0.43
54:DZ:56:LEU:HA	54:DZ:59:GLU:HG2	2.01	0.43
1:BA:77:A:H2'	1:BA:78:A:C8	2.54	0.43
31:CA:1716:U:H2'	31:CA:1717:A:C8	2.54	0.43
31:CA:357:C:H2'	31:CA:358:U:C6	2.54	0.43
33:DA:1394:U:H4'	33:DA:1603:A:H4'	2.01	0.43
33:DA:819:A:C4	33:DA:1189:A:C2	3.07	0.43
37:DH:41:LYS:HA	37:DH:44:ILE:HG12	2.00	0.43
55:DI:67:THR:CG2	55:DI:68:PRO:HA	2.48	0.43
39:DK:7:LYS:O	39:DK:11:VAL:HG23	2.18	0.43
1:AA:1137:C:H1'	1:AA:1138:G:N2	2.34	0.42
7:AG:59:LEU:H	7:AG:59:LEU:HG	1.65	0.42
14:AN:53:ARG:HH21	19:AS:37:ARG:HH22	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1137:C:H1'	1:BA:1138:G:N2	2.34	0.42
2:BB:100:MET:HA	2:BB:107:VAL:HG21	2.01	0.42
5:BE:47:GLY:HA3	5:BE:71:MET:HG2	2.01	0.42
31:CA:2822:G:H2'	31:CA:2823:A:H5''	2.00	0.42
29:CC:107:PRO:HD2	29:CC:110:LEU:HD22	2.01	0.42
37:CH:71:LYS:HB3	37:CH:108:VAL:HG22	2.00	0.42
37:CH:41:LYS:HA	37:CH:44:ILE:HG12	2.00	0.42
41:CM:19:LEU:HD23	41:CM:31:GLY:O	2.19	0.42
47:CS:59:ILE:HG12	47:CS:101:ILE:HD13	2.01	0.42
13:BM:11:ASP:HA	13:BM:45:ILE:HD13	2.00	0.42
54:CZ:56:LEU:HA	54:CZ:59:GLU:HG2	2.01	0.42
33:DA:1171:G:H1'	33:DA:1179:G:H22	1.83	0.42
33:DA:419:U:H2'	33:DA:420:C:C6	2.53	0.42
33:DA:588:U:H2'	33:DA:589:U:C6	2.54	0.42
1:AA:246:A:N3	1:AA:247:G:H1'	2.33	0.42
5:AE:47:GLY:HA3	5:AE:71:MET:HG2	2.01	0.42
7:AG:132:GLY:H	7:AG:135:VAL:HG22	1.84	0.42
10:BJ:65:TYR:HB2	14:BN:96:LEU:HD11	2.02	0.42
41:CM:77:ILE:HD12	41:CM:109:LYS:O	2.18	0.42
33:DA:1680:U:H2'	33:DA:1681:G:O4'	2.19	0.42
33:DA:1746:A:H2'	33:DA:1747:U:C6	2.54	0.42
55:DI:132:TYR:N	55:DI:133:GLU:HB2	2.33	0.42
38:DJ:56:PRO:HD3	38:DJ:74:PRO:HA	2.01	0.42
47:DS:59:ILE:HG12	47:DS:101:ILE:HD13	2.01	0.42
49:DU:11:LEU:HD12	49:DU:50:LEU:HD12	2.01	0.42
19:AS:29:LYS:HB3	19:AS:30:PRO:HD2	2.02	0.42
1:BA:1305:G:HO2'	1:BA:1306:A:H8	1.63	0.42
1:BA:629:A:H2'	1:BA:630:A:O4'	2.19	0.42
7:BG:130:ASN:HA	7:BG:135:VAL:HG11	2.01	0.42
9:BI:19:VAL:HG11	9:BI:83:ILE:HA	2.01	0.42
31:CA:1454:C:H5'	43:CO:63:ARG:HH21	1.85	0.42
30:CD:13:ARG:NH1	31:CA:2683:C:H4'	2.35	0.42
29:CC:210:ALA:HA	29:CC:213:TRP:CE2	2.55	0.42
31:CA:586:A:H5'	34:CE:84:THR:HG21	2.00	0.42
31:CA:1131:G:OP1	39:CK:82:GLY:HA2	2.19	0.42
45:CQ:106:LYS:HA	45:CQ:109:ARG:HD3	2.01	0.42
69:DB:321:HOH:O	44:DP:103:VAL:HG23	2.19	0.42
53:DY:59:ILE:HG12	53:DY:67:VAL:HG21	2.01	0.42
1:AA:528:C:H5''	1:AA:528:C:H6	1.84	0.42
8:AH:18:GLN:HG2	8:AH:63:LEU:HD21	2.01	0.42
1:BA:524:G:H2'	1:BA:525:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BE:81:LEU:HB3	5:BE:147:MET:SD	2.59	0.42
7:BG:132:GLY:H	7:BG:135:VAL:HG22	1.84	0.42
12:BL:65:SER:HB2	12:BL:82:ILE:HD11	2.01	0.42
31:CA:128:C:H2'	31:CA:129:C:C6	2.55	0.42
31:CA:1881:C:H2'	31:CA:1882:U:O4'	2.20	0.42
47:CS:78:ARG:HB2	47:CS:83:TYR:HD1	1.85	0.42
33:DA:1381:G:H1'	33:DA:1571:A:N1	2.35	0.42
33:DA:1716:U:H2'	33:DA:1717:A:C8	2.55	0.42
33:DA:2215:C:H2'	33:DA:2216:G:C8	2.54	0.42
32:DD:13:ARG:NH1	33:DA:2683:C:H4'	2.35	0.42
32:DD:121:THR:HB	32:DD:127:PHE:CD2	2.55	0.42
42:DN:30:SER:H	42:DN:106:ASP:HB3	1.84	0.42
1:BA:728:A:H2'	1:BA:729:A:C8	2.54	0.42
1:BA:1313:U:OP2	19:BS:6:LYS:HB3	2.19	0.42
31:CA:2271:G:H2'	31:CA:2272:U:C6	2.55	0.42
40:CL:35:VAL:CG1	40:CL:106:GLU:HG2	2.49	0.42
27:D0:45:ARG:HH12	27:D0:59:GLU:CD	2.22	0.42
32:DD:133:THR:HG21	33:DA:1676:A:H1'	2.02	0.42
33:DA:1938:A:H2'	69:DA:7933:HOH:O	2.19	0.42
33:DA:2577:A:H5''	33:DA:2578:G:H5'	2.00	0.42
29:DC:227:PRO:HA	29:DC:233:GLY:HA2	2.01	0.42
35:DF:14:LYS:O	35:DF:18:THR:HG22	2.19	0.42
62:DA:3207:EDO:H22	57:DR:203:PG4:H21	2.02	0.42
1:AA:1182:G:H5'	1:AA:1184:G:H5'	2.02	0.42
3:AC:153:VAL:HG12	3:AC:198:VAL:HG22	2.00	0.42
1:BA:1530:G:H2'	1:BA:1531:A:C8	2.55	0.42
13:BM:86:TYR:CZ	13:BM:90:ARG:HD2	2.54	0.42
31:CA:1101:U:H2'	31:CA:1102:C:H6	1.85	0.42
31:CA:1434:A:H2'	31:CA:1435:G:H8	1.84	0.42
31:CA:2377:A:H2'	31:CA:2378:A:C8	2.55	0.42
29:CC:78:VAL:HG21	29:CC:110:LEU:HD21	2.00	0.42
38:CJ:11:LEU:HD22	38:CJ:24:VAL:HG23	2.02	0.42
50:CV:14:LEU:HD11	50:CV:71:ALA:HB2	2.01	0.42
33:DA:1425:G:H2'	33:DA:1426:G:O4'	2.20	0.42
29:DC:219:THR:O	33:DA:1789:A:H5''	2.20	0.42
34:DE:21:ARG:HD2	69:DE:417:HOH:O	2.18	0.42
1:AA:300:A:H2'	1:AA:301:G:O4'	2.20	0.42
4:BD:170:TRP:CD2	4:BD:186:PRO:HB3	2.54	0.42
5:BE:24:THR:HA	5:BE:29:ARG:HA	2.02	0.42
31:CA:722:A:H2'	31:CA:723:C:O4'	2.19	0.42
31:CA:686:U:H6	31:CA:788:A:N1	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:CY:59:ILE:HG12	53:CY:67:VAL:HG21	2.02	0.42
33:DA:832:U:H2'	33:DA:833:A:C8	2.55	0.42
40:DL:113:MET:CE	40:DL:116:ILE:HD11	2.49	0.42
20:AT:44:LYS:HG3	20:AT:44:LYS:H	1.53	0.42
21:BU:28:VAL:O	21:BU:32:VAL:HG23	2.20	0.42
31:CA:2345:G:N3	31:CA:2381:A:H2'	2.35	0.42
29:CC:174:LEU:HD21	29:CC:184:VAL:HB	2.02	0.42
38:CJ:56:PRO:HD3	38:CJ:74:PRO:HA	2.01	0.42
33:DA:118:A:C8	33:DA:119:A:C8	3.07	0.42
33:DA:514:A:H5'	46:DR:11:ARG:NH1	2.34	0.42
33:DA:593:U:H2'	33:DA:594:U:C6	2.55	0.42
69:DA:5611:HOH:O	34:DE:42:GLY:HA2	2.19	0.42
1:AA:1239:A:H62	1:AA:1299:A:H62	1.68	0.42
1:AA:312:C:H2'	1:AA:313:A:C8	2.55	0.42
9:AI:19:VAL:HG11	9:AI:83:ILE:HA	2.02	0.42
14:AN:46:LEU:HA	14:AN:49:GLN:HE21	1.85	0.42
1:BA:1239:A:H62	1:BA:1299:A:H62	1.67	0.42
1:BA:300:A:H2'	1:BA:301:G:O4'	2.20	0.42
16:BP:40:ASN:O	16:BP:43:ALA:HB2	2.20	0.42
19:BS:29:LYS:HB3	19:BS:30:PRO:HD2	2.02	0.42
31:CA:1974:C:H2'	31:CA:1975:G:H8	1.85	0.42
31:CA:825:A:H2'	31:CA:826:U:O4'	2.20	0.42
43:CO:33:ILE:HB	43:CO:118:ARG:HD2	2.02	0.42
33:DA:1101:U:H2'	33:DA:1102:C:H6	1.84	0.42
33:DA:1442:U:H2'	33:DA:1443:U:C6	2.54	0.42
33:DA:2678:C:H2'	33:DA:2679:A:O4'	2.19	0.42
33:DA:492:A:H2'	33:DA:493:G:O4'	2.20	0.42
1:AA:1530:G:H2'	1:AA:1531:A:C8	2.55	0.41
2:AB:100:MET:HA	2:AB:107:VAL:HG21	2.01	0.41
7:AG:130:ASN:HA	7:AG:135:VAL:HG11	2.01	0.41
14:BN:31:ILE:HG23	14:BN:42:TRP:CZ2	2.54	0.41
31:CA:2101:A:H2'	31:CA:2102:G:H8	1.84	0.41
31:CA:2298:A:C2	31:CA:2321:U:N3	2.87	0.41
31:CA:2502:G:H5''	31:CA:2503:2MA:H5''	2.02	0.41
31:CA:35:G:H2'	31:CA:36:G:O4'	2.19	0.41
31:CA:586:A:H1'	31:CA:672:C:H1'	2.02	0.41
29:CC:227:PRO:HA	29:CC:233:GLY:HA2	2.02	0.41
30:CD:4:LEU:HD13	30:CD:29:VAL:HG11	2.02	0.41
35:CF:31:VAL:CG1	35:CF:97:TRP:CH2	3.03	0.41
33:DA:2123:G:H1	33:DA:2175:C:H42	1.68	0.41
33:DA:2193:G:H2'	33:DA:2194:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:DE:126:VAL:HA	58:DE:301:MPD:H13	2.01	0.41
42:DN:33:LEU:HD13	42:DN:117:PHE:HB3	2.02	0.41
48:DT:36:LEU:HD13	48:DT:48:LYS:HA	2.00	0.41
1:AA:728:A:H2'	1:AA:729:A:C8	2.56	0.41
1:AA:8:A:C6	4:AD:206:LYS:HB3	2.55	0.41
13:AM:86:TYR:CZ	13:AM:90:ARG:HD2	2.54	0.41
1:BA:227:G:H2'	1:BA:228:A:O4'	2.20	0.41
1:BA:677:U:H3	1:BA:713:G:H22	1.68	0.41
5:BE:23:LYS:HB3	5:BE:30:ILE:HG23	2.02	0.41
20:BT:67:ILE:O	20:BT:68:HIS:HB2	2.19	0.41
31:CA:1310:G:H2'	31:CA:1311:G:O4'	2.21	0.41
31:CA:1442:U:H2'	31:CA:1443:U:C6	2.55	0.41
35:CF:138:PHE:HE1	35:CF:152:LEU:HD21	1.85	0.41
31:CA:514:A:H4'	46:CR:11:ARG:HH12	1.85	0.41
1:AA:620:C:H2'	1:AA:621:A:O4'	2.20	0.41
4:AD:170:TRP:CD2	4:AD:186:PRO:HB3	2.54	0.41
11:AK:34:ILE:HB	11:AK:74:VAL:HG11	2.02	0.41
31:CA:737:C:H2'	31:CA:738:G:O4'	2.20	0.41
41:CM:28:GLY:O	41:CM:29:LYS:C	2.58	0.41
53:CY:37:ARG:HG2	53:CY:48:THR:HG22	2.01	0.41
33:DA:1590:A:H2'	33:DA:1591:A:C8	2.55	0.41
33:DA:357:C:H2'	33:DA:358:U:C6	2.55	0.41
55:DI:94:ARG:HG2	55:DI:127:ALA:HA	2.02	0.41
1:AA:1216:A:H5''	14:AN:5:SER:HB3	2.03	0.41
1:BA:1417:G:C6	1:BA:1482:G:C6	3.08	0.41
1:BA:522:C:H41	12:BL:50:ARG:NH2	2.18	0.41
31:CA:1196:C:H1'	31:CA:1226:A:C4	2.55	0.41
31:CA:1274:A:N3	31:CA:1297:C:H1'	2.35	0.41
31:CA:1957:C:H5'	31:CA:1984:G:O2'	2.21	0.41
31:CA:2304:G:H22	31:CA:2312:U:H3	1.68	0.41
29:CC:245:VAL:HG12	29:CC:251:GLN:HA	2.02	0.41
30:CD:106:LYS:HD3	30:CD:174:SER:HB3	2.01	0.41
38:CJ:24:VAL:HG22	38:CJ:28:LEU:HD22	2.03	0.41
39:CK:7:LYS:O	39:CK:11:VAL:HG23	2.21	0.41
41:CM:28:GLY:O	41:CM:29:LYS:O	2.39	0.41
31:CA:1808:A:N1	53:CY:28:ARG:HD2	2.36	0.41
33:DA:1011:G:OP1	46:DR:75:SER:HB2	2.20	0.41
33:DA:2026:U:H2'	33:DA:2027:G:O4'	2.20	0.41
33:DA:2101:A:H2'	33:DA:2102:G:H8	1.86	0.41
35:DF:5:HIS:HD1	35:DF:97:TRP:HE1	1.66	0.41
48:DT:29:VAL:HB	48:DT:55:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:413:G:H5''	1:AA:414:A:H5'	2.01	0.41
11:AK:101:ASN:HD22	11:AK:107:ILE:HG12	1.84	0.41
10:AJ:65:TYR:HB2	14:AN:96:LEU:HD11	2.01	0.41
8:BH:87:LYS:HB2	8:BH:125:ILE:CD1	2.45	0.41
13:BM:4:ILE:HA	13:BM:57:ARG:HG2	2.03	0.41
31:CA:1835:2MG:HM23	31:CA:1836:C:H1'	2.02	0.41
31:CA:188:G:H1	31:CA:208:C:H42	1.68	0.41
31:CA:582:A:H2'	31:CA:583:G:C8	2.55	0.41
33:DA:1482:G:H1'	33:DA:1509:A:H61	1.85	0.41
33:DA:2633:G:H2'	33:DA:2634:A:O4'	2.21	0.41
29:DC:245:VAL:HG12	29:DC:251:GLN:HA	2.03	0.41
55:DI:50:VAL:HG13	55:DI:85:VAL:HG22	2.02	0.41
33:DA:2428:G:H22	41:DM:60:ARG:NH2	2.15	0.41
43:DO:51:LEU:HD22	43:DO:51:LEU:HA	1.94	0.41
1:AA:910:C:H6	1:AA:910:C:O5'	2.04	0.41
5:AE:76:LEU:HD11	5:AE:120:VAL:HG22	2.03	0.41
31:CA:1587:G:H2'	31:CA:1588:G:H8	1.86	0.41
31:CA:1785:A:H2'	31:CA:1787:A:N7	2.35	0.41
31:CA:2114:A:N6	31:CA:2119:A:H62	2.18	0.41
31:CA:460:A:H2'	31:CA:461:C:O4'	2.20	0.41
41:CM:79:LEU:HD11	41:CM:112:LEU:HD12	2.01	0.41
25:D4:54:ASP:HB3	41:DM:57:LEU:HD22	2.02	0.41
37:DH:104:THR:HG22	37:DH:109:GLU:HA	2.02	0.41
1:AA:268:U:H2'	1:AA:269:C:C6	2.56	0.41
7:AG:57:SER:HB3	7:AG:60:GLU:HB2	2.03	0.41
1:BA:1053:G:N7	1:BA:1200:C:H5''	2.36	0.41
9:BI:36:GLU:HA	9:BI:45:ARG:HE	1.85	0.41
1:BA:1216:A:H5''	14:BN:5:SER:HB3	2.03	0.41
20:BT:24:ARG:O	20:BT:27:MET:HG3	2.20	0.41
31:CA:1590:A:H2'	31:CA:1591:A:C8	2.56	0.41
31:CA:2688:G:H1'	31:CA:2721:A:H61	1.85	0.41
31:CA:453:A:H4'	31:CA:472:A:H62	1.85	0.41
43:CO:53:THR:HA	43:CO:56:LYS:HD2	2.01	0.41
22:D1:54:VAL:HG23	22:D1:55:ILE:HG12	2.03	0.41
33:DA:118:A:N3	33:DA:178:G:H1'	2.36	0.41
29:DC:50:THR:O	33:DA:1805:A:H1'	2.21	0.41
1:AA:1338:G:H2'	1:AA:1339:A:C8	2.56	0.41
1:AA:604:G:H2'	1:AA:605:U:O4'	2.21	0.41
1:AA:438:U:H5'	4:AD:120:HIS:HB3	2.03	0.41
1:BA:429:U:H1'	1:BA:430:A:H5''	2.03	0.41
1:BA:23:C:H5	1:BA:561:U:O4	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:754:U:H2'	31:CA:755:U:C6	2.56	0.41
44:CP:28:VAL:HG11	44:CP:103:VAL:HG13	2.03	0.41
33:DA:1172:C:C5	33:DA:1173:U:H1'	2.56	0.41
33:DA:225:C:H2'	33:DA:226:A:O4'	2.20	0.41
42:DN:63:ILE:HG12	42:DN:105:MET:HG3	2.03	0.41
51:DW:12:GLN:HB3	69:DW:126:HOH:O	2.20	0.41
7:AG:22:LEU:HD12	7:AG:62:PHE:HE2	1.86	0.41
1:BA:978:A:O2'	1:BA:1322:C:H5	2.04	0.41
1:BA:438:U:H5'	4:BD:120:HIS:HB3	2.02	0.41
31:CA:1998:A:O3'	31:CA:2724:U:H4'	2.20	0.41
34:CE:108:ILE:HG21	34:CE:181:ILE:HD11	2.02	0.41
29:DC:107:PRO:HD2	29:DC:110:LEU:HD22	2.03	0.41
43:DO:33:ILE:HB	43:DO:118:ARG:HD2	2.02	0.41
43:DO:53:THR:HA	43:DO:56:LYS:HD2	2.03	0.41
1:AA:721:G:H4'	1:AA:722:G:O4'	2.20	0.41
17:AQ:15:ASP:HA	17:AQ:21:ILE:HG22	2.03	0.41
1:BA:374:A:H5''	1:BA:452:A:N1	2.36	0.41
2:BB:39:HIS:HB2	2:BB:189:THR:HG21	2.03	0.41
22:C1:6:ASN:ND2	31:CA:2020:A:H62	2.18	0.41
31:CA:2182:U:H2'	31:CA:2183:A:C8	2.56	0.41
31:CA:2798:U:H4'	31:CA:2799:A:H5'	2.02	0.41
31:CA:600:G:H2'	31:CA:601:C:O4'	2.20	0.41
34:CE:117:ARG:HA	34:CE:185:LYS:HD3	2.03	0.41
49:CU:11:LEU:HD12	49:CU:50:LEU:HD12	2.03	0.41
33:DA:128:C:H2'	33:DA:129:C:C6	2.55	0.41
32:DD:56:LYS:O	32:DD:60:VAL:HG23	2.20	0.41
10:AJ:26:VAL:HG21	10:AJ:39:PRO:HD3	2.01	0.41
11:AK:34:ILE:HG21	11:AK:74:VAL:HG21	2.02	0.41
1:BA:502:A:H2'	1:BA:503:C:O4'	2.21	0.41
1:BA:580:C:H2'	1:BA:581:G:O4'	2.21	0.41
2:BB:130:THR:H	2:BB:133:GLU:HB2	1.85	0.41
19:BS:32:ARG:HA	19:BS:50:ALA:HB3	2.03	0.41
33:DA:1957:C:H5'	33:DA:1984:G:O2'	2.21	0.41
33:DA:2182:U:H2'	33:DA:2183:A:C8	2.56	0.41
9:AI:36:GLU:HA	9:AI:45:ARG:HE	1.86	0.40
1:BA:1356:G:H2'	1:BA:1357:A:C8	2.55	0.40
4:BD:91:LEU:HD21	4:BD:195:ILE:HG21	2.03	0.40
31:CA:2819:G:H2'	31:CA:2821:A:N7	2.36	0.40
43:CO:44:LEU:HD23	43:CO:113:ILE:HD13	2.02	0.40
33:DA:839:U:H1'	33:DA:1191:G:H1'	2.02	0.40
33:DA:600:G:H2'	33:DA:601:C:O4'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DA:754:U:H2'	33:DA:755:U:C6	2.57	0.40
29:DC:160:THR:HG21	33:DA:1819:A:H5''	2.03	0.40
1:AA:59:A:H5''	1:AA:387:U:H5''	2.03	0.40
1:AA:81:A:H2	1:AA:88:U:H3	1.69	0.40
3:AC:7:PRO:HD2	3:AC:184:TYR:CD1	2.56	0.40
6:AF:74:LEU:O	6:AF:77:THR:HG22	2.21	0.40
1:BA:868:C:H2'	1:BA:869:G:O4'	2.21	0.40
17:BQ:12:VAL:HG12	17:BQ:55:ILE:HA	2.04	0.40
31:CA:1556:C:H2'	31:CA:1557:C:C6	2.56	0.40
31:CA:1810:A:H2'	31:CA:1811:G:O4'	2.20	0.40
31:CA:2193:G:H2'	31:CA:2194:U:C6	2.56	0.40
31:CA:545:U:H2'	31:CA:546:U:O3'	2.20	0.40
48:CT:66:ILE:HA	48:CT:69:LEU:HD22	2.04	0.40
33:DA:1169:A:H2'	33:DA:1170:C:O4'	2.22	0.40
33:DA:2544:G:H2'	33:DA:2545:G:O4'	2.20	0.40
33:DA:414:C:H2'	33:DA:415:A:C8	2.56	0.40
37:DH:4:ILE:HD11	37:DH:44:ILE:HG22	2.03	0.40
42:DN:57:VAL:HA	42:DN:112:LEU:HD21	2.03	0.40
48:DT:17:VAL:HB	48:DT:76:VAL:HG11	2.03	0.40
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.56	0.40
1:AA:502:A:H2'	1:AA:503:C:O4'	2.21	0.40
3:AC:47:LEU:HD22	3:AC:76:VAL:HG22	2.04	0.40
10:BJ:6:ILE:HD11	10:BJ:79:PRO:HB3	2.02	0.40
13:BM:90:ARG:HD3	13:BM:97:VAL:HA	2.03	0.40
31:CA:1430:G:H2'	31:CA:1431:A:O4'	2.21	0.40
31:CA:796:C:H2'	31:CA:797:G:H8	1.86	0.40
41:CM:132:ARG:HG3	41:CM:142:ILE:HD13	2.04	0.40
48:CT:17:VAL:HB	48:CT:76:VAL:HG11	2.03	0.40
25:D4:33:LEU:HD23	25:D4:36:LYS:HD2	2.03	0.40
33:DA:2377:A:H2'	33:DA:2378:A:C8	2.56	0.40
33:DA:742:A:H2'	33:DA:743:A:C8	2.57	0.40
37:DH:50:ARG:HD3	37:DH:53:GLU:HG2	2.03	0.40
1:AA:621:A:H2'	1:AA:622:A:O4'	2.21	0.40
1:AA:957:U:O2	1:AA:959:A:H8	2.05	0.40
5:AE:16:ILE:HD13	5:AE:137:VAL:HG11	2.03	0.40
11:AK:16:VAL:HG23	11:AK:79:ILE:HG13	2.02	0.40
1:BA:1126:U:O2	1:BA:1280:A:H5'	2.22	0.40
1:BA:1289:A:H3'	1:BA:1290:G:H8	1.86	0.40
15:BO:29:VAL:HG13	15:BO:63:ARG:HG3	2.04	0.40
31:CA:942:G:H4'	31:CA:1190:G:H5'	2.02	0.40
31:CA:29:U:H2'	31:CA:30:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C3:1:MET:HG2	31:CA:753:A:OP1	2.21	0.40
29:CC:158:ALA:HB3	31:CA:1820:U:O2'	2.21	0.40
1:AA:629:A:H2'	1:AA:630:A:O4'	2.22	0.40
1:AA:892:A:O2'	1:AA:1415:G:H4'	2.21	0.40
19:AS:32:ARG:HA	19:AS:50:ALA:HB3	2.02	0.40
31:CA:516:C:H1'	31:CA:1261:C:O2'	2.21	0.40
31:CA:2552:OMU:H6	31:CA:2552:OMU:O5'	2.22	0.40
31:CA:2571:U:C4	31:CA:2574:G:C8	3.10	0.40
31:CA:634:C:H2'	31:CA:635:C:H6	1.86	0.40
31:CA:824:U:H3	31:CA:833:A:H61	1.69	0.40
37:CH:27:ARG:HD3	37:CH:27:ARG:HA	1.82	0.40
33:DA:1125:G:C6	33:DA:1126:A:N6	2.90	0.40
33:DA:1759:A:H2'	33:DA:1760:C:C6	2.56	0.40
33:DA:319:G:OP2	34:DE:132:LYS:HE2	2.22	0.40
29:DC:21:ASN:OD1	29:DC:23:GLU:HB2	2.22	0.40
32:DD:3:GLY:HA3	32:DD:204:LYS:HG2	2.04	0.40
34:DE:117:ARG:HA	34:DE:185:LYS:HD3	2.03	0.40
46:DR:90:ILE:HG22	46:DR:95:LEU:HG	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	209 (94%)	8 (4%)	5 (2%)	8	36
2	BB	222/224 (99%)	209 (94%)	8 (4%)	5 (2%)	8	36
3	AC	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	19	59
3	BC	204/206 (99%)	193 (95%)	8 (4%)	3 (2%)	13	47
4	AD	203/205 (99%)	192 (95%)	11 (5%)	0	100	100
4	BD	203/205 (99%)	193 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AE	153/155 (99%)	144 (94%)	7 (5%)	2 (1%)	15	51
5	BE	148/155 (96%)	130 (88%)	15 (10%)	3 (2%)	9	39
6	AF	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
6	BF	98/106 (92%)	89 (91%)	7 (7%)	2 (2%)	9	39
7	AG	149/151 (99%)	135 (91%)	13 (9%)	1 (1%)	26	67
7	BG	149/151 (99%)	139 (93%)	10 (7%)	0	100	100
8	AH	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	24	64
8	BH	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
9	AI	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
9	BI	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
10	AJ	97/99 (98%)	89 (92%)	5 (5%)	3 (3%)	5	28
10	BJ	96/99 (97%)	76 (79%)	14 (15%)	6 (6%)	2	10
11	AK	115/117 (98%)	103 (90%)	10 (9%)	2 (2%)	11	44
11	BK	115/117 (98%)	103 (90%)	10 (9%)	2 (2%)	11	44
12	AL	120/123 (98%)	116 (97%)	3 (2%)	1 (1%)	24	64
12	BL	120/123 (98%)	114 (95%)	4 (3%)	2 (2%)	11	44
13	AM	112/114 (98%)	101 (90%)	7 (6%)	4 (4%)	4	24
13	BM	112/114 (98%)	100 (89%)	6 (5%)	6 (5%)	2	14
14	AN	98/100 (98%)	88 (90%)	8 (8%)	2 (2%)	9	39
14	BN	98/100 (98%)	90 (92%)	6 (6%)	2 (2%)	9	39
15	AO	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
15	BO	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	16	53
16	AP	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	15	51
16	BP	80/82 (98%)	68 (85%)	10 (12%)	2 (2%)	7	33
17	AQ	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	15	51
17	BQ	78/80 (98%)	73 (94%)	2 (3%)	3 (4%)	4	23
18	AR	53/55 (96%)	53 (100%)	0	0	100	100
18	BR	53/55 (96%)	51 (96%)	1 (2%)	1 (2%)	10	41
19	AS	77/79 (98%)	68 (88%)	8 (10%)	1 (1%)	15	51
19	BS	77/79 (98%)	65 (84%)	11 (14%)	1 (1%)	15	51
20	AT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	BT	83/86 (96%)	79 (95%)	3 (4%)	1 (1%)	16	53
21	AU	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
21	BU	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
22	C1	54/56 (96%)	48 (89%)	3 (6%)	3 (6%)	2	13
22	D1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
23	C2	48/51 (94%)	42 (88%)	5 (10%)	1 (2%)	9	38
23	D2	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
24	C3	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	8	36
24	D3	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
25	C4	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
25	D4	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
26	C5	36/38 (95%)	36 (100%)	0	0	100	100
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	4	24
27	D0	57/58 (98%)	55 (96%)	2 (4%)	0	100	100
29	CC	269/271 (99%)	250 (93%)	14 (5%)	5 (2%)	10	41
29	DC	269/271 (99%)	253 (94%)	15 (6%)	1 (0%)	39	77
30	CD	207/209 (99%)	193 (93%)	14 (7%)	0	100	100
32	DD	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
34	CE	199/201 (99%)	187 (94%)	9 (4%)	3 (2%)	13	47
34	DE	199/201 (99%)	191 (96%)	7 (4%)	1 (0%)	34	73
35	CF	175/177 (99%)	165 (94%)	9 (5%)	1 (1%)	30	70
35	DF	175/177 (99%)	164 (94%)	10 (6%)	1 (1%)	30	70
36	CG	174/176 (99%)	158 (91%)	12 (7%)	4 (2%)	8	36
36	DG	174/176 (99%)	160 (92%)	13 (8%)	1 (1%)	30	70
37	CH	147/149 (99%)	132 (90%)	11 (8%)	4 (3%)	6	31
37	DH	147/149 (99%)	135 (92%)	10 (7%)	2 (1%)	14	49
38	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	5	29
38	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	5	29
39	CK	140/142 (99%)	132 (94%)	5 (4%)	3 (2%)	9	38
39	DK	140/142 (99%)	134 (96%)	4 (3%)	2 (1%)	14	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	CL	120/123 (98%)	112 (93%)	7 (6%)	1 (1%)	24	64
40	DL	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
41	CM	142/144 (99%)	130 (92%)	8 (6%)	4 (3%)	6	31
41	DM	142/144 (99%)	136 (96%)	4 (3%)	2 (1%)	14	49
42	CN	133/136 (98%)	123 (92%)	9 (7%)	1 (1%)	24	64
42	DN	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
43	CO	118/125 (94%)	107 (91%)	8 (7%)	3 (2%)	7	33
43	DO	123/125 (98%)	113 (92%)	9 (7%)	1 (1%)	24	64
44	CP	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
44	DP	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
45	CQ	112/114 (98%)	104 (93%)	7 (6%)	1 (1%)	21	62
45	DQ	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	21	62
46	CR	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
46	DR	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
47	CS	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	5	29
47	DS	101/103 (98%)	95 (94%)	5 (5%)	1 (1%)	19	59
48	CT	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
48	DT	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
49	CU	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
49	DU	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
50	CV	100/102 (98%)	86 (86%)	10 (10%)	4 (4%)	4	21
50	DV	100/102 (98%)	95 (95%)	3 (3%)	2 (2%)	9	39
51	CW	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
51	DW	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
52	CX	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
52	DX	75/76 (99%)	72 (96%)	3 (4%)	0	100	100
53	CY	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
53	DY	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
54	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11	44
54	DZ	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
55	DI	133/135 (98%)	114 (86%)	14 (10%)	5 (4%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	11407/11629 (98%)	10635 (93%)	633 (6%)	139 (1%)	16	53

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE
3	AC	156	ARG
5	AE	162	GLU
13	AM	5	ALA
22	C1	25	VAL
27	C0	14	ILE
2	BB	126	PHE
3	BC	156	ARG
10	BJ	91	ASP
13	BM	7	ILE
13	BM	114	LYS
19	BS	6	LYS
20	BT	5	LYS
34	CE	83	VAL
36	CG	119	ALA
36	CG	175	LYS
36	CG	176	LYS
37	CH	10	ALA
38	CJ	19	ASN
39	CK	81	ILE
41	CM	29	LYS
42	CN	70	ASP
43	CO	118	ARG
50	CV	7	ARG
50	CV	16	GLY
50	CV	17	LYS
38	DJ	19	ASN
50	DV	52	LEU
55	DI	91	ALA
2	AB	95	ARG
5	AE	109	GLY
10	AJ	57	VAL
11	AK	54	GLY
13	AM	105	ASN
14	AN	38	ASP
17	AQ	82	ALA
2	BB	95	ARG

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Mol	Chain	Res	Type
3	BC	61	ALA
5	BE	103	THR
5	BE	110	ALA
6	BF	98	GLU
10	BJ	38	GLY
10	BJ	57	VAL
11	BK	54	GLY
12	BL	44	LYS
13	BM	5	ALA
13	BM	105	ASN
14	BN	38	ASP
16	BP	80	LYS
17	BQ	70	THR
17	BQ	82	ALA
29	CC	158	ALA
34	CE	82	GLY
36	CG	46	ALA
38	CJ	25	GLY
39	CK	25	LEU
39	CK	95	ARG
40	CL	35	VAL
41	CM	30	THR
41	CM	69	ARG
43	CO	119	SER
45	CQ	105	GLY
36	DG	46	ALA
37	DH	11	ASN
38	DJ	25	GLY
39	DK	95	ARG
45	DQ	105	GLY
47	DS	44	GLY
2	AB	127	ASP
7	AG	56	LYS
11	AK	89	PRO
19	AS	6	LYS
22	C1	26	THR
22	C1	27	SER
24	C3	45	SER
27	C0	4	THR
2	BB	127	ASP
6	BF	92	THR
10	BJ	36	VAL

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Mol	Chain	Res	Type
11	BK	89	PRO
15	BO	88	ARG
29	CC	108	LYS
29	CC	197	ASN
37	CH	122	LEU
41	CM	36	LYS
37	DH	122	LEU
39	DK	25	LEU
41	DM	29	LYS
41	DM	36	LYS
55	DI	70	GLU
55	DI	130	PRO
2	AB	125	THR
12	AL	74	LEU
13	AM	47	GLU
16	AP	45	GLU
23	C2	51	GLU
2	BB	125	THR
10	BJ	95	GLY
12	BL	74	LEU
13	BM	47	GLU
17	BQ	17	MET
37	CH	9	VAL
37	CH	11	ASN
38	CJ	23	PRO
47	CS	53	PHE
50	CV	89	ASP
38	DJ	23	PRO
50	DV	89	ASP
55	DI	88	HIS
10	AJ	33	GLY
13	AM	7	ILE
14	AN	81	ARG
13	BM	4	ILE
29	CC	233	GLY
34	CE	6	LYS
38	CJ	32	GLY
47	CS	55	ASP
34	DE	6	LYS
38	DJ	32	GLY
55	DI	108	VAL
3	AC	107	ARG

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Mol	Chain	Res	Type
10	BJ	93	ALA
14	BN	81	ARG
16	BP	44	SER
18	BR	66	SER
29	CC	251	GLN
29	DC	233	GLY
47	CS	43	ASN
35	DF	176	PRO
35	CF	176	PRO
43	CO	116	VAL
54	CZ	62	GLY
43	DO	116	VAL
8	AH	68	GLY
3	BC	108	LYS
5	BE	105	ILE
2	AB	71	GLY
2	BB	71	GLY
10	AJ	39	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/186 (100%)	172 (92%)	14 (8%)	17	51
2	BB	186/186 (100%)	173 (93%)	13 (7%)	19	54
3	AC	170/170 (100%)	160 (94%)	10 (6%)	24	60
3	BC	170/170 (100%)	156 (92%)	14 (8%)	14	47
4	AD	172/172 (100%)	164 (95%)	8 (5%)	32	70
4	BD	172/172 (100%)	162 (94%)	10 (6%)	25	61
5	AE	118/118 (100%)	98 (83%)	20 (17%)	2	11
5	BE	113/118 (96%)	92 (81%)	21 (19%)	2	9
6	AF	92/92 (100%)	85 (92%)	7 (8%)	16	51
6	BF	87/92 (95%)	78 (90%)	9 (10%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AG	124/124 (100%)	110 (89%)	14 (11%)	7	29
7	BG	124/124 (100%)	105 (85%)	19 (15%)	3	14
8	AH	104/104 (100%)	92 (88%)	12 (12%)	7	28
8	BH	104/104 (100%)	93 (89%)	11 (11%)	8	31
9	AI	105/105 (100%)	99 (94%)	6 (6%)	25	62
9	BI	105/105 (100%)	99 (94%)	6 (6%)	25	62
10	AJ	87/87 (100%)	80 (92%)	7 (8%)	15	48
10	BJ	86/87 (99%)	77 (90%)	9 (10%)	8	32
11	AK	90/90 (100%)	89 (99%)	1 (1%)	80	93
11	BK	90/90 (100%)	85 (94%)	5 (6%)	26	63
12	AL	102/102 (100%)	96 (94%)	6 (6%)	24	60
12	BL	102/102 (100%)	93 (91%)	9 (9%)	12	43
13	AM	92/92 (100%)	84 (91%)	8 (9%)	13	44
13	BM	92/92 (100%)	85 (92%)	7 (8%)	16	51
14	AN	83/83 (100%)	80 (96%)	3 (4%)	42	78
14	BN	83/83 (100%)	81 (98%)	2 (2%)	57	85
15	AO	76/76 (100%)	69 (91%)	7 (9%)	11	40
15	BO	76/76 (100%)	66 (87%)	10 (13%)	5	21
16	AP	65/65 (100%)	64 (98%)	1 (2%)	72	90
16	BP	65/65 (100%)	62 (95%)	3 (5%)	33	70
17	AQ	74/74 (100%)	68 (92%)	6 (8%)	15	47
17	BQ	74/74 (100%)	67 (90%)	7 (10%)	11	38
18	AR	48/48 (100%)	46 (96%)	2 (4%)	36	73
18	BR	48/48 (100%)	48 (100%)	0	100	100
19	AS	70/70 (100%)	62 (89%)	8 (11%)	7	28
19	BS	70/70 (100%)	64 (91%)	6 (9%)	13	45
20	AT	65/65 (100%)	57 (88%)	8 (12%)	6	24
20	BT	65/65 (100%)	54 (83%)	11 (17%)	2	11
21	AU	48/48 (100%)	45 (94%)	3 (6%)	22	58
21	BU	48/48 (100%)	45 (94%)	3 (6%)	22	58
22	C1	47/47 (100%)	46 (98%)	1 (2%)	61	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	D1	47/47 (100%)	45 (96%)	2 (4%)	35	73
23	C2	45/46 (98%)	42 (93%)	3 (7%)	20	56
23	D2	45/46 (98%)	40 (89%)	5 (11%)	8	30
24	C3	38/38 (100%)	35 (92%)	3 (8%)	15	49
24	D3	38/38 (100%)	36 (95%)	2 (5%)	28	65
25	C4	51/51 (100%)	47 (92%)	4 (8%)	16	50
25	D4	51/51 (100%)	47 (92%)	4 (8%)	16	50
26	C5	34/34 (100%)	33 (97%)	1 (3%)	50	82
26	D5	34/34 (100%)	34 (100%)	0	100	100
27	C0	48/48 (100%)	39 (81%)	9 (19%)	2	8
27	D0	49/48 (102%)	45 (92%)	4 (8%)	14	47
29	CC	216/216 (100%)	204 (94%)	12 (6%)	26	63
29	DC	216/216 (100%)	207 (96%)	9 (4%)	36	73
30	CD	164/164 (100%)	159 (97%)	5 (3%)	48	81
32	DD	163/163 (100%)	159 (98%)	4 (2%)	55	84
34	CE	165/165 (100%)	150 (91%)	15 (9%)	12	40
34	DE	165/165 (100%)	159 (96%)	6 (4%)	42	78
35	CF	148/148 (100%)	133 (90%)	15 (10%)	9	34
35	DF	148/148 (100%)	134 (90%)	14 (10%)	11	38
36	CG	137/137 (100%)	132 (96%)	5 (4%)	42	78
36	DG	137/137 (100%)	132 (96%)	5 (4%)	42	78
37	CH	114/114 (100%)	101 (89%)	13 (11%)	7	28
37	DH	114/114 (100%)	102 (90%)	12 (10%)	8	32
38	CJ	104/104 (100%)	99 (95%)	5 (5%)	31	69
38	DJ	104/104 (100%)	99 (95%)	5 (5%)	31	69
39	CK	116/116 (100%)	111 (96%)	5 (4%)	35	73
39	DK	116/116 (100%)	112 (97%)	4 (3%)	44	79
40	CL	103/104 (99%)	98 (95%)	5 (5%)	31	69
40	DL	104/104 (100%)	97 (93%)	7 (7%)	20	56
41	CM	103/103 (100%)	95 (92%)	8 (8%)	16	50
41	DM	103/103 (100%)	98 (95%)	5 (5%)	31	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	CN	108/108 (100%)	102 (94%)	6 (6%)	26	63
42	DN	109/108 (101%)	106 (97%)	3 (3%)	51	82
43	CO	100/102 (98%)	94 (94%)	6 (6%)	24	60
43	DO	102/102 (100%)	97 (95%)	5 (5%)	31	69
44	CP	86/87 (99%)	81 (94%)	5 (6%)	25	61
44	DP	87/87 (100%)	83 (95%)	4 (5%)	33	70
45	CQ	99/99 (100%)	94 (95%)	5 (5%)	29	66
45	DQ	99/99 (100%)	95 (96%)	4 (4%)	38	75
46	CR	89/89 (100%)	85 (96%)	4 (4%)	34	71
46	DR	89/89 (100%)	86 (97%)	3 (3%)	44	79
47	CS	84/84 (100%)	79 (94%)	5 (6%)	24	60
47	DS	84/84 (100%)	83 (99%)	1 (1%)	78	92
48	CT	93/93 (100%)	90 (97%)	3 (3%)	46	80
48	DT	93/93 (100%)	92 (99%)	1 (1%)	80	93
49	CU	80/80 (100%)	73 (91%)	7 (9%)	12	43
49	DU	80/80 (100%)	75 (94%)	5 (6%)	22	58
50	CV	83/83 (100%)	77 (93%)	6 (7%)	18	53
50	DV	83/83 (100%)	77 (93%)	6 (7%)	18	53
51	CW	78/78 (100%)	72 (92%)	6 (8%)	16	50
51	DW	78/78 (100%)	74 (95%)	4 (5%)	29	66
52	CX	56/58 (97%)	53 (95%)	3 (5%)	27	64
52	DX	58/58 (100%)	53 (91%)	5 (9%)	13	45
53	CY	67/67 (100%)	63 (94%)	4 (6%)	24	60
53	DY	67/67 (100%)	62 (92%)	5 (8%)	17	51
54	CZ	54/54 (100%)	51 (94%)	3 (6%)	26	63
54	DZ	54/54 (100%)	53 (98%)	1 (2%)	65	88
55	DI	103/103 (100%)	100 (97%)	3 (3%)	50	82
All	All	9461/9478 (100%)	8825 (93%)	636 (7%)	20	56

All (636) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	23	TRP

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Mol	Chain	Res	Type
2	AB	44	GLU
2	AB	57	LEU
2	AB	93	ASN
2	AB	105	LYS
2	AB	125	THR
2	AB	129	LEU
2	AB	135	LEU
2	AB	147	SER
2	AB	161	LEU
2	AB	168	HIS
2	AB	201	PRO
2	AB	205	ASP
2	AB	207	ILE
3	AC	3	GLN
3	AC	21	THR
3	AC	33	LEU
3	AC	75	ILE
3	AC	107	ARG
3	AC	128	VAL
3	AC	168	TYR
3	AC	178	LEU
3	AC	185	ASN
3	AC	186	THR
4	AD	17	THR
4	AD	22	LYS
4	AD	26	ARG
4	AD	48	LEU
4	AD	50	ASP
4	AD	142	VAL
4	AD	151	LYS
4	AD	194	ASP
5	AE	11	LEU
5	AE	14	LYS
5	AE	46	VAL
5	AE	76	LEU
5	AE	78	ASN
5	AE	81	LEU
5	AE	82	GLN
5	AE	88	VAL
5	AE	100	SER
5	AE	106	ILE
5	AE	123	VAL

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Mol	Chain	Res	Type
5	AE	126	LYS
5	AE	131	THR
5	AE	134	ILE
5	AE	137	VAL
5	AE	142	ASP
5	AE	149	SER
5	AE	159	LYS
5	AE	160	SER
5	AE	162	GLU
6	AF	39	LEU
6	AF	68	GLN
6	AF	69	GLU
6	AF	71	ILE
6	AF	72	ASP
6	AF	89	VAL
6	AF	93	LYS
7	AG	18	PHE
7	AG	30	LEU
7	AG	36	LYS
7	AG	58	GLU
7	AG	59	LEU
7	AG	63	GLU
7	AG	83	SER
7	AG	92	ARG
7	AG	95	ARG
7	AG	109	ARG
7	AG	120	LEU
7	AG	131	LYS
7	AG	133	THR
7	AG	142	HIS
8	AH	3	MET
8	AH	31	LYS
8	AH	38	ASN
8	AH	47	GLU
8	AH	54	ASP
8	AH	55	THR
8	AH	60	GLU
8	AH	63	LEU
8	AH	83	LEU
8	AH	90	ASP
8	AH	96	MET
8	AH	107	SER

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Mol	Chain	Res	Type
9	AI	11	ARG
9	AI	36	GLU
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	69	THR
10	AJ	88	MET
10	AJ	89	ARG
10	AJ	90	LEU
11	AK	55	SER
12	AL	3	THR
12	AL	24	LEU
12	AL	40	THR
12	AL	82	ILE
12	AL	110	ARG
12	AL	121	ARG
13	AM	3	ARG
13	AM	7	ILE
13	AM	13	LYS
13	AM	27	LYS
13	AM	48	LEU
13	AM	58	ASP
13	AM	71	ARG
13	AM	101	ARG
14	AN	31	ILE
14	AN	40	ASP
14	AN	69	ARG
15	AO	2	SER
15	AO	4	SER
15	AO	40	GLN
15	AO	70	LEU
15	AO	84	ARG
15	AO	88	ARG
15	AO	89	ARG
16	AP	18	GLN
17	AQ	5	ILE
17	AQ	16	LYS
17	AQ	38	ILE

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Mol	Chain	Res	Type
17	AQ	40	ARG
17	AQ	75	LEU
17	AQ	83	VAL
18	AR	47	THR
18	AR	66	SER
19	AS	5	LEU
19	AS	7	LYS
19	AS	11	ILE
19	AS	13	LEU
19	AS	27	ASP
19	AS	33	THR
19	AS	37	ARG
19	AS	63	THR
20	AT	5	LYS
20	AT	15	GLU
20	AT	24	ARG
20	AT	27	MET
20	AT	44	LYS
20	AT	48	GLN
20	AT	66	LEU
20	AT	85	LYS
21	AU	13	ASP
21	AU	16	LEU
21	AU	56	HIS
22	C1	40	ARG
23	C2	9	ILE
23	C2	46	HIS
23	C2	47	VAL
24	C3	1	MET
24	C3	24	THR
24	C3	34	ARG
25	C4	15	LYS
25	C4	31	HIS
25	C4	51	SER
25	C4	52	LYS
26	C5	26	ILE
27	C0	3	LYS
27	C0	4	THR
27	C0	5	ILE
27	C0	19	LYS
27	C0	25	LEU
27	C0	36	VAL

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Mol	Chain	Res	Type
27	C0	39	GLU
27	C0	45	ARG
27	C0	59	GLU
2	BB	44	GLU
2	BB	57	LEU
2	BB	93	ASN
2	BB	105	LYS
2	BB	125	THR
2	BB	129	LEU
2	BB	135	LEU
2	BB	147	SER
2	BB	161	LEU
2	BB	167	ASP
2	BB	168	HIS
2	BB	205	ASP
2	BB	207	ILE
3	BC	3	GLN
3	BC	21	THR
3	BC	33	LEU
3	BC	36	ASP
3	BC	37	PHE
3	BC	38	LYS
3	BC	75	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	17	THR
4	BD	22	LYS
4	BD	26	ARG
4	BD	47	ARG
4	BD	48	LEU
4	BD	50	ASP
4	BD	142	VAL
4	BD	151	LYS
4	BD	173	VAL
4	BD	194	ASP
5	BE	11	LEU
5	BE	14	LYS

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Mol	Chain	Res	Type
5	BE	22	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	105	ILE
5	BE	114	VAL
5	BE	115	LEU
5	BE	123	VAL
5	BE	126	LYS
5	BE	134	ILE
5	BE	137	VAL
5	BE	142	ASP
5	BE	149	SER
5	BE	151	GLU
5	BE	159	LYS
6	BF	14	GLN
6	BF	16	GLU
6	BF	39	LEU
6	BF	53	LYS
6	BF	68	GLN
6	BF	69	GLU
6	BF	71	ILE
6	BF	72	ASP
6	BF	89	VAL
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	58	GLU
7	BG	59	LEU
7	BG	63	GLU
7	BG	72	THR
7	BG	83	SER
7	BG	92	ARG
7	BG	95	ARG

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Mol	Chain	Res	Type
7	BG	109	ARG
7	BG	120	LEU
7	BG	131	LYS
7	BG	133	THR
7	BG	142	HIS
8	BH	3	MET
8	BH	38	ASN
8	BH	47	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	96	MET
8	BH	107	SER
9	BI	11	ARG
9	BI	36	GLU
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	59	LYS
10	BJ	62	ARG
10	BJ	63	ASP
10	BJ	78	GLU
10	BJ	89	ARG
10	BJ	90	LEU
10	BJ	91	ASP
11	BK	18	ASP
11	BK	22	HIS
11	BK	31	ILE
11	BK	38	GLN
11	BK	72	ASP
12	BL	3	THR
12	BL	24	LEU
12	BL	44	LYS
12	BL	49	LEU
12	BL	58	THR
12	BL	86	ARG

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Mol	Chain	Res	Type
12	BL	108	LYS
12	BL	110	ARG
12	BL	121	ARG
13	BM	11	ASP
13	BM	16	VAL
13	BM	27	LYS
13	BM	29	ARG
13	BM	48	LEU
13	BM	54	ASP
13	BM	101	ARG
14	BN	26	GLU
14	BN	69	ARG
15	BO	2	SER
15	BO	4	SER
15	BO	17	ARG
15	BO	40	GLN
15	BO	64	ARG
15	BO	66	LEU
15	BO	70	LEU
15	BO	84	ARG
15	BO	87	LEU
15	BO	88	ARG
16	BP	20	VAL
16	BP	36	VAL
16	BP	46	LYS
17	BQ	17	MET
17	BQ	21	ILE
17	BQ	26	GLU
17	BQ	38	ILE
17	BQ	51	ASN
17	BQ	67	LEU
17	BQ	75	LEU
19	BS	6	LYS
19	BS	7	LYS
19	BS	11	ILE
19	BS	13	LEU
19	BS	37	ARG
19	BS	63	THR
20	BT	12	ILE
20	BT	15	GLU
20	BT	48	GLN
20	BT	54	MET

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Mol	Chain	Res	Type
20	BT	58	VAL
20	BT	64	LYS
20	BT	66	LEU
20	BT	67	ILE
20	BT	69	LYS
20	BT	84	ASN
20	BT	85	LYS
21	BU	13	ASP
21	BU	16	LEU
21	BU	56	HIS
22	D1	26	THR
22	D1	55	ILE
23	D2	5	ILE
23	D2	9	ILE
23	D2	46	HIS
23	D2	47	VAL
23	D2	48	ILE
24	D3	1	MET
24	D3	24	THR
25	D4	8	ARG
25	D4	15	LYS
25	D4	31	HIS
25	D4	52	LYS
27	D0	10	THR
27	D0	19	LYS
27	D0	36	VAL
27	D0	39	GLU
29	CC	97	LYS
29	CC	117	GLN
29	CC	118	SER
29	CC	120	VAL
29	CC	130	LEU
29	CC	157	SER
29	CC	168	ASP
29	CC	192	LEU
29	CC	195	VAL
29	CC	204	VAL
29	CC	236	GLU
29	CC	258	ARG
30	CD	18	ASP
30	CD	32	ASN
30	CD	95	SER

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Mol	Chain	Res	Type
30	CD	138	LEU
30	CD	150	GLN
29	DC	43	ARG
29	DC	70	ASN
29	DC	97	LYS
29	DC	117	GLN
29	DC	118	SER
29	DC	120	VAL
29	DC	130	LEU
29	DC	192	LEU
29	DC	236	GLU
32	DD	18	ASP
32	DD	32	ASN
32	DD	95	SER
32	DD	138	LEU
34	CE	7	ASP
34	CE	12	LEU
34	CE	25	GLU
34	CE	44	ARG
34	CE	72	SER
34	CE	78	TRP
34	CE	80	SER
34	CE	83	VAL
34	CE	107	SER
34	CE	122	GLU
34	CE	127	GLU
34	CE	149	ILE
34	CE	152	GLU
34	CE	176	ASP
34	CE	189	THR
35	CF	35	THR
35	CF	36	LEU
35	CF	50	LEU
35	CF	57	LEU
35	CF	72	LYS
35	CF	80	ARG
35	CF	94	GLU
35	CF	117	LEU
35	CF	123	ASP
35	CF	134	GLU
35	CF	136	ILE
35	CF	141	ILE

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Mol	Chain	Res	Type
35	CF	149	VAL
35	CF	152	LEU
35	CF	174	ASP
36	CG	18	LYS
36	CG	72	LEU
36	CG	105	LEU
36	CG	127	THR
36	CG	155	GLU
37	CH	7	ASP
37	CH	15	LEU
37	CH	21	VAL
37	CH	44	ILE
37	CH	48	GLU
37	CH	51	ARG
37	CH	53	GLU
37	CH	55	GLU
37	CH	62	LEU
37	CH	75	LEU
37	CH	89	LYS
37	CH	127	GLU
37	CH	145	ASN
38	CJ	13	VAL
38	CJ	28	LEU
38	CJ	53	LEU
38	CJ	55	ILE
38	CJ	113	LYS
39	CK	5	THR
39	CK	45	THR
39	CK	90	GLU
39	CK	124	VAL
39	CK	142	ILE
40	CL	35	VAL
40	CL	49	ARG
40	CL	58	LEU
40	CL	70	ARG
40	CL	76	VAL
41	CM	33	ARG
41	CM	92	LEU
41	CM	94	THR
41	CM	100	ILE
41	CM	103	ILE
41	CM	107	PHE

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Mol	Chain	Res	Type
41	CM	115	GLU
41	CM	120	VAL
42	CN	6	ARG
42	CN	14	LYS
42	CN	20	LEU
42	CN	55	ARG
42	CN	59	ARG
42	CN	75	GLU
43	CO	2	ARG
43	CO	14	SER
43	CO	51	LEU
43	CO	53	THR
43	CO	71	ARG
43	CO	95	THR
44	CP	38	GLN
44	CP	45	SER
44	CP	48	LEU
44	CP	78	VAL
44	CP	115	LEU
45	CQ	39	ARG
45	CQ	65	SER
45	CQ	96	LYS
45	CQ	102	GLU
45	CQ	114	LEU
46	CR	5	LYS
46	CR	9	ILE
46	CR	51	ARG
46	CR	52	GLN
47	CS	12	HIS
47	CS	18	GLN
47	CS	46	GLU
47	CS	48	LYS
47	CS	51	VAL
48	CT	7	HIS
48	CT	29	VAL
48	CT	86	MET
49	CU	1	MET
49	CU	2	ILE
49	CU	3	ARG
49	CU	30	ILE
49	CU	69	ARG
49	CU	73	ARG

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Mol	Chain	Res	Type
49	CU	93	LEU
50	CV	9	ASP
50	CV	34	VAL
50	CV	61	LYS
50	CV	67	VAL
50	CV	81	ASP
50	CV	98	SER
51	CW	1	MET
51	CW	7	GLU
51	CW	10	LYS
51	CW	18	ARG
51	CW	61	LEU
51	CW	90	ASP
52	CX	39	ARG
52	CX	78	LYS
52	CX	82	ILE
53	CY	5	CYS
53	CY	25	THR
53	CY	35	SER
53	CY	71	LEU
54	CZ	18	LEU
54	CZ	19	LEU
54	CZ	58	ASN
34	DE	12	LEU
34	DE	80	SER
34	DE	107	SER
34	DE	127	GLU
34	DE	176	ASP
34	DE	189	THR
35	DF	10	ASP
35	DF	35	THR
35	DF	50	LEU
35	DF	57	LEU
35	DF	72	LYS
35	DF	94	GLU
35	DF	117	LEU
35	DF	120	LYS
35	DF	134	GLU
35	DF	136	ILE
35	DF	141	ILE
35	DF	149	VAL
35	DF	152	LEU

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Mol	Chain	Res	Type
35	DF	174	ASP
36	DG	18	LYS
36	DG	72	LEU
36	DG	105	LEU
36	DG	127	THR
36	DG	155	GLU
37	DH	7	ASP
37	DH	15	LEU
37	DH	44	ILE
37	DH	48	GLU
37	DH	53	GLU
37	DH	58	LEU
37	DH	60	GLU
37	DH	62	LEU
37	DH	75	LEU
37	DH	89	LYS
37	DH	127	GLU
37	DH	145	ASN
38	DJ	13	VAL
38	DJ	28	LEU
38	DJ	53	LEU
38	DJ	55	ILE
38	DJ	113	LYS
39	DK	45	THR
39	DK	101	ILE
39	DK	124	VAL
39	DK	142	ILE
40	DL	49	ARG
40	DL	58	LEU
40	DL	70	ARG
40	DL	108	ARG
40	DL	109	SER
40	DL	110	GLU
40	DL	123	LEU
41	DM	91	ASP
41	DM	92	LEU
41	DM	94	THR
41	DM	107	PHE
41	DM	120	VAL
42	DN	58	LYS
42	DN	75	GLU
42	DN	100	LYS

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Mol	Chain	Res	Type
43	DO	2	ARG
43	DO	14	SER
43	DO	51	LEU
43	DO	53	THR
43	DO	119	SER
44	DP	45	SER
44	DP	49	VAL
44	DP	78	VAL
44	DP	115	LEU
45	DQ	40	LEU
45	DQ	65	SER
45	DQ	96	LYS
45	DQ	102	GLU
46	DR	5	LYS
46	DR	9	ILE
46	DR	51	ARG
47	DS	38	VAL
48	DT	86	MET
49	DU	1	MET
49	DU	2	ILE
49	DU	3	ARG
49	DU	25	GLU
49	DU	74	ILE
50	DV	34	VAL
50	DV	52	LEU
50	DV	61	LYS
50	DV	67	VAL
50	DV	72	ILE
50	DV	81	ASP
51	DW	7	GLU
51	DW	53	LYS
51	DW	61	LEU
51	DW	90	ASP
52	DX	38	VAL
52	DX	39	ARG
52	DX	41[A]	ARG
52	DX	41[B]	ARG
52	DX	82	ILE
53	DY	5	CYS
53	DY	11	ARG
53	DY	25	THR
53	DY	35	SER

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Mol	Chain	Res	Type
53	DY	48	THR
54	DZ	19	LEU
55	DI	16	SER
55	DI	53	ARG
55	DI	60	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	93	ASN
2	AB	120	GLN
2	AB	177	ASN
2	AB	178	ASN
4	AD	136	GLN
6	AF	63	ASN
7	AG	97	ASN
8	AH	4	GLN
11	AK	101	ASN
16	AP	63	GLN
20	AT	48	GLN
22	C1	6	ASN
22	C1	42	HIS
27	C0	20	HIS
2	BB	39	HIS
2	BB	93	ASN
2	BB	120	GLN
2	BB	177	ASN
2	BB	178	ASN
5	BE	70	ASN
6	BF	3	HIS
6	BF	14	GLN
7	BG	97	ASN
8	BH	4	GLN
11	BK	101	ASN
16	BP	9	HIS
16	BP	63	GLN
17	BQ	51	ASN
20	BT	3	ASN
20	BT	78	ASN
29	CC	251	GLN
29	DC	251	GLN
35	CF	27	GLN

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Mol	Chain	Res	Type
36	CG	38	ASN
39	CK	138	GLN
43	CO	107	ASN
50	CV	74	ASN
54	CZ	45	GLN
34	DE	90	GLN
36	DG	116	GLN
37	DH	28	ASN
39	DK	47	HIS
50	DV	74	ASN
55	DI	88	HIS
55	DI	122	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	265 (17%)	38 (2%)
1	BA	1529/1534 (99%)	263 (17%)	44 (2%)
28	CB	117/120 (97%)	12 (10%)	0
28	DB	119/120 (99%)	12 (10%)	0
31	CA	2892/2904 (99%)	511 (17%)	94 (3%)
33	DA	2880/2903 (99%)	441 (15%)	72 (2%)
All	All	9067/9115 (99%)	1504 (16%)	248 (2%)

All (1504) 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	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	49	U
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	69	G

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Mol	Chain	Res	Type
1	AA	71	A
1	AA	72	A
1	AA	74	A
1	AA	80	A
1	AA	81	A
1	AA	82	G
1	AA	83	C
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	88	U
1	AA	89	U
1	AA	90	C
1	AA	92	U
1	AA	94	G
1	AA	95	C
1	AA	108	G
1	AA	116	A
1	AA	120	A
1	AA	127	G
1	AA	128	G
1	AA	130	A
1	AA	131	A
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	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	251	G

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Mol	Chain	Res	Type
1	AA	262	A
1	AA	266	G
1	AA	267	C
1	AA	281	G
1	AA	289	G
1	AA	321	A
1	AA	328	C
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	346	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	382	A
1	AA	384	G
1	AA	388	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	439	U
1	AA	451	A
1	AA	457	G
1	AA	458	U
1	AA	466	A
1	AA	467	U
1	AA	468	A
1	AA	474	G
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	505	G

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Mol	Chain	Res	Type
1	AA	509	A
1	AA	511	C
1	AA	524	G
1	AA	527	G7M
1	AA	528	C
1	AA	531	U
1	AA	533	A
1	AA	547	A
1	AA	559	A
1	AA	564	C
1	AA	568	G
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	596	A
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	675	A
1	AA	682	G
1	AA	687	A
1	AA	702	A
1	AA	703	G
1	AA	721	G
1	AA	723	U
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	764	C
1	AA	774	G
1	AA	777	A
1	AA	793	U
1	AA	794	A
1	AA	809	G
1	AA	814	A
1	AA	815	A
1	AA	817	C
1	AA	818	G

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Mol	Chain	Res	Type
1	AA	821	G
1	AA	828	U
1	AA	832	G
1	AA	836	G
1	AA	839	C
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	934	C
1	AA	935	A
1	AA	936	C
1	AA	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	987	G
1	AA	992	U
1	AA	993	G
1	AA	996	A
1	AA	1004	A
1	AA	1009	U
1	AA	1015	G
1	AA	1019	A
1	AA	1026	G
1	AA	1027	C
1	AA	1029	U
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	G
1	AA	1036	A
1	AA	1037	C
1	AA	1043	G
1	AA	1046	A
1	AA	1053	G

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Mol	Chain	Res	Type
1	AA	1054	C
1	AA	1065	U
1	AA	1066	C
1	AA	1086	U
1	AA	1094	G
1	AA	1095	U
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
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	1200	C
1	AA	1201	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

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Mol	Chain	Res	Type
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	1318	A
1	AA	1320	C
1	AA	1323	G
1	AA	1346	A
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1379	G
1	AA	1381	U
1	AA	1419	G
1	AA	1441	A
1	AA	1446	A
1	AA	1447	A
1	AA	1448	C
1	AA	1451	U
1	AA	1452	C
1	AA	1453	G
1	AA	1475	G
1	AA	1487	G
1	AA	1492	A
1	AA	1493	A
1	AA	1497	G
1	AA	1499	A
1	AA	1503	A
1	AA	1505	G
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1533	C
1	AA	1534	A
1	BA	4	U

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Mol	Chain	Res	Type
1	BA	5	U
1	BA	9	G
1	BA	22	G
1	BA	31	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
1	BA	116	A
1	BA	120	A
1	BA	127	G
1	BA	128	G
1	BA	130	A
1	BA	131	A
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

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Mol	Chain	Res	Type
1	BA	168	G
1	BA	177	G
1	BA	197	A
1	BA	200	G
1	BA	205	A
1	BA	210	C
1	BA	211	G
1	BA	212	G
1	BA	226	G
1	BA	240	G
1	BA	245	U
1	BA	247	G
1	BA	251	G
1	BA	262	A
1	BA	266	G
1	BA	267	C
1	BA	281	G
1	BA	289	G
1	BA	306	A
1	BA	321	A
1	BA	328	C
1	BA	329	A
1	BA	330	C
1	BA	332	G
1	BA	346	G
1	BA	352	C
1	BA	354	G
1	BA	367	U
1	BA	372	C
1	BA	373	A
1	BA	382	A
1	BA	384	G
1	BA	398	U
1	BA	406	G
1	BA	411	A
1	BA	412	A
1	BA	413	G
1	BA	421	U
1	BA	422	C
1	BA	424	G
1	BA	429	U
1	BA	451	A

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Mol	Chain	Res	Type
1	BA	457	G
1	BA	458	U
1	BA	467	U
1	BA	468	A
1	BA	474	G
1	BA	481	G
1	BA	484	G
1	BA	486	U
1	BA	495	A
1	BA	505	G
1	BA	509	A
1	BA	511	C
1	BA	524	G
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	560	A
1	BA	562	U
1	BA	564	C
1	BA	568	G
1	BA	572	A
1	BA	573	A
1	BA	576	C
1	BA	577	G
1	BA	596	A
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	675	A
1	BA	682	G
1	BA	687	A
1	BA	702	A
1	BA	703	G
1	BA	721	G
1	BA	723	U
1	BA	734	G

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Mol	Chain	Res	Type
1	BA	748	G
1	BA	755	G
1	BA	774	G
1	BA	777	A
1	BA	793	U
1	BA	794	A
1	BA	809	G
1	BA	814	A
1	BA	815	A
1	BA	817	C
1	BA	818	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	936	C
1	BA	960	U
1	BA	966	2MG
1	BA	969	A
1	BA	975	A
1	BA	976	G
1	BA	977	A
1	BA	987	G
1	BA	993	G
1	BA	996	A
1	BA	1004	A
1	BA	1008	U
1	BA	1009	U
1	BA	1015	G
1	BA	1019	A
1	BA	1026	G

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Mol	Chain	Res	Type
1	BA	1027	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	1086	U
1	BA	1094	G
1	BA	1095	U
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	1200	C
1	BA	1201	A
1	BA	1212	U
1	BA	1213	A
1	BA	1214	C
1	BA	1215	G

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Mol	Chain	Res	Type
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	1261	A
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	1318	A
1	BA	1320	C
1	BA	1323	G
1	BA	1346	A
1	BA	1353	G
1	BA	1362	A
1	BA	1363	A
1	BA	1370	G
1	BA	1379	G
1	BA	1381	U
1	BA	1398	A
1	BA	1419	G
1	BA	1441	A
1	BA	1446	A
1	BA	1447	A
1	BA	1448	C
1	BA	1451	U
1	BA	1452	C
1	BA	1453	G
1	BA	1475	G
1	BA	1487	G
1	BA	1494	G
1	BA	1497	G

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Mol	Chain	Res	Type
1	BA	1499	A
1	BA	1503	A
1	BA	1505	G
1	BA	1506	U
1	BA	1507	A
1	BA	1517	G
1	BA	1529	G
1	BA	1530	G
1	BA	1533	C
1	BA	1534	A
28	CB	9	G
28	CB	25	U
28	CB	35	C
28	CB	44	G
28	CB	45	A
28	CB	56	G
28	CB	57	A
28	CB	88	C
28	CB	89	U
28	CB	90	C
28	CB	99	A
28	CB	109	A
31	CA	10	A
31	CA	34	U
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	86	G
31	CA	101	A
31	CA	102	U
31	CA	118	A
31	CA	119	A
31	CA	120	U
31	CA	138	U

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Mol	Chain	Res	Type
31	CA	139	U
31	CA	140	C
31	CA	141	G
31	CA	142	A
31	CA	177	G
31	CA	178	G
31	CA	181	A
31	CA	196	A
31	CA	197	A
31	CA	215	G
31	CA	216	A
31	CA	221	A
31	CA	222	A
31	CA	248	G
31	CA	250	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	310	A
31	CA	311	A
31	CA	329	G
31	CA	330	A
31	CA	343	C
31	CA	345	A
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	387	U
31	CA	399	U
31	CA	403	U
31	CA	404	A
31	CA	405	U
31	CA	406	G
31	CA	411	G

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Mol	Chain	Res	Type
31	CA	412	A
31	CA	420	C
31	CA	424	G
31	CA	451	U
31	CA	454	A
31	CA	455	C
31	CA	456	C
31	CA	457	A
31	CA	480	A
31	CA	481	G
31	CA	491	G
31	CA	496	G
31	CA	501	A
31	CA	503	A
31	CA	504	A
31	CA	505	A
31	CA	508	A
31	CA	517	C
31	CA	526	A
31	CA	528	A
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	572	A
31	CA	573	U
31	CA	575	A
31	CA	586	A
31	CA	603	A
31	CA	613	A
31	CA	614	A
31	CA	615	U
31	CA	622	G
31	CA	627	A

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Mol	Chain	Res	Type
31	CA	634	C
31	CA	637	A
31	CA	645	C
31	CA	647	G
31	CA	653	U
31	CA	654	A
31	CA	655	A
31	CA	670	A
31	CA	684	G
31	CA	685	A
31	CA	686	U
31	CA	695	G
31	CA	696	G
31	CA	701	G
31	CA	702	U
31	CA	717	C
31	CA	730	A
31	CA	740	C
31	CA	746	PSU
31	CA	747	5MU
31	CA	764	A
31	CA	765	C
31	CA	775	G
31	CA	776	G
31	CA	782	A
31	CA	783	A
31	CA	784	G
31	CA	785	G
31	CA	792	A
31	CA	798	G
31	CA	800	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	856	G
31	CA	858	G

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Mol	Chain	Res	Type
31	CA	859	G
31	CA	866	A
31	CA	869	G
31	CA	878	A
31	CA	883	G
31	CA	896	A
31	CA	897	C
31	CA	907	G
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	971	G
31	CA	973	A
31	CA	974	G
31	CA	981	A
31	CA	983	A
31	CA	984	A
31	CA	985	C
31	CA	995	C
31	CA	996	A
31	CA	1005	C
31	CA	1012	U
31	CA	1013	C
31	CA	1022	G
31	CA	1026	G
31	CA	1033	U
31	CA	1040	A
31	CA	1045	C
31	CA	1046	A
31	CA	1047	G
31	CA	1051	G
31	CA	1061	U
31	CA	1062	G
31	CA	1069	A
31	CA	1070	A
31	CA	1073	A

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Mol	Chain	Res	Type
31	CA	1083	U
31	CA	1088	A
31	CA	1089	A
31	CA	1090	A
31	CA	1096	A
31	CA	1097	U
31	CA	1111	A
31	CA	1112	G
31	CA	1119	U
31	CA	1129	A
31	CA	1132	U
31	CA	1133	A
31	CA	1135	C
31	CA	1136	G
31	CA	1142	A
31	CA	1143	A
31	CA	1168	G
31	CA	1169	A
31	CA	1171	G
31	CA	1175	A
31	CA	1176	U
31	CA	1177	G
31	CA	1179	G
31	CA	1180	U
31	CA	1182	G
31	CA	1186	G
31	CA	1195	G
31	CA	1212	G
31	CA	1227	G
31	CA	1236	G
31	CA	1238	G
31	CA	1247	A
31	CA	1248	G
31	CA	1253	A
31	CA	1256	G
31	CA	1262	A
31	CA	1266	G
31	CA	1271	G
31	CA	1272	A
31	CA	1273	U
31	CA	1300	G
31	CA	1301	A

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Mol	Chain	Res	Type
31	CA	1306	C
31	CA	1312	U
31	CA	1313	U
31	CA	1320	C
31	CA	1321	A
31	CA	1328	A
31	CA	1329	U
31	CA	1341	G
31	CA	1344	U
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	1386	C
31	CA	1395	A
31	CA	1403	A
31	CA	1416	G
31	CA	1417	C
31	CA	1419	A
31	CA	1420	A
31	CA	1428	C
31	CA	1434	A
31	CA	1437	C
31	CA	1438	U
31	CA	1452	G
31	CA	1453	A
31	CA	1458	U
31	CA	1460	U
31	CA	1482	G
31	CA	1490	A
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	1522	A
31	CA	1523	U
31	CA	1532	A
31	CA	1534	U

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Mol	Chain	Res	Type
31	CA	1535	A
31	CA	1536	C
31	CA	1537	G
31	CA	1565	C
31	CA	1569	A
31	CA	1578	U
31	CA	1583	A
31	CA	1584	U
31	CA	1585	C
31	CA	1607	C
31	CA	1608	A
31	CA	1609	A
31	CA	1610	A
31	CA	1616	A
31	CA	1617	C
31	CA	1647	U
31	CA	1648	U
31	CA	1649	G
31	CA	1660	G
31	CA	1674	G
31	CA	1675	C
31	CA	1694	C
31	CA	1695	G
31	CA	1703	G
31	CA	1715	G
31	CA	1729	U
31	CA	1730	C
31	CA	1732	C
31	CA	1738	G
31	CA	1744	A
31	CA	1750	G
31	CA	1758	U
31	CA	1764	C
31	CA	1773	A
31	CA	1782	U
31	CA	1786	A
31	CA	1800	C
31	CA	1801	A
31	CA	1808	A
31	CA	1816	C
31	CA	1826	G
31	CA	1828	G

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Mol	Chain	Res	Type
31	CA	1829	A
31	CA	1833	C
31	CA	1834	U
31	CA	1839	G
31	CA	1869	G
31	CA	1870	C
31	CA	1871	A
31	CA	1872	A
31	CA	1873	G
31	CA	1889	A
31	CA	1900	A
31	CA	1901	A
31	CA	1903	G
31	CA	1906	G
31	CA	1907	G
31	CA	1914	C
31	CA	1929	G
31	CA	1930	G
31	CA	1931	U
31	CA	1937	A
31	CA	1938	A
31	CA	1955	U
31	CA	1967	C
31	CA	1970	A
31	CA	1972	G
31	CA	1991	U
31	CA	1993	U
31	CA	1997	C
31	CA	2022	U
31	CA	2023	C
31	CA	2033	A
31	CA	2035	G
31	CA	2036	C
31	CA	2043	C
31	CA	2049	G
31	CA	2051	A
31	CA	2055	C
31	CA	2056	G
31	CA	2060	A
31	CA	2061	G
31	CA	2062	A
31	CA	2069	G7M

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Mol	Chain	Res	Type
31	CA	2072	C
31	CA	2080	A
31	CA	2093	G
31	CA	2095	A
31	CA	2100	G
31	CA	2108	A
31	CA	2110	G
31	CA	2111	U
31	CA	2112	G
31	CA	2113	U
31	CA	2115	G
31	CA	2117	A
31	CA	2118	U
31	CA	2119	A
31	CA	2124	G
31	CA	2125	G
31	CA	2126	A
31	CA	2127	G
31	CA	2128	G
31	CA	2131	U
31	CA	2132	U
31	CA	2133	G
31	CA	2146	C
31	CA	2147	A
31	CA	2157	G
31	CA	2158	A
31	CA	2159	G
31	CA	2160	C
31	CA	2162	G
31	CA	2164	C
31	CA	2165	C
31	CA	2171	A
31	CA	2172	U
31	CA	2173	A
31	CA	2174	C
31	CA	2178	C
31	CA	2183	A
31	CA	2190	G
31	CA	2195	U
31	CA	2198	A
31	CA	2203	U
31	CA	2204	G

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Mol	Chain	Res	Type
31	CA	2211	A
31	CA	2225	A
31	CA	2226	C
31	CA	2238	G
31	CA	2239	G
31	CA	2259	U
31	CA	2268	A
31	CA	2278	A
31	CA	2279	G
31	CA	2280	G
31	CA	2282	G
31	CA	2283	C
31	CA	2287	A
31	CA	2288	A
31	CA	2305	U
31	CA	2311	A
31	CA	2322	A
31	CA	2326	C
31	CA	2327	A
31	CA	2331	G
31	CA	2333	A
31	CA	2335	A
31	CA	2343	U
31	CA	2345	G
31	CA	2347	C
31	CA	2350	C
31	CA	2354	C
31	CA	2357	G
31	CA	2361	G
31	CA	2383	G
31	CA	2385	C
31	CA	2388	A
31	CA	2393	U
31	CA	2402	U
31	CA	2403	C
31	CA	2406	A
31	CA	2410	G
31	CA	2424	C
31	CA	2425	A
31	CA	2426	A
31	CA	2429	G
31	CA	2430	A

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Mol	Chain	Res	Type
31	CA	2435	A
31	CA	2436	G
31	CA	2441	U
31	CA	2448	A
31	CA	2465	C
31	CA	2476	A
31	CA	2484	G
31	CA	2491	U
31	CA	2494	G
31	CA	2498	OMC
31	CA	2502	G
31	CA	2505	G
31	CA	2518	A
31	CA	2520	C
31	CA	2529	G
31	CA	2547	A
31	CA	2549	G
31	CA	2554	U
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	2599	G
31	CA	2603	G
31	CA	2606	C
31	CA	2609	U
31	CA	2613	U
31	CA	2629	U
31	CA	2630	G
31	CA	2634	A
31	CA	2645	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	2693	G
31	CA	2714	G

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Mol	Chain	Res	Type
31	CA	2726	A
31	CA	2727	A
31	CA	2733	A
31	CA	2739	U
31	CA	2744	G
31	CA	2748	A
31	CA	2751	G
31	CA	2762	C
31	CA	2769	U
31	CA	2776	A
31	CA	2777	G
31	CA	2778	A
31	CA	2779	U
31	CA	2791	G
31	CA	2794	C
31	CA	2799	A
31	CA	2820	A
31	CA	2825	G
31	CA	2835	A
31	CA	2836	U
31	CA	2849	U
31	CA	2850	A
31	CA	2861	U
31	CA	2867	G
31	CA	2877	G
31	CA	2883	A
31	CA	2886	A
31	CA	2891	U
31	CA	2903	U
28	DB	9	G
28	DB	25	U
28	DB	35	C
28	DB	44	G
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
28	DB	120	U
33	DA	10	A

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Mol	Chain	Res	Type
33	DA	12	U
33	DA	13	A
33	DA	34	U
33	DA	46	G
33	DA	51	G
33	DA	58	G
33	DA	63	A
33	DA	71	A
33	DA	74	A
33	DA	75	G
33	DA	80	G
33	DA	84	A
33	DA	86	G
33	DA	101	A
33	DA	102	U
33	DA	118	A
33	DA	119	A
33	DA	120	U
33	DA	138	U
33	DA	139	U
33	DA	140	C
33	DA	141	G
33	DA	142	A
33	DA	196	A
33	DA	199	A
33	DA	200	U
33	DA	215	G
33	DA	216	A
33	DA	221	A
33	DA	222	A
33	DA	248	G
33	DA	265	A
33	DA	266	G
33	DA	272	A
33	DA	276	U
33	DA	277	G
33	DA	278	A
33	DA	302	C
33	DA	308	G
33	DA	310	A
33	DA	311	A
33	DA	312	G

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Mol	Chain	Res	Type
33	DA	329	G
33	DA	330	A
33	DA	343	C
33	DA	345	A
33	DA	346	A
33	DA	352	A
33	DA	353	C
33	DA	362	A
33	DA	370	G
33	DA	372	G
33	DA	386	G
33	DA	387	U
33	DA	399	U
33	DA	403	U
33	DA	406	G
33	DA	411	G
33	DA	412	A
33	DA	420	C
33	DA	424	G
33	DA	451	U
33	DA	454	A
33	DA	455	C
33	DA	456	C
33	DA	459	U
33	DA	460	A
33	DA	480	A
33	DA	481	G
33	DA	491	G
33	DA	496	G
33	DA	503	A
33	DA	504	A
33	DA	505	A
33	DA	508	A
33	DA	518	G
33	DA	531	C
33	DA	532	A
33	DA	533	G
33	DA	543	G
33	DA	544	C
33	DA	546	U
33	DA	547	A
33	DA	548	G

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Mol	Chain	Res	Type
33	DA	549	G
33	DA	550	C
33	DA	551	G
33	DA	563	A
33	DA	573	U
33	DA	575	A
33	DA	586	A
33	DA	603	A
33	DA	613	A
33	DA	614	A
33	DA	615	U
33	DA	627	A
33	DA	634	C
33	DA	637	A
33	DA	645	C
33	DA	647	G
33	DA	653	U
33	DA	654	A
33	DA	655	A
33	DA	686	U
33	DA	687	C
33	DA	702	U
33	DA	717	C
33	DA	730	A
33	DA	747	5MU
33	DA	758	C
33	DA	764	A
33	DA	765	C
33	DA	775	G
33	DA	776	G
33	DA	782	A
33	DA	784	G
33	DA	785	G
33	DA	790	U
33	DA	792	A
33	DA	802	A
33	DA	805	G
33	DA	812	C
33	DA	827	U
33	DA	828	U
33	DA	858	G
33	DA	859	G

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Mol	Chain	Res	Type
33	DA	866	A
33	DA	870	U
33	DA	878	A
33	DA	883	G
33	DA	885	C
33	DA	896	A
33	DA	897	C
33	DA	910	A
33	DA	915	C
33	DA	931	U
33	DA	932	U
33	DA	946	C
33	DA	961	C
33	DA	974	G
33	DA	983	A
33	DA	984	A
33	DA	985	C
33	DA	996	A
33	DA	1005	C
33	DA	1012	U
33	DA	1013	C
33	DA	1022	G
33	DA	1023	U
33	DA	1026	G
33	DA	1033	U
33	DA	1040	A
33	DA	1047	G
33	DA	1061	U
33	DA	1062	G
33	DA	1069	A
33	DA	1070	A
33	DA	1073	A
33	DA	1083	U
33	DA	1088	A
33	DA	1090	A
33	DA	1096	A
33	DA	1097	U
33	DA	1112	G
33	DA	1128	G
33	DA	1129	A
33	DA	1130	U
33	DA	1132	U

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Mol	Chain	Res	Type
33	DA	1133	A
33	DA	1135	C
33	DA	1136	G
33	DA	1142	A
33	DA	1168	G
33	DA	1172	C
33	DA	1174	U
33	DA	1176	U
33	DA	1177	G
33	DA	1180	U
33	DA	1182	G
33	DA	1210	G
33	DA	1227	G
33	DA	1238	G
33	DA	1253	A
33	DA	1256	G
33	DA	1271	G
33	DA	1272	A
33	DA	1273	U
33	DA	1284	A
33	DA	1300	G
33	DA	1301	A
33	DA	1306	C
33	DA	1321	A
33	DA	1329	U
33	DA	1341	G
33	DA	1352	U
33	DA	1365	A
33	DA	1376	C
33	DA	1379	U
33	DA	1380	G
33	DA	1383	A
33	DA	1386	C
33	DA	1403	A
33	DA	1416	G
33	DA	1417	C
33	DA	1420	A
33	DA	1427	A
33	DA	1428	C
33	DA	1434	A
33	DA	1452	G
33	DA	1453	A

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Mol	Chain	Res	Type
33	DA	1458	U
33	DA	1460	U
33	DA	1482	G
33	DA	1490	A
33	DA	1493	C
33	DA	1494	A
33	DA	1497	U
33	DA	1508	A
33	DA	1509	A
33	DA	1510	G
33	DA	1515	A
33	DA	1523	U
33	DA	1532	A
33	DA	1534	U
33	DA	1535	A
33	DA	1536	C
33	DA	1537	G
33	DA	1569	A
33	DA	1578	U
33	DA	1583	A
33	DA	1584	U
33	DA	1585	C
33	DA	1607	C
33	DA	1608	A
33	DA	1609	A
33	DA	1610	A
33	DA	1616	A
33	DA	1639	C
33	DA	1647	U
33	DA	1648	U
33	DA	1649	G
33	DA	1660	G
33	DA	1674	G
33	DA	1694	C
33	DA	1715	G
33	DA	1729	U
33	DA	1730	C
33	DA	1732	C
33	DA	1738	G
33	DA	1744	A
33	DA	1758	U
33	DA	1764	C

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Mol	Chain	Res	Type
33	DA	1773	A
33	DA	1782	U
33	DA	1800	C
33	DA	1801	A
33	DA	1808	A
33	DA	1816	C
33	DA	1826	G
33	DA	1869	G
33	DA	1870	C
33	DA	1871	A
33	DA	1872	A
33	DA	1873	G
33	DA	1900	A
33	DA	1906	G
33	DA	1907	G
33	DA	1913	A
33	DA	1914	C
33	DA	1929	G
33	DA	1930	G
33	DA	1931	U
33	DA	1937	A
33	DA	1938	A
33	DA	1939	5MU
33	DA	1955	U
33	DA	1965	C
33	DA	1967	C
33	DA	1970	A
33	DA	1972	G
33	DA	1991	U
33	DA	1993	U
33	DA	1997	C
33	DA	2018	G
33	DA	2023	C
33	DA	2028	U
33	DA	2031	A
33	DA	2033	A
33	DA	2043	C
33	DA	2049	G
33	DA	2055	C
33	DA	2056	G
33	DA	2060	A
33	DA	2061	G

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Mol	Chain	Res	Type
33	DA	2062	A
33	DA	2069	G7M
33	DA	2080	A
33	DA	2093	G
33	DA	2097	A
33	DA	2100	G
33	DA	2105	U
33	DA	2111	U
33	DA	2112	G
33	DA	2113	U
33	DA	2116	G
33	DA	2117	A
33	DA	2118	U
33	DA	2119	A
33	DA	2120	G
33	DA	2123	G
33	DA	2125	G
33	DA	2126	A
33	DA	2128	G
33	DA	2131	U
33	DA	2132	U
33	DA	2133	G
33	DA	2134	A
33	DA	2135	A
33	DA	2145	C
33	DA	2146	C
33	DA	2148	G
33	DA	2158	A
33	DA	2159	G
33	DA	2160	C
33	DA	2161	C
33	DA	2162	G
33	DA	2163	A
33	DA	2164	C
33	DA	2165	C
33	DA	2167	U
33	DA	2168	G
33	DA	2169	A
33	DA	2170	A
33	DA	2171	A
33	DA	2172	U
33	DA	2173	A

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Mol	Chain	Res	Type
33	DA	2178	C
33	DA	2179	C
33	DA	2181	U
33	DA	2183	A
33	DA	2185	U
33	DA	2186	G
33	DA	2190	G
33	DA	2195	U
33	DA	2198	A
33	DA	2203	U
33	DA	2204	G
33	DA	2211	A
33	DA	2225	A
33	DA	2238	G
33	DA	2239	G
33	DA	2243	U
33	DA	2268	A
33	DA	2279	G
33	DA	2280	G
33	DA	2283	C
33	DA	2286	G
33	DA	2287	A
33	DA	2288	A
33	DA	2305	U
33	DA	2308	G
33	DA	2322	A
33	DA	2325	G
33	DA	2331	G
33	DA	2333	A
33	DA	2335	A
33	DA	2345	G
33	DA	2347	C
33	DA	2354	C
33	DA	2357	G
33	DA	2383	G
33	DA	2385	C
33	DA	2393	U
33	DA	2402	U
33	DA	2403	C
33	DA	2406	A
33	DA	2407	A
33	DA	2410	G

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Mol	Chain	Res	Type
33	DA	2423	U
33	DA	2424	C
33	DA	2425	A
33	DA	2435	A
33	DA	2441	U
33	DA	2445	2MG
33	DA	2448	A
33	DA	2476	A
33	DA	2484	G
33	DA	2491	U
33	DA	2494	G
33	DA	2502	G
33	DA	2505	G
33	DA	2518	A
33	DA	2529	G
33	DA	2547	A
33	DA	2566	A
33	DA	2567	G
33	DA	2573	C
33	DA	2585	U
33	DA	2586	U
33	DA	2603	G
33	DA	2609	U
33	DA	2613	U
33	DA	2623	G
33	DA	2629	U
33	DA	2630	G
33	DA	2634	A
33	DA	2661	G
33	DA	2663	G
33	DA	2682	A
33	DA	2689	U
33	DA	2690	U
33	DA	2691	C
33	DA	2714	G
33	DA	2718	G
33	DA	2719	G
33	DA	2720	U
33	DA	2726	A
33	DA	2733	A
33	DA	2739	U
33	DA	2744	G

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Mol	Chain	Res	Type
33	DA	2748	A
33	DA	2751	G
33	DA	2762	C
33	DA	2765	A
33	DA	2778	A
33	DA	2791	G
33	DA	2798	U
33	DA	2799	A
33	DA	2820	A
33	DA	2821	A
33	DA	2823	A
33	DA	2825	G
33	DA	2835	A
33	DA	2836	U
33	DA	2861	U
33	DA	2867	G
33	DA	2877	G
33	DA	2883	A
33	DA	2891	U
33	DA	2903	U

All (248) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	7	A
1	AA	30	U
1	AA	70	U
1	AA	88	U
1	AA	89	U
1	AA	181	A
1	AA	209	U
1	AA	281	G
1	AA	305	G
1	AA	367	U
1	AA	413	G
1	AA	422	C
1	AA	438	U
1	AA	485	U
1	AA	653	U
1	AA	702	A
1	AA	733	G

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Mol	Chain	Res	Type
1	AA	793	U
1	AA	841	C
1	AA	872	A
1	AA	884	U
1	AA	992	U
1	AA	1086	U
1	AA	1094	G
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1224	U
1	AA	1225	A
1	AA	1281	C
1	AA	1299	A
1	AA	1319	A
1	AA	1380	U
1	AA	1397	C
1	AA	1447	A
1	AA	1452	C
1	BA	5	U
1	BA	7	A
1	BA	30	U
1	BA	70	U
1	BA	86	G
1	BA	89	U
1	BA	181	A
1	BA	209	U
1	BA	246	A
1	BA	281	G
1	BA	305	G
1	BA	367	U
1	BA	411	A
1	BA	422	C
1	BA	438	U
1	BA	485	U
1	BA	559	A
1	BA	561	U
1	BA	653	U
1	BA	702	A
1	BA	733	G
1	BA	793	U

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Mol	Chain	Res	Type
1	BA	842	U
1	BA	872	A
1	BA	884	U
1	BA	992	U
1	BA	1008	U
1	BA	1086	U
1	BA	1094	G
1	BA	1137	C
1	BA	1139	G
1	BA	1140	C
1	BA	1141	C
1	BA	1224	U
1	BA	1225	A
1	BA	1281	C
1	BA	1299	A
1	BA	1319	A
1	BA	1362	A
1	BA	1363	A
1	BA	1380	U
1	BA	1447	A
1	BA	1452	C
1	BA	1493	A
31	CA	33	C
31	CA	62	U
31	CA	83	A
31	CA	138	U
31	CA	139	U
31	CA	141	G
31	CA	177	G
31	CA	196	A
31	CA	199	A
31	CA	228	C
31	CA	271	G
31	CA	278	A
31	CA	310	A
31	CA	345	A
31	CA	361	G
31	CA	386	G
31	CA	387	U
31	CA	403	U
31	CA	404	A
31	CA	411	G

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Mol	Chain	Res	Type
31	CA	455	C
31	CA	503	A
31	CA	506	G
31	CA	527	C
31	CA	555	G
31	CA	620	G
31	CA	684	G
31	CA	685	A
31	CA	764	A
31	CA	784	G
31	CA	846	U
31	CA	913	U
31	CA	961	C
31	CA	973	A
31	CA	980	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	1133	A
31	CA	1141	U
31	CA	1253	A
31	CA	1288	G
31	CA	1300	G
31	CA	1320	C
31	CA	1329	U
31	CA	1379	U
31	CA	1396	U
31	CA	1452	G
31	CA	1490	A
31	CA	1497	U
31	CA	1509	A
31	CA	1535	A
31	CA	1536	C
31	CA	1607	C
31	CA	1609	A
31	CA	1647	U

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Mol	Chain	Res	Type
31	CA	1730	C
31	CA	1786	A
31	CA	1800	C
31	CA	1818	U
31	CA	1870	C
31	CA	1871	A
31	CA	1900	A
31	CA	1966	A
31	CA	2035	G
31	CA	2043	C
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	2517	C
31	CA	2645	G
31	CA	2680	U
31	CA	2681	C
31	CA	2778	A
31	CA	2779	U
31	CA	2790	U
31	CA	2849	U
31	CA	2873	A
31	CA	2893	A
33	DA	62	U
33	DA	101	A
33	DA	138	U
33	DA	141	G
33	DA	177	G
33	DA	196	A
33	DA	199	A
33	DA	228	C
33	DA	271	G
33	DA	278	A

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Mol	Chain	Res	Type
33	DA	310	A
33	DA	345	A
33	DA	370	G
33	DA	387	U
33	DA	403	U
33	DA	455	C
33	DA	503	A
33	DA	532	A
33	DA	620	G
33	DA	764	A
33	DA	784	G
33	DA	961	C
33	DA	984	A
33	DA	1046	A
33	DA	1061	U
33	DA	1069	A
33	DA	1070	A
33	DA	1089	A
33	DA	1128	G
33	DA	1133	A
33	DA	1141	U
33	DA	1171	G
33	DA	1175	A
33	DA	1253	A
33	DA	1286	A
33	DA	1288	G
33	DA	1300	G
33	DA	1396	U
33	DA	1490	A
33	DA	1497	U
33	DA	1509	A
33	DA	1523	U
33	DA	1535	A
33	DA	1536	C
33	DA	1565	C
33	DA	1607	C
33	DA	1609	A
33	DA	1647	U
33	DA	1730	C
33	DA	1800	C
33	DA	1870	C
33	DA	1871	A

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Mol	Chain	Res	Type
33	DA	1939	5MU
33	DA	2097	A
33	DA	2119	A
33	DA	2127	G
33	DA	2146	C
33	DA	2157	G
33	DA	2158	A
33	DA	2164	C
33	DA	2282	G
33	DA	2286	G
33	DA	2311	A
33	DA	2406	A
33	DA	2423	U
33	DA	2585	U
33	DA	2778	A
33	DA	2779	U
33	DA	2790	U
33	DA	2798	U
33	DA	2849	U
33	DA	2873	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	2MG	AA	1207	1	18,26,27	1.04	1 (5%)	21,38,41	2.60	4 (19%)
1	4OC	AA	1402	1	15,23,24	0.75	0	21,32,35	1.48	2 (9%)
1	5MC	AA	1407	1	14,22,23	0.85	1 (7%)	17,32,35	0.75	1 (5%)
1	UR3	AA	1498	1	13,22,23	0.87	1 (7%)	18,32,35	0.56	0
1	2MG	AA	1516	1	18,26,27	1.14	2 (11%)	21,38,41	2.45	4 (19%)
1	MA6	AA	1518	1	18,26,27	0.61	0	15,38,41	0.57	0
1	MA6	AA	1519	1	18,26,27	0.72	0	15,38,41	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	AA	516	1,56	15,21,22	1.18	2 (13%)	16,30,33	3.46	1 (6%)
1	G7M	AA	527	1	18,26,27	1.07	2 (11%)	21,39,42	3.48	5 (23%)
1	2MG	AA	966	1	18,26,27	1.21	2 (11%)	21,38,41	2.55	3 (14%)
1	5MC	AA	967	1	14,22,23	0.85	1 (7%)	17,32,35	0.65	1 (5%)
12	D2T	AL	89	12	4,9,10	0.45	0	4,11,13	1.35	0
1	2MG	BA	1207	1	18,26,27	1.08	1 (5%)	21,38,41	2.58	4 (19%)
1	4OC	BA	1402	1	15,23,24	0.79	0	21,32,35	1.43	2 (9%)
1	5MC	BA	1407	1	14,22,23	0.91	1 (7%)	17,32,35	0.72	1 (5%)
1	UR3	BA	1498	1	13,22,23	1.03	1 (7%)	18,32,35	0.63	0
1	2MG	BA	1516	1	18,26,27	1.12	1 (5%)	21,38,41	2.47	4 (19%)
1	MA6	BA	1518	1	18,26,27	0.60	0	15,38,41	0.56	0
1	MA6	BA	1519	1	18,26,27	0.68	0	15,38,41	0.72	0
1	PSU	BA	516	1	15,21,22	1.17	2 (13%)	16,30,33	3.46	1 (6%)
1	G7M	BA	527	1	18,26,27	1.00	1 (5%)	21,39,42	3.70	6 (28%)
1	2MG	BA	966	1	18,26,27	1.13	2 (11%)	21,38,41	2.56	4 (19%)
1	5MC	BA	967	1	14,22,23	0.87	1 (7%)	17,32,35	0.65	1 (5%)
12	D2T	BL	89	12	4,9,10	0.68	0	4,11,13	1.35	0
31	6MZ	CA	1618	31	17,25,26	0.70	0	15,36,39	0.75	1 (6%)
31	2MG	CA	1835	31	18,26,27	1.11	1 (5%)	21,38,41	2.50	4 (19%)
31	PSU	CA	1911	31	15,21,22	1.17	2 (13%)	16,30,33	3.48	2 (12%)
31	3TD	CA	1915	31	15,22,23	1.02	2 (13%)	17,32,35	0.99	1 (5%)
31	PSU	CA	1917	31	15,21,22	1.18	2 (13%)	16,30,33	3.52	1 (6%)
31	5MU	CA	1939	31	13,22,23	1.12	1 (7%)	16,32,35	4.77	3 (18%)
31	5MC	CA	1962	31	14,22,23	0.75	1 (7%)	17,32,35	0.66	1 (5%)
31	6MZ	CA	2030	31	17,25,26	0.77	0	15,36,39	0.81	1 (6%)
31	G7M	CA	2069	31	18,26,27	0.94	1 (5%)	21,39,42	3.57	5 (23%)
31	OMG	CA	2251	31	18,26,27	1.25	2 (11%)	21,38,41	2.84	4 (19%)
31	2MG	CA	2445	31	18,26,27	1.13	2 (11%)	21,38,41	2.62	4 (19%)
31	PSU	CA	2457	31	15,21,22	1.28	3 (20%)	16,30,33	3.51	2 (12%)
31	OMC	CA	2498	31,56	15,22,23	0.83	0	20,31,34	0.51	0
31	2MA	CA	2503	31	17,25,26	0.82	0	18,37,40	1.17	3 (16%)
31	PSU	CA	2504	31	15,21,22	1.20	2 (13%)	16,30,33	3.52	2 (12%)
31	OMU	CA	2552	31	14,22,23	1.28	2 (14%)	19,31,34	2.92	2 (10%)
31	PSU	CA	2580	31	15,21,22	1.24	2 (13%)	16,30,33	3.51	2 (12%)
31	PSU	CA	2605	31	15,21,22	1.17	2 (13%)	16,30,33	3.51	1 (6%)
31	1MG	CA	745	31	17,26,27	1.07	1 (5%)	19,39,42	1.04	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PSU	CA	746	31,56	15,21,22	1.32	2 (13%)	16,30,33	3.55	2 (12%)
31	5MU	CA	747	31	13,22,23	1.08	1 (7%)	16,32,35	4.74	3 (18%)
31	PSU	CA	955	31	15,21,22	1.12	2 (13%)	16,30,33	3.47	1 (6%)
42	4D4	CN	81	42	7,11,12	0.72	0	5,13,15	0.95	0
33	6MZ	DA	1618	33	17,25,26	0.72	0	15,36,39	0.93	1 (6%)
33	2MG	DA	1835	33	18,26,27	1.08	1 (5%)	21,38,41	2.51	4 (19%)
33	PSU	DA	1911	33	15,21,22	1.17	2 (13%)	16,30,33	3.46	2 (12%)
33	3TD	DA	1915	33	15,22,23	0.97	1 (6%)	17,32,35	1.03	1 (5%)
33	PSU	DA	1917	33	15,21,22	1.28	2 (13%)	16,30,33	3.49	1 (6%)
33	5MU	DA	1939	33	13,22,23	1.29	3 (23%)	16,32,35	4.78	3 (18%)
33	5MC	DA	1962	33	14,22,23	0.78	1 (7%)	17,32,35	0.71	1 (5%)
33	6MZ	DA	2030	33	17,25,26	0.93	1 (5%)	15,36,39	0.94	1 (6%)
33	G7M	DA	2069	33	18,26,27	1.07	1 (5%)	21,39,42	3.21	5 (23%)
33	OMG	DA	2251	33	18,26,27	0.99	1 (5%)	21,38,41	2.66	4 (19%)
33	2MG	DA	2445	33	18,26,27	1.10	1 (5%)	21,38,41	2.53	4 (19%)
33	H2U	DA	2449	33	17,21,22	0.72	0	23,30,33	0.44	0
33	PSU	DA	2457	33	15,21,22	1.25	2 (13%)	16,30,33	3.48	2 (12%)
33	OMC	DA	2498	33,56	15,22,23	0.91	1 (6%)	20,31,34	0.53	0
33	2MA	DA	2503	33,56	17,25,26	0.84	0	18,37,40	1.27	4 (22%)
33	PSU	DA	2504	33	15,21,22	1.36	3 (20%)	16,30,33	3.49	1 (6%)
33	OMU	DA	2552	33	14,22,23	1.17	2 (14%)	19,31,34	2.92	2 (10%)
33	PSU	DA	2580	33	15,21,22	1.35	2 (13%)	16,30,33	3.49	2 (12%)
33	PSU	DA	2604	33	15,21,22	1.20	2 (13%)	16,30,33	3.57	2 (12%)
33	PSU	DA	2605	33	15,21,22	1.12	2 (13%)	16,30,33	3.50	1 (6%)
33	1MG	DA	745	33	17,26,27	1.08	1 (5%)	19,39,42	1.00	2 (10%)
33	PSU	DA	746	33,56	15,21,22	1.72	5 (33%)	16,30,33	3.54	2 (12%)
33	5MU	DA	747	33	13,22,23	1.12	1 (7%)	16,32,35	4.77	3 (18%)
33	PSU	DA	955	33	15,21,22	1.28	2 (13%)	16,30,33	3.46	1 (6%)
32	MEQ	DD	150[A]	32	7,9,10	0.37	0	8,10,12	1.50	2 (25%)
32	MEQ	DD	150[B]	32	7,9,10	1.31	1 (14%)	8,10,12	1.70	2 (25%)
42	4D4	DN	81[A]	-	7,11,12	0.58	0	5,13,15	1.12	0
42	4D4	DN	81[B]	-	7,11,12	0.80	0	5,13,15	0.91	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	AA	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	AA	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	AA	516	1,56	-	0/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	0/3/25/26	0/3/3/3
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
1	5MC	AA	967	1	-	0/3/25/26	0/2/2/2
12	D2T	AL	89	12	-	0/2/12/14	0/0/0/0
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	BA	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	BA	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	BA	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	BA	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	BA	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
1	G7M	BA	527	1	-	0/3/25/26	0/3/3/3
1	2MG	BA	966	1	-	0/5/27/28	0/3/3/3
1	5MC	BA	967	1	-	0/3/25/26	0/2/2/2
12	D2T	BL	89	12	-	0/2/12/14	0/0/0/0
31	6MZ	CA	1618	31	-	0/5/27/28	0/3/3/3
31	2MG	CA	1835	31	-	0/5/27/28	0/3/3/3
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
31	5MU	CA	1939	31	-	0/3/25/26	0/2/2/2
31	5MC	CA	1962	31	-	0/3/25/26	0/2/2/2
31	6MZ	CA	2030	31	-	0/5/27/28	0/3/3/3
31	G7M	CA	2069	31	-	0/3/25/26	0/3/3/3
31	OMG	CA	2251	31	-	0/5/27/28	0/3/3/3
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
31	OMC	CA	2498	31,56	-	0/5/27/28	0/2/2/2
31	2MA	CA	2503	31	-	0/3/25/26	0/3/3/3
31	PSU	CA	2504	31	-	0/7/25/26	0/2/2/2
31	OMU	CA	2552	31	-	0/5/27/28	0/2/2/2
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
31	PSU	CA	746	31,56	-	0/7/25/26	0/2/2/2
31	5MU	CA	747	31	-	0/3/25/26	0/2/2/2
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
42	4D4	CN	81	42	-	0/8/12/14	0/0/0/0
33	6MZ	DA	1618	33	-	0/5/27/28	0/3/3/3
33	2MG	DA	1835	33	-	0/5/27/28	0/3/3/3
33	PSU	DA	1911	33	-	0/7/25/26	0/2/2/2
33	3TD	DA	1915	33	-	0/7/25/26	0/2/2/2
33	PSU	DA	1917	33	-	0/7/25/26	0/2/2/2
33	5MU	DA	1939	33	-	0/3/25/26	0/2/2/2
33	5MC	DA	1962	33	-	0/3/25/26	0/2/2/2
33	6MZ	DA	2030	33	-	0/5/27/28	0/3/3/3
33	G7M	DA	2069	33	-	0/3/25/26	0/3/3/3
33	OMG	DA	2251	33	-	0/5/27/28	0/3/3/3
33	2MG	DA	2445	33	-	0/5/27/28	0/3/3/3
33	H2U	DA	2449	33	-	0/7/38/39	0/2/2/2
33	PSU	DA	2457	33	-	0/7/25/26	0/2/2/2
33	OMC	DA	2498	33,56	-	0/5/27/28	0/2/2/2
33	2MA	DA	2503	33,56	-	0/3/25/26	0/3/3/3
33	PSU	DA	2504	33	-	0/7/25/26	0/2/2/2
33	OMU	DA	2552	33	-	0/5/27/28	0/2/2/2
33	PSU	DA	2580	33	-	0/7/25/26	0/2/2/2
33	PSU	DA	2604	33	-	0/7/25/26	0/2/2/2
33	PSU	DA	2605	33	-	0/7/25/26	0/2/2/2
33	1MG	DA	745	33	-	0/3/25/26	0/3/3/3
33	PSU	DA	746	33,56	-	0/7/25/26	0/2/2/2
33	5MU	DA	747	33	-	0/3/25/26	0/2/2/2
33	PSU	DA	955	33	-	0/7/25/26	0/2/2/2
32	MEQ	DD	150[A]	32	-	0/7/9/11	0/0/0/0
32	MEQ	DD	150[B]	32	-	0/7/9/11	0/0/0/0
42	4D4	DN	81[A]	-	-	0/8/12/14	0/0/0/0
42	4D4	DN	81[B]	-	-	0/8/12/14	0/0/0/0

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	DA	746	PSU	O4'-C1'	-3.36	1.39	1.44
33	DA	746	PSU	C2'-C1'	-3.10	1.50	1.53
31	CA	746	PSU	O4'-C1'	-2.47	1.40	1.44
33	DA	746	PSU	C5-C1'	-2.47	1.50	1.52
33	DA	2580	PSU	C6-C5	-2.21	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	DA	2504	PSU	C6-C5	-2.19	1.35	1.38
33	DA	2457	PSU	C6-C5	-2.19	1.35	1.38
1	AA	516	PSU	C6-C5	-2.17	1.35	1.38
31	CA	2457	PSU	C6-C5	-2.15	1.35	1.38
1	BA	516	PSU	C6-C5	-2.15	1.35	1.38
31	CA	1915	3TD	C6-C5	-2.13	1.35	1.38
33	DA	1915	3TD	C6-C5	-2.13	1.35	1.38
33	DA	1911	PSU	C6-C5	-2.12	1.35	1.38
31	CA	1917	PSU	C6-C5	-2.12	1.35	1.38
33	DA	2504	PSU	C5-C1'	-2.11	1.50	1.52
33	DA	955	PSU	C6-C5	-2.10	1.35	1.38
33	DA	1917	PSU	C6-C5	-2.09	1.35	1.38
31	CA	2605	PSU	C6-C5	-2.08	1.35	1.38
33	DA	1962	5MC	C6-C5	-2.08	1.34	1.40
31	CA	955	PSU	C6-C5	-2.08	1.35	1.38
1	BA	1407	5MC	C6-C5	-2.07	1.34	1.40
1	BA	967	5MC	C6-C5	-2.06	1.34	1.40
33	DA	2604	PSU	C6-C5	-2.05	1.35	1.38
33	DA	746	PSU	C6-C5	-2.05	1.35	1.38
31	CA	2504	PSU	C6-C5	-2.05	1.35	1.38
1	AA	1407	5MC	C6-C5	-2.04	1.34	1.40
33	DA	2605	PSU	C6-C5	-2.04	1.35	1.38
31	CA	1911	PSU	C6-C5	-2.04	1.35	1.38
1	AA	967	5MC	C6-C5	-2.04	1.34	1.40
33	DA	1939	5MU	C6-C5	-2.02	1.34	1.40
31	CA	2457	PSU	C5-C1'	-2.02	1.50	1.52
33	DA	1939	5MU	C2'-C1'	-2.02	1.50	1.53
33	DA	2030	6MZ	O3'-C3'	-2.02	1.38	1.43
31	CA	1962	5MC	C6-C5	-2.01	1.34	1.40
31	CA	2580	PSU	C6-C5	-2.00	1.35	1.38
1	AA	1516	2MG	C6-C5	2.09	1.45	1.41
33	DA	2498	OMC	C6-N1	2.12	1.38	1.35
33	DA	2552	OMU	C6-N1	2.18	1.38	1.35
1	AA	527	G7M	C6-C5	2.24	1.45	1.41
31	CA	1915	3TD	C4-N3	2.29	1.41	1.38
1	BA	1498	UR3	C4-N3	2.34	1.41	1.38
31	CA	2445	2MG	C6-C5	2.35	1.46	1.41
1	AA	1498	UR3	C4-N3	2.42	1.41	1.38
1	BA	966	2MG	C6-C5	2.44	1.46	1.41
31	CA	2552	OMU	C6-N1	2.50	1.39	1.35
33	DA	1835	2MG	C6-N1	2.88	1.38	1.33
33	DA	2445	2MG	C6-N1	2.99	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	DA	2604	PSU	C4-N3	3.00	1.38	1.33
1	AA	966	2MG	C6-C5	3.01	1.47	1.41
33	DA	2251	OMG	C6-N1	3.03	1.38	1.33
31	CA	745	1MG	C6-C5	3.10	1.46	1.40
1	AA	1207	2MG	C6-N1	3.11	1.38	1.33
33	DA	2552	OMU	C4-N3	3.13	1.38	1.33
1	BA	527	G7M	C6-N1	3.14	1.38	1.33
33	DA	2457	PSU	C4-N3	3.15	1.38	1.33
33	DA	1939	5MU	C4-N3	3.16	1.38	1.33
31	CA	2605	PSU	C4-N3	3.17	1.38	1.33
31	CA	2251	OMG	C6-C5	3.19	1.47	1.41
33	DA	2580	PSU	C4-N3	3.21	1.38	1.33
1	BA	516	PSU	C4-N3	3.21	1.38	1.33
1	BA	1207	2MG	C6-N1	3.23	1.38	1.33
31	CA	2457	PSU	C4-N3	3.23	1.38	1.33
31	CA	2069	G7M	C6-N1	3.24	1.38	1.33
33	DA	2605	PSU	C4-N3	3.24	1.38	1.33
31	CA	747	5MU	C4-N3	3.24	1.38	1.33
31	CA	955	PSU	C4-N3	3.26	1.38	1.33
31	CA	2445	2MG	C6-N1	3.27	1.38	1.33
33	DA	2504	PSU	C4-N3	3.28	1.38	1.33
31	CA	1835	2MG	C6-N1	3.29	1.39	1.33
1	AA	516	PSU	C4-N3	3.30	1.39	1.33
33	DA	955	PSU	C4-N3	3.31	1.39	1.33
32	DD	150[B]	MEQ	CB-CA	3.31	1.58	1.53
33	DA	1911	PSU	C4-N3	3.31	1.39	1.33
31	CA	2504	PSU	C4-N3	3.32	1.39	1.33
33	DA	2069	G7M	C6-N1	3.32	1.39	1.33
33	DA	747	5MU	C4-N3	3.32	1.39	1.33
1	AA	1516	2MG	C6-N1	3.32	1.39	1.33
33	DA	1917	PSU	C4-N3	3.34	1.39	1.33
31	CA	1911	PSU	C4-N3	3.35	1.39	1.33
31	CA	1917	PSU	C4-N3	3.35	1.39	1.33
1	BA	966	2MG	C6-N1	3.35	1.39	1.33
31	CA	2251	OMG	C6-N1	3.36	1.39	1.33
33	DA	746	PSU	C4-N3	3.37	1.39	1.33
31	CA	1939	5MU	C4-N3	3.38	1.39	1.33
31	CA	2580	PSU	C4-N3	3.40	1.39	1.33
1	AA	527	G7M	C6-N1	3.41	1.39	1.33
1	BA	1516	2MG	C6-N1	3.44	1.39	1.33
31	CA	746	PSU	C4-N3	3.47	1.39	1.33
31	CA	2552	OMU	C4-N3	3.49	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	966	2MG	C6-N1	3.51	1.39	1.33
33	DA	745	1MG	C6-C5	3.52	1.47	1.40

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	DA	1939	5MU	C5-C4-N3	-12.15	115.16	125.35
33	DA	747	5MU	C5-C4-N3	-12.09	115.20	125.35
31	CA	1939	5MU	C5-C4-N3	-12.08	115.21	125.35
31	CA	747	5MU	C5-C4-N3	-12.07	115.22	125.35
31	CA	2069	G7M	C5-C6-N1	-10.03	110.42	123.52
1	BA	527	G7M	C5-C6-N1	-9.85	110.64	123.52
33	DA	2069	G7M	C5-C6-N1	-9.80	110.70	123.52
1	BA	527	G7M	C6-C5-C4	-9.80	109.66	120.86
1	AA	527	G7M	C5-C6-N1	-9.73	110.80	123.52
31	CA	2069	G7M	C6-C5-C4	-9.52	109.97	120.86
31	CA	2251	OMG	C5-C6-N1	-8.89	111.91	123.52
31	CA	2445	2MG	C5-C6-N1	-8.86	111.94	123.52
1	AA	966	2MG	C5-C6-N1	-8.63	112.23	123.52
1	AA	1207	2MG	C5-C6-N1	-8.63	112.24	123.52
33	DA	2445	2MG	C5-C6-N1	-8.63	112.24	123.52
1	BA	966	2MG	C5-C6-N1	-8.60	112.28	123.52
33	DA	2251	OMG	C5-C6-N1	-8.42	112.52	123.52
1	BA	1207	2MG	C5-C6-N1	-8.40	112.54	123.52
33	DA	1835	2MG	C5-C6-N1	-8.31	112.66	123.52
1	BA	1516	2MG	C5-C6-N1	-8.26	112.72	123.52
31	CA	1835	2MG	C5-C6-N1	-8.25	112.74	123.52
1	AA	1516	2MG	C5-C6-N1	-8.22	112.78	123.52
1	AA	527	G7M	C6-C5-C4	-8.07	111.63	120.86
33	DA	2069	G7M	C6-C5-C4	-4.73	115.46	120.86
1	AA	527	G7M	N3-C2-N1	-4.35	121.64	127.56
1	BA	527	G7M	N3-C2-N1	-3.99	122.14	127.56
31	CA	2069	G7M	N3-C2-N1	-3.91	122.23	127.56
33	DA	2069	G7M	N3-C2-N1	-3.66	122.58	127.56
31	CA	2552	OMU	C5-C4-N3	-3.47	114.76	123.28
33	DA	2552	OMU	C5-C4-N3	-3.46	114.78	123.28
33	DA	2251	OMG	N3-C2-N1	-3.12	123.31	127.56
31	CA	1915	3TD	C5-C4-N3	-3.01	116.19	118.65
1	AA	966	2MG	C6-C5-C4	-3.00	117.42	120.86
33	DA	1915	3TD	C5-C4-N3	-3.00	116.20	118.65
32	DD	150[A]	MEQ	CG-CB-CA	-3.00	107.22	114.03
33	DA	2604	PSU	C4-C5-C1'	-2.94	116.26	121.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	DA	745	1MG	C6-C5-C4	-2.93	117.84	119.93
31	CA	2251	OMG	C6-C5-C4	-2.86	117.59	120.86
31	CA	745	1MG	C6-C5-C4	-2.84	117.90	119.93
31	CA	2251	OMG	N3-C2-N1	-2.83	123.71	127.56
33	DA	745	1MG	C5-C6-N1	-2.78	114.71	118.35
1	AA	1516	2MG	C6-C5-C4	-2.77	117.70	120.86
1	BA	1516	2MG	C6-C5-C4	-2.76	117.71	120.86
31	CA	1835	2MG	C6-C5-C4	-2.75	117.71	120.86
31	CA	2445	2MG	C6-C5-C4	-2.74	117.72	120.86
1	BA	1207	2MG	C6-C5-C4	-2.74	117.73	120.86
33	DA	746	PSU	C4-C5-C1'	-2.71	116.66	121.22
1	BA	966	2MG	C6-C5-C4	-2.71	117.76	120.86
33	DA	1835	2MG	C6-C5-C4	-2.66	117.82	120.86
31	CA	746	PSU	C4-C5-C1'	-2.62	116.81	121.22
31	CA	745	1MG	C5-C6-N1	-2.59	114.96	118.35
1	AA	1207	2MG	C6-C5-C4	-2.54	117.96	120.86
32	DD	150[B]	MEQ	O-C-CA	-2.48	119.08	125.72
33	DA	2251	OMG	C6-C5-C4	-2.31	118.21	120.86
32	DD	150[A]	MEQ	O-C-CA	-2.31	119.53	125.72
33	DA	2445	2MG	C6-C5-C4	-2.29	118.24	120.86
33	DA	2503	2MA	C6-C5-C4	-2.22	115.69	119.67
33	DA	2503	2MA	N3-C2-N1	-2.14	121.39	125.60
31	CA	2504	PSU	C4-C5-C1'	-2.09	117.69	121.22
1	BA	527	G7M	C1'-N9-C4	-2.09	124.47	126.81
31	CA	2503	2MA	C6-C5-C4	-2.07	115.96	119.67
33	DA	2503	2MA	CM2-C2-N3	2.03	120.67	117.22
31	CA	1939	5MU	C5M-C5-C6	2.09	122.86	118.63
31	CA	2503	2MA	C1'-N9-C4	2.13	129.19	126.81
31	CA	747	5MU	C5M-C5-C6	2.15	122.98	118.63
33	DA	1939	5MU	C5M-C5-C6	2.16	123.00	118.63
31	CA	2445	2MG	N2-C2-N3	2.16	119.45	116.94
33	DA	2580	PSU	O4'-C1'-C2'	2.16	107.03	104.69
1	BA	1407	5MC	CM5-C5-C6	2.16	123.01	118.63
33	DA	747	5MU	C5M-C5-C6	2.17	123.03	118.63
1	AA	967	5MC	CM5-C5-C6	2.19	123.06	118.63
1	BA	967	5MC	CM5-C5-C6	2.20	123.10	118.63
31	CA	1618	6MZ	C2-N1-C6	2.21	118.06	116.47
1	BA	1516	2MG	N2-C2-N3	2.22	119.52	116.94
33	DA	1962	5MC	CM5-C5-C6	2.24	123.16	118.63
33	DA	1911	PSU	O4'-C1'-C2'	2.24	107.12	104.69
33	DA	2445	2MG	N2-C2-N3	2.26	119.57	116.94
31	CA	1962	5MC	CM5-C5-C6	2.28	123.26	118.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1407	5MC	CM5-C5-C6	2.28	123.26	118.63
31	CA	2457	PSU	O4'-C1'-C2'	2.29	107.17	104.69
1	AA	1516	2MG	N2-C2-N3	2.30	119.61	116.94
33	DA	2457	PSU	O4'-C1'-C2'	2.32	107.20	104.69
31	CA	1911	PSU	O4'-C1'-C2'	2.36	107.24	104.69
31	CA	2580	PSU	O4'-C1'-C2'	2.41	107.29	104.69
1	BA	966	2MG	N2-C2-N3	2.44	119.77	116.94
1	AA	1207	2MG	N2-C2-N3	2.50	119.84	116.94
31	CA	1835	2MG	N2-C2-N3	2.57	119.92	116.94
33	DA	1618	6MZ	C2-N1-C6	2.57	118.32	116.47
33	DA	1835	2MG	N2-C2-N3	2.58	119.94	116.94
31	CA	2503	2MA	C2-N3-C4	2.60	116.54	115.29
33	DA	2030	6MZ	C2-N1-C6	2.60	118.34	116.47
1	BA	1207	2MG	N2-C2-N3	2.64	120.01	116.94
31	CA	2030	6MZ	C2-N1-C6	2.65	118.38	116.47
33	DA	2503	2MA	C2-N3-C4	3.18	116.82	115.29
32	DD	150[B]	MEQ	CB-CA-N	3.27	119.73	110.54
31	CA	2069	G7M	O4'-C1'-N9	3.31	114.36	108.11
1	AA	1402	4OC	C2-N3-C4	4.02	120.55	115.43
1	AA	527	G7M	O4'-C1'-N9	4.03	115.72	108.11
1	BA	1402	4OC	C2-N3-C4	4.05	120.58	115.43
1	BA	1402	4OC	CM4-N4-C4	4.54	126.70	122.87
1	BA	527	G7M	O4'-C1'-N9	4.80	117.17	108.11
1	AA	1402	4OC	CM4-N4-C4	4.98	127.07	122.87
33	DA	2069	G7M	O4'-C1'-N9	5.43	118.36	108.11
1	AA	1516	2MG	C6-N1-C2	6.22	124.15	115.24
1	BA	1516	2MG	C6-N1-C2	6.30	124.27	115.24
31	CA	1835	2MG	C6-N1-C2	6.44	124.46	115.24
33	DA	2445	2MG	C6-N1-C2	6.45	124.48	115.24
33	DA	1835	2MG	C6-N1-C2	6.50	124.54	115.24
1	AA	966	2MG	C6-N1-C2	6.55	124.62	115.24
1	BA	966	2MG	C6-N1-C2	6.64	124.75	115.24
1	BA	1207	2MG	C6-N1-C2	6.70	124.83	115.24
1	AA	1207	2MG	C6-N1-C2	6.75	124.91	115.24
31	CA	2069	G7M	C6-N1-C2	6.76	123.80	115.88
31	CA	2445	2MG	C6-N1-C2	6.78	124.94	115.24
1	BA	527	G7M	C6-N1-C2	6.83	123.89	115.88
33	DA	2069	G7M	C6-N1-C2	7.11	124.22	115.88
1	AA	527	G7M	C6-N1-C2	7.21	124.33	115.88
33	DA	2251	OMG	C6-N1-C2	7.69	124.89	115.88
31	CA	2251	OMG	C6-N1-C2	8.21	125.50	115.88
33	DA	2552	OMU	C4-N3-C2	12.06	126.92	114.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2552	OMU	C4-N3-C2	12.07	126.93	114.21
33	DA	955	PSU	C4-N3-C2	13.44	126.37	115.16
33	DA	2580	PSU	C4-N3-C2	13.47	126.40	115.16
31	CA	955	PSU	C4-N3-C2	13.48	126.41	115.16
33	DA	2605	PSU	C4-N3-C2	13.49	126.41	115.16
33	DA	2457	PSU	C4-N3-C2	13.50	126.42	115.16
33	DA	1911	PSU	C4-N3-C2	13.50	126.42	115.16
31	CA	1911	PSU	C4-N3-C2	13.53	126.45	115.16
33	DA	1917	PSU	C4-N3-C2	13.53	126.45	115.16
33	DA	2504	PSU	C4-N3-C2	13.54	126.45	115.16
1	AA	516	PSU	C4-N3-C2	13.54	126.45	115.16
1	BA	516	PSU	C4-N3-C2	13.54	126.46	115.16
31	CA	746	PSU	C4-N3-C2	13.54	126.46	115.16
31	CA	2605	PSU	C4-N3-C2	13.56	126.47	115.16
33	DA	2604	PSU	C4-N3-C2	13.56	126.47	115.16
31	CA	2504	PSU	C4-N3-C2	13.57	126.48	115.16
31	CA	2457	PSU	C4-N3-C2	13.59	126.50	115.16
31	CA	2580	PSU	C4-N3-C2	13.60	126.50	115.16
33	DA	746	PSU	C4-N3-C2	13.62	126.52	115.16
31	CA	1917	PSU	C4-N3-C2	13.65	126.55	115.16
33	DA	1939	5MU	C4-N3-C2	14.38	127.16	115.16
31	CA	747	5MU	C4-N3-C2	14.40	127.17	115.16
31	CA	1939	5MU	C4-N3-C2	14.49	127.25	115.16
33	DA	747	5MU	C4-N3-C2	14.51	127.27	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1518	MA6	1	0
1	AA	1519	MA6	1	0
12	AL	89	D2T	1	0
1	BA	1518	MA6	1	0
1	BA	1519	MA6	1	0
12	BL	89	D2T	1	0
31	CA	1835	2MG	1	0
31	CA	2030	6MZ	1	0
31	CA	2251	OMG	1	0
31	CA	2503	2MA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	CA	2552	OMU	1	0
33	DA	2030	6MZ	1	0
33	DA	2503	2MA	1	0
32	DD	150[A]	MEQ	2	0
32	DD	150[B]	MEQ	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 549 ligands modelled in this entry, 469 are monoatomic - leaving 80 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	PG4	AA	1670	-	12,12,12	0.26	0	11,11,11	0.22	0
58	MPD	AA	1671	-	6,7,7	0.36	0	6,10,10	0.43	0
59	PUT	AA	1672	-	5,5,5	0.23	0	4,4,4	0.15	0
59	PUT	AA	1673	-	5,5,5	0.15	0	4,4,4	0.19	0
59	PUT	AA	1674	-	5,5,5	0.20	0	4,4,4	0.15	0
59	PUT	AA	1675	-	5,5,5	0.26	0	4,4,4	0.10	0
58	MPD	AA	1676	-	6,7,7	0.43	0	6,10,10	0.33	0
61	PEG	AL	201	-	6,6,6	0.22	0	5,5,5	0.08	0
57	PG4	BA	1642	-	12,12,12	0.18	0	11,11,11	0.16	0
62	EDO	D0	101	-	3,3,3	0.62	0	2,2,2	0.31	0
62	EDO	D1	101	-	3,3,3	0.62	0	2,2,2	0.09	0
61	PEG	D1	102	-	6,6,6	0.27	0	5,5,5	0.05	0
63	PGE	D3	101	-	9,9,9	0.19	0	8,8,8	0.08	0
61	PEG	D3	102	-	6,6,6	0.27	0	5,5,5	0.16	0
62	EDO	DA	3001	-	3,3,3	0.55	0	2,2,2	0.48	0
64	SPD	DA	3182	-	9,9,9	0.11	0	8,8,8	0.17	0
59	PUT	DA	3183	-	5,5,5	0.18	0	4,4,4	0.19	0
65	1PE	DA	3184	-	15,15,15	0.19	0	14,14,14	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	PGE	DA	3185	-	9,9,9	0.25	0	8,8,8	0.33	0
64	SPD	DA	3186	-	9,9,9	0.15	0	8,8,8	0.16	0
59	PUT	DA	3187	-	5,5,5	0.33	0	4,4,4	0.20	0
59	PUT	DA	3188	-	5,5,5	0.30	0	4,4,4	0.14	0
58	MPD	DA	3189	-	6,7,7	0.37	0	6,10,10	0.44	0
66	ACY	DA	3190	-	0,3,3	0.00	-	0,3,3	0.00	-
58	MPD	DA	3191	-	6,7,7	0.41	0	6,10,10	0.42	0
57	PG4	DA	3192	-	12,12,12	0.21	0	11,11,11	0.21	0
62	EDO	DA	3193	-	3,3,3	0.53	0	2,2,2	0.36	0
59	PUT	DA	3194	-	5,5,5	0.36	0	4,4,4	0.32	0
66	ACY	DA	3195	-	0,3,3	0.00	-	0,3,3	0.00	-
62	EDO	DA	3196	-	3,3,3	0.61	0	2,2,2	0.33	0
62	EDO	DA	3197	-	3,3,3	0.60	0	2,2,2	0.17	0
61	PEG	DA	3198	-	6,6,6	0.18	0	5,5,5	0.08	0
61	PEG	DA	3199	-	6,6,6	0.23	0	5,5,5	0.15	0
66	ACY	DA	3200	-	0,3,3	0.00	-	0,3,3	0.00	-
65	1PE	DA	3201	-	15,15,15	0.32	0	14,14,14	0.38	0
58	MPD	DA	3202	-	6,7,7	0.38	0	6,10,10	0.49	0
59	PUT	DA	3203	-	5,5,5	0.15	0	4,4,4	0.19	0
64	SPD	DA	3204	-	9,9,9	0.21	0	8,8,8	0.20	0
58	MPD	DA	3205	-	6,7,7	0.39	0	6,10,10	0.52	0
62	EDO	DA	3206	-	3,3,3	0.75	0	2,2,2	0.09	0
62	EDO	DA	3207	-	3,3,3	0.62	0	2,2,2	0.29	0
58	MPD	DA	3208	-	6,7,7	0.46	0	6,10,10	0.35	0
67	GUN	DA	3209	-	9,12,12	1.55	2 (22%)	7,17,17	4.82	5 (71%)
59	PUT	DA	3210	-	5,5,5	0.24	0	4,4,4	0.06	0
59	PUT	DA	3211	-	5,5,5	0.23	0	4,4,4	0.13	0
63	PGE	DA	3212	-	9,9,9	0.12	0	8,8,8	0.09	0
62	EDO	DA	3213	-	3,3,3	0.61	0	2,2,2	0.42	0
57	PG4	DA	3214	-	12,12,12	0.15	0	11,11,11	0.17	0
63	PGE	DA	3215	-	9,9,9	0.17	0	8,8,8	0.13	0
61	PEG	DA	3216	-	6,6,6	0.17	0	5,5,5	0.06	0
59	PUT	DA	3217	-	5,5,5	0.24	0	4,4,4	0.20	0
68	TRS	DA	3218	-	7,7,7	0.38	0	9,9,9	0.32	0
59	PUT	DA	3219	-	5,5,5	0.21	0	4,4,4	0.13	0
59	PUT	DA	3220	-	5,5,5	0.24	0	4,4,4	0.29	0
59	PUT	DA	3221	-	5,5,5	0.20	0	4,4,4	0.15	0
64	SPD	DA	3222	-	9,9,9	0.14	0	8,8,8	0.34	0
63	PGE	DA	3223	-	9,9,9	0.16	0	8,8,8	0.28	0
61	PEG	DA	3224	-	6,6,6	0.21	0	5,5,5	0.08	0
61	PEG	DA	3225	-	6,6,6	0.30	0	5,5,5	0.16	0
59	PUT	DA	3227	-	5,5,5	0.16	0	4,4,4	0.14	0
62	EDO	DA	3228	-	3,3,3	0.57	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	MPD	DA	3229	-	6,7,7	0.42	0	6,10,10	0.23	0
62	EDO	DB	210	-	3,3,3	0.57	0	2,2,2	0.25	0
62	EDO	DB	211	-	3,3,3	0.57	0	2,2,2	0.32	0
63	PGE	DD	302	-	9,9,9	0.18	0	8,8,8	0.11	0
58	MPD	DE	301	-	6,7,7	0.43	0	6,10,10	0.41	0
58	MPD	DE	302	-	6,7,7	0.45	0	6,10,10	0.32	0
58	MPD	DK	201	-	6,7,7	0.46	0	6,10,10	0.34	0
61	PEG	DL	201	-	6,6,6	0.19	0	5,5,5	0.06	0
58	MPD	DN	201	-	6,7,7	0.55	0	6,10,10	0.33	0
61	PEG	DP	201	-	6,6,6	0.15	0	5,5,5	0.05	0
61	PEG	DQ	201	-	6,6,6	0.14	0	5,5,5	0.09	0
57	PG4	DQ	202	-	12,12,12	0.20	0	11,11,11	0.13	0
57	PG4	DR	203	-	12,12,12	0.22	0	11,11,11	0.21	0
63	PGE	DS	201	-	9,9,9	0.31	0	8,8,8	0.20	0
57	PG4	DS	202	-	12,12,12	0.30	0	11,11,11	0.21	0
58	MPD	DS	203	-	6,7,7	0.27	0	6,10,10	0.37	0
63	PGE	DT	201	-	9,9,9	0.16	0	8,8,8	0.12	0
58	MPD	DT	202	-	6,7,7	0.34	0	6,10,10	0.35	0
63	PGE	DU	101	-	9,9,9	0.26	0	8,8,8	0.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PG4	AA	1670	-	-	0/10/10/10	0/0/0/0
58	MPD	AA	1671	-	-	0/5/5/5	0/0/0/0
59	PUT	AA	1672	-	-	0/3/3/3	0/0/0/0
59	PUT	AA	1673	-	-	0/3/3/3	0/0/0/0
59	PUT	AA	1674	-	-	0/3/3/3	0/0/0/0
59	PUT	AA	1675	-	-	0/3/3/3	0/0/0/0
58	MPD	AA	1676	-	-	0/5/5/5	0/0/0/0
61	PEG	AL	201	-	-	0/4/4/4	0/0/0/0
57	PG4	BA	1642	-	-	0/10/10/10	0/0/0/0
62	EDO	D0	101	-	-	0/1/1/1	0/0/0/0
62	EDO	D1	101	-	-	0/1/1/1	0/0/0/0
61	PEG	D1	102	-	-	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
64	SPD	DA	3182	-	-	0/7/7/7	0/0/0/0
59	PUT	DA	3183	-	-	0/3/3/3	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
65	1PE	DA	3184	-	-	0/13/13/13	0/0/0/0
63	PGE	DA	3185	-	-	0/7/7/7	0/0/0/0
64	SPD	DA	3186	-	-	0/7/7/7	0/0/0/0
59	PUT	DA	3187	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3188	-	-	0/3/3/3	0/0/0/0
58	MPD	DA	3189	-	-	0/5/5/5	0/0/0/0
66	ACY	DA	3190	-	-	0/0/0/0	0/0/0/0
58	MPD	DA	3191	-	-	0/5/5/5	0/0/0/0
57	PG4	DA	3192	-	-	0/10/10/10	0/0/0/0
62	EDO	DA	3193	-	-	0/1/1/1	0/0/0/0
59	PUT	DA	3194	-	-	0/3/3/3	0/0/0/0
66	ACY	DA	3195	-	-	0/0/0/0	0/0/0/0
62	EDO	DA	3196	-	-	0/1/1/1	0/0/0/0
62	EDO	DA	3197	-	-	0/1/1/1	0/0/0/0
61	PEG	DA	3198	-	-	0/4/4/4	0/0/0/0
61	PEG	DA	3199	-	-	0/4/4/4	0/0/0/0
66	ACY	DA	3200	-	-	0/0/0/0	0/0/0/0
65	1PE	DA	3201	-	-	0/13/13/13	0/0/0/0
58	MPD	DA	3202	-	-	0/5/5/5	0/0/0/0
59	PUT	DA	3203	-	-	0/3/3/3	0/0/0/0
64	SPD	DA	3204	-	-	0/7/7/7	0/0/0/0
58	MPD	DA	3205	-	-	0/5/5/5	0/0/0/0
62	EDO	DA	3206	-	-	0/1/1/1	0/0/0/0
62	EDO	DA	3207	-	-	0/1/1/1	0/0/0/0
58	MPD	DA	3208	-	-	0/5/5/5	0/0/0/0
67	GUN	DA	3209	-	-	0/0/0/0	0/2/2/2
59	PUT	DA	3210	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3211	-	-	0/3/3/3	0/0/0/0
63	PGE	DA	3212	-	-	0/7/7/7	0/0/0/0
62	EDO	DA	3213	-	-	0/1/1/1	0/0/0/0
57	PG4	DA	3214	-	-	0/10/10/10	0/0/0/0
63	PGE	DA	3215	-	-	0/7/7/7	0/0/0/0
61	PEG	DA	3216	-	-	0/4/4/4	0/0/0/0
59	PUT	DA	3217	-	-	0/3/3/3	0/0/0/0
68	TRS	DA	3218	-	-	0/9/9/9	0/0/0/0
59	PUT	DA	3219	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3220	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3221	-	-	0/3/3/3	0/0/0/0
64	SPD	DA	3222	-	-	0/7/7/7	0/0/0/0
63	PGE	DA	3223	-	-	0/7/7/7	0/0/0/0
61	PEG	DA	3224	-	-	0/4/4/4	0/0/0/0
61	PEG	DA	3225	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PUT	DA	3227	-	-	0/3/3/3	0/0/0/0
62	EDO	DA	3228	-	-	0/1/1/1	0/0/0/0
58	MPD	DA	3229	-	-	0/5/5/5	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	302	-	-	0/7/7/7	0/0/0/0
58	MPD	DE	301	-	-	0/5/5/5	0/0/0/0
58	MPD	DE	302	-	-	0/5/5/5	0/0/0/0
58	MPD	DK	201	-	-	0/5/5/5	0/0/0/0
61	PEG	DL	201	-	-	0/4/4/4	0/0/0/0
58	MPD	DN	201	-	-	0/5/5/5	0/0/0/0
61	PEG	DP	201	-	-	0/4/4/4	0/0/0/0
61	PEG	DQ	201	-	-	0/4/4/4	0/0/0/0
57	PG4	DQ	202	-	-	0/10/10/10	0/0/0/0
57	PG4	DR	203	-	-	0/10/10/10	0/0/0/0
63	PGE	DS	201	-	-	0/7/7/7	0/0/0/0
57	PG4	DS	202	-	-	0/10/10/10	0/0/0/0
58	MPD	DS	203	-	-	0/5/5/5	0/0/0/0
63	PGE	DT	201	-	-	0/7/7/7	0/0/0/0
58	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	3209	GUN	C6-C5	2.30	1.45	1.41
67	DA	3209	GUN	C6-N1	3.33	1.39	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	DA	3209	GUN	C5-C6-N1	-8.61	112.27	123.52
67	DA	3209	GUN	N3-C2-N1	-3.00	123.48	127.56
67	DA	3209	GUN	C5-C4-N9	-2.81	106.13	111.12
67	DA	3209	GUN	C6-C5-C4	-2.48	118.02	120.86
67	DA	3209	GUN	C6-N1-C2	8.02	125.28	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	1670	PG4	1	0
58	AA	1671	MPD	1	0
57	BA	1642	PG4	1	0
61	D1	102	PEG	2	0
65	DA	3184	1PE	1	0
58	DA	3191	MPD	1	0
57	DA	3192	PG4	1	0
59	DA	3194	PUT	1	0
62	DA	3207	EDO	1	0
59	DA	3211	PUT	1	0
68	DA	3218	TRS	1	0
63	DA	3223	PGE	2	0
58	DE	301	MPD	1	0
57	DR	203	PG4	3	0
63	DS	201	PGE	2	0
57	DS	202	PG4	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%)	-0.13	22 (1%) 78 61	40, 90, 219, 296	0
1	BA	1522/1534 (99%)	0.45	137 (9%) 12 4	46, 131, 271, 279	0
2	AB	224/224 (100%)	0.27	6 (2%) 58 35	65, 116, 194, 247	0
2	BB	224/224 (100%)	0.57	17 (7%) 17 6	91, 129, 190, 236	0
3	AC	206/206 (100%)	-0.07	0 100 100	67, 95, 126, 146	0
3	BC	206/206 (100%)	0.64	18 (8%) 13 4	86, 134, 172, 196	0
4	AD	205/205 (100%)	-0.04	0 100 100	63, 99, 125, 146	0
4	BD	205/205 (100%)	-0.35	0 100 100	42, 72, 104, 134	0
5	AE	155/155 (100%)	-0.05	0 100 100	48, 82, 118, 155	0
5	BE	150/155 (96%)	-0.04	1 (0%) 89 79	60, 83, 132, 206	0
6	AF	106/106 (100%)	-0.01	1 (0%) 85 73	68, 94, 118, 143	0
6	BF	100/106 (94%)	0.23	1 (1%) 84 70	79, 114, 141, 155	0
7	AG	151/151 (100%)	0.39	9 (5%) 25 10	81, 116, 143, 156	0
7	BG	151/151 (100%)	1.85	64 (42%) 0 0	125, 189, 206, 220	0
8	AH	129/129 (100%)	-0.12	1 (0%) 87 75	54, 84, 111, 121	0
8	BH	129/129 (100%)	0.38	10 (7%) 16 5	76, 108, 142, 160	0
9	AI	127/127 (100%)	0.39	3 (2%) 62 40	76, 114, 149, 158	0
9	BI	127/127 (100%)	1.20	23 (18%) 2 1	125, 158, 188, 202	0
10	AJ	99/99 (100%)	0.37	4 (4%) 42 20	70, 106, 135, 146	0
10	BJ	98/99 (98%)	2.21	49 (50%) 0 0	121, 165, 189, 199	0
11	AK	117/117 (100%)	0.52	7 (5%) 25 10	54, 106, 141, 153	0
11	BK	117/117 (100%)	0.44	3 (2%) 59 37	80, 117, 144, 170	0
12	AL	122/123 (99%)	-0.12	1 (0%) 87 75	49, 69, 99, 124	0
12	BL	122/123 (99%)	0.25	2 (1%) 74 55	62, 90, 116, 145	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.60	5 (4%) 38 17	89, 118, 154, 171	0
13	BM	114/114 (100%)	3.09	81 (71%) 0 0	195, 227, 238, 248	0
14	AN	100/100 (100%)	0.41	8 (8%) 15 5	71, 104, 179, 193	0
14	BN	100/100 (100%)	1.75	38 (38%) 0 0	114, 173, 217, 228	0
15	AO	88/88 (100%)	-0.03	1 (1%) 82 67	58, 81, 108, 136	0
15	BO	88/88 (100%)	0.37	2 (2%) 64 41	70, 111, 132, 159	0
16	AP	82/82 (100%)	0.29	5 (6%) 25 10	62, 82, 127, 146	0
16	BP	82/82 (100%)	1.18	17 (20%) 1 0	95, 114, 151, 162	0
17	AQ	80/80 (100%)	0.31	5 (6%) 23 9	54, 79, 116, 139	0
17	BQ	80/80 (100%)	1.21	17 (21%) 1 0	82, 125, 147, 160	0
18	AR	55/55 (100%)	0.02	0 100 100	53, 87, 117, 153	0
18	BR	55/55 (100%)	0.40	4 (7%) 18 7	60, 88, 124, 154	0
19	AS	79/79 (100%)	0.58	4 (5%) 32 13	90, 114, 145, 152	0
19	BS	79/79 (100%)	2.95	56 (70%) 0 0	200, 222, 234, 239	0
20	AT	86/86 (100%)	0.19	1 (1%) 81 65	64, 83, 113, 136	0
20	BT	85/86 (98%)	1.66	30 (35%) 0 0	108, 138, 167, 180	0
21	AU	56/56 (100%)	1.18	10 (17%) 2 1	93, 124, 166, 180	0
21	BU	56/56 (100%)	0.38	1 (1%) 71 50	81, 107, 154, 167	0
22	C1	56/56 (100%)	2.23	25 (44%) 0 0	124, 162, 181, 184	0
22	D1	56/56 (100%)	-0.41	0 100 100	14, 39, 71, 99	0
23	C2	50/51 (98%)	3.30	34 (68%) 0 0	139, 161, 173, 186	0
23	D2	51/51 (100%)	0.29	0 100 100	54, 67, 101, 110	0
24	C3	46/46 (100%)	1.98	21 (45%) 0 0	119, 143, 157, 165	0
24	D3	46/46 (100%)	-0.41	0 100 100	29, 40, 64, 112	0
25	C4	64/64 (100%)	1.59	17 (26%) 1 0	116, 138, 155, 161	0
25	D4	64/64 (100%)	-0.38	0 100 100	26, 41, 53, 73	0
26	C5	38/38 (100%)	1.72	16 (42%) 0 0	108, 126, 139, 143	0
26	D5	38/38 (100%)	-0.35	0 100 100	33, 45, 69, 87	0
27	C0	58/58 (100%)	1.36	17 (29%) 1 0	115, 135, 151, 156	0
27	D0	58/58 (100%)	-0.38	0 100 100	17, 33, 61, 95	0
28	CB	118/120 (98%)	0.97	13 (11%) 7 2	135, 190, 241, 251	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	120/120 (100%)	-0.25	0 100 100	28, 57, 87, 143	0
29	CC	271/271 (100%)	0.49	19 (7%) 19 7	80, 113, 143, 167	0
29	DC	271/271 (100%)	-0.38	1 (0%) 93 86	23, 53, 84, 113	0
30	CD	209/209 (100%)	1.52	60 (28%) 1 0	102, 136, 165, 177	0
31	CA	2876/2904 (99%)	1.06	437 (15%) 3 1	69, 185, 272, 290	0
32	DD	208/209 (99%)	-0.45	0 100 100	15, 40, 73, 98	0
33	DA	2873/2903 (98%)	-0.14	70 (2%) 62 40	13, 46, 203, 298	0
34	CE	201/201 (100%)	2.38	108 (53%) 0 0	121, 176, 206, 224	0
34	DE	201/201 (100%)	-0.26	0 100 100	17, 57, 103, 139	0
35	CF	177/177 (100%)	2.87	116 (65%) 0 0	194, 215, 226, 232	0
35	DF	177/177 (100%)	-0.15	1 (0%) 90 81	52, 80, 120, 145	0
36	CG	176/176 (100%)	2.56	97 (55%) 0 0	146, 178, 208, 222	0
36	DG	176/176 (100%)	-0.10	2 (1%) 82 67	33, 70, 99, 136	0
37	CH	149/149 (100%)	1.06	27 (18%) 2 1	89, 149, 170, 178	0
37	DH	149/149 (100%)	0.85	17 (11%) 7 2	73, 154, 190, 203	0
38	CJ	134/134 (100%)	5.26	121 (90%) 0 0	236, 254, 265, 273	0
38	DJ	134/134 (100%)	3.51	97 (72%) 0 0	193, 222, 235, 242	0
39	CK	142/142 (100%)	1.40	42 (29%) 1 0	106, 132, 169, 195	0
39	DK	142/142 (100%)	-0.44	0 100 100	18, 35, 66, 88	0
40	CL	122/123 (99%)	1.09	29 (23%) 1 0	96, 118, 151, 168	0
40	DL	123/123 (100%)	-0.45	0 100 100	26, 44, 70, 112	0
41	CM	144/144 (100%)	2.14	61 (42%) 0 0	117, 169, 227, 247	0
41	DM	144/144 (100%)	-0.34	1 (0%) 89 79	14, 54, 87, 128	0
42	CN	135/136 (99%)	0.98	20 (14%) 3 1	92, 125, 151, 178	0
42	DN	135/136 (99%)	-0.46	0 100 100	20, 41, 73, 89	0
43	CO	120/125 (96%)	2.19	54 (45%) 0 0	110, 141, 163, 197	0
43	DO	125/125 (100%)	-0.34	1 (0%) 87 75	18, 36, 84, 137	0
44	CP	116/117 (99%)	2.10	56 (48%) 0 0	140, 171, 187, 195	0
44	DP	117/117 (100%)	-0.31	0 100 100	34, 55, 88, 95	0
45	CQ	114/114 (100%)	1.45	26 (22%) 1 0	113, 131, 157, 180	0
45	DQ	114/114 (100%)	-0.41	0 100 100	29, 51, 80, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
46	CR	117/117 (100%)	1.53	37 (31%) 1 0	108, 137, 166, 175	0
46	DR	117/117 (100%)	-0.42	0 100 100	14, 30, 51, 80	0
47	CS	103/103 (100%)	2.36	53 (51%) 0 0	124, 149, 173, 187	0
47	DS	103/103 (100%)	-0.42	1 (0%) 84 70	19, 43, 76, 103	0
48	CT	110/110 (100%)	2.28	54 (49%) 0 0	123, 155, 177, 188	0
48	DT	110/110 (100%)	-0.48	0 100 100	19, 33, 66, 126	0
49	CU	93/93 (100%)	2.41	42 (45%) 0 0	136, 168, 193, 201	0
49	DU	93/93 (100%)	0.02	2 (2%) 65 43	26, 55, 126, 141	0
50	CV	102/102 (100%)	3.49	73 (71%) 0 0	147, 176, 207, 219	0
50	DV	102/102 (100%)	-0.12	1 (0%) 84 70	41, 62, 104, 139	0
51	CW	94/94 (100%)	1.29	24 (25%) 1 0	128, 153, 165, 173	0
51	DW	94/94 (100%)	-0.31	1 (1%) 82 67	29, 54, 86, 99	0
52	CX	75/76 (98%)	2.32	43 (57%) 0 0	109, 140, 152, 186	0
52	DX	76/76 (100%)	-0.33	1 (1%) 79 63	22, 40, 74, 114	0
53	CY	77/77 (100%)	1.42	20 (25%) 1 0	108, 123, 156, 170	0
53	DY	77/77 (100%)	-0.22	0 100 100	32, 55, 88, 98	0
54	CZ	62/62 (100%)	2.35	32 (51%) 0 0	161, 179, 190, 196	0
54	DZ	62/62 (100%)	-0.12	1 (1%) 74 55	44, 74, 108, 140	0
55	DI	135/135 (100%)	1.46	41 (30%) 1 0	78, 153, 204, 224	1 (0%)
All	All	20634/20744 (99%)	0.60	2696 (13%) 5 2	13, 111, 241, 298	1 (0%)

All (2696) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
38	DJ	54	PRO	19.7
38	CJ	76	ALA	16.9
38	DJ	53	LEU	15.5
38	CJ	69	PHE	15.0
38	CJ	54	PRO	12.1
38	CJ	14	ALA	11.5
38	CJ	80	LEU	11.5
23	C2	52	ALA	11.3
38	CJ	51	LYS	10.8
35	CF	128	TYR	10.7
48	CT	5	ALA	10.5

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Mol	Chain	Res	Type	RSRZ
50	CV	3	ALA	10.2
38	CJ	11	LEU	10.2
35	CF	23	ASN	10.0
22	C1	27	SER	9.8
38	CJ	31	GLN	9.7
38	DJ	21	SER	9.5
38	CJ	32	GLY	9.5
7	BG	8	GLY	9.3
9	BI	128	SER	9.2
19	BS	14	HIS	9.2
49	CU	72	GLN	9.1
44	CP	107	ALA	9.1
38	CJ	120	ALA	8.9
41	CM	92	LEU	8.9
38	DJ	23	PRO	8.8
38	CJ	121	ASP	8.8
38	CJ	13	VAL	8.8
31	CA	1537	G	8.8
47	CS	96	VAL	8.7
38	CJ	116	ASP	8.6
1	BA	1030	U	8.6
35	CF	155	THR	8.5
47	CS	50	GLY	8.5
38	DJ	52	GLY	8.5
35	CF	153	ASP	8.5
50	CV	31	SER	8.5
36	CG	103	ILE	8.4
1	BA	211	G	8.4
50	CV	35	ILE	8.4
19	BS	24	GLU	8.4
31	CA	1067	A	8.4
38	DJ	87	LYS	8.3
38	CJ	55	ILE	8.3
38	CJ	131	GLY	8.2
18	BR	20	GLU	8.2
38	DJ	13	VAL	8.1
33	DA	2132	U	8.1
10	BJ	76	ILE	8.1
38	CJ	89	GLY	8.1
49	CU	71	GLY	8.0
38	CJ	124	ALA	7.9
38	DJ	79	LEU	7.9

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Mol	Chain	Res	Type	RSRZ
10	BJ	75	ASP	7.9
38	CJ	115	ALA	7.8
41	CM	144	GLU	7.8
1	BA	207	C	7.8
13	BM	45	ILE	7.8
48	CT	48	LYS	7.8
43	CO	26	GLY	7.8
50	CV	29	LEU	7.8
1	BA	1032	G	7.7
38	CJ	23	PRO	7.7
1	BA	208	U	7.7
38	DJ	24	VAL	7.7
1	BA	209	U	7.7
38	CJ	99	GLY	7.7
34	CE	131	THR	7.7
50	CV	27	ASN	7.7
31	CA	1068	G	7.7
36	CG	102	VAL	7.6
38	CJ	60	THR	7.6
38	CJ	53	LEU	7.6
38	CJ	83	ALA	7.6
38	CJ	94	ASN	7.6
31	CA	1175	A	7.6
38	CJ	126	THR	7.6
38	DJ	88	SER	7.5
23	C2	47	VAL	7.5
38	DJ	12	GLN	7.5
14	BN	43	ASN	7.5
36	CG	57	GLY	7.5
31	CA	1087	G	7.5
23	C2	50	LYS	7.4
33	DA	2120	G	7.4
38	CJ	33	VAL	7.4
50	CV	77	THR	7.4
38	DJ	59	ILE	7.4
10	BJ	74	VAL	7.4
19	BS	49	ILE	7.4
34	CE	119	ILE	7.4
50	CV	26	LYS	7.3
36	CG	52	PHE	7.3
33	DA	2131	U	7.3
24	C3	1	MET	7.2

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Mol	Chain	Res	Type	RSRZ
49	CU	15	HIS	7.2
13	BM	84	GLY	7.2
20	BT	4	ILE	7.2
49	CU	55	VAL	7.2
50	CV	36	VAL	7.2
2	BB	123	ASP	7.1
35	CF	85	ILE	7.1
35	CF	126	GLY	7.1
38	CJ	82	LYS	7.1
50	CV	48	PRO	7.1
31	CA	1095	A	7.0
38	CJ	79	LEU	7.0
50	CV	25	VAL	7.0
34	CE	128	ALA	7.0
23	C2	53	LYS	6.9
38	CJ	113	LYS	6.9
42	CN	136	MET	6.9
31	CA	331	C	6.9
38	CJ	87	LYS	6.9
38	CJ	129	ILE	6.9
9	BI	130	ARG	6.8
38	CJ	59	ILE	6.8
36	CG	112	PRO	6.8
19	BS	66	MET	6.8
43	CO	63	ARG	6.8
35	CF	144	ASP	6.8
35	CF	156	ILE	6.8
36	CG	166	ASP	6.8
35	CF	40	VAL	6.8
38	CJ	73	THR	6.7
38	CJ	67	PHE	6.7
38	CJ	75	PRO	6.7
38	DJ	19	ASN	6.7
34	CE	17	THR	6.7
33	DA	2111	U	6.7
34	CE	144	GLU	6.7
13	BM	46	SER	6.7
43	CO	25	ALA	6.7
38	DJ	67	PHE	6.7
48	CT	3	THR	6.7
38	CJ	38	PHE	6.7
34	CE	127	GLU	6.6

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Mol	Chain	Res	Type	RSRZ
52	CX	54	GLY	6.6
44	CP	64	TYR	6.6
35	CF	119	ALA	6.6
35	CF	86	GLY	6.6
50	CV	39	ILE	6.6
19	BS	29	LYS	6.6
49	CU	47	VAL	6.6
50	CV	13	VAL	6.6
38	DJ	80	LEU	6.6
41	CM	81	ASP	6.6
13	BM	29	ARG	6.5
38	CJ	42	PHE	6.5
10	BJ	77	VAL	6.5
34	CE	33	VAL	6.5
38	DJ	20	PRO	6.5
44	CP	63	LYS	6.4
38	DJ	55	ILE	6.4
50	CV	83	VAL	6.4
19	BS	39	THR	6.4
13	BM	48	LEU	6.4
35	CF	116	GLY	6.4
36	CG	104	ASN	6.4
50	CV	32	GLY	6.3
13	BM	77	ILE	6.3
50	CV	78	GLY	6.3
48	CT	4	ILE	6.3
23	C2	36	LEU	6.3
49	CU	1	MET	6.3
33	DA	2110	G	6.3
13	BM	33	ILE	6.3
38	CJ	22	PRO	6.2
7	BG	73	VAL	6.2
24	C3	42	LEU	6.2
52	CX	70	GLU	6.2
33	DA	2166	U	6.2
41	CM	114	GLY	6.2
31	CA	345	A	6.2
50	CV	30	SER	6.2
54	CZ	11	VAL	6.2
31	CA	228	C	6.2
38	CJ	61	VAL	6.1
38	DJ	96	ASP	6.1

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Mol	Chain	Res	Type	RSRZ
47	CS	27	ILE	6.1
47	CS	20	VAL	6.1
33	DA	2163	A	6.1
38	CJ	132	THR	6.1
55	DI	121	SER	6.1
49	CU	67	VAL	6.1
31	CA	1103	A	6.1
50	CV	52	LEU	6.0
14	BN	44	ALA	6.0
55	DI	114	GLU	6.0
38	CJ	17	MET	6.0
19	BS	71	LEU	6.0
38	CJ	125	MET	6.0
36	CG	172	LYS	6.0
38	CJ	98	VAL	6.0
13	BM	24	GLY	6.0
50	CV	40	ASN	6.0
36	CG	56	ASP	6.0
48	CT	40	ASN	6.0
23	C2	37	LYS	6.0
13	BM	96	PRO	6.0
54	CZ	45	GLN	6.0
43	CO	24	MET	5.9
38	CJ	56	PRO	5.9
38	DJ	51	LYS	5.9
10	BJ	26	VAL	5.9
13	BM	99	GLY	5.9
34	CE	129	PRO	5.9
13	BM	108	THR	5.9
13	BM	2	ALA	5.9
13	BM	47	GLU	5.9
31	CA	289	G	5.9
35	CF	41	GLY	5.8
43	CO	98	LEU	5.8
45	CQ	9	GLU	5.8
23	C2	43	VAL	5.8
31	CA	1211	C	5.8
31	CA	1066	U	5.8
38	DJ	22	PRO	5.8
36	CG	32	GLU	5.8
31	CA	1078	U	5.8
7	BG	77	SER	5.8

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Mol	Chain	Res	Type	RSRZ
31	CA	846	U	5.8
35	CF	129	SER	5.8
7	BG	65	ALA	5.8
36	CG	9	VAL	5.7
49	CU	43	ILE	5.7
44	CP	66	GLY	5.7
45	CQ	110	ILE	5.7
38	CJ	50	GLU	5.7
36	CG	2	SER	5.7
7	BG	69	VAL	5.7
36	CG	45	HIS	5.7
38	CJ	12	GLN	5.7
38	CJ	122	ILE	5.7
38	CJ	110	ALA	5.6
43	CO	28	LEU	5.6
1	BA	79	G	5.6
35	CF	35	THR	5.6
35	CF	29	PRO	5.6
38	CJ	62	TYR	5.6
38	CJ	44	ALA	5.6
38	CJ	138	LEU	5.6
19	BS	48	THR	5.6
35	CF	37	ASN	5.6
1	BA	203	G	5.6
34	CE	89	PRO	5.6
50	CV	79	LYS	5.6
43	CO	29	VAL	5.6
31	CA	2168	G	5.6
52	CX	52	GLY	5.6
15	BO	89	ARG	5.5
1	BA	94	G	5.5
14	AN	21	PHE	5.5
38	DJ	14	ALA	5.5
54	CZ	22	LEU	5.5
54	CZ	63	ALA	5.5
54	CZ	15	ASN	5.5
1	AA	1030	U	5.5
38	DJ	135	SER	5.5
30	CD	25	THR	5.5
38	DJ	50	GLU	5.5
48	CT	105	VAL	5.5
10	BJ	8	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
13	BM	11	ASP	5.5
41	CM	28	GLY	5.5
55	DI	128	THR	5.5
13	BM	64	VAL	5.5
54	CZ	59	GLU	5.5
38	DJ	28	LEU	5.5
9	BI	127	PHE	5.5
38	CJ	52	GLY	5.5
38	CJ	35	ILE	5.5
38	DJ	71	THR	5.4
38	CJ	85	GLY	5.4
31	CA	1090	A	5.4
38	CJ	21	SER	5.4
43	CO	120	GLU	5.4
52	CX	53	CYS	5.4
50	CV	28	VAL	5.4
10	BJ	41	PRO	5.4
14	BN	23	LYS	5.4
7	BG	103	TRP	5.4
38	CJ	68	THR	5.4
38	CJ	24	VAL	5.4
38	DJ	98	VAL	5.4
50	CV	42	VAL	5.4
25	C4	61	CYS	5.4
7	BG	62	PHE	5.4
41	CM	15	ALA	5.4
10	BJ	87	LEU	5.3
41	CM	79	LEU	5.3
44	CP	29	HIS	5.3
13	BM	105	ASN	5.3
20	BT	47	ALA	5.3
44	CP	117	PHE	5.3
30	CD	180	VAL	5.3
50	CV	84	GLY	5.3
2	AB	123	ASP	5.3
50	CV	75	ALA	5.3
38	CJ	130	GLU	5.3
1	BA	204	G	5.3
33	DA	2116	G	5.3
35	CF	122	PHE	5.3
33	DA	896	A	5.3
38	CJ	88	SER	5.3

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Mol	Chain	Res	Type	RSRZ
13	BM	94	GLY	5.3
35	CF	174	ASP	5.3
38	CJ	123	GLU	5.3
38	CJ	58	VAL	5.3
34	CE	88	ARG	5.3
47	CS	87	GLN	5.3
43	CO	93	GLY	5.3
51	CW	84	PRO	5.3
23	C2	21	TYR	5.2
42	CN	29	GLY	5.2
35	CF	28	VAL	5.2
7	BG	79	ARG	5.2
1	AA	86	G	5.2
1	BA	213	G	5.2
36	CG	7	ALA	5.2
41	CM	1	MET	5.2
35	CF	76	GLY	5.2
13	BM	95	LEU	5.2
36	CG	40	ALA	5.2
50	CV	64	ALA	5.2
13	BM	23	TYR	5.2
34	CE	10	SER	5.2
36	CG	50	LEU	5.2
31	CA	2797	U	5.2
38	CJ	45	LYS	5.1
17	BQ	83	VAL	5.1
34	CE	126	VAL	5.1
33	DA	2175	C	5.1
35	CF	22	TYR	5.1
47	CS	26	ASP	5.1
38	CJ	57	VAL	5.1
43	CO	73	ASN	5.1
36	CG	43	VAL	5.1
41	CM	101	ILE	5.1
48	CT	44	ALA	5.1
54	CZ	29	ARG	5.1
34	CE	157	LEU	5.1
34	CE	188	MET	5.1
10	BJ	35	GLN	5.1
31	CA	1089	A	5.1
50	CV	95	PHE	5.1
49	CU	60	THR	5.1

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Mol	Chain	Res	Type	RSRZ
36	CG	175	LYS	5.0
41	CM	80	SER	5.0
7	BG	42	ILE	5.0
34	CE	12	LEU	5.0
54	CZ	58	ASN	5.0
13	BM	97	VAL	5.0
46	CR	29	SER	5.0
41	CM	20	GLY	5.0
47	CS	32	THR	5.0
30	CD	96	ILE	5.0
50	CV	18	ASP	5.0
30	CD	74	GLU	5.0
1	BA	1024	G	5.0
38	CJ	97	LYS	5.0
1	BA	85	U	5.0
19	BS	28	LYS	5.0
50	CV	2	ALA	4.9
36	CG	83	PHE	4.9
34	CE	172	ALA	4.9
30	CD	10	GLY	4.9
33	DA	1067	A	4.9
41	CM	89	VAL	4.9
34	CE	118	LEU	4.9
50	CV	89	ASP	4.9
41	CM	102	GLY	4.9
38	CJ	47	ASP	4.9
7	AG	8	GLY	4.9
13	BM	93	ARG	4.9
17	BQ	8	LEU	4.9
50	CV	88	GLU	4.9
34	CE	104	ALA	4.9
36	CG	167	GLU	4.9
54	CZ	60	LYS	4.9
22	C1	6	ASN	4.9
14	BN	37	SER	4.9
36	CG	105	LEU	4.8
50	CV	51	ALA	4.8
38	CJ	43	ASN	4.8
14	BN	47	LYS	4.8
22	C1	34	SER	4.8
13	BM	83	LEU	4.8
47	CS	19	THR	4.8

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Mol	Chain	Res	Type	RSRZ
33	DA	2125	G	4.8
14	BN	60	GLN	4.8
34	CE	171	ASP	4.8
13	BM	40	ALA	4.8
23	C2	35	GLU	4.8
49	DU	1	MET	4.8
31	CA	357	C	4.8
55	DI	130	PRO	4.8
1	AA	1032	G	4.8
38	CJ	81	LYS	4.8
52	CX	63	ALA	4.8
38	CJ	96	ASP	4.8
47	CS	30	GLY	4.8
7	BG	75	VAL	4.8
1	BA	1020	G	4.8
26	C5	19	ARG	4.8
48	CT	49	LYS	4.8
9	AI	130	ARG	4.8
1	BA	1022	A	4.8
38	CJ	111	GLN	4.8
36	CG	10	VAL	4.7
33	DA	2167	U	4.7
35	CF	164	GLU	4.7
12	AL	124	ALA	4.7
30	CD	55	LYS	4.7
38	DJ	68	THR	4.7
47	CS	67	GLY	4.7
40	CL	89	ASN	4.7
14	BN	45	VAL	4.7
10	BJ	37	ARG	4.7
13	BM	19	LEU	4.7
13	BM	10	PRO	4.7
38	CJ	64	ASP	4.7
49	CU	2	ILE	4.7
31	CA	1086	A	4.7
33	DA	2174	C	4.7
19	BS	60	VAL	4.7
36	CG	169	VAL	4.7
46	CR	99	ALA	4.7
31	CA	2110	G	4.7
38	DJ	94	ASN	4.7
50	CV	33	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
31	CA	1064	C	4.7
38	DJ	49	ILE	4.7
45	CQ	115	ASN	4.7
35	CF	150	ARG	4.7
1	BA	1031	C	4.7
47	CS	31	GLU	4.7
38	CJ	34	ASN	4.7
1	BA	1307	U	4.7
17	BQ	70	THR	4.7
31	CA	1171	G	4.7
35	CF	165	GLU	4.7
23	C2	49	TYR	4.7
54	CZ	18	LEU	4.6
31	CA	1228	G	4.6
33	DA	2124	G	4.6
1	BA	1534	A	4.6
43	CO	72	ASP	4.6
36	CG	171	THR	4.6
52	CX	56	ASP	4.6
13	BM	43	VAL	4.6
44	CP	60	GLU	4.6
19	BS	12	ASP	4.6
31	CA	1535	A	4.6
41	CM	120	VAL	4.6
31	CA	138	U	4.6
9	BI	38	TYR	4.6
23	C2	46	HIS	4.6
23	C2	45	GLN	4.6
35	CF	173	PHE	4.6
35	CF	152	LEU	4.6
14	BN	39	GLU	4.6
45	CQ	19	SER	4.6
34	CE	102	ARG	4.6
38	CJ	77	ALA	4.6
31	CA	440	C	4.6
38	DJ	100	LYS	4.6
44	CP	88	LYS	4.6
55	DI	122	GLN	4.6
35	CF	24	SER	4.6
36	CG	174	ALA	4.6
38	CJ	25	GLY	4.6
38	CJ	20	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
49	CU	70	HIS	4.6
38	DJ	36	MET	4.5
43	CO	111	ALA	4.5
1	BA	985	C	4.5
23	C2	34	LEU	4.5
1	BA	1016	A	4.5
34	CE	37	ALA	4.5
54	CZ	33	ALA	4.5
36	CG	58	TYR	4.5
35	CF	67	ILE	4.5
38	DJ	76	ALA	4.5
38	CJ	139	VAL	4.5
46	CR	106	PHE	4.5
38	DJ	73	THR	4.5
50	CV	81	ASP	4.5
44	CP	40	ILE	4.5
1	AA	844	G	4.5
10	BJ	90	LEU	4.5
23	C2	23	THR	4.5
50	CV	53	ASN	4.5
35	CF	149	VAL	4.5
38	CJ	74	PRO	4.5
7	BG	53	ARG	4.5
31	CA	1201	U	4.5
37	DH	137	GLU	4.5
49	CU	69	ARG	4.5
38	CJ	141	GLU	4.5
1	BA	212	G	4.5
36	CG	17	VAL	4.5
44	CP	54	VAL	4.5
14	BN	30	ILE	4.4
31	CA	1082	U	4.4
48	CT	47	VAL	4.4
38	CJ	48	SER	4.4
38	DJ	97	LYS	4.4
45	CQ	112	GLU	4.4
35	CF	170	LEU	4.4
38	CJ	71	THR	4.4
19	BS	18	LYS	4.4
54	DZ	63	ALA	4.4
23	C2	24	THR	4.4
30	CD	176	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	BA	999	C	4.4
31	CA	549	G	4.4
41	CM	115	GLU	4.4
50	CV	43	LYS	4.4
52	CX	57	HIS	4.4
31	CA	1083	U	4.4
19	BS	37	ARG	4.4
31	CA	2125	G	4.4
50	CV	71	ALA	4.4
31	CA	1084	A	4.4
48	CT	93	ALA	4.4
10	BJ	102	LEU	4.4
13	BM	80	LEU	4.4
31	CA	613	A	4.4
16	BP	17	TYR	4.4
31	CA	2892	G	4.4
41	CM	70	LYS	4.4
31	CA	1174	U	4.4
35	CF	130	MET	4.4
38	CJ	128	SER	4.4
38	CJ	136	MET	4.4
46	CR	37	GLN	4.4
19	BS	40	ILE	4.4
44	CP	78	VAL	4.4
33	DA	2109	U	4.4
31	CA	1205	A	4.4
53	CY	55	GLY	4.4
34	CE	186	VAL	4.4
44	CP	61	GLN	4.4
53	CY	29	PHE	4.3
1	BA	1302	C	4.3
10	BJ	80	THR	4.3
38	CJ	41	ALA	4.3
44	CP	62	LEU	4.3
43	CO	27	SER	4.3
9	BI	129	LYS	4.3
10	BJ	73	LEU	4.3
50	CV	58	ILE	4.3
34	CE	55	SER	4.3
40	CL	14	SER	4.3
34	CE	201	ALA	4.3
19	BS	81	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
41	CM	78	ARG	4.3
48	CT	37	THR	4.3
49	CU	16	VAL	4.3
36	CG	62	TRP	4.3
36	CG	68	ALA	4.3
43	CO	83	LEU	4.3
31	CA	1407	G	4.3
33	DA	2127	G	4.3
26	C5	1	MET	4.3
31	CA	1172	C	4.3
22	C1	55	ILE	4.3
35	CF	8	TYR	4.3
45	CQ	85	SER	4.3
31	CA	1173	U	4.3
43	CO	23	ASN	4.3
19	BS	72	GLY	4.3
31	CA	2172	U	4.3
49	CU	77	ARG	4.3
52	CX	32	LEU	4.3
23	C2	39	PHE	4.3
31	CA	1088	A	4.3
40	CL	56	ASP	4.3
44	CP	108	ASP	4.3
19	BS	68	GLY	4.3
31	CA	1093	G	4.3
19	BS	74	PHE	4.3
41	CM	77	ILE	4.3
39	CK	98	GLU	4.3
38	CJ	63	ALA	4.3
1	BA	205	A	4.2
30	CD	26	VAL	4.2
34	CE	193	VAL	4.2
38	CJ	18	ALA	4.2
34	CE	13	THR	4.2
38	DJ	83	ALA	4.2
31	CA	882	G	4.2
38	CJ	112	THR	4.2
41	CM	121	THR	4.2
34	CE	30	GLN	4.2
48	CT	73	LYS	4.2
38	CJ	46	THR	4.2
7	BG	151	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
35	CF	162	SER	4.2
1	BA	1021	A	4.2
38	DJ	116	ASP	4.2
31	CA	885	C	4.2
34	CE	64	GLY	4.2
38	CJ	9	VAL	4.2
38	CJ	78	VAL	4.2
34	CE	161	ALA	4.2
42	CN	56	ALA	4.2
38	DJ	38	PHE	4.2
41	CM	107	PHE	4.2
13	BM	106	ALA	4.2
55	DI	131	THR	4.2
24	C3	33	ARG	4.2
1	AA	87	C	4.2
36	CG	154	PRO	4.2
1	BA	1025	U	4.2
53	CY	78	TYR	4.2
52	CX	55	ARG	4.2
48	CT	45	VAL	4.2
43	CO	77	ALA	4.2
34	CE	147	LEU	4.2
8	BH	123	GLY	4.2
12	BL	124	ALA	4.2
36	CG	51	THR	4.2
36	CG	6	LYS	4.2
43	CO	76	VAL	4.2
34	CE	122	GLU	4.2
35	CF	47	LYS	4.1
7	BG	15	ASP	4.1
48	CT	69	LEU	4.1
51	CW	6	ALA	4.1
22	C1	2	ALA	4.1
38	DJ	66	SER	4.1
30	CD	6	GLY	4.1
31	CA	1076	C	4.1
13	BM	39	ILE	4.1
13	BM	32	ALA	4.1
14	AN	22	ALA	4.1
31	CA	88	G	4.1
48	CT	108	SER	4.1
22	C1	57	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
31	CA	2181	U	4.1
19	BS	52	HIS	4.1
30	CD	186	LEU	4.1
50	CV	76	ALA	4.1
52	CX	33	ALA	4.1
25	C4	36	LYS	4.1
34	CE	14	VAL	4.1
38	DJ	99	GLY	4.1
38	DJ	42	PHE	4.1
44	CP	52	SER	4.1
7	BG	66	LEU	4.1
35	CF	27	GLN	4.1
31	CA	896	A	4.1
19	BS	30	PRO	4.1
38	CJ	114	ALA	4.1
52	CX	51	VAL	4.1
11	BK	13	ARG	4.1
44	CP	51	ALA	4.1
14	BN	27	LEU	4.1
41	CM	71	ALA	4.1
34	CE	143	LEU	4.1
35	CF	154	ILE	4.1
38	CJ	28	LEU	4.1
36	CG	84	THR	4.1
7	BG	91	VAL	4.1
23	C2	31	PRO	4.1
7	BG	148	ASN	4.1
19	BS	43	ASN	4.1
31	CA	2112	G	4.1
31	CA	2174	C	4.1
34	CE	43	THR	4.0
34	CE	183	PHE	4.0
38	CJ	127	ARG	4.0
46	CR	21	ALA	4.0
55	DI	134	GLU	4.0
31	CA	2124	G	4.0
44	CP	25	ARG	4.0
44	CP	65	THR	4.0
39	CK	142	ILE	4.0
39	CK	87	ALA	4.0
41	CM	90	VAL	4.0
7	BG	71	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
31	CA	2890	G	4.0
38	DJ	103	ARG	4.0
49	CU	12	ARG	4.0
34	CE	121	VAL	4.0
47	CS	63	VAL	4.0
38	DJ	114	ALA	4.0
43	CO	79	LEU	4.0
31	CA	329	G	4.0
31	CA	1530	G	4.0
20	BT	87	ALA	4.0
7	BG	72	THR	4.0
35	CF	147	ASP	4.0
35	CF	177	PHE	4.0
36	CG	162	VAL	4.0
13	BM	109	ARG	4.0
38	CJ	117	MET	4.0
44	CP	53	THR	4.0
47	CS	35	PHE	4.0
47	CS	55	ASP	4.0
31	CA	646	U	4.0
33	DA	2118	U	4.0
41	CM	100	ILE	4.0
52	CX	50	ASN	4.0
34	CE	47	LYS	4.0
52	CX	78	LYS	4.0
35	CF	20	PHE	4.0
39	CK	128	ASN	4.0
46	CR	6	ARG	4.0
31	CA	45	G	4.0
36	CG	148	LEU	4.0
38	CJ	95	LYS	4.0
48	CT	6	LYS	4.0
36	CG	22	GLN	4.0
13	BM	63	PHE	4.0
13	BM	113	ARG	4.0
51	CW	70	ILE	4.0
50	CV	37	GLU	3.9
55	DI	84	TYR	3.9
31	CA	2904	U	3.9
38	CJ	29	GLY	3.9
33	DA	2133	G	3.9
48	CT	92	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
47	CS	37	GLU	3.9
38	DJ	89	GLY	3.9
35	CF	75	ALA	3.9
31	CA	1536	C	3.9
49	CU	75	GLY	3.9
31	CA	288	U	3.9
47	CS	52	PRO	3.9
49	CU	10	VAL	3.9
30	CD	31	ALA	3.9
33	DA	138	U	3.9
48	CT	36	LEU	3.9
10	BJ	25	ILE	3.9
31	CA	75	G	3.9
46	CR	81	ASN	3.9
31	CA	2126	A	3.9
27	C0	56	LYS	3.9
26	C5	25	VAL	3.9
39	CK	119	PHE	3.9
50	CV	38	GLY	3.9
23	C2	48	ILE	3.9
31	CA	1065	U	3.9
41	CM	75	ALA	3.9
34	CE	72	SER	3.9
45	CQ	111	LYS	3.9
31	CA	2602	A	3.9
31	CA	291	G	3.9
31	CA	881	G	3.9
35	CF	92	ARG	3.9
44	CP	30	ARG	3.9
45	CQ	84	ILE	3.9
47	CS	103	ALA	3.9
38	CJ	66	SER	3.9
31	CA	515	A	3.9
36	CG	173	GLU	3.9
14	BN	36	ALA	3.9
19	BS	36	ARG	3.8
38	DJ	78	VAL	3.8
25	C4	2	PRO	3.8
37	CH	136	SER	3.8
51	CW	69	GLU	3.8
11	AK	18	ASP	3.8
33	DA	1175	A	3.8

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Mol	Chain	Res	Type	RSRZ
31	CA	318	C	3.8
41	CM	21	ARG	3.8
48	CT	110	ARG	3.8
17	AQ	53	CYS	3.8
31	CA	528	A	3.8
23	C2	32	GLU	3.8
13	BM	81	MET	3.8
31	CA	394	C	3.8
13	BM	12	HIS	3.8
14	BN	22	ALA	3.8
19	BS	75	ALA	3.8
38	DJ	61	VAL	3.8
13	BM	98	ARG	3.8
1	BA	196	A	3.8
41	CM	142	ILE	3.8
16	AP	82	ALA	3.8
31	CA	1278	C	3.8
35	CF	69	LYS	3.8
31	CA	1245	G	3.8
36	CG	25	THR	3.8
49	CU	8	LEU	3.8
31	CA	441	U	3.8
7	BG	88	PRO	3.8
35	CF	117	LEU	3.8
46	CR	117	LEU	3.8
13	BM	22	ILE	3.8
38	DJ	17	MET	3.8
46	CR	2	ALA	3.8
1	BA	1034	G	3.8
31	CA	1538	G	3.8
33	DA	2172	U	3.8
48	CT	38	TYR	3.8
16	BP	57	ILE	3.8
19	BS	41	PHE	3.8
26	C5	38	GLY	3.8
38	CJ	30	GLN	3.8
31	CA	1059	G	3.8
23	C2	40	ASP	3.8
1	BA	1035	A	3.8
44	CP	56	LYS	3.8
50	CV	50	PRO	3.8
50	CV	62	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
50	CV	12	ILE	3.8
51	CW	94	ALA	3.8
34	CE	150	THR	3.8
34	CE	181	ILE	3.8
40	CL	75	SER	3.8
31	CA	1468	U	3.7
34	CE	199	MET	3.7
55	DI	120	ALA	3.7
9	BI	37	GLN	3.7
40	CL	99	ILE	3.7
22	C1	5	GLN	3.7
54	CZ	14	LEU	3.7
38	DJ	81	LYS	3.7
14	BN	24	ARG	3.7
19	BS	63	THR	3.7
1	BA	63	C	3.7
44	CP	87	ILE	3.7
34	CE	103	GLY	3.7
27	C0	2	ALA	3.7
7	BG	52	GLN	3.7
14	BN	49	GLN	3.7
31	CA	1077	A	3.7
34	CE	168	ASP	3.7
34	CE	180	LEU	3.7
36	CG	157	TYR	3.7
41	CM	19	LEU	3.7
48	CT	7	HIS	3.7
38	CJ	118	THR	3.7
48	CT	43	ALA	3.7
22	C1	46	ASP	3.7
25	C4	58	VAL	3.7
1	BA	1001	C	3.7
45	CQ	34	GLU	3.7
36	CG	80	THR	3.7
50	CV	72	ILE	3.7
55	DI	96	PHE	3.7
21	AU	2	PRO	3.7
16	BP	80	LYS	3.7
40	CL	110	GLU	3.7
48	CT	2	GLU	3.7
39	CK	86	GLN	3.7
38	CJ	93	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
23	C2	44	ARG	3.7
36	CG	20	ASN	3.7
41	CM	113	ALA	3.7
50	CV	5	ILE	3.7
2	BB	130	THR	3.7
38	DJ	85	GLY	3.7
52	CX	47	ALA	3.7
54	CZ	56	LEU	3.7
35	CF	143	TYR	3.7
38	CJ	86	ILE	3.7
16	BP	3	THR	3.7
17	BQ	17	MET	3.7
53	CY	12	PRO	3.7
54	CZ	6	LEU	3.7
35	CF	120	LYS	3.7
38	CJ	133	ALA	3.7
31	CA	1202	G	3.7
11	AK	82	LEU	3.7
20	BT	5	LYS	3.7
38	DJ	138	LEU	3.7
13	BM	4	ILE	3.7
38	CJ	65	ARG	3.7
22	C1	35	GLY	3.6
28	CB	18	G	3.6
31	CA	12	U	3.6
10	BJ	39	PRO	3.6
14	BN	51	LEU	3.6
46	CR	35	ALA	3.6
33	DA	2114	A	3.6
30	CD	8	LYS	3.6
30	CD	90	PHE	3.6
31	CA	356	G	3.6
1	AA	1492	A	3.6
1	BA	80	A	3.6
1	BA	1441	A	3.6
35	CF	81	GLN	3.6
36	CG	101	ASN	3.6
7	BG	152	ALA	3.6
34	CE	124	PHE	3.6
52	CX	26	PHE	3.6
22	C1	26	THR	3.6
31	CA	1094	U	3.6

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Mol	Chain	Res	Type	RSRZ
48	CT	106	VAL	3.6
10	BJ	19	ASP	3.6
34	CE	154	ASP	3.6
22	C1	36	GLU	3.6
25	C4	64	TYR	3.6
31	CA	290	U	3.6
46	CR	45	TYR	3.6
35	CF	113	ASP	3.6
26	C5	10	LEU	3.6
49	CU	46	ALA	3.6
1	BA	153	C	3.6
54	CZ	8	GLU	3.6
7	BG	49	THR	3.6
19	BS	27	ASP	3.6
45	CQ	8	LEU	3.6
37	DH	136	SER	3.6
20	BT	45	ALA	3.6
7	BG	78	ARG	3.6
49	CU	76	ARG	3.6
13	BM	104	THR	3.6
14	BN	54	ASP	3.6
34	CE	173	THR	3.6
7	BG	90	GLU	3.6
31	CA	409	G	3.6
31	CA	2402	U	3.6
53	CY	18	ARG	3.6
16	BP	60	TRP	3.6
50	CV	82	ARG	3.6
31	CA	2180	U	3.6
2	BB	135	LEU	3.6
46	CR	7	GLY	3.6
19	BS	51	VAL	3.6
34	CE	196	VAL	3.6
55	DI	124	ASP	3.6
19	BS	69	HIS	3.6
38	CJ	16	GLY	3.6
2	BB	131	LYS	3.6
37	DH	94	ILE	3.6
36	CG	129	THR	3.6
19	BS	80	TYR	3.6
28	CB	19	C	3.5
43	CO	113	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
48	CT	52	GLU	3.5
10	BJ	91	ASP	3.5
14	BN	58	SER	3.5
34	CE	18	THR	3.5
41	CM	117	THR	3.5
51	CW	45	ASP	3.5
43	CO	103	ARG	3.5
37	CH	137	GLU	3.5
39	CK	97	PRO	3.5
40	CL	103	VAL	3.5
33	DA	1730	C	3.5
50	CV	74	ASN	3.5
45	CQ	35	GLY	3.5
35	CF	157	THR	3.5
35	CF	151	GLY	3.5
45	CQ	97	LEU	3.5
20	BT	3	ASN	3.5
34	CE	116	ASP	3.5
7	BG	83	SER	3.5
10	BJ	22	THR	3.5
36	CG	8	PRO	3.5
43	CO	118	ARG	3.5
31	CA	431	U	3.5
36	CG	161	GLY	3.5
7	BG	85	TYR	3.5
31	CA	879	G	3.5
35	CF	42	GLU	3.5
7	BG	16	PRO	3.5
14	BN	4	GLN	3.5
35	CF	65	PRO	3.5
38	DJ	25	GLY	3.5
38	DJ	104	ALA	3.5
31	CA	2803	G	3.5
34	CE	40	ARG	3.5
34	CE	175	ILE	3.5
36	CG	44	LYS	3.5
36	CG	106	SER	3.5
36	CG	116	GLN	3.5
48	CT	31	GLN	3.5
52	CX	74	PRO	3.5
30	CD	73	VAL	3.5
30	CD	95	SER	3.5

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Mol	Chain	Res	Type	RSRZ
35	CF	39	GLY	3.5
54	CZ	36	GLN	3.5
7	BG	131	LYS	3.5
31	CA	101	A	3.5
14	BN	52	PRO	3.5
30	CD	97	SER	3.5
44	CP	80	GLU	3.5
39	CK	140	LEU	3.5
3	BC	159	GLY	3.5
33	DA	2176	A	3.5
30	CD	46	ARG	3.5
31	CA	2891	U	3.5
35	CF	95	ARG	3.5
39	CK	60	ASP	3.5
52	CX	42	GLY	3.5
20	BT	35	VAL	3.5
36	CG	107	LEU	3.5
55	DI	72	LEU	3.5
35	CF	175	PHE	3.5
47	CS	1	MET	3.5
31	CA	2123	G	3.5
1	BA	219	U	3.5
35	CF	36	LEU	3.5
36	CG	99	LYS	3.5
43	CO	56	LYS	3.5
47	CS	66	HIS	3.5
31	CA	1870	C	3.4
35	CF	54	ALA	3.5
1	BA	1026	G	3.4
13	BM	79	ARG	3.4
31	CA	446	G	3.4
39	CK	15	TRP	3.4
13	BM	103	LYS	3.4
55	DI	136	ILE	3.4
30	CD	158	GLY	3.4
41	CM	131	ALA	3.4
1	AA	1031	C	3.4
31	CA	275	C	3.4
31	CA	355	U	3.4
31	CA	1247	A	3.4
31	CA	1277	G	3.4
36	DG	177	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
52	CX	62	LYS	3.4
44	CP	115	LEU	3.4
1	BA	206	C	3.4
38	CJ	36	MET	3.4
29	CC	48	ARG	3.4
50	CV	14	LEU	3.4
24	C3	26	ASN	3.4
38	CJ	101	ILE	3.4
44	CP	93	ASP	3.4
52	CX	80	ILE	3.4
23	C2	18	GLY	3.4
13	BM	55	THR	3.4
1	BA	175	C	3.4
13	BM	70	ARG	3.4
38	CJ	90	SER	3.4
35	CF	136	ILE	3.4
10	BJ	97	ASP	3.4
30	CD	166	GLY	3.4
38	DJ	69	PHE	3.4
14	AN	23	LYS	3.4
31	CA	653	U	3.4
31	CA	2132	U	3.4
47	CS	61	ALA	3.4
38	CJ	8	TYR	3.4
38	DJ	33	VAL	3.4
23	C2	7	GLU	3.4
24	C3	43	THR	3.4
33	DA	2180	U	3.4
38	DJ	107	GLN	3.4
13	BM	13	LYS	3.4
24	C3	7	PRO	3.4
39	CK	137	PRO	3.4
31	CA	1508	A	3.4
47	CS	83	TYR	3.4
31	CA	1224	U	3.4
38	CJ	91	GLY	3.4
7	BG	111	ARG	3.4
55	DI	129	LEU	3.4
35	CF	159	THR	3.4
47	CS	49	ILE	3.4
14	BN	28	LYS	3.4
20	BT	56	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
55	DI	106	PHE	3.4
36	CG	111	HIS	3.4
1	BA	1000	A	3.4
20	BT	34	LYS	3.4
25	C4	49	MET	3.4
48	CT	90	LYS	3.4
44	CP	103	VAL	3.4
31	CA	2120	G	3.4
38	CJ	37	GLU	3.4
54	CZ	40	SER	3.4
7	BG	87	VAL	3.3
13	BM	58	ASP	3.3
35	CF	56	ASP	3.3
43	CO	99	LYS	3.3
47	CS	88	GLY	3.3
31	CA	1639	C	3.3
31	CA	1529	G	3.3
3	BC	196	ILE	3.3
35	CF	83	TYR	3.3
38	DJ	101	ILE	3.3
7	BG	112	GLY	3.3
38	DJ	29	GLY	3.3
31	CA	139	U	3.3
52	CX	23	VAL	3.3
1	BA	216	U	3.3
38	CJ	140	VAL	3.3
7	AG	4	ARG	3.3
33	DA	2121	G	3.3
34	CE	21	ARG	3.3
38	DJ	117	MET	3.3
48	CT	99	ARG	3.3
49	CU	44	LYS	3.3
50	CV	47	LYS	3.3
31	CA	213	A	3.3
20	BT	79	LEU	3.3
24	C3	14	ARG	3.3
34	CE	4	VAL	3.3
47	CS	48	LYS	3.3
31	CA	72	U	3.3
31	CA	1057	A	3.3
16	BP	52	LEU	3.3
48	CT	34	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
48	CT	94	ASP	3.3
31	CA	1052	C	3.3
31	CA	546	U	3.3
34	CE	73	ILE	3.3
37	DH	105	ALA	3.3
48	CT	39	THR	3.3
37	CH	133	GLN	3.3
45	CQ	16	ASP	3.3
7	BG	46	ALA	3.3
30	CD	88	GLU	3.3
36	CG	121	ILE	3.3
38	DJ	131	GLY	3.3
49	CU	35	ALA	3.3
1	BA	1136	C	3.3
10	BJ	7	ARG	3.3
14	BN	48	LEU	3.3
41	CM	74	THR	3.3
9	AI	21	ILE	3.3
31	CA	2814	A	3.3
37	CH	72	ILE	3.3
20	BT	24	ARG	3.3
28	CB	41	G	3.3
47	CS	79	ARG	3.3
26	C5	13	ASN	3.3
35	CF	50	LEU	3.3
19	BS	61	PHE	3.3
22	C1	8	PRO	3.3
31	CA	1727	C	3.3
31	CA	2743	U	3.3
44	CP	38	GLN	3.3
7	BG	7	ILE	3.3
17	BQ	61	ILE	3.3
34	CE	145	ASP	3.3
52	CX	59	LEU	3.3
31	CA	321	U	3.3
13	BM	28	THR	3.3
46	CR	44	GLN	3.3
38	DJ	123	GLU	3.3
52	CX	17	GLU	3.3
25	C4	37	ALA	3.3
38	DJ	133	ALA	3.3
31	CA	89	A	3.2

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Mol	Chain	Res	Type	RSRZ
38	DJ	31	GLN	3.2
52	CX	25	ARG	3.2
31	CA	2118	U	3.2
36	CG	65	ALA	3.2
38	DJ	137	GLY	3.2
1	BA	82	G	3.2
7	BG	4	ARG	3.2
34	CE	24	ASN	3.2
43	CO	62	ASN	3.2
31	CA	1325	U	3.2
34	CE	190	ALA	3.2
44	CP	110	ALA	3.2
10	BJ	36	VAL	3.2
30	CD	131	ASP	3.2
44	CP	39	VAL	3.2
38	DJ	37	GLU	3.2
41	CM	35	HIS	3.2
23	C2	41	PRO	3.2
25	C4	21	GLY	3.2
37	CH	11	ASN	3.2
43	CO	33	ILE	3.2
43	CO	81	ASN	3.2
46	CR	23	GLY	3.2
20	AT	87	ALA	3.2
21	AU	26	ALA	3.2
35	CF	171	ALA	3.2
53	CY	22	LEU	3.2
31	CA	1396	U	3.2
41	CM	91	ASP	3.2
22	C1	15	MET	3.2
38	DJ	72	LYS	3.2
37	DH	65	ALA	3.2
40	CL	83	ALA	3.2
27	C0	41	THR	3.2
3	BC	206	GLU	3.2
31	CA	1046	A	3.2
7	AG	7	ILE	3.2
31	CA	281	C	3.2
7	AG	6	VAL	3.2
22	C1	11	SER	3.2
13	BM	31	LYS	3.2
16	BP	53	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
19	BS	21	LYS	3.2
31	CA	1406	U	3.2
19	BS	32	ARG	3.2
50	CV	6	ARG	3.2
31	CA	1328	A	3.2
31	CA	33	C	3.2
31	CA	76	C	3.2
31	CA	1075	C	3.2
22	C1	45	ALA	3.2
36	CG	13	ALA	3.2
45	CQ	95	ALA	3.2
14	BN	19	LYS	3.2
20	BT	36	TYR	3.2
51	CW	27	PRO	3.2
47	CS	46	GLU	3.2
33	DA	1727	C	3.2
50	CV	20	GLY	3.2
1	BA	121	U	3.2
17	BQ	78	VAL	3.2
31	CA	1539	U	3.2
31	CA	2111	U	3.2
39	CK	56	VAL	3.2
27	C0	39	GLU	3.2
11	AK	81	ASN	3.2
10	BJ	38	GLY	3.2
29	CC	233	GLY	3.2
31	CA	1085	A	3.2
38	DJ	34	ASN	3.2
34	CE	120	VAL	3.2
44	CP	109	ALA	3.2
30	CD	179	ARG	3.2
52	CX	82	ILE	3.2
33	DA	879	G	3.2
1	BA	172	A	3.2
31	CA	2766	A	3.2
35	CF	132	VAL	3.2
44	CP	59	ALA	3.2
46	CR	31	VAL	3.2
31	CA	2045	C	3.2
14	BN	21	PHE	3.2
45	CQ	91	ALA	3.2
47	CS	102	SER	3.2

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Mol	Chain	Res	Type	RSRZ
53	CY	17	ASN	3.2
7	BG	80	VAL	3.2
35	CF	105	THR	3.2
38	DJ	9	VAL	3.2
1	BA	134	G	3.2
31	CA	1551	A	3.2
14	AN	31	ILE	3.1
33	DA	2130	U	3.1
30	CD	101	PHE	3.1
30	CD	60	VAL	3.1
13	BM	85	CYS	3.1
31	CA	344	A	3.1
38	DJ	86	ILE	3.1
43	CO	52	ILE	3.1
31	CA	1719	G	3.1
31	CA	2165	C	3.1
31	CA	2819	G	3.1
33	DA	2123	G	3.1
7	AG	79	ARG	3.1
14	BN	18	ASP	3.1
34	CE	29	HIS	3.1
47	CS	22	LEU	3.1
53	CY	20	HIS	3.1
39	CK	118	MET	3.1
50	CV	87	PHE	3.1
31	CA	1322	A	3.1
31	CA	2169	A	3.1
48	CT	107	VAL	3.1
31	CA	1079	C	3.1
34	CE	41	GLN	3.1
34	CE	178	VAL	3.1
44	CP	85	LYS	3.1
13	BM	41	GLU	3.1
49	CU	85	VAL	3.1
7	BG	70	ARG	3.1
10	BJ	99	GLN	3.1
31	CA	877	A	3.1
33	DA	1065	U	3.1
31	CA	2895	G	3.1
39	CK	21	THR	3.1
9	BI	64	TYR	3.1
20	BT	48	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
27	C0	48	ILE	3.1
10	BJ	63	ASP	3.1
36	CG	132	VAL	3.1
1	AA	81	A	3.1
31	CA	2799	A	3.1
36	CG	54	PRO	3.1
40	CL	37	ASP	3.1
50	CV	63	ALA	3.1
17	BQ	5	ILE	3.1
39	CK	93	ILE	3.1
34	CE	105	LEU	3.1
31	CA	128	C	3.1
31	CA	504	A	3.1
33	DA	2164	C	3.1
52	CX	69	PHE	3.1
34	CE	164	LEU	3.1
38	DJ	60	THR	3.1
41	CM	103	ILE	3.1
36	CG	163	ARG	3.1
55	DI	119	PRO	3.1
46	CR	25	TYR	3.1
30	CD	91	THR	3.1
42	CN	132	THR	3.1
46	CR	17	ILE	3.1
24	C3	37	LYS	3.1
34	CE	28	VAL	3.1
1	BA	1492	A	3.1
31	CA	866	A	3.1
31	CA	1111	A	3.1
34	CE	45	ALA	3.1
38	CJ	104	ALA	3.1
39	CK	47	HIS	3.1
10	AJ	75	ASP	3.0
7	BG	43	VAL	3.0
24	C3	35	ARG	3.0
31	CA	1250	G	3.0
10	BJ	94	ALA	3.0
51	CW	10	LYS	3.0
11	AK	17	SER	3.0
35	CF	146	VAL	3.0
34	CE	44	ARG	3.0
14	BN	6	MET	3.0

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Mol	Chain	Res	Type	RSRZ
17	BQ	53	CYS	3.0
38	DJ	40	LYS	3.0
1	BA	198	G	3.0
16	BP	42	ILE	3.0
31	CA	1524	G	3.0
31	CA	2802	G	3.0
44	CP	58	ILE	3.0
31	CA	878	A	3.0
33	DA	1847	A	3.0
35	CF	115	ARG	3.0
46	CR	102	ASP	3.0
50	CV	98	SER	3.0
35	CF	91	LEU	3.0
49	CU	29	THR	3.0
10	BJ	23	ALA	3.0
38	CJ	84	ALA	3.0
55	DI	51	TYR	3.0
1	BA	78	A	3.0
31	CA	502	A	3.0
39	CK	20	ALA	3.0
44	CP	82	ALA	3.0
55	DI	104	ALA	3.0
41	CM	106	GLU	3.0
35	CF	9	LYS	3.0
19	BS	38	SER	3.0
38	DJ	64	ASP	3.0
25	C4	22	PHE	3.0
1	BA	844	G	3.0
1	BA	1005	A	3.0
1	BA	1306	A	3.0
31	CA	1047	G	3.0
31	CA	1179	G	3.0
31	CA	1533	C	3.0
31	CA	1734	G	3.0
36	CG	61	GLY	3.0
36	CG	158	LYS	3.0
49	CU	68	LYS	3.0
7	BG	74	GLU	3.0
55	DI	110	ALA	3.0
7	BG	76	LYS	3.0
31	CA	1092	C	3.0
30	CD	4	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
7	AG	151	PHE	3.0
13	BM	51	GLY	3.0
35	CF	10	ASP	3.0
19	BS	35	SER	3.0
35	CF	60	ILE	3.0
38	DJ	48	SER	3.0
41	CM	116	VAL	3.0
1	AA	1037	C	3.0
1	BA	1314	C	3.0
17	BQ	63	GLU	3.0
23	C2	15	ALA	3.0
27	C0	44	ILE	3.0
33	DA	2115	G	3.0
38	DJ	63	ALA	3.0
38	DJ	121	ASP	3.0
50	CV	57	GLY	3.0
21	AU	56	HIS	3.0
30	CD	68	PHE	3.0
31	CA	34	U	3.0
21	AU	27	GLY	3.0
31	CA	1072	C	3.0
31	CA	2793	C	3.0
34	CE	11	ALA	3.0
37	CH	94	ILE	3.0
1	BA	949	A	3.0
22	C1	3	VAL	3.0
31	CA	603	A	3.0
42	CN	6	ARG	3.0
1	AA	1026	G	3.0
42	CN	80	VAL	3.0
43	CO	94	TYR	3.0
19	BS	5	LEU	3.0
31	CA	513	A	3.0
31	CA	1073	A	3.0
27	C0	10	THR	3.0
48	CT	86	MET	3.0
2	BB	67	ILE	2.9
14	BN	31	ILE	2.9
31	CA	2801	G	2.9
47	CS	100	GLY	2.9
34	CE	87	ALA	2.9
34	CE	5	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
35	CF	25	VAL	2.9
34	CE	98	LYS	2.9
35	CF	169	LEU	2.9
36	CG	4	VAL	2.9
49	CU	83	ALA	2.9
30	CD	154	LYS	2.9
31	CA	1105	U	2.9
29	CC	272	SER	2.9
31	CA	1045	C	2.9
27	C0	59	GLU	2.9
31	CA	514	A	2.9
31	CA	1532	A	2.9
37	CH	149	GLU	2.9
13	BM	56	LEU	2.9
17	BQ	22	VAL	2.9
34	CE	200	LEU	2.9
1	BA	1356	G	2.9
20	BT	43	ASP	2.9
31	CA	931	U	2.9
54	CZ	49	ASP	2.9
16	BP	47	GLU	2.9
49	CU	42	GLU	2.9
35	CF	12	VAL	2.9
36	CG	141	ILE	2.9
55	DI	126	LEU	2.9
46	CR	11	ARG	2.9
31	CA	880	G	2.9
51	CW	5	ASN	2.9
23	C2	17	THR	2.9
31	CA	2313	C	2.9
19	BS	10	PHE	2.9
34	CE	191	ASP	2.9
50	CV	44	LYS	2.9
51	CW	43	ASP	2.9
31	CA	405	U	2.9
21	AU	16	LEU	2.9
48	CT	85	ILE	2.9
31	CA	1091	G	2.9
35	CF	30	ARG	2.9
55	DI	67	THR	2.9
54	CZ	17	GLU	2.9
11	AK	19	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
13	BM	42	ASP	2.9
37	DH	107	GLY	2.9
1	AA	85	U	2.9
31	CA	2585	U	2.9
35	CF	176	PRO	2.9
37	CH	140	ALA	2.9
41	CM	94	THR	2.9
43	CO	84	GLY	2.9
48	CT	103	ILE	2.9
54	CZ	37	LEU	2.9
55	DI	29	ASP	2.9
31	CA	1509	A	2.9
35	CF	118	SER	2.9
54	CZ	41	HIS	2.9
43	CO	7	GLY	2.9
38	CJ	70	VAL	2.9
1	BA	220	G	2.9
19	BS	76	PRO	2.9
26	C5	33	HIS	2.9
31	CA	117	G	2.9
35	CF	84	PRO	2.9
31	CA	1169	A	2.9
13	BM	17	ILE	2.9
13	BM	52	GLN	2.9
34	CE	9	GLN	2.9
37	CH	139	PHE	2.9
29	DC	272	SER	2.9
1	BA	989	U	2.9
31	CA	451	U	2.9
21	AU	53	VAL	2.9
31	CA	2872	A	2.9
34	CE	153	LEU	2.9
48	CT	71	VAL	2.9
3	BC	193	TYR	2.9
29	CC	180	GLU	2.9
53	CY	76	GLU	2.9
13	BM	30	SER	2.9
29	CC	27	GLY	2.9
49	CU	40	LYS	2.9
54	CZ	54	LYS	2.9
28	CB	110	C	2.9
30	CD	188	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
36	CG	24	ILE	2.9
55	DI	38	MET	2.9
55	DI	113	PHE	2.9
31	CA	476	G	2.9
3	BC	85	GLU	2.9
36	CG	151	TYR	2.9
39	CK	120	ARG	2.9
39	CK	61	LYS	2.9
47	CS	24	LYS	2.9
37	CH	15	LEU	2.9
52	CX	45	PHE	2.8
10	BJ	89	ARG	2.8
10	BJ	78	GLU	2.8
14	BN	20	TYR	2.8
23	C2	33	LYS	2.8
38	DJ	82	LYS	2.8
1	BA	380	G	2.8
7	BG	82	GLY	2.8
31	CA	1439	A	2.8
10	BJ	15	HIS	2.8
53	CY	49	LEU	2.8
36	CG	26	ILE	2.8
41	CM	18	ARG	2.8
49	CU	51	PHE	2.8
44	CP	46	GLU	2.8
47	CS	62	GLU	2.8
52	CX	83	GLU	2.8
33	DA	2108	A	2.8
43	CO	22	ARG	2.8
31	CA	2159	G	2.8
54	CZ	32	ALA	2.8
41	CM	82	LEU	2.8
33	DA	2178	C	2.8
47	CS	78	ARG	2.8
34	CE	23	PHE	2.8
46	CR	14	HIS	2.8
41	CM	76	GLU	2.8
34	CE	75	SER	2.8
46	CR	42	ALA	2.8
31	CA	1215	G	2.8
31	CA	1633	G	2.8
1	AA	209	U	2.8

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Mol	Chain	Res	Type	RSRZ
31	CA	114	U	2.8
45	CQ	43	PHE	2.8
39	CK	136	GLN	2.8
35	CF	161	LYS	2.8
41	CM	4	ASN	2.8
47	CS	69	GLY	2.8
52	CX	73	GLY	2.8
55	DI	73	LYS	2.8
7	BG	89	VAL	2.8
13	BM	102	THR	2.8
49	CU	62	VAL	2.8
31	CA	548	G	2.8
31	CA	1311	G	2.8
31	CA	2127	G	2.8
36	CG	165	ALA	2.8
36	CG	177	LYS	2.8
31	CA	262	A	2.8
31	CA	1522	A	2.8
31	CA	2147	A	2.8
9	BI	126	GLN	2.8
35	CF	131	GLY	2.8
45	CQ	12	GLN	2.8
53	CY	30	LEU	2.8
31	CA	315	G	2.8
31	CA	495	G	2.8
37	DH	110	VAL	2.8
39	CK	55	ILE	2.8
53	CY	13	VAL	2.8
1	BA	93	U	2.8
20	BT	86	LEU	2.8
27	C0	17	LEU	2.8
31	CA	347	A	2.8
31	CA	2106	U	2.8
22	C1	30	VAL	2.8
41	CM	38	GLN	2.8
2	BB	132	LYS	2.8
31	CA	561	G	2.8
31	CA	1726	C	2.8
35	CF	26	MET	2.8
40	CL	51	LYS	2.8
1	BA	1004	A	2.8
1	BA	1362	A	2.8

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Mol	Chain	Res	Type	RSRZ
22	C1	37	LYS	2.8
35	CF	71	ARG	2.8
31	CA	795	C	2.8
34	CE	160	ALA	2.8
44	CP	50	ALA	2.8
47	CS	28	ALA	2.8
26	C5	20	ASP	2.8
31	CA	361	G	2.8
55	DI	66	GLY	2.8
31	CA	1214	A	2.8
16	BP	81	ALA	2.8
51	CW	67	GLY	2.8
1	BA	1218	C	2.8
1	BA	1226	C	2.8
13	BM	14	HIS	2.8
17	AQ	9	GLN	2.7
20	BT	32	ILE	2.7
33	DA	2146	C	2.8
40	CL	111	LYS	2.8
49	CU	79	ASP	2.8
49	DU	91	GLN	2.7
45	CQ	11	GLU	2.7
31	CA	448	U	2.7
9	BI	68	LYS	2.7
39	CK	89	PHE	2.7
43	CO	36	THR	2.7
47	CS	82	HIS	2.7
35	CF	163	ASP	2.7
10	BJ	86	ALA	2.7
28	CB	16	G	2.7
36	CG	94	TYR	2.7
39	CK	124	VAL	2.7
50	DV	53	ASN	2.7
3	BC	79	LYS	2.7
13	BM	6	GLY	2.7
31	CA	1319	C	2.7
27	C0	43	ALA	2.7
44	CP	99	TYR	2.7
46	CR	32	TYR	2.7
52	CX	38	VAL	2.7
10	BJ	27	GLU	2.7
34	CE	125	SER	2.7

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Mol	Chain	Res	Type	RSRZ
47	CS	101	ILE	2.7
36	CG	127	THR	2.7
9	BI	72	ILE	2.7
13	BM	115	PRO	2.7
26	C5	9	LYS	2.7
31	CA	1217	U	2.7
35	CF	80	ARG	2.7
38	CJ	92	LYS	2.7
41	CM	132	ARG	2.7
8	BH	121	LEU	2.7
47	CS	29	THR	2.7
1	BA	977	A	2.7
1	BA	1018	G	2.7
1	BA	1033	G	2.7
31	CA	501	A	2.7
31	CA	508	A	2.7
31	CA	2792	A	2.7
42	CN	79	ALA	2.7
1	BA	83	C	2.7
7	BG	144	MET	2.7
9	BI	31	ASN	2.7
20	BT	51	PHE	2.7
22	C1	23	THR	2.7
24	C3	17	GLY	2.7
40	CL	68	GLY	2.7
29	CC	245	VAL	2.7
50	CV	80	ALA	2.7
1	AA	1000	A	2.7
33	DA	2153	C	2.7
34	CE	165	HIS	2.7
40	CL	28	SER	2.7
48	CT	97	LEU	2.7
31	CA	475	C	2.7
31	CA	884	U	2.7
41	CM	50	PHE	2.7
30	CD	9	VAL	2.7
3	BC	170	GLU	2.7
41	CM	5	THR	2.7
19	BS	15	LEU	2.7
27	C0	9	GLN	2.7
1	BA	68	G	2.7
1	BA	108	G	2.7

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Mol	Chain	Res	Type	RSRZ
47	CS	80	ARG	2.7
9	BI	17	ALA	2.7
14	AN	33	ASP	2.7
25	C4	27	ALA	2.7
34	CE	51	GLU	2.7
35	CF	21	ASN	2.7
34	CE	91	ASP	2.7
36	CG	19	ILE	2.7
36	CG	46	ALA	2.7
36	CG	48	ASN	2.7
34	CE	134	LEU	2.7
7	BG	137	LYS	2.7
38	DJ	16	GLY	2.7
50	CV	55	PRO	2.7
21	AU	8	GLU	2.7
20	BT	39	ILE	2.7
31	CA	1058	U	2.7
33	DA	546	U	2.7
55	DI	118	ILE	2.7
1	BA	202	G	2.7
1	BA	976	G	2.7
1	BA	998	C	2.7
1	BA	1209	C	2.7
7	BG	99	LEU	2.7
20	BT	85	LYS	2.7
10	BJ	16	ARG	2.7
7	BG	132	GLY	2.7
9	BI	32	GLN	2.7
27	C0	55	VAL	2.7
52	CX	46	HIS	2.7
44	CP	57	ALA	2.7
10	BJ	10	LEU	2.7
29	CC	37	ASN	2.7
31	CA	505	A	2.7
19	BS	67	VAL	2.7
38	DJ	108	GLU	2.7
49	CU	14	PRO	2.7
7	BG	134	ALA	2.7
34	CE	132	LYS	2.6
55	DI	132	TYR	2.6
39	CK	78	THR	2.6
8	BH	120	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
31	CA	1866	A	2.6
35	CF	62	GLY	2.6
50	CV	60	GLU	2.6
54	CZ	31	GLN	2.6
31	CA	1625	C	2.6
30	CD	184	ARG	2.6
35	CF	55	ALA	2.6
31	CA	488	G	2.6
13	BM	54	ASP	2.6
37	CH	132	PHE	2.6
47	CS	43	ASN	2.6
33	DA	1094	U	2.6
53	CY	8	THR	2.6
55	DI	21	GLY	2.6
53	CY	28	ARG	2.6
16	BP	54	LEU	2.6
19	BS	16	LEU	2.6
30	CD	132	ALA	2.6
38	DJ	106	LEU	2.6
44	CP	26	LEU	2.6
44	CP	41	ALA	2.6
31	CA	22	C	2.6
21	AU	9	ASN	2.6
26	C5	35	GLN	2.6
31	CA	537	G	2.6
31	CA	1026	G	2.6
31	CA	1332	G	2.6
35	CF	17	MET	2.6
36	CG	42	GLU	2.6
38	DJ	46	THR	2.6
42	CN	134	THR	2.6
10	BJ	100	ILE	2.6
31	CA	2817	U	2.6
20	BT	11	ALA	2.6
31	CA	1069	A	2.6
35	CF	97	TRP	2.6
29	CC	234	GLY	2.6
31	CA	1104	C	2.6
31	CA	1606	C	2.6
35	CF	32	GLU	2.6
1	BA	69	G	2.6
1	BA	1003	G	2.6

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Mol	Chain	Res	Type	RSRZ
1	BA	1017	U	2.6
31	CA	1017	G	2.6
31	CA	1271	G	2.6
38	DJ	120	ALA	2.6
48	CT	54	ALA	2.6
7	BG	6	VAL	2.6
9	BI	122	ARG	2.6
14	BN	41	ARG	2.6
50	CV	70	VAL	2.6
31	CA	353	C	2.6
31	CA	1320	C	2.6
22	C1	44	THR	2.6
25	C4	52	LYS	2.6
39	CK	125	TYR	2.6
31	CA	2506	U	2.6
44	CP	92	PHE	2.6
10	BJ	81	GLU	2.6
23	C2	42	VAL	2.6
27	C0	37	GLU	2.6
39	CK	62	VAL	2.6
13	AM	19	LEU	2.6
22	C1	20	ASP	2.6
30	CD	200	ASP	2.6
31	CA	44	A	2.6
31	CA	443	A	2.6
31	CA	1614	A	2.6
31	CA	2883	A	2.6
31	CA	335	C	2.6
37	DH	106	ALA	2.6
38	CJ	15	ALA	2.6
36	CG	152	ARG	2.6
33	DA	2122	U	2.6
36	CG	168	VAL	2.6
53	CY	56	MET	2.6
43	CO	97	ILE	2.6
1	BA	86	G	2.6
33	DA	1068	G	2.6
38	DJ	110	ALA	2.6
1	BA	1019	A	2.6
44	CP	67	ASN	2.6
7	BG	60	GLU	2.6
9	BI	43	THR	2.6

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Mol	Chain	Res	Type	RSRZ
16	BP	50	THR	2.6
31	CA	531	C	2.6
31	CA	1547	C	2.6
31	CA	810	U	2.6
10	BJ	6	ILE	2.6
34	CE	177	PRO	2.6
36	CG	41	VAL	2.6
37	DH	87	GLU	2.6
1	BA	954	G	2.6
10	BJ	28	THR	2.6
24	C3	11	LYS	2.6
31	CA	1099	G	2.6
36	CG	69	ARG	2.6
49	CU	24	MET	2.6
46	CR	38	ALA	2.6
38	DJ	58	VAL	2.6
46	CR	34	VAL	2.6
37	DH	77	THR	2.6
53	CY	74	ARG	2.6
22	C1	42	HIS	2.6
25	C4	4	ILE	2.6
40	CL	38	ILE	2.6
31	CA	1213	A	2.6
1	BA	90	C	2.6
9	BI	16	ALA	2.6
43	CO	74	GLU	2.6
44	CP	27	VAL	2.6
48	CT	91	GLY	2.6
51	CW	59	GLU	2.6
3	BC	195	VAL	2.6
19	BS	23	VAL	2.6
39	CK	141	ASP	2.6
52	CX	71	VAL	2.6
17	BQ	45	HIS	2.6
20	BT	80	THR	2.6
24	C3	22	MET	2.6
41	CM	8	PRO	2.6
35	CF	34	ILE	2.6
24	C3	18	PHE	2.5
11	AK	66	ALA	2.5
14	AN	39	GLU	2.5
18	BR	51	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
34	CE	50	ALA	2.5
46	CR	118	ALA	2.5
1	BA	988	G	2.5
31	CA	1607	C	2.5
35	CF	112	ARG	2.5
50	CV	49	VAL	2.5
50	CV	9	ASP	2.5
19	BS	42	PRO	2.5
50	CV	15	THR	2.5
37	CH	102	ALA	2.5
39	CK	83	GLY	2.5
36	CG	18	LYS	2.5
48	CT	42	LYS	2.5
1	BA	1305	G	2.5
31	CA	266	G	2.5
20	BT	68	HIS	2.5
10	AJ	35	GLN	2.5
13	BM	100	GLN	2.5
30	CD	77	ARG	2.5
35	CF	68	THR	2.5
39	CK	88	THR	2.5
41	CM	126	ARG	2.5
53	CY	14	THR	2.5
35	CF	31	VAL	2.5
38	CJ	106	LEU	2.5
13	AM	11	ASP	2.5
17	BQ	21	ILE	2.5
31	CA	2105	U	2.5
43	CO	106	ASP	2.5
1	BA	983	A	2.5
31	CA	2666	C	2.5
10	AJ	36	VAL	2.5
27	C0	8	THR	2.5
36	CG	49	THR	2.5
48	CT	58	ALA	2.5
31	CA	539	G	2.5
31	CA	1334	G	2.5
47	CS	14	VAL	2.5
25	C4	14	PHE	2.5
35	CF	102	ARG	2.5
43	CO	102	PHE	2.5
1	BA	1211	U	2.5

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Mol	Chain	Res	Type	RSRZ
8	BH	2	SER	2.5
10	BJ	93	ALA	2.5
1	BA	67	C	2.5
1	BA	1210	C	2.5
20	BT	42	GLY	2.5
23	C2	12	VAL	2.5
35	CF	107	ALA	2.5
31	CA	1548	A	2.5
33	DA	2165	C	2.5
37	CH	142	VAL	2.5
1	BA	104	G	2.5
1	BA	378	G	2.5
31	CA	205	G	2.5
7	BG	37	SER	2.5
44	CP	32	PRO	2.5
48	CT	101	SER	2.5
1	BA	842	U	2.5
1	BA	1308	U	2.5
31	CA	2796	U	2.5
38	CJ	105	GLN	2.5
49	CU	61	LEU	2.5
1	BA	210	C	2.5
1	BA	980	C	2.5
31	CA	316	C	2.5
31	CA	352	A	2.5
31	CA	1251	C	2.5
31	CA	2753	A	2.5
31	CA	2820	A	2.5
16	AP	47	GLU	2.5
43	CO	78	LYS	2.5
51	CW	7	GLU	2.5
38	DJ	57	VAL	2.5
1	BA	1008	U	2.5
31	CA	387	U	2.5
37	CH	58	LEU	2.5
9	AI	129	LYS	2.5
1	BA	222	C	2.5
31	CA	680	C	2.5
11	BK	73	ALA	2.5
35	CF	13	VAL	2.5
37	CH	74	ALA	2.5
38	DJ	47	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
39	CK	73	VAL	2.5
14	BN	46	LEU	2.5
40	CL	84	CYS	2.5
43	CO	18	GLN	2.5
49	CU	87	LEU	2.5
24	C3	13	ASN	2.5
31	CA	2871	U	2.5
31	CA	2671	G	2.5
52	CX	72	LYS	2.5
13	BM	71	ARG	2.5
36	CG	82	GLY	2.5
1	BA	1137	C	2.5
31	CA	478	A	2.5
33	DA	2104	C	2.5
45	CQ	74	PHE	2.5
36	CG	131	ILE	2.5
36	CG	130	GLU	2.5
55	DI	40	GLU	2.5
43	CO	71	ARG	2.5
20	BT	72	ALA	2.5
21	AU	52	ALA	2.5
30	CD	47	ALA	2.5
34	CE	36	ALA	2.5
47	CS	57	GLY	2.5
16	BP	38	PHE	2.5
7	BG	123	GLU	2.5
31	CA	2163	A	2.5
31	CA	2175	C	2.5
35	CF	121	SER	2.5
19	BS	3	ARG	2.5
36	CG	55	ARG	2.5
42	CN	105	MET	2.5
36	CG	79	VAL	2.5
36	CG	108	GLY	2.5
55	DI	22	ALA	2.5
2	BB	126	PHE	2.5
35	CF	135	GLN	2.5
36	CG	126	PRO	2.5
19	BS	73	GLU	2.5
28	CB	20	G	2.5
31	CA	1216	G	2.5
43	CO	3	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
47	CS	68	ARG	2.5
53	CY	34	HIS	2.5
1	BA	215	C	2.4
31	CA	509	C	2.4
31	CA	1764	C	2.4
39	CK	92	MET	2.4
31	CA	631	A	2.4
36	CG	125	CYS	2.4
1	AA	88	U	2.4
38	CJ	27	ALA	2.4
45	CQ	59	PHE	2.4
42	CN	50	ARG	2.4
52	DX	85	GLU	2.4
9	BI	63	LEU	2.4
17	AQ	4	LYS	2.4
51	CW	48	MET	2.4
31	CA	30	G	2.4
31	CA	585	G	2.4
31	CA	1233	C	2.4
31	CA	1408	G	2.4
31	CA	1867	G	2.4
47	CS	72	VAL	2.4
49	CU	31	VAL	2.4
44	CP	77	ALA	2.4
31	CA	87	U	2.4
31	CA	892	A	2.4
35	CF	106	ILE	2.4
40	CL	48	PRO	2.4
52	CX	68	LYS	2.4
11	BK	43	GLY	2.4
34	CE	179	SER	2.4
7	BG	18	PHE	2.4
29	CC	2	ALA	2.4
35	CF	178	ARG	2.4
29	CC	46	ASN	2.4
1	BA	1312	G	2.4
31	CA	124	G	2.4
31	CA	343	C	2.4
31	CA	686	U	2.4
33	DA	1176	U	2.4
2	BB	14	VAL	2.4
30	CD	39	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
34	CE	100	MET	2.4
35	CF	74	VAL	2.4
50	CV	93	VAL	2.4
3	BC	29	PHE	2.4
38	DJ	62	TYR	2.4
42	CN	110	GLU	2.4
43	DO	123	GLU	2.4
34	CE	90	GLN	2.4
1	BA	135	C	2.4
1	BA	1364	U	2.4
28	CB	37	C	2.4
33	DA	2170	A	2.4
53	CY	11	ARG	2.4
8	BH	113	ASP	2.4
31	CA	7	G	2.4
31	CA	859	G	2.4
31	CA	1248	G	2.4
31	CA	2621	G	2.4
14	BN	17	ALA	2.4
43	CO	119	SER	2.4
26	C5	12	ARG	2.4
31	CA	240	C	2.4
31	CA	267	C	2.4
33	DA	1726	C	2.4
51	CW	71	LYS	2.4
52	CX	75	LYS	2.4
13	BM	37	ALA	2.4
31	CA	2860	A	2.4
31	CA	1324	G	2.4
31	CA	2828	G	2.4
45	CQ	109	ARG	2.4
7	BG	47	LEU	2.4
38	DJ	11	LEU	2.4
44	CP	106	LEU	2.4
38	DJ	75	PRO	2.4
41	CM	141	LYS	2.4
47	CS	85	LYS	2.4
52	CX	60	PHE	2.4
31	CA	29	U	2.4
46	CR	113	ALA	2.4
1	BA	1214	C	2.4
10	BJ	72	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
33	DA	1072	C	2.4
30	CD	199	SER	2.4
40	CL	2	ILE	2.4
1	BA	66	A	2.4
31	CA	883	G	2.4
31	CA	1107	G	2.4
31	CA	2162	G	2.4
37	DH	96	THR	2.4
23	C2	19	HIS	2.4
34	CE	49	ARG	2.4
39	CK	9	GLU	2.4
39	CK	75	TYR	2.4
52	CX	37	ILE	2.4
43	CO	20	MET	2.4
51	CW	1	MET	2.4
54	CZ	25	GLN	2.4
2	BB	201	PRO	2.4
47	CS	94	THR	2.4
1	BA	1475	G	2.4
31	CA	230	G	2.4
39	CK	76	HIS	2.4
39	CK	49	ASP	2.4
22	C1	29	SER	2.4
43	CO	101	GLY	2.4
31	CA	1100	C	2.4
31	CA	2129	C	2.4
13	BM	112	PRO	2.4
31	CA	222	A	2.4
35	CF	111	ILE	2.4
36	CG	27	LYS	2.4
38	DJ	113	LYS	2.4
43	CO	68	ALA	2.4
48	CT	66	ILE	2.4
48	CT	72	THR	2.4
55	DI	63	ALA	2.4
13	BM	65	VAL	2.4
46	CR	4	VAL	2.4
1	BA	133	U	2.4
16	BP	39	PHE	2.4
31	CA	1060	U	2.4
41	CM	60	ARG	2.4
1	BA	1028	C	2.4

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Mol	Chain	Res	Type	RSRZ
1	BA	1322	C	2.4
2	BB	31	ILE	2.4
3	BC	207	ILE	2.4
31	CA	444	C	2.4
31	CA	2178	C	2.4
55	DI	135	ALA	2.4
1	BA	1257	A	2.3
13	BM	25	VAL	2.3
17	AQ	54	GLY	2.3
31	CA	2158	A	2.3
33	DA	2169	A	2.3
35	CF	142	ASP	2.3
38	DJ	30	GLN	2.3
50	CV	85	PHE	2.3
31	CA	2786	U	2.3
34	CE	16	GLU	2.3
1	BA	1221	G	2.3
3	BC	71	ALA	2.3
13	BM	35	ALA	2.3
31	CA	551	G	2.3
31	CA	976	G	2.3
33	DA	882	G	2.3
35	CF	168	ALA	2.3
3	BC	197	GLY	2.3
7	BG	64	VAL	2.3
31	CA	2767	C	2.3
36	DG	111	HIS	2.3
43	CO	37	THR	2.3
44	CP	75	GLY	2.3
43	CO	40	LYS	2.3
50	CV	101	GLU	2.3
1	BA	1286	U	2.3
5	BE	149	SER	2.3
31	CA	545	U	2.3
35	CF	104	ILE	2.3
46	CR	24	TYR	2.3
51	CW	23	ALA	2.3
2	AB	37	LYS	2.3
13	BM	111	GLY	2.3
31	CA	411	G	2.3
31	CA	1071	G	2.3
31	CA	1300	G	2.3

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Mol	Chain	Res	Type	RSRZ
31	CA	2877	G	2.3
33	DA	883	G	2.3
46	CR	26	GLY	2.3
30	CD	148	GLN	2.3
31	CA	31	C	2.3
31	CA	2150	C	2.3
35	CF	46	ASP	2.3
54	CZ	5	GLU	2.3
2	BB	166	ALA	2.3
13	BM	5	ALA	2.3
31	CA	2835	A	2.3
33	DA	1098	A	2.3
30	CD	56	LYS	2.3
46	CR	8	VAL	2.3
31	CA	85	G	2.3
45	CQ	108	ALA	2.3
16	BP	16	PHE	2.3
17	BQ	46	VAL	2.3
34	CE	15	SER	2.3
45	CQ	17	VAL	2.3
46	CR	39	VAL	2.3
54	CZ	4	LYS	2.3
31	CA	1729	U	2.3
34	CE	42	GLY	2.3
38	DJ	119	GLY	2.3
3	BC	28	GLU	2.3
9	BI	59	GLU	2.3
35	CF	11	GLU	2.3
10	BJ	83	THR	2.3
30	CD	35	THR	2.3
44	CP	24	THR	2.3
3	BC	103	ILE	2.3
13	BM	44	LYS	2.3
20	BT	46	ALA	2.3
41	CM	138	ALA	2.3
48	CT	16	LYS	2.3
8	BH	122	GLY	2.3
9	BI	39	PHE	2.3
22	C1	51	GLY	2.3
23	C2	13	SER	2.3
24	C3	15	SER	2.3
44	CP	86	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
52	CX	79	PHE	2.3
28	CB	24	G	2.3
28	CB	117	G	2.3
31	CA	35	G	2.3
31	CA	1622	G	2.3
31	CA	2630	G	2.3
33	DA	2156	G	2.3
55	DI	89	PRO	2.3
49	CU	4	GLU	2.3
34	CE	138	LEU	2.3
37	CH	6	LEU	2.3
9	BI	124	ARG	2.3
25	C4	47	LYS	2.3
30	CD	38	LYS	2.3
31	CA	456	C	2.3
31	CA	2164	C	2.3
48	CT	1	MET	2.3
31	CA	277	G	2.3
31	CA	474	G	2.3
33	DA	1093	G	2.3
50	CV	46	GLN	2.3
1	AA	1441	A	2.3
24	C3	24	THR	2.3
31	CA	270	A	2.3
31	CA	1321	A	2.3
38	DJ	8	TYR	2.3
45	CQ	32	VAL	2.3
52	CX	84	ALA	2.3
14	BN	16	LEU	2.3
20	BT	25	ARG	2.3
20	BT	41	ALA	2.3
20	BT	52	ASN	2.3
30	CD	75	ALA	2.3
31	CA	1176	U	2.3
37	CH	36	ALA	2.3
47	CS	42	ALA	2.3
39	CK	50	THR	2.3
48	CT	104	THR	2.3
55	DI	50	VAL	2.3
1	BA	959	A	2.3
31	CA	38	A	2.3
31	CA	259	G	2.3

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Mol	Chain	Res	Type	RSRZ
31	CA	332	A	2.3
31	CA	469	G	2.3
31	CA	472	A	2.3
31	CA	1227	G	2.3
40	CL	101	GLY	2.3
41	CM	143	GLU	2.3
38	DJ	93	PRO	2.3
2	BB	129	LEU	2.3
10	BJ	40	ILE	2.3
24	C3	19	ARG	2.3
36	CG	170	ARG	2.3
26	C5	8	LYS	2.3
31	CA	550	C	2.3
49	CU	64	LYS	2.3
48	CT	109	ASP	2.3
1	BA	1275	A	2.3
31	CA	126	A	2.3
19	BS	78	ARG	2.3
31	CA	2004	G	2.3
43	CO	30	ARG	2.3
44	CP	19	GLN	2.3
47	CS	84	ARG	2.3
10	BJ	21	ALA	2.3
24	C3	23	ALA	2.3
26	C5	32	LYS	2.3
29	CC	92	ALA	2.3
30	CD	104	VAL	2.3
43	CO	32	GLU	2.3
1	BA	1325	C	2.3
31	CA	2755	C	2.3
16	BP	51	ARG	2.3
47	CS	25	LEU	2.3
27	C0	14	ILE	2.3
7	BG	141	VAL	2.3
19	BS	25	SER	2.3
14	BN	42	TRP	2.2
31	CA	497	A	2.3
31	CA	1572	A	2.3
31	CA	39	G	2.2
38	DJ	91	GLY	2.2
6	AF	1	MET	2.2
27	C0	11	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	895	U	2.2
48	CT	84	ARG	2.2
31	CA	2787	C	2.2
49	CU	74	ILE	2.2
51	CW	2	PHE	2.2
54	CZ	26	PHE	2.2
7	BG	86	GLN	2.2
13	AM	32	ALA	2.2
55	DI	112	ALA	2.2
1	BA	958	A	2.2
1	BA	1274	A	2.2
14	BN	13	ARG	2.2
31	CA	1285	A	2.2
31	CA	1654	A	2.2
2	BB	117	LEU	2.2
19	BS	31	LEU	2.2
42	CN	88	ASN	2.2
46	CR	22	LYS	2.2
55	DI	117	LEU	2.2
1	BA	1006	G	2.2
31	CA	971	G	2.2
31	CA	1038	G	2.2
37	CH	119	ASN	2.2
1	AA	1025	U	2.2
7	AG	62	PHE	2.2
35	CF	114	PHE	2.2
40	CL	95	ILE	2.2
42	CN	9	PHE	2.2
47	CS	47	VAL	2.2
31	CA	57	C	2.2
33	DA	1172	C	2.2
44	CP	113	ALA	2.2
2	BB	128	LYS	2.2
10	BJ	82	LYS	2.2
1	AA	1016	A	2.2
30	CD	48	ILE	2.2
31	CA	330	A	2.2
31	CA	2873	A	2.2
33	DA	2147	A	2.2
47	CS	95	ASP	2.2
48	CT	57	ASN	2.2
51	CW	66	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
18	BR	23	TYR	2.2
30	CD	36	GLN	2.2
30	CD	71	ALA	2.2
35	CF	43	ALA	2.2
38	DJ	77	ALA	2.2
41	CM	130	GLY	2.2
52	CX	61	ALA	2.2
36	CG	176	LYS	2.2
14	AN	27	LEU	2.2
30	CD	139	SER	2.2
31	CA	1170	C	2.2
31	CA	1730	C	2.2
13	BM	9	ILE	2.2
19	BS	19	VAL	2.2
1	BA	174	A	2.2
14	BN	57	PRO	2.2
35	CF	133	ARG	2.2
40	CL	53	LYS	2.2
41	CM	24	GLY	2.2
54	CZ	7	ARG	2.2
24	C3	36	ALA	2.2
1	BA	218	U	2.2
31	CA	26	G	2.2
31	CA	512	G	2.2
31	CA	1252	G	2.2
31	CA	2791	G	2.2
33	DA	2168	G	2.2
1	BA	214	C	2.2
1	BA	979	C	2.2
33	DA	2161	C	2.2
7	BG	5	ARG	2.2
48	CT	98	LYS	2.2
51	CW	34	LYS	2.2
7	AG	68	ASN	2.2
36	CG	59	ALA	2.2
36	CG	145	ALA	2.2
37	DH	66	ASN	2.2
37	DH	104	THR	2.2
46	CR	71	GLN	2.2
8	BH	99	LEU	2.2
18	BR	74	HIS	2.2
31	CA	526	A	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	1108	U	2.2
31	CA	2660	A	2.2
33	DA	1077	A	2.2
48	CT	19	LEU	2.2
3	BC	51	SER	2.2
22	C1	7	LYS	2.2
30	CD	189	VAL	2.2
34	CE	148	ILE	2.2
41	CM	42	SER	2.2
51	DW	69	GLU	2.2
28	CB	21	G	2.2
31	CA	1389	G	2.2
31	CA	1444	G	2.2
31	CA	1653	G	2.2
31	CA	2128	G	2.2
31	CA	2808	G	2.2
17	BQ	9	GLN	2.2
38	DJ	115	ALA	2.2
42	CN	106	ASP	2.2
50	CV	69	ASN	2.2
10	BJ	30	LYS	2.2
34	CE	79	ARG	2.2
38	CJ	72	LYS	2.2
43	CO	80	PHE	2.2
7	BG	54	SER	2.2
35	CF	19	GLU	2.2
37	CH	130	VAL	2.2
39	CK	17	VAL	2.2
30	CD	76	GLY	2.2
2	BB	134	ALA	2.2
35	CF	53	ALA	2.2
45	CQ	98	TYR	2.2
1	BA	379	C	2.2
29	CC	33	LEU	2.2
7	BG	84	THR	2.2
19	AS	55	ARG	2.2
29	CC	239	ASN	2.2
30	CD	167	ASN	2.2
31	CA	445	C	2.2
31	CA	81	G	2.2
31	CA	327	G	2.2
37	CH	27	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
46	CR	30	ARG	2.2
50	CV	86	ARG	2.2
30	CD	27	ILE	2.2
30	CD	89	GLU	2.2
13	BM	74	SER	2.2
31	CA	2131	U	2.2
34	CE	155	GLU	2.2
31	CA	1254	A	2.2
36	CG	149	ARG	2.2
38	CJ	100	LYS	2.2
48	CT	68	ASP	2.2
1	BA	1132	C	2.2
37	DH	11	ASN	2.2
52	CX	43	THR	2.2
16	AP	78	VAL	2.2
17	AQ	83	VAL	2.2
31	CA	1303	G	2.2
39	CK	66	GLY	2.2
41	CM	88	GLY	2.2
10	BJ	71	LEU	2.2
23	C2	14	SER	2.2
26	C5	2	LYS	2.2
26	C5	34	LYS	2.2
34	CE	182	ALA	2.2
35	CF	45	ALA	2.2
51	CW	58	SER	2.2
53	CY	77	LYS	2.2
1	BA	197	A	2.2
13	AM	115	PRO	2.2
14	BN	40	ASP	2.2
37	CH	47	PHE	2.2
45	CQ	18	PRO	2.2
7	BG	38	THR	2.2
26	C5	30	GLU	2.2
8	BH	89	LYS	2.2
31	CA	32	C	2.2
8	BH	130	ALA	2.2
29	CC	202	LEU	2.2
36	CG	72	LEU	2.2
34	CE	70	SER	2.2
1	BA	1013	G	2.2
28	CB	64	G	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	494	G	2.2
34	CE	46	GLN	2.2
11	AK	79	ILE	2.2
49	CU	53	VAL	2.2
52	CX	85	GLU	2.2
7	BG	68	ASN	2.2
13	BM	62	LYS	2.2
14	BN	53	ARG	2.2
19	BS	79	THR	2.2
29	CC	90	ASN	2.2
30	CD	59	ARG	2.2
36	CG	33	LEU	2.1
9	BI	44	ALA	2.1
31	CA	145	C	2.1
31	CA	1102	C	2.1
31	CA	1507	C	2.1
31	CA	1531	C	2.1
8	AH	2	SER	2.1
14	BN	55	SER	2.1
40	CL	3	GLN	2.1
1	BA	324	G	2.1
31	CA	1540	G	2.1
31	CA	412	A	2.1
31	CA	2173	A	2.1
40	CL	60	ALA	2.1
13	BM	107	ARG	2.1
15	AO	89	ARG	2.1
19	BS	58	VAL	2.1
24	C3	30	VAL	2.1
31	CA	876	C	2.1
36	CG	90	VAL	2.1
50	CV	21	LYS	2.1
31	CA	235	U	2.1
31	CA	2903	U	2.1
33	DA	884	U	2.1
43	CO	105	GLY	2.1
41	CM	3	LEU	2.1
8	BH	55	THR	2.1
16	AP	22	ALA	2.1
25	C4	65	ALA	2.1
44	CP	34	HIS	2.1
49	CU	92	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	1382	G	2.1
31	CA	2742	G	2.1
31	CA	2812	G	2.1
31	CA	2862	G	2.1
34	CE	198	GLU	2.1
40	CL	98	ARG	2.1
37	DH	99	ILE	2.1
41	CM	127	VAL	2.1
50	CV	100	SER	2.1
1	BA	1009	U	2.1
17	BQ	44	LEU	2.1
31	CA	113	U	2.1
33	DA	1729	U	2.1
24	C3	34	ARG	2.1
41	CM	84	LYS	2.1
43	CO	70	THR	2.1
2	AB	60	ILE	2.1
10	AJ	74	VAL	2.1
23	C2	9	ILE	2.1
29	CC	251	GLN	2.1
1	AA	1036	A	2.1
19	BS	44	MET	2.1
31	CA	244	A	2.1
31	CA	914	G	2.1
31	CA	1098	A	2.1
31	CA	1287	A	2.1
31	CA	2108	A	2.1
14	BN	61	ARG	2.1
19	BS	22	ALA	2.1
31	CA	1015	U	2.1
31	CA	1018	U	2.1
38	DJ	70	VAL	2.1
44	CP	28	VAL	2.1
43	CO	100	CYS	2.1
3	BC	87	LEU	2.1
7	BG	23	LEU	2.1
30	CD	187	LEU	2.1
21	BU	55	ARG	2.1
39	CK	99	ARG	2.1
51	CW	46	LYS	2.1
19	AS	50	ALA	2.1
30	CD	206	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	71	A	2.1
31	CA	675	A	2.1
1	BA	89	U	2.1
29	CC	232	HIS	2.1
31	CA	1	G	2.1
31	CA	70	G	2.1
31	CA	1534	U	2.1
31	CA	1720	U	2.1
33	DA	139	U	2.1
33	DA	1731	G	2.1
28	CB	35	C	2.1
29	CC	64	ILE	2.1
30	CD	24	VAL	2.1
31	CA	2146	C	2.1
31	CA	2527	C	2.1
49	CU	28	ASN	2.1
52	CX	58	THR	2.1
36	CG	35	ARG	2.1
14	AN	37	SER	2.1
29	CC	30	PHE	2.1
37	CH	14	SER	2.1
1	AA	1044	A	2.1
13	BM	38	GLY	2.1
25	C4	16	LYS	2.1
31	CA	306	U	2.1
31	CA	1542	U	2.1
31	CA	2058	A	2.1
37	CH	108	VAL	2.1
42	CN	135	VAL	2.1
31	CA	16	C	2.1
31	CA	245	G	2.1
31	CA	312	G	2.1
31	CA	1323	C	2.1
31	CA	2156	G	2.1
35	CF	93	GLY	2.1
48	CT	46	LEU	2.1
52	CX	34	GLY	2.1
54	CZ	30	MET	2.1
9	BI	112	GLU	2.1
13	BM	21	SER	2.1
20	BT	38	ALA	2.1
27	C0	40	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
34	CE	149	ILE	2.1
37	DH	142	VAL	2.1
10	BJ	95	GLY	2.1
19	BS	13	LEU	2.1
1	BA	1014	A	2.1
30	CD	1	MET	2.1
30	CD	49	GLN	2.1
37	CH	107	GLY	2.1
54	CZ	35	GLY	2.1
31	CA	25	U	2.1
19	BS	77	THR	2.1
31	CA	1276	A	2.1
33	DA	613	A	2.1
40	CL	13	ASN	2.1
1	BA	1454	G	2.1
3	BC	42	TYR	2.1
7	BG	61	ALA	2.1
31	CA	242	G	2.1
31	CA	307	G	2.1
31	CA	393	C	2.1
31	CA	1197	G	2.1
31	CA	1335	C	2.1
31	CA	1517	G	2.1
31	CA	2318	G	2.1
31	CA	2874	C	2.1
39	CK	8	PRO	2.1
38	DJ	124	ALA	2.1
41	DM	144	GLU	2.1
16	AP	46	LYS	2.1
20	BT	8	LYS	2.1
55	DI	111	ALA	2.1
16	BP	4	ILE	2.1
37	CH	110	VAL	2.1
55	DI	71	CYS	2.1
44	CP	114	GLY	2.1
1	BA	1240	U	2.1
17	BQ	74	THR	2.1
31	CA	292	U	2.1
31	CA	2739	U	2.1
1	BA	325	A	2.1
1	BA	1287	A	2.1
13	BM	110	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	845	A	2.1
33	DA	654	A	2.1
37	DH	39	ALA	2.1
42	CN	8	LYS	2.1
44	CP	55	GLU	2.1
55	DI	133	GLU	2.1
17	BQ	79	VAL	2.1
31	CA	517	C	2.1
38	CJ	49	ILE	2.1
1	AA	1015	G	2.1
13	BM	69	LEU	2.1
50	CV	90	GLY	2.1
43	CO	21	PHE	2.1
46	CR	59	GLN	2.1
47	CS	93	PHE	2.1
1	BA	843	U	2.1
31	CA	2818	U	2.1
12	BL	24	LEU	2.1
13	AM	33	ILE	2.1
31	CA	278	A	2.1
31	CA	2309	A	2.1
43	CO	75	ILE	2.1
41	CM	124	GLY	2.1
42	CN	124	LEU	2.1
50	CV	103	ILE	2.1
7	BG	9	GLN	2.0
31	CA	564	C	2.1
31	CA	2830	C	2.1
42	CN	60	GLN	2.0
46	CR	36	PHE	2.0
13	BM	92	ARG	2.0
15	BO	17	ARG	2.0
1	BA	107	G	2.0
1	BA	1309	G	2.0
31	CA	2732	G	2.0
34	CE	34	ALA	2.0
37	CH	106	ALA	2.0
39	CK	53	TYR	2.0
1	BA	1023	U	2.0
6	BF	92	THR	2.0
31	CA	2690	U	2.0
40	CL	69	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
40	CL	88	ASN	2.0
50	CV	41	LEU	2.0
55	DI	123	ILE	2.0
1	BA	344	A	2.0
7	AG	9	GLN	2.0
13	BM	76	SER	2.0
13	BM	90	ARG	2.0
19	BS	55	ARG	2.0
31	CA	340	A	2.0
31	CA	439	A	2.0
31	CA	1134	A	2.0
31	CA	2154	A	2.0
34	CE	158	PHE	2.0
35	CF	100	PHE	2.0
46	CR	33	ARG	2.0
33	DA	885	C	2.0
33	DA	1064	C	2.0
47	DS	45	GLU	2.0
39	CK	59	ALA	2.0
41	CM	83	ALA	2.0
51	CW	57	TYR	2.0
2	BB	10	LEU	2.0
10	BJ	92	LEU	2.0
25	C4	57	LEU	2.0
1	BA	103	U	2.0
31	CA	1435	G	2.0
2	AB	6	MET	2.0
19	AS	32	ARG	2.0
40	CL	108	ARG	2.0
34	CE	197	GLU	2.0
38	CJ	107	GLN	2.0
44	CP	69	ASP	2.0
54	CZ	24	GLU	2.0
31	CA	1080	A	2.0
31	CA	1204	A	2.0
33	DA	2154	A	2.0
40	CL	52	VAL	2.0
31	CA	1330	C	2.0
36	CG	133	LEU	2.0
40	CL	118	LEU	2.0
51	CW	63	ILE	2.0
2	AB	156	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
31	CA	1460	U	2.0
34	CE	1	MET	2.0
1	AA	1024	G	2.0
1	BA	1222	G	2.0
10	BJ	24	GLU	2.0
19	BS	34	TRP	2.0
31	CA	496	G	2.0
31	CA	2838	G	2.0
19	AS	81	ARG	2.0
28	CB	52	A	2.0
31	CA	2725	A	2.0
30	CD	133	THR	2.0
31	CA	2712	C	2.0
38	DJ	118	THR	2.0
21	AU	36	GLU	2.0
3	BC	122	SER	2.0
9	BI	58	VAL	2.0
23	C2	38	LYS	2.0
31	CA	2109	U	2.0
47	CS	33	VAL	2.0
47	CS	89	HIS	2.0
2	BB	34	ALA	2.0
7	BG	39	ALA	2.0
35	DF	2	ALA	2.0
1	AA	79	G	2.0
1	BA	1270	G	2.0
31	CA	2010	G	2.0
33	DA	2128	G	2.0
41	CM	22	GLY	2.0
30	CD	58	ASN	2.0
31	CA	794	A	2.0
31	CA	1253	A	2.0
34	CE	141	MET	2.0
31	CA	812	C	2.0
31	CA	1289	C	2.0
42	CN	7	THR	2.0
42	CN	84	LYS	2.0
2	AB	221	VAL	2.0
37	CH	122	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	PSU	DA	2504	20/21	0.99	0.17	-	29,34,37,41	0
33	2MG	DA	1835	24/25	0.97	0.18	-	44,48,54,61	0
1	2MG	AA	966	24/25	0.95	0.13	-	83,86,88,88	0
31	5MC	CA	1962	21/22	0.95	0.15	-	76,79,80,85	0
33	2MG	DA	2445	24/25	0.98	0.19	-	16,25,30,31	0
33	PSU	DA	1911	20/21	0.96	0.13	-	86,90,91,92	0
1	2MG	BA	966	24/25	0.91	0.25	-	140,144,153,153	0
31	OMC	CA	2498	21/22	0.96	0.22	-	98,104,108,109	0
31	2MA	CA	2503	23/24	0.86	0.25	-	101,104,114,114	0
1	5MC	AA	967	21/22	0.95	0.16	-	84,88,89,89	0
31	G7M	CA	2069	24/25	0.86	0.21	-	105,111,117,118	0
42	4D4	DN	81[B]	12/13	0.97	0.26	-	13,22,30,31	9
31	6MZ	CA	1618	23/24	0.84	0.26	-	165,167,172,173	0
12	D2T	BL	89	10/11	0.92	0.25	-	79,85,97,98	0
31	PSU	CA	2605	20/21	0.91	0.22	-	81,87,95,96	0
33	OMG	DA	2251	24/25	0.99	0.16	-	28,30,40,44	0
1	G7M	AA	527	24/25	0.97	0.14	-	57,62,67,70	0
1	UR3	BA	1498	21/22	0.95	0.20	-	83,84,89,89	0
1	5MC	BA	1407	21/22	0.90	0.20	-	93,96,104,107	0
1	MA6	AA	1519	24/25	0.97	0.20	-	46,51,55,59	0
31	PSU	CA	955	20/21	0.74	0.24	-	108,113,117,117	0
33	2MA	DA	2503	23/24	0.98	0.18	-	16,28,36,40	0
31	PSU	CA	2457	20/21	0.88	0.21	-	109,112,117,118	0
31	5MU	CA	747	21/22	0.86	0.27	-	129,137,142,144	0
33	H2U	DA	2449	20/21	0.99	0.17	-	12,22,32,33	0
33	5MC	DA	1962	21/22	0.98	0.18	-	40,46,48,48	0
31	6MZ	CA	2030	23/24	0.80	0.26	-	117,125,129,130	0
33	1MG	DA	745	24/25	0.99	0.16	-	26,32,36,38	0
33	OMU	DA	2552	21/22	0.98	0.18	-	25,30,35,42	0
1	2MG	AA	1516	24/25	0.97	0.14	-	51,53,55,57	0
33	5MU	DA	747	21/22	0.99	0.17	-	26,28,35,37	0
32	MEQ	DD	150[B]	10/11	0.98	0.20	-	26,31,38,40	10
31	5MU	CA	1939	21/22	0.94	0.14	-	79,86,88,89	0
1	5MC	AA	1407	21/22	0.97	0.14	-	54,55,57,58	0
33	6MZ	DA	1618	23/24	0.99	0.15	-	17,28,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MEQ	DD	150[A]	10/11	0.98	0.20	-	9,14,29,29	10
33	3TD	DA	1915	21/22	0.93	0.16	-	110,116,120,122	0
33	PSU	DA	2580	20/21	0.99	0.17	-	18,26,29,31	0
1	PSU	BA	516	20/21	0.93	0.17	-	78,85,90,91	0
31	3TD	CA	1915	21/22	0.86	0.18	-	139,145,147,148	0
31	PSU	CA	2580	20/21	0.88	0.27	-	105,112,116,117	0
42	4D4	CN	81	12/13	0.89	0.32	-	99,103,115,116	0
31	OMU	CA	2552	21/22	0.88	0.31	-	100,103,113,115	0
31	PSU	CA	2504	20/21	0.89	0.27	-	91,98,101,102	0
33	6MZ	DA	2030	23/24	0.99	0.17	-	16,20,26,27	0
33	PSU	DA	2604	20/21	0.98	0.16	-	31,43,54,56	0
1	UR3	AA	1498	21/22	0.97	0.18	-	54,58,62,64	0
31	OMG	CA	2251	24/25	0.89	0.24	-	95,101,105,106	0
33	5MU	DA	1939	21/22	0.97	0.21	-	38,40,48,50	0
33	PSU	DA	955	20/21	0.99	0.17	-	17,22,24,25	0
1	2MG	AA	1207	24/25	0.93	0.13	-	90,100,107,107	0
1	MA6	AA	1518	24/25	0.97	0.16	-	45,48,54,54	0
33	PSU	DA	2605	20/21	0.99	0.16	-	33,40,41,41	0
1	MA6	BA	1519	24/25	0.94	0.23	-	78,82,85,85	0
1	2MG	BA	1516	24/25	0.91	0.18	-	82,87,93,93	0
33	G7M	DA	2069	24/25	0.99	0.15	-	34,37,43,45	0
31	1MG	CA	745	24/25	0.87	0.35	-	117,123,124,126	0
42	4D4	DN	81[A]	12/13	0.97	0.26	-	29,36,47,49	9
1	G7M	BA	527	24/25	0.95	0.15	-	69,73,78,78	0
1	4OC	AA	1402	22/23	0.96	0.16	-	60,63,64,65	0
33	PSU	DA	2457	20/21	0.98	0.15	-	24,25,30,32	0
31	PSU	CA	1911	20/21	0.89	0.17	-	128,136,137,138	0
33	OMC	DA	2498	21/22	0.99	0.17	-	15,20,26,33	0
1	4OC	BA	1402	22/23	0.96	0.19	-	72,74,77,78	0
31	PSU	CA	746	20/21	0.84	0.28	-	127,129,130,130	0
1	5MC	BA	967	21/22	0.87	0.26	-	135,141,145,145	0
12	D2T	AL	89	10/11	0.95	0.23	-	59,63,78,81	0
31	2MG	CA	1835	24/25	0.95	0.15	-	76,80,82,83	0
1	MA6	BA	1518	24/25	0.93	0.24	-	71,77,85,86	0
33	PSU	DA	1917	20/21	0.95	0.12	-	83,86,95,95	0
31	PSU	CA	1917	20/21	0.85	0.15	-	120,122,127,127	0
31	2MG	CA	2445	24/25	0.89	0.27	-	79,94,103,104	0
1	PSU	AA	516	20/21	0.96	0.13	-	77,81,84,85	0
1	2MG	BA	1207	24/25	0.86	0.24	-	154,155,158,161	0
33	PSU	DA	746	20/21	0.99	0.15	-	16,22,31,32	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
58	MPD	DA	3202	8/8	0.78	0.95	81.33	125,126,127,128	0
59	PUT	AA	1674	6/6	0.62	0.65	67.68	108,109,110,110	0
62	EDO	DA	3197	4/4	0.80	0.41	45.57	86,88,89,89	0
61	PEG	DA	3199	7/7	0.77	0.52	40.92	118,120,124,124	0
61	PEG	D3	102	7/7	0.70	0.86	38.26	105,109,110,111	0
59	PUT	DA	3211	6/6	0.80	0.41	35.76	108,110,112,113	0
59	PUT	DA	3194	6/6	0.73	0.48	35.37	88,90,92,92	0
59	PUT	DA	3183	6/6	0.87	0.29	31.96	77,78,80,80	0
56	MG	DA	3171	1/1	0.76	0.51	29.54	79,79,79,79	0
56	MG	BA	1612	1/1	0.86	0.45	29.32	200,200,200,200	0
56	MG	CA	3003	1/1	0.67	1.68	28.78	280,280,280,280	0
59	PUT	DA	3217	6/6	0.80	0.38	25.40	71,72,72,72	0
59	PUT	DA	3219	6/6	0.80	0.39	21.40	122,122,123,123	0
61	PEG	DA	3216	7/7	0.85	0.36	20.50	126,128,134,135	0
57	PG4	DA	3214	13/13	0.79	0.43	20.26	101,107,112,112	0
62	EDO	D0	101	4/4	0.95	0.38	19.18	67,67,68,69	0
56	MG	AA	1612	1/1	0.72	0.39	18.07	59,59,59,59	0
56	MG	DA	3126	1/1	0.96	0.38	18.01	48,48,48,48	0
56	MG	CA	3110	1/1	0.27	1.10	17.14	168,168,168,168	0
64	SPD	DA	3222	10/10	0.91	0.29	16.62	47,58,65,68	0
65	1PE	DA	3201	16/16	0.89	0.39	16.10	62,67,77,77	0
63	PGE	DT	201	10/10	0.77	0.56	15.06	137,138,140,140	0
59	PUT	DA	3220	6/6	0.84	0.37	14.84	55,57,61,62	0
61	PEG	DQ	201	7/7	0.60	0.72	14.07	118,119,121,121	0
63	PGE	DA	3215	10/10	0.94	0.25	13.59	81,82,84,85	0
63	PGE	DA	3212	10/10	0.88	0.34	13.47	81,82,90,93	0
58	MPD	AA	1676	8/8	0.94	0.39	12.73	96,98,102,102	0
59	PUT	DA	3210	6/6	0.72	0.37	12.43	80,83,87,88	0
56	MG	CA	3133	1/1	0.64	0.63	12.33	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
62	EDO	DA	3207	4/4	0.60	0.54	10.21	104,104,105,105	0
58	MPD	DE	301	8/8	0.58	1.01	9.66	151,152,153,153	0
59	PUT	AA	1672	6/6	0.76	0.42	9.49	88,89,89,90	0
59	PUT	DA	3203	6/6	0.84	0.39	8.77	95,96,96,96	0
57	PG4	BA	1642	13/13	0.85	0.32	8.50	94,97,106,107	0
58	MPD	DE	302	8/8	0.80	0.40	8.44	116,118,121,121	0
56	MG	DA	3146	1/1	0.94	0.24	8.03	58,58,58,58	0
63	PGE	DD	302	10/10	0.92	0.29	7.88	75,77,78,79	0
64	SPD	DA	3182	10/10	0.92	0.28	7.56	66,69,73,73	0
57	PG4	DA	3192	13/13	0.87	0.55	7.33	76,87,103,103	0
64	SPD	DA	3204	10/10	0.87	0.24	6.76	93,98,105,106	0
57	PG4	AA	1670	13/13	0.88	0.25	6.60	77,84,91,92	0
56	MG	CA	3039	1/1	0.89	0.54	6.43	203,203,203,203	0
59	PUT	AA	1673	6/6	0.84	0.36	6.30	91,92,94,95	0
58	MPD	DA	3191	8/8	0.94	0.47	6.17	99,100,101,101	0
58	MPD	AA	1671	8/8	0.86	0.67	5.71	110,112,114,115	0
63	PGE	D3	101	10/10	0.85	0.31	5.40	93,97,100,100	0
58	MPD	DA	3205	8/8	0.87	0.39	5.34	93,94,97,97	0
56	MG	CA	3026	1/1	0.52	0.57	5.31	201,201,201,201	0
66	ACY	DA	3200	4/4	0.94	0.21	5.27	83,84,85,85	0
57	PG4	DS	202	13/13	0.87	0.29	5.07	73,75,77,77	0
63	PGE	DS	201	10/10	0.79	0.40	4.64	68,74,77,77	0
56	MG	AA	1608	1/1	0.91	0.28	4.31	83,83,83,83	0
59	PUT	DA	3227	6/6	0.93	0.23	4.14	74,74,75,75	0
61	PEG	DL	201	7/7	0.90	0.30	3.93	78,80,83,84	0
56	MG	CA	3123	1/1	0.30	0.55	3.56	200,200,200,200	0
62	EDO	DA	3196	4/4	0.93	0.29	3.48	71,73,74,75	0
59	PUT	DA	3188	6/6	0.92	0.20	3.06	36,42,42,42	0
56	MG	CA	3136	1/1	0.96	0.29	3.05	66,66,66,66	0
61	PEG	AL	201	7/7	0.82	0.31	2.83	78,79,84,85	0
61	PEG	D1	102	7/7	0.90	0.23	2.78	61,65,68,69	0
56	MG	AA	1642	1/1	0.85	0.23	2.75	173,173,173,173	0
63	PGE	DA	3185	10/10	0.93	0.19	2.63	39,51,60,63	0
65	1PE	DA	3184	16/16	0.94	0.24	2.54	46,56,86,87	0
59	PUT	DA	3221	6/6	0.95	0.24	2.52	77,80,81,81	0
63	PGE	DU	101	10/10	0.95	0.23	2.43	79,83,88,88	0
56	MG	CA	3022	1/1	0.82	0.57	2.25	235,235,235,235	0
56	MG	DA	3176	1/1	0.97	0.19	2.09	47,47,47,47	0
56	MG	DA	3127	1/1	0.98	0.19	1.97	55,55,55,55	0
56	MG	DA	3036	1/1	0.98	0.17	1.79	16,16,16,16	0
64	SPD	DA	3186	10/10	0.94	0.20	1.48	52,53,57,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3018	1/1	0.96	0.36	1.16	131,131,131,131	0
57	PG4	DQ	202	13/13	0.83	0.25	1.05	65,68,81,81	0
67	GUN	DA	3209	11/11	0.92	0.23	0.98	111,112,113,113	0
56	MG	DA	3034	1/1	0.97	0.18	0.84	28,28,28,28	0
56	MG	BA	1624	1/1	0.61	0.56	0.74	274,274,274,274	0
56	MG	AA	1663	1/1	0.95	0.23	0.61	65,65,65,65	0
56	MG	CA	3153	1/1	0.95	0.23	0.50	49,49,49,49	0
56	MG	DA	3124	1/1	0.99	0.19	0.09	37,37,37,37	0
56	MG	CA	3105	1/1	0.79	0.36	-0.03	254,254,254,254	0
56	MG	AA	1669	1/1	0.93	0.23	-0.03	91,91,91,91	0
56	MG	CA	3032	1/1	-0.01	0.48	-0.05	257,257,257,257	0
56	MG	CA	3037	1/1	0.93	0.28	-0.12	206,206,206,206	0
56	MG	DA	3042	1/1	0.96	0.16	-0.18	24,24,24,24	0
56	MG	DA	3011	1/1	0.99	0.19	-0.21	9,9,9,9	0
56	MG	AA	1661	1/1	0.80	0.17	-0.40	166,166,166,166	0
56	MG	DA	3062	1/1	0.98	0.16	-0.55	110,110,110,110	0
58	MPD	DS	203	8/8	0.98	0.19	-0.57	59,60,62,64	0
56	MG	BA	1626	1/1	0.92	0.16	-0.73	138,138,138,138	0
56	MG	DA	3147	1/1	0.96	0.12	-0.74	117,117,117,117	0
62	EDO	D1	101	4/4	0.93	0.16	-0.84	53,53,53,54	0
56	MG	DA	3049	1/1	0.98	0.17	-1.08	10,10,10,10	0
56	MG	CA	3101	1/1	0.78	0.19	-1.15	164,164,164,164	0
60	ZN	D5	101	1/1	1.00	0.11	-1.17	55,55,55,55	0
56	MG	CA	3102	1/1	0.95	0.16	-1.18	92,92,92,92	0
56	MG	CA	3099	1/1	0.95	0.26	-1.19	189,189,189,189	0
56	MG	CA	3054	1/1	0.79	0.18	-1.26	180,180,180,180	0
56	MG	BA	1622	1/1	0.96	0.14	-1.26	150,150,150,150	0
56	MG	DA	3028	1/1	0.97	0.18	-1.26	21,21,21,21	0
56	MG	DA	3098	1/1	0.97	0.17	-1.30	19,19,19,19	0
56	MG	DA	3140	1/1	0.98	0.16	-1.47	73,73,73,73	0
56	MG	DA	3093	1/1	0.95	0.16	-1.54	17,17,17,17	0
56	MG	CA	3051	1/1	0.84	0.16	-1.54	183,183,183,183	0
56	MG	AA	1677	1/1	0.96	0.15	-1.67	121,121,121,121	0
56	MG	CB	202	1/1	0.93	0.09	-1.68	123,123,123,123	0
56	MG	DB	201	1/1	0.96	0.12	-1.80	66,66,66,66	0
56	MG	CA	3061	1/1	0.36	0.13	-1.83	264,264,264,264	0
60	ZN	C5	101	1/1	0.93	0.07	-1.83	149,149,149,149	0
60	ZN	AB	301	1/1	0.94	0.06	-1.84	125,125,125,125	0
56	MG	CA	3011	1/1	0.88	0.17	-1.85	68,68,68,68	0
56	MG	DA	3046	1/1	0.99	0.14	-1.87	46,46,46,46	0
56	MG	DA	3109	1/1	0.99	0.16	-1.90	13,13,13,13	0
56	MG	DA	3069	1/1	0.98	0.13	-1.97	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3019	1/1	0.64	0.16	-2.01	71,71,71,71	0
56	MG	BA	1614	1/1	0.90	0.13	-2.02	127,127,127,127	0
56	MG	CA	3009	1/1	0.95	0.14	-2.05	271,271,271,271	0
56	MG	CA	3103	1/1	0.95	0.13	-2.09	93,93,93,93	0
56	MG	AA	1656	1/1	0.81	0.12	-2.14	132,132,132,132	0
56	MG	CA	3033	1/1	0.92	0.23	-2.30	154,154,154,154	0
56	MG	CA	3006	1/1	0.56	0.19	-2.33	240,240,240,240	0
56	MG	CA	3063	1/1	0.86	0.19	-2.40	181,181,181,181	0
56	MG	CA	3088	1/1	0.89	0.14	-2.42	75,75,75,75	0
56	MG	AA	1657	1/1	0.88	0.08	-2.45	152,152,152,152	0
56	MG	BA	1601	1/1	0.93	0.10	-2.45	140,140,140,140	0
56	MG	CA	3100	1/1	0.97	0.18	-2.49	104,104,104,104	0
56	MG	DA	3022	1/1	0.99	0.14	-2.50	21,21,21,21	0
56	MG	AA	1611	1/1	0.90	0.12	-2.59	50,50,50,50	0
56	MG	AA	1659	1/1	0.96	0.10	-2.71	94,94,94,94	0
56	MG	DA	3060	1/1	0.95	0.17	-2.74	32,32,32,32	0
56	MG	BA	1632	1/1	0.92	0.11	-2.87	72,72,72,72	0
56	MG	CA	3079	1/1	0.89	0.16	-2.93	156,156,156,156	0
56	MG	DA	3162	1/1	0.95	0.11	-2.99	48,48,48,48	0
56	MG	CA	3094	1/1	0.61	0.21	-3.05	139,139,139,139	0
56	MG	DA	3226	1/1	0.97	0.12	-3.08	14,14,14,14	0
56	MG	AA	1668	1/1	0.96	0.09	-3.18	62,62,62,62	0
56	MG	DA	3016	1/1	0.96	0.06	-3.30	32,32,32,32	0
56	MG	DA	3089	1/1	0.98	0.15	-3.42	16,16,16,16	0
56	MG	AA	1648	1/1	0.97	0.07	-3.43	55,55,55,55	0
56	MG	BA	1613	1/1	0.95	0.12	-3.44	86,86,86,86	0
56	MG	CA	3085	1/1	0.93	0.14	-3.49	67,67,67,67	0
56	MG	CB	201	1/1	0.82	0.09	-3.49	169,169,169,169	0
56	MG	CA	3044	1/1	0.92	0.10	-3.51	102,102,102,102	0
56	MG	DA	3015	1/1	0.97	0.14	-3.54	28,28,28,28	0
56	MG	DA	3007	1/1	0.99	0.09	-3.61	19,19,19,19	0
56	MG	CA	3091	1/1	0.96	0.11	-3.62	137,137,137,137	0
56	MG	CA	3041	1/1	0.88	0.07	-3.78	47,47,47,47	0
56	MG	DB	204	1/1	0.94	0.12	-3.85	56,56,56,56	0
56	MG	BA	1615	1/1	0.99	0.08	-3.90	44,44,44,44	0
56	MG	CA	3031	1/1	0.88	0.06	-3.91	102,102,102,102	0
56	MG	BA	1617	1/1	0.81	0.07	-3.95	160,160,160,160	0
56	MG	DA	3023	1/1	0.99	0.14	-3.98	29,29,29,29	0
56	MG	CA	3013	1/1	0.81	0.22	-4.00	91,91,91,91	0
56	MG	BA	1610	1/1	0.92	0.06	-4.05	97,97,97,97	0
56	MG	BA	1602	1/1	0.80	0.07	-4.13	79,79,79,79	0
56	MG	DA	3091	1/1	0.99	0.11	-4.16	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3144	1/1	0.93	0.06	-4.25	54,54,54,54	0
56	MG	AA	1631	1/1	0.96	0.10	-4.35	42,42,42,42	0
56	MG	DA	3057	1/1	0.97	0.09	-4.41	33,33,33,33	0
56	MG	DA	3005	1/1	0.99	0.13	-4.51	78,78,78,78	0
56	MG	CA	3086	1/1	0.80	0.11	-4.55	67,67,67,67	0
56	MG	AA	1653	1/1	0.97	0.07	-4.63	32,32,32,32	0
56	MG	BA	1608	1/1	0.87	0.09	-4.66	122,122,122,122	0
56	MG	BA	1605	1/1	0.96	0.07	-4.68	58,58,58,58	0
56	MG	DA	3021	1/1	0.99	0.11	-5.07	9,9,9,9	0
56	MG	AA	1637	1/1	0.97	0.06	-5.36	47,47,47,47	0
56	MG	DA	3045	1/1	0.97	0.11	-5.36	25,25,25,25	0
56	MG	CA	3040	1/1	0.89	0.10	-5.62	134,134,134,134	0
56	MG	DA	3150	1/1	0.96	0.06	-5.71	38,38,38,38	0
56	MG	AA	1644	1/1	0.85	0.11	-6.06	123,123,123,123	0
56	MG	BA	1620	1/1	0.96	0.08	-6.18	90,90,90,90	0
56	MG	DA	3135	1/1	0.94	0.10	-6.21	120,120,120,120	0
56	MG	CA	3020	1/1	0.98	0.04	-6.21	73,73,73,73	0
56	MG	DA	3094	1/1	0.99	0.10	-6.28	54,54,54,54	0
56	MG	DA	3092	1/1	0.99	0.12	-6.36	11,11,11,11	0
56	MG	DA	3002	1/1	0.98	0.08	-6.49	77,77,77,77	0
56	MG	CA	3089	1/1	0.89	0.16	-6.79	69,69,69,69	0
56	MG	AA	1643	1/1	0.98	0.10	-6.87	65,65,65,65	0
56	MG	DA	3025	1/1	0.96	0.08	-7.52	74,74,74,74	0
56	MG	DA	3063	1/1	0.98	0.08	-7.78	83,83,83,83	0
56	MG	DA	3101	1/1	0.98	0.12	-7.79	26,26,26,26	0
56	MG	DA	3026	1/1	0.91	0.14	-7.92	39,39,39,39	0
56	MG	CA	3030	1/1	0.91	0.06	-8.10	76,76,76,76	0
56	MG	DA	3083	1/1	0.98	0.10	-8.21	23,23,23,23	0
56	MG	DA	3065	1/1	0.97	0.12	-8.52	24,24,24,24	0
56	MG	DA	3012	1/1	0.98	0.14	-8.66	18,18,18,18	0
56	MG	DA	3096	1/1	0.98	0.09	-9.01	36,36,36,36	0
56	MG	AA	1649	1/1	0.98	0.05	-9.36	62,62,62,62	0
56	MG	AA	1639	1/1	0.98	0.04	-9.39	82,82,82,82	0
56	MG	DA	3108	1/1	0.99	0.12	-9.55	36,36,36,36	0
56	MG	DA	3030	1/1	0.97	0.16	-9.81	26,26,26,26	0
56	MG	AA	1646	1/1	0.99	0.07	-10.67	50,50,50,50	0
56	MG	AA	1629	1/1	0.94	0.07	-10.69	100,100,100,100	0
56	MG	DA	3038	1/1	0.99	0.07	-11.10	29,29,29,29	0
56	MG	DA	3111	1/1	0.94	0.15	-15.70	21,21,21,21	0
56	MG	CA	3008	1/1	0.62	0.55	-	251,251,251,251	0
56	MG	DA	3168	1/1	0.95	0.13	-	23,23,23,23	0
59	PUT	AA	1675	6/6	0.56	0.61	-	111,112,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3126	1/1	0.86	0.13	-	74,74,74,74	0
56	MG	DA	3024	1/1	0.99	0.11	-	45,45,45,45	0
56	MG	CA	3118	1/1	0.83	0.40	-	52,52,52,52	0
56	MG	DR	202	1/1	0.89	0.40	-	29,29,29,29	0
56	MG	CA	3083	1/1	0.82	0.29	-	263,263,263,263	0
56	MG	CA	3090	1/1	0.95	0.29	-	222,222,222,222	0
56	MG	CA	3042	1/1	0.97	0.07	-	93,93,93,93	0
56	MG	BA	1607	1/1	0.90	0.20	-	203,203,203,203	0
56	MG	DA	3102	1/1	0.94	0.11	-	38,38,38,38	0
56	MG	DA	3009	1/1	0.98	0.11	-	29,29,29,29	0
56	MG	CA	3111	1/1	0.77	0.69	-	121,121,121,121	0
56	MG	CA	3002	1/1	0.79	0.27	-	273,273,273,273	0
56	MG	CA	3142	1/1	0.67	0.22	-	73,73,73,73	0
56	MG	AA	1602	1/1	0.82	0.51	-	80,80,80,80	0
56	MG	AA	1617	1/1	0.83	0.34	-	63,63,63,63	0
56	MG	CA	3001	1/1	0.85	0.21	-	294,294,294,294	0
56	MG	DA	3020	1/1	0.99	0.13	-	23,23,23,23	0
56	MG	DA	3019	1/1	0.99	0.07	-	54,54,54,54	0
56	MG	BA	1638	1/1	0.88	0.41	-	64,64,64,64	0
59	PUT	DA	3187	6/6	0.94	0.20	-	44,49,50,51	0
56	MG	CA	3016	1/1	0.97	0.17	-	107,107,107,107	0
56	MG	DA	3061	1/1	0.97	0.07	-	209,209,209,209	0
56	MG	AA	1651	1/1	0.99	0.07	-	61,61,61,61	0
56	MG	CA	3055	1/1	0.86	0.13	-	145,145,145,145	0
56	MG	CA	3028	1/1	0.79	0.10	-	263,263,263,263	0
56	MG	DB	206	1/1	0.90	0.23	-	61,61,61,61	0
56	MG	DA	3031	1/1	0.97	0.15	-	16,16,16,16	0
56	MG	CA	3059	1/1	0.86	0.17	-	120,120,120,120	0
56	MG	CA	3137	1/1	0.89	0.33	-	137,137,137,137	0
56	MG	AA	1634	1/1	0.90	0.07	-	141,141,141,141	0
56	MG	AA	1622	1/1	0.77	0.58	-	70,70,70,70	0
56	MG	DA	3106	1/1	0.97	0.13	-	32,32,32,32	0
56	MG	DA	3145	1/1	0.98	0.17	-	65,65,65,65	0
56	MG	DA	3170	1/1	0.67	0.49	-	86,86,86,86	0
56	MG	CA	3071	1/1	0.70	0.13	-	230,230,230,230	0
56	MG	CA	3114	1/1	0.92	0.28	-	40,40,40,40	0
56	MG	DA	3115	1/1	0.96	0.11	-	32,32,32,32	0
56	MG	BA	1606	1/1	0.41	0.17	-	249,249,249,249	0
56	MG	AA	1627	1/1	0.87	0.25	-	55,55,55,55	0
56	MG	DA	3040	1/1	0.98	0.25	-	10,10,10,10	0
56	MG	DA	3035	1/1	0.97	0.17	-	15,15,15,15	0
56	MG	DA	3178	1/1	0.75	0.33	-	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3147	1/1	0.88	0.24	-	50,50,50,50	1
56	MG	CA	3155	1/1	0.81	0.31	-	196,196,196,196	0
56	MG	DA	3157	1/1	0.95	0.09	-	45,45,45,45	0
56	MG	DA	3142	1/1	0.92	0.24	-	46,46,46,46	0
56	MG	DB	209	1/1	0.77	0.38	-	105,105,105,105	0
56	MG	DA	3125	1/1	0.87	0.23	-	59,59,59,59	0
56	MG	DA	3085	1/1	0.99	0.10	-	27,27,27,27	0
56	MG	DA	3130	1/1	0.67	0.29	-	46,46,46,46	0
56	MG	CA	3046	1/1	0.89	0.12	-	123,123,123,123	0
56	MG	DA	3064	1/1	0.99	0.11	-	24,24,24,24	0
56	MG	CA	3098	1/1	0.79	0.15	-	101,101,101,101	0
56	MG	CA	3024	1/1	0.87	0.14	-	153,153,153,153	0
56	MG	DA	3131	1/1	0.71	0.53	-	76,76,76,76	0
56	MG	DA	3066	1/1	0.95	0.08	-	49,49,49,49	0
56	MG	AA	1616	1/1	0.81	0.44	-	55,55,55,55	0
56	MG	AA	1666	1/1	0.95	0.07	-	56,56,56,56	0
56	MG	CA	3140	1/1	0.81	0.50	-	112,112,112,112	0
56	MG	DA	3231	1/1	0.98	0.05	-	60,60,60,60	0
56	MG	CA	3134	1/1	0.91	0.18	-	134,134,134,134	0
56	MG	BA	1639	1/1	0.72	0.28	-	70,70,70,70	0
56	MG	DA	3139	1/1	0.94	0.14	-	43,43,43,43	0
56	MG	BA	1629	1/1	0.97	0.41	-	195,195,195,195	0
56	MG	DA	3112	1/1	0.95	0.10	-	94,94,94,94	0
56	MG	BA	1631	1/1	0.92	0.08	-	42,42,42,42	0
56	MG	CA	3131	1/1	0.74	0.35	-	75,75,75,75	0
56	MG	CA	3029	1/1	0.85	0.21	-	181,181,181,181	0
56	MG	CA	3129	1/1	0.27	0.22	-	109,109,109,109	0
56	MG	CA	3152	1/1	0.81	0.23	-	167,167,167,167	0
58	MPD	DA	3208	8/8	0.91	0.35	-	64,70,73,78	0
56	MG	DA	3123	1/1	0.95	0.23	-	66,66,66,66	0
66	ACY	DA	3190	4/4	0.97	0.18	-	65,66,66,67	0
56	MG	DA	3006	1/1	0.96	0.07	-	118,118,118,118	0
56	MG	AA	1630	1/1	0.94	0.16	-	124,124,124,124	0
56	MG	BA	1635	1/1	0.85	0.14	-	96,96,96,96	0
56	MG	CA	3148	1/1	0.93	0.14	-	27,27,27,27	1
56	MG	CA	3014	1/1	0.73	0.24	-	256,256,256,256	0
56	MG	DA	3080	1/1	0.98	0.09	-	28,28,28,28	0
56	MG	DA	3027	1/1	0.96	0.10	-	136,136,136,136	0
56	MG	DA	3119	1/1	0.96	0.28	-	56,56,56,56	0
56	MG	AA	1664	1/1	0.82	0.15	-	147,147,147,147	0
56	MG	CA	3146	1/1	0.74	0.30	-	220,220,220,220	0
56	MG	DA	3008	1/1	0.99	0.09	-	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3155	1/1	0.91	0.13	-	62,62,62,62	0
56	MG	DA	3104	1/1	0.99	0.12	-	20,20,20,20	0
58	MPD	DA	3229	8/8	0.91	0.23	-	92,96,99,99	0
56	MG	DA	3158	1/1	0.85	0.30	-	67,67,67,67	0
56	MG	DA	3163	1/1	0.98	0.23	-	50,50,50,50	0
56	MG	BA	1641	1/1	0.86	0.15	-	72,72,72,72	0
56	MG	CA	3141	1/1	0.87	0.31	-	72,72,72,72	0
62	EDO	DA	3193	4/4	0.94	0.24	-	92,92,93,94	0
56	MG	AA	1654	1/1	0.97	0.14	-	200,200,200,200	0
56	MG	CA	3121	1/1	0.94	0.26	-	63,63,63,63	0
56	MG	CA	3113	1/1	0.94	0.31	-	50,50,50,50	0
56	MG	DA	3079	1/1	0.98	0.07	-	44,44,44,44	0
56	MG	DA	3180	1/1	0.87	0.34	-	56,56,56,56	0
56	MG	DA	3082	1/1	1.00	0.05	-	64,64,64,64	0
56	MG	CA	3021	1/1	0.93	0.49	-	272,272,272,272	0
56	MG	CA	3093	1/1	0.80	0.14	-	140,140,140,140	0
56	MG	DA	3047	1/1	0.99	0.14	-	47,47,47,47	0
56	MG	CB	203	1/1	0.74	0.07	-	106,106,106,106	0
56	MG	CA	3154	1/1	0.38	0.70	-	132,132,132,132	0
56	MG	DA	3033	1/1	0.99	0.11	-	10,10,10,10	0
56	MG	DR	201	1/1	0.60	0.35	-	228,228,228,228	0
56	MG	DA	3037	1/1	0.99	0.11	-	26,26,26,26	0
56	MG	AA	1620	1/1	0.79	0.43	-	79,79,79,79	0
62	EDO	DB	211	4/4	0.91	0.45	-	96,96,96,96	0
56	MG	CA	3150	1/1	0.93	0.13	-	50,50,50,50	0
56	MG	DA	3143	1/1	0.83	0.31	-	58,58,58,58	0
63	PGE	DA	3223	10/10	0.84	0.41	-	79,90,99,99	0
56	MG	AA	1607	1/1	0.99	0.26	-	52,52,52,52	0
56	MG	CA	3127	1/1	0.91	0.17	-	71,71,71,71	0
56	MG	BA	1627	1/1	0.93	0.32	-	109,109,109,109	0
56	MG	DA	3160	1/1	0.87	0.63	-	60,60,60,60	0
56	MG	CA	3047	1/1	0.83	0.26	-	230,230,230,230	0
56	MG	BA	1636	1/1	0.94	0.64	-	91,91,91,91	0
56	MG	CA	3067	1/1	0.83	0.56	-	283,283,283,283	0
58	MPD	DN	201	8/8	0.84	0.50	-	90,95,96,96	0
56	MG	DA	3071	1/1	0.94	0.22	-	102,102,102,102	0
58	MPD	DK	201	8/8	0.71	0.47	-	138,140,140,141	0
56	MG	CA	3138	1/1	0.88	0.14	-	67,67,67,67	0
56	MG	CA	3107	1/1	0.97	0.36	-	67,67,67,67	0
56	MG	DA	3173	1/1	0.95	0.19	-	48,48,48,48	0
56	MG	CA	3027	1/1	0.70	0.17	-	118,118,118,118	0
56	MG	DA	3100	1/1	0.99	0.18	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DB	203	1/1	0.97	0.10	-	27,27,27,27	0
56	MG	AA	1645	1/1	0.93	0.12	-	54,54,54,54	0
56	MG	DA	3014	1/1	0.95	0.13	-	56,56,56,56	0
56	MG	DA	3175	1/1	0.88	0.43	-	99,99,99,99	0
56	MG	DA	3128	1/1	0.97	0.54	-	24,24,24,24	0
56	MG	CA	3115	1/1	0.69	0.25	-	85,85,85,85	0
56	MG	CA	3004	1/1	0.94	0.17	-	203,203,203,203	0
56	MG	CA	3104	1/1	0.55	0.41	-	234,234,234,234	0
56	MG	DA	3136	1/1	0.96	0.16	-	25,25,25,25	0
56	MG	CA	3050	1/1	0.84	0.12	-	58,58,58,58	0
56	MG	AA	1635	1/1	0.91	0.19	-	209,209,209,209	0
56	MG	CA	3112	1/1	0.91	0.35	-	85,85,85,85	0
56	MG	AA	1614	1/1	0.68	0.13	-	81,81,81,81	0
56	MG	CA	3058	1/1	0.95	0.22	-	203,203,203,203	0
56	MG	DA	3232	1/1	0.99	0.22	-	43,43,43,43	0
56	MG	CA	3007	1/1	-0.18	0.84	-	256,256,256,256	0
56	MG	DA	3086	1/1	0.95	0.17	-	17,17,17,17	0
56	MG	AA	1641	1/1	0.96	0.06	-	44,44,44,44	0
56	MG	CA	3070	1/1	0.96	0.10	-	94,94,94,94	0
56	MG	BA	1609	1/1	0.74	0.16	-	203,203,203,203	0
56	MG	DA	3041	1/1	0.99	0.07	-	25,25,25,25	0
56	MG	CA	3025	1/1	0.97	0.20	-	109,109,109,109	0
56	MG	AA	1619	1/1	0.51	0.56	-	98,98,98,98	0
56	MG	DA	3078	1/1	0.97	0.14	-	127,127,127,127	0
58	MPD	DT	202	8/8	0.81	0.28	-	117,118,119,119	0
62	EDO	DA	3001	4/4	0.76	0.34	-	95,95,95,96	0
56	MG	BA	1621	1/1	0.93	0.17	-	13,13,13,13	0
56	MG	CA	3077	1/1	0.41	0.79	-	240,240,240,240	0
56	MG	DA	3044	1/1	0.97	0.12	-	73,73,73,73	0
56	MG	DA	3052	1/1	0.99	0.07	-	53,53,53,53	0
56	MG	CA	3053	1/1	0.91	0.09	-	84,84,84,84	0
56	MG	AA	1638	1/1	0.98	0.12	-	105,105,105,105	0
56	MG	DA	3117	1/1	0.98	0.07	-	43,43,43,43	0
56	MG	DB	208	1/1	0.90	0.20	-	60,60,60,60	0
56	MG	CA	3097	1/1	0.86	0.21	-	123,123,123,123	0
56	MG	CA	3082	1/1	0.88	0.20	-	152,152,152,152	0
56	MG	CA	3084	1/1	0.83	0.12	-	196,196,196,196	0
56	MG	DA	3068	1/1	0.96	0.15	-	52,52,52,52	0
61	PEG	DP	201	7/7	0.47	1.70	-	136,137,140,141	0
56	MG	DB	207	1/1	0.81	0.26	-	74,74,74,74	0
56	MG	DA	3164	1/1	0.78	0.27	-	70,70,70,70	0
56	MG	DD	301	1/1	0.92	0.22	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1625	1/1	0.75	0.36	-	61,61,61,61	0
56	MG	CA	3075	1/1	0.74	0.80	-	241,241,241,241	0
56	MG	BA	1637	1/1	0.92	0.23	-	63,63,63,63	0
56	MG	DA	3144	1/1	0.61	1.43	-	111,111,111,111	0
56	MG	DA	3161	1/1	0.93	0.48	-	87,87,87,87	0
61	PEG	DA	3198	7/7	0.79	0.46	-	91,99,102,102	0
66	ACY	DA	3195	4/4	0.94	0.20	-	52,56,56,58	0
56	MG	DA	3132	1/1	0.96	0.15	-	43,43,43,43	0
56	MG	DA	3075	1/1	0.98	0.15	-	26,26,26,26	0
56	MG	CA	3068	1/1	0.90	0.34	-	266,266,266,266	0
56	MG	DA	3121	1/1	0.96	0.47	-	51,51,51,51	0
56	MG	DA	3090	1/1	0.99	0.11	-	11,11,11,11	0
56	MG	CA	3045	1/1	0.96	0.14	-	78,78,78,78	0
56	MG	CA	3106	1/1	0.92	0.18	-	81,81,81,81	0
56	MG	CA	3120	1/1	0.83	0.35	-	135,135,135,135	0
56	MG	CA	3048	1/1	0.85	0.23	-	112,112,112,112	0
56	MG	DA	3172	1/1	0.85	0.72	-	106,106,106,106	0
56	MG	BA	1640	1/1	0.88	0.16	-	131,131,131,131	0
56	MG	DA	3116	1/1	0.98	0.14	-	33,33,33,33	0
56	MG	DA	3179	1/1	0.89	0.74	-	105,105,105,105	0
56	MG	CA	3076	1/1	0.55	0.23	-	214,214,214,214	0
56	MG	DA	3074	1/1	0.98	0.10	-	26,26,26,26	0
56	MG	BA	1611	1/1	0.98	0.10	-	31,31,31,31	0
56	MG	CA	3143	1/1	0.85	0.18	-	54,54,54,54	0
56	MG	AA	1603	1/1	0.57	0.62	-	91,91,91,91	0
56	MG	AA	1609	1/1	0.81	0.36	-	72,72,72,72	0
56	MG	BA	1628	1/1	0.94	0.10	-	80,80,80,80	0
56	MG	CA	3096	1/1	0.90	0.17	-	105,105,105,105	0
56	MG	AA	1636	1/1	0.96	0.13	-	89,89,89,89	0
56	MG	AA	1605	1/1	0.71	0.89	-	98,98,98,98	0
56	MG	DA	3010	1/1	0.88	0.25	-	145,145,145,145	0
56	MG	DA	3050	1/1	0.93	0.17	-	44,44,44,44	0
56	MG	DA	3103	1/1	0.99	0.16	-	22,22,22,22	0
56	MG	DA	3055	1/1	0.99	0.17	-	19,19,19,19	0
56	MG	CA	3043	1/1	0.78	0.10	-	72,72,72,72	0
56	MG	DA	3138	1/1	0.98	0.36	-	29,29,29,29	1
56	MG	AA	1632	1/1	0.98	0.05	-	88,88,88,88	0
56	MG	CA	3156	1/1	0.58	0.24	-	252,252,252,252	0
56	MG	CA	3060	1/1	0.17	0.57	-	259,259,259,259	0
62	EDO	DA	3206	4/4	0.93	0.24	-	79,82,83,83	0
68	TRS	DA	3218	8/8	0.70	0.78	-	149,150,153,155	0
56	MG	DB	202	1/1	0.99	0.12	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1658	1/1	0.93	0.06	-	58,58,58,58	0
56	MG	CA	3073	1/1	0.92	0.26	-	212,212,212,212	0
56	MG	DA	3053	1/1	0.96	0.12	-	68,68,68,68	0
56	MG	DA	3059	1/1	0.97	0.15	-	25,25,25,25	0
56	MG	CA	3135	1/1	0.72	0.77	-	96,96,96,96	0
56	MG	BA	1604	1/1	0.65	0.18	-	218,218,218,218	0
56	MG	AA	1606	1/1	0.25	0.52	-	106,106,106,106	0
56	MG	DA	3181	1/1	0.86	0.45	-	72,72,72,72	0
56	MG	DA	3018	1/1	0.99	0.28	-	10,10,10,10	0
56	MG	DA	3017	1/1	0.98	0.07	-	53,53,53,53	0
56	MG	AA	1610	1/1	0.90	0.46	-	76,76,76,76	0
56	MG	AA	1633	1/1	0.97	0.08	-	76,76,76,76	0
56	MG	CA	3049	1/1	0.89	0.14	-	53,53,53,53	0
56	MG	BA	1618	1/1	0.96	0.18	-	91,91,91,91	0
56	MG	DA	3084	1/1	0.95	0.11	-	56,56,56,56	0
56	MG	AA	1662	1/1	0.96	0.14	-	66,66,66,66	0
56	MG	CA	3066	1/1	0.88	0.24	-	133,133,133,133	0
56	MG	DA	3087	1/1	1.00	0.09	-	58,58,58,58	0
56	MG	CA	3125	1/1	0.58	0.46	-	85,85,85,85	0
56	MG	DA	3169	1/1	0.85	0.34	-	47,47,47,47	0
56	MG	AA	1650	1/1	0.97	0.07	-	149,149,149,149	0
56	MG	DB	205	1/1	0.82	0.29	-	64,64,64,64	0
56	MG	CA	3078	1/1	0.79	0.09	-	128,128,128,128	0
56	MG	CA	3139	1/1	0.68	0.56	-	100,100,100,100	0
56	MG	CA	3036	1/1	0.82	0.26	-	194,194,194,194	0
56	MG	BA	1603	1/1	0.90	0.17	-	254,254,254,254	0
56	MG	BA	1625	1/1	0.91	0.36	-	269,269,269,269	0
56	MG	DA	3141	1/1	0.94	0.27	-	54,54,54,54	0
56	MG	CA	3072	1/1	0.94	1.10	-	273,273,273,273	0
56	MG	CA	3130	1/1	0.87	0.19	-	75,75,75,75	0
56	MG	AA	1621	1/1	0.77	0.30	-	59,59,59,59	0
56	MG	DA	3097	1/1	0.95	0.16	-	187,187,187,187	0
56	MG	DA	3095	1/1	0.99	0.15	-	14,14,14,14	0
56	MG	DA	3067	1/1	0.96	0.14	-	43,43,43,43	0
56	MG	CA	3012	1/1	0.59	0.29	-	130,130,130,130	0
56	MG	DA	3167	1/1	-0.03	0.32	-	141,141,141,141	0
56	MG	DA	3058	1/1	0.99	0.11	-	22,22,22,22	0
56	MG	DA	3148	1/1	0.90	0.17	-	46,46,46,46	0
56	MG	DA	3088	1/1	0.96	0.16	-	13,13,13,13	0
56	MG	AA	1628	1/1	-0.09	0.89	-	177,177,177,177	0
56	MG	CA	3038	1/1	-0.46	0.32	-	250,250,250,250	0
56	MG	CA	3064	1/1	0.77	0.41	-	283,283,283,283	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	DA	3039	1/1	0.99	0.07	-	43,43,43,43	0
56	MG	AA	1660	1/1	0.94	0.55	-	278,278,278,278	0
56	MG	DA	3133	1/1	0.90	0.27	-	57,57,57,57	0
56	MG	DA	3177	1/1	0.87	0.19	-	59,59,59,59	0
56	MG	DA	3081	1/1	0.96	0.05	-	80,80,80,80	0
56	MG	DA	3013	1/1	0.98	0.21	-	92,92,92,92	0
56	MG	BA	1616	1/1	0.91	0.12	-	169,169,169,169	0
56	MG	DA	3137	1/1	0.64	0.52	-	91,91,91,91	0
56	MG	DA	3073	1/1	0.97	0.06	-	37,37,37,37	0
56	MG	CA	3069	1/1	0.90	0.10	-	81,81,81,81	0
56	MG	CA	3109	1/1	0.88	0.25	-	80,80,80,80	0
56	MG	CA	3052	1/1	0.93	0.07	-	80,80,80,80	0
56	MG	BA	1630	1/1	0.91	0.08	-	165,165,165,165	0
56	MG	CA	3092	1/1	0.67	0.17	-	210,210,210,210	0
56	MG	CA	3151	1/1	0.81	0.33	-	81,81,81,81	0
57	PG4	DR	203	13/13	0.82	0.40	-	151,153,155,155	0
56	MG	CA	3074	1/1	0.90	0.09	-	142,142,142,142	0
56	MG	DA	3174	1/1	0.90	0.30	-	73,73,73,73	0
56	MG	DA	3048	1/1	0.99	0.12	-	67,67,67,67	0
56	MG	DA	3120	1/1	0.98	0.15	-	64,64,64,64	0
56	MG	AA	1665	1/1	0.92	0.17	-	153,153,153,153	0
56	MG	DA	3043	1/1	0.96	0.07	-	84,84,84,84	0
56	MG	CA	3034	1/1	0.63	0.33	-	239,239,239,239	0
56	MG	DA	3099	1/1	0.98	0.18	-	9,9,9,9	0
56	MG	CA	3116	1/1	0.81	0.41	-	62,62,62,62	0
56	MG	CA	3128	1/1	0.95	0.21	-	65,65,65,65	0
56	MG	BA	1634	1/1	0.92	0.08	-	133,133,133,133	0
56	MG	DA	3070	1/1	0.96	0.11	-	58,58,58,58	0
56	MG	CA	3023	1/1	0.79	0.41	-	206,206,206,206	0
56	MG	DA	3113	1/1	0.99	0.11	-	30,30,30,30	0
56	MG	AA	1626	1/1	0.65	0.84	-	77,77,77,77	0
56	MG	DA	3077	1/1	0.99	0.05	-	34,34,34,34	0
56	MG	DA	3152	1/1	0.91	0.35	-	82,82,82,82	0
56	MG	CA	3145	1/1	0.88	0.15	-	50,50,50,50	0
56	MG	DA	3156	1/1	0.84	0.32	-	47,47,47,47	0
56	MG	CA	3062	1/1	0.95	0.03	-	191,191,191,191	0
62	EDO	DA	3213	4/4	0.88	0.29	-	72,73,74,75	0
56	MG	DA	3159	1/1	0.96	0.15	-	61,61,61,61	0
56	MG	DA	3051	1/1	0.96	0.10	-	52,52,52,52	0
56	MG	CA	3122	1/1	0.91	0.55	-	81,81,81,81	0
56	MG	AA	1623	1/1	0.92	0.20	-	60,60,60,60	0
56	MG	CA	3005	1/1	0.62	0.72	-	250,250,250,250	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	CA	3035	1/1	0.90	0.18	-	102,102,102,102	0
56	MG	DA	3032	1/1	0.98	0.19	-	21,21,21,21	0
56	MG	CA	3108	1/1	0.91	0.20	-	74,74,74,74	0
56	MG	DA	3230	1/1	0.94	0.06	-	45,45,45,45	0
56	MG	CA	3080	1/1	0.96	0.37	-	160,160,160,160	0
56	MG	DA	3029	1/1	0.99	0.20	-	68,68,68,68	0
56	MG	CA	3057	1/1	0.80	0.15	-	143,143,143,143	0
56	MG	DA	3072	1/1	0.97	0.14	-	26,26,26,26	0
56	MG	DA	3118	1/1	0.94	0.20	-	62,62,62,62	0
61	PEG	DA	3225	7/7	0.88	0.28	-	75,76,78,79	0
56	MG	DA	3056	1/1	0.98	0.12	-	7,7,7,7	0
56	MG	CA	3015	1/1	0.95	0.19	-	59,59,59,59	0
56	MG	CA	3095	1/1	0.95	0.13	-	80,80,80,80	0
56	MG	CA	3065	1/1	0.88	0.25	-	151,151,151,151	0
56	MG	BA	1619	1/1	0.94	0.17	-	198,198,198,198	0
56	MG	CA	3117	1/1	0.90	0.43	-	64,64,64,64	0
56	MG	AA	1655	1/1	0.91	0.10	-	101,101,101,101	0
56	MG	AA	1640	1/1	0.84	0.11	-	80,80,80,80	0
56	MG	BA	1623	1/1	0.90	0.29	-	193,193,193,193	0
56	MG	AA	1667	1/1	0.98	0.12	-	33,33,33,33	0
56	MG	AA	1618	1/1	0.79	0.51	-	57,57,57,57	0
56	MG	DA	3153	1/1	0.95	0.18	-	59,59,59,59	0
56	MG	CA	3149	1/1	0.89	0.49	-	52,52,52,52	0
56	MG	DA	3076	1/1	0.98	0.09	-	34,34,34,34	0
56	MG	CA	3119	1/1	0.95	0.17	-	68,68,68,68	0
56	MG	DA	3134	1/1	0.92	0.25	-	55,55,55,55	0
56	MG	DA	3054	1/1	0.99	0.20	-	27,27,27,27	0
56	MG	DA	3149	1/1	0.96	0.23	-	34,34,34,34	0
58	MPD	DA	3189	8/8	0.89	0.29	-	91,94,96,98	0
56	MG	AA	1652	1/1	0.99	0.20	-	18,18,18,18	0
56	MG	AA	1613	1/1	0.88	0.35	-	52,52,52,52	0
56	MG	CA	3056	1/1	0.87	0.30	-	48,48,48,48	0
61	PEG	DA	3224	7/7	0.90	0.26	-	82,82,84,85	0
56	MG	BA	1633	1/1	0.87	0.25	-	248,248,248,248	0
56	MG	CA	3010	1/1	0.76	0.28	-	250,250,250,250	0
56	MG	AA	1624	1/1	0.94	0.23	-	85,85,85,85	0
56	MG	DA	3165	1/1	0.96	0.43	-	78,78,78,78	0
56	MG	CA	3087	1/1	0.68	0.18	-	196,196,196,196	0
56	MG	DA	3114	1/1	0.99	0.17	-	7,7,7,7	0
56	MG	CA	3017	1/1	0.87	0.08	-	87,87,87,87	0
56	MG	CA	3124	1/1	0.37	0.69	-	165,165,165,165	0
56	MG	DA	3004	1/1	0.98	0.09	-	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	AA	1615	1/1	0.58	0.44	-	110,110,110,110	0
62	EDO	DA	3228	4/4	0.57	0.52	-	123,124,125,126	0
56	MG	AA	1647	1/1	0.98	0.28	-	217,217,217,217	0
56	MG	DA	3129	1/1	0.75	0.15	-	52,52,52,52	0
56	MG	DA	3105	1/1	0.98	0.12	-	11,11,11,11	0
56	MG	DA	3154	1/1	0.92	0.22	-	47,47,47,47	0
56	MG	CA	3132	1/1	0.71	0.38	-	116,116,116,116	0
56	MG	AA	1604	1/1	0.87	0.36	-	57,57,57,57	0
56	MG	AA	1601	1/1	0.92	0.32	-	48,48,48,48	0
56	MG	DA	3122	1/1	0.73	0.40	-	86,86,86,86	0
56	MG	DA	3003	1/1	0.93	0.09	-	93,93,93,93	0
56	MG	CA	3081	1/1	0.91	0.10	-	117,117,117,117	0
56	MG	DA	3110	1/1	0.86	0.36	-	273,273,273,273	0
62	EDO	DB	210	4/4	0.78	0.39	-	87,88,89,90	0
56	MG	DA	3107	1/1	0.97	0.06	-	26,26,26,26	0
56	MG	DA	3166	1/1	0.74	0.31	-	118,118,118,118	0
56	MG	DA	3151	1/1	0.96	0.20	-	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.