



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:02 pm BST

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

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

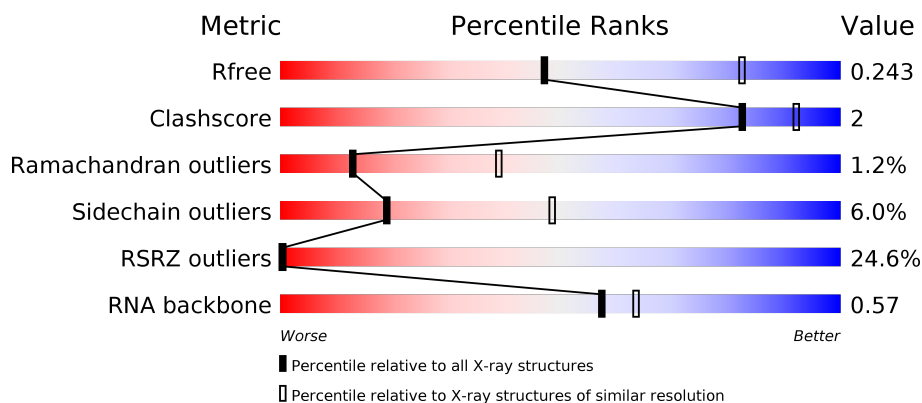
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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

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

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Mol	Chain	Length	Quality of chain
3	AC	206	<div> <div>9%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
3	BC	206	<div> <div>40%</div> <div>83%</div> <div>17%</div> </div>
4	AD	205	<div> <div>3%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
4	BD	205	<div> <div>%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
5	AE	155	<div> <div>4%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>
5	BE	155	<div> <div>12%</div> <div>63%</div> <div>29%</div> <div>5%</div> <div>..</div> </div>
6	AF	106	<div> <div>12%</div> <div>85%</div> <div>15%</div> </div>
6	BF	106	<div> <div>8%</div> <div>72%</div> <div>22%</div> <div>6%</div> </div>
7	AG	151	<div> <div>28%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
7	BG	151	<div> <div>72%</div> <div>86%</div> <div>14%</div> </div>
8	AH	129	<div> <div>5%</div> <div>81%</div> <div>19%</div> </div>
8	BH	129	<div> <div>14%</div> <div>85%</div> <div>15%</div> </div>
9	AI	127	<div> <div>36%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
9	BI	127	<div> <div>61%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
10	AJ	99	<div> <div>21%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
10	BJ	99	<div> <div>74%</div> <div>73%</div> <div>23%</div> <div>..</div> </div>
11	AK	117	<div> <div>24%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
11	BK	117	<div> <div>21%</div> <div>74%</div> <div>22%</div> <div>.</div> </div>
12	AL	123	<div> <div>2%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
12	BL	123	<div> <div>24%</div> <div>81%</div> <div>13%</div> <div>6%</div> </div>
13	AM	114	<div> <div>41%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
13	BM	114	<div> <div>93%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
14	AN	100	<div> <div>21%</div> <div>88%</div> <div>12%</div> </div>
14	BN	100	<div> <div>73%</div> <div>88%</div> <div>12%</div> </div>
15	AO	88	<div> <div>8%</div> <div>92%</div> <div>8%</div> </div>

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

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


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Mol	Chain	Length	Quality of chain
41	CO	125	
41	DO	125	
42	CP	117	
42	DP	117	
43	CQ	114	
43	DQ	114	
44	CR	117	
44	DR	117	
45	CS	103	
45	DS	103	
46	CT	110	
46	DT	110	
47	CU	93	
47	DU	93	
48	CV	102	
48	DV	102	
49	CW	94	
49	DW	94	
50	CX	76	
50	DX	76	
51	CY	77	
51	DY	77	
52	CZ	62	
52	DZ	62	
53	DI	135	

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Mol	Chain	Length	Quality of chain
54	DA	2904	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	1601	-	-	-	X
55	MG	AA	1603	-	-	-	X
55	MG	AA	1605	-	-	-	X
55	MG	AA	1606	-	-	-	X
55	MG	AA	1610	-	-	-	X
55	MG	AA	1614	-	-	-	X
55	MG	AA	1615	-	-	-	X
55	MG	AA	1616	-	-	-	X
55	MG	AA	1617	-	-	-	X
55	MG	AA	1621	-	-	-	X
55	MG	AA	1622	-	-	-	X
55	MG	AA	1623	-	-	-	X
55	MG	AA	1624	-	-	-	X
55	MG	AA	1626	-	-	-	X
55	MG	AA	1628	-	-	-	X
55	MG	AA	1642	-	-	-	X
55	MG	AA	1661	-	-	-	X
55	MG	BA	1625	-	-	-	X
55	MG	BA	1629	-	-	-	X
55	MG	BA	1640	-	-	-	X
55	MG	C3	101	-	-	-	X
55	MG	CA	3002	-	-	-	X
55	MG	CA	3004	-	-	-	X
55	MG	CA	3006	-	-	-	X
55	MG	CA	3025	-	-	-	X
55	MG	CA	3031	-	-	-	X
55	MG	CA	3033	-	-	-	X
55	MG	CA	3037	-	-	-	X
55	MG	CA	3038	-	-	-	X
55	MG	CA	3046	-	-	-	X
55	MG	CA	3055	-	-	-	X
55	MG	CA	3059	-	-	-	X
55	MG	CA	3063	-	-	-	X
55	MG	CA	3066	-	-	-	X
55	MG	CA	3074	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	CA	3076	-	-	-	X
55	MG	CA	3079	-	-	-	X
55	MG	CA	3106	-	-	-	X
55	MG	CA	3109	-	-	-	X
55	MG	CA	3110	-	-	-	X
55	MG	CA	3111	-	-	-	X
55	MG	CA	3116	-	-	-	X
55	MG	CA	3118	-	-	-	X
55	MG	CA	3119	-	-	-	X
55	MG	CA	3121	-	-	-	X
55	MG	CA	3122	-	-	-	X
55	MG	CA	3128	-	-	-	X
55	MG	CA	3129	-	-	-	X
55	MG	CA	3131	-	-	-	X
55	MG	CA	3132	-	-	-	X
55	MG	CA	3133	-	-	-	X
55	MG	CA	3134	-	-	-	X
55	MG	CA	3136	-	-	-	X
55	MG	CA	3138	-	-	-	X
55	MG	CA	3139	-	-	-	X
55	MG	CA	3140	-	-	-	X
55	MG	CA	3141	-	-	-	X
55	MG	CA	3145	-	-	-	X
55	MG	CA	3146	-	-	-	X
55	MG	CA	3147	-	-	-	X
55	MG	CA	3148	-	-	-	X
55	MG	CA	3153	-	-	-	X
55	MG	DA	3112	-	-	-	X
55	MG	DA	3125	-	-	-	X
55	MG	DA	3129	-	-	-	X
55	MG	DA	3145	-	-	-	X
55	MG	DA	3155	-	-	-	X
55	MG	DA	3157	-	-	-	X
55	MG	DA	3159	-	-	-	X
55	MG	DA	3166	-	-	-	X
55	MG	DA	3167	-	-	-	X
55	MG	DA	3168	-	-	-	X
55	MG	DA	3170	-	-	-	X
55	MG	DA	3171	-	-	-	X
55	MG	DA	3172	-	-	-	X
55	MG	DA	3173	-	-	-	X
55	MG	DA	3175	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3176	-	-	-	X
55	MG	DA	3178	-	-	-	X
55	MG	DA	3179	-	-	-	X
55	MG	DA	3180	-	-	-	X
55	MG	DA	3181	-	-	-	X
55	MG	DA	3182	-	-	-	X
55	MG	DB	206	-	-	-	X
55	MG	DB	209	-	-	-	X
55	MG	DR	201	-	-	-	X
56	PG4	DR	202	-	-	-	X
57	MPD	AA	1676	-	-	-	X
57	MPD	DA	3203	-	-	-	X
57	MPD	DA	3206	-	-	-	X
57	MPD	DE	301	-	-	-	X
57	MPD	DE	302	-	-	-	X
57	MPD	DT	202	-	-	-	X
58	PUT	AA	1672	-	-	-	X
58	PUT	AA	1674	-	-	-	X
58	PUT	AA	1675	-	-	-	X
58	PUT	DA	3218	-	-	-	X
58	PUT	DA	3221	-	-	-	X
61	PEG	D3	102	-	-	-	X
61	PEG	DA	3200	-	-	-	X
61	PEG	DA	3217	-	-	-	X
61	PEG	DP	201	-	-	-	X
61	PEG	DQ	201	-	-	-	X
62	EDO	DA	3004	-	-	-	X
62	EDO	DA	3208	-	-	-	X
63	PGE	D1	102	-	-	-	X
63	PGE	D3	101	-	-	-	X
68	TRS	DA	3219	-	-	-	X

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 32 is a protein called 50S ribosomal protein L4.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

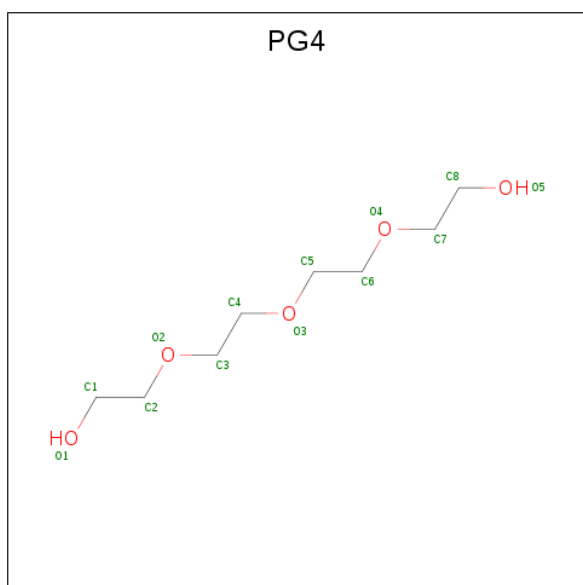
There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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



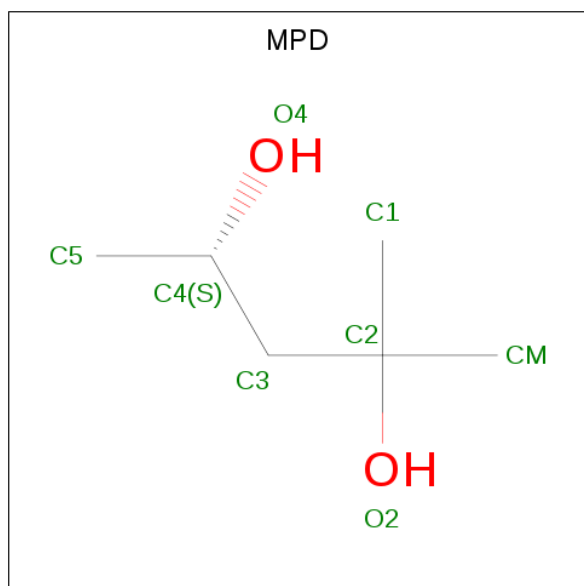
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	C	O	0	0
			13	8	5		
56	BA	1	Total	C	O	0	0
			13	8	5		

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

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



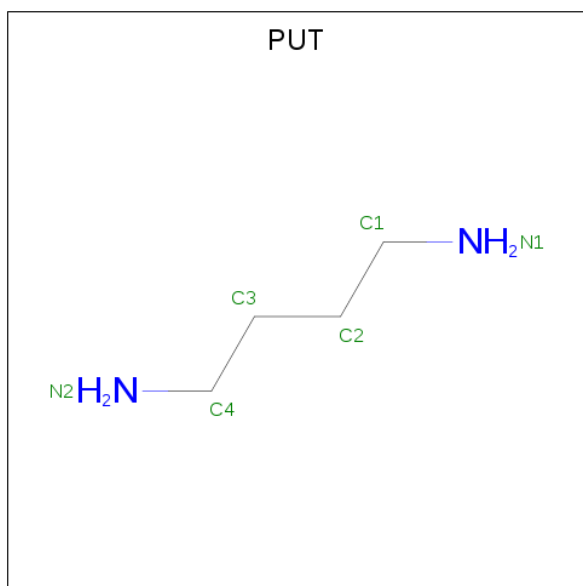
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			8	6	2		
57	AA	1	Total	C	O	0	0
			8	6	2		
57	DE	1	Total	C	O	0	0
			8	6	2		
57	DE	1	Total	C	O	0	0
			8	6	2		
57	DK	1	Total	C	O	0	0
			8	6	2		
57	DN	1	Total	C	O	0	0
			8	6	2		

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

- Molecule 58 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



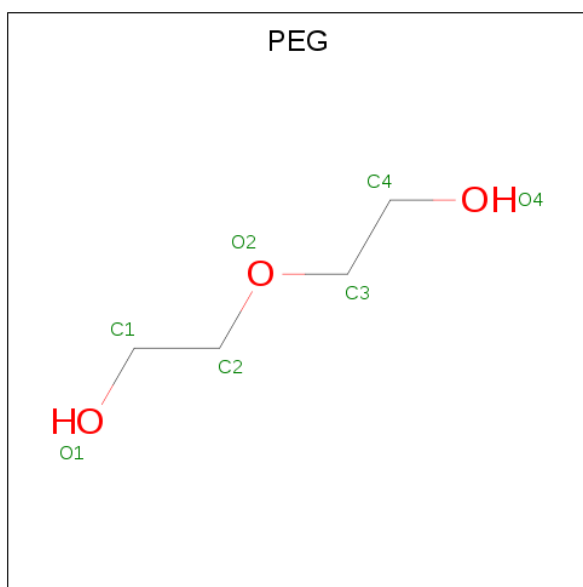
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AA	1	Total	C	N	0	0
			6	4	2		
58	AA	1	Total	C	N	0	0
			6	4	2		
58	AA	1	Total	C	N	0	0
			6	4	2		

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

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



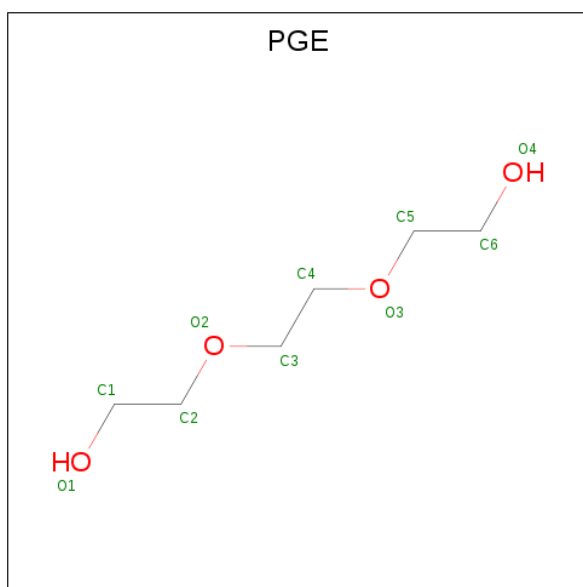
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	D1	1	Total	C	O	0	0
			7	4	3		
61	D3	1	Total	C	O	0	0
			7	4	3		
61	DL	1	Total	C	O	0	0
			7	4	3		
61	DP	1	Total	C	O	0	0
			7	4	3		
61	DQ	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7	4	3		
61	DA	1	Total	C	O	0	0
			7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

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



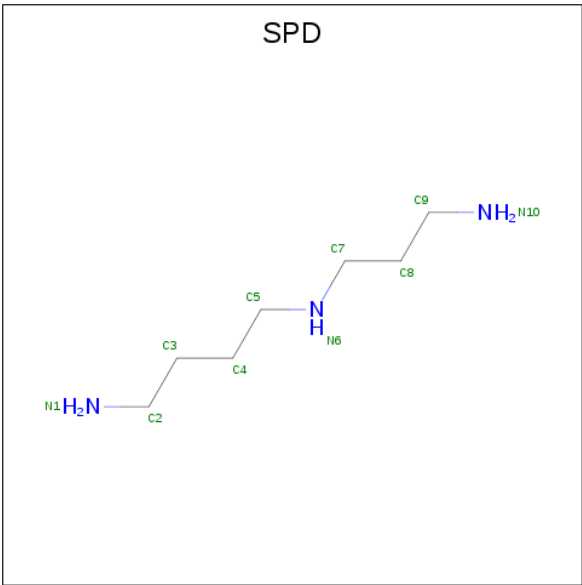
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	D1	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4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

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



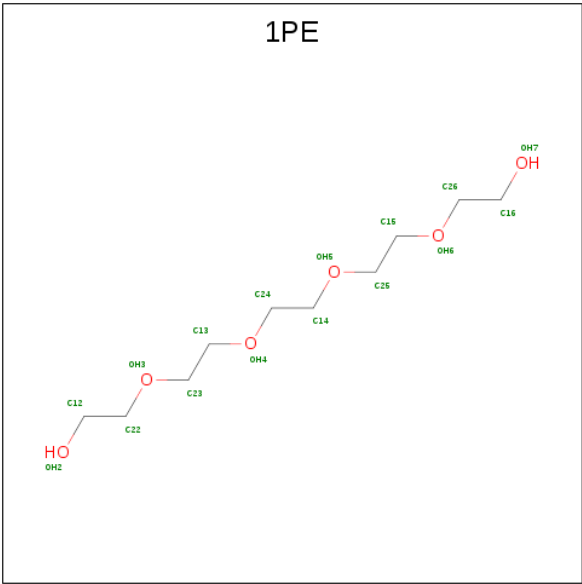
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			10	6	4		
63	D3	1	Total	C	O	0	0
			10	6	4		
63	DD	1	Total	C	O	0	0
			10	6	4		
63	DS	1	Total	C	O	0	0
			10	6	4		
63	DU	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0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

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



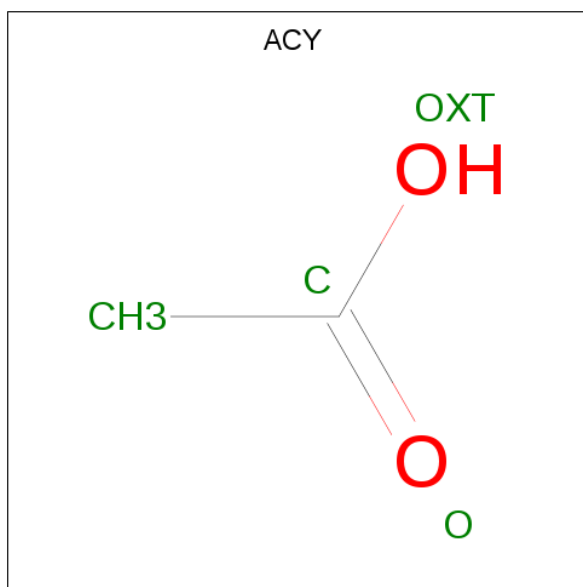
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		

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



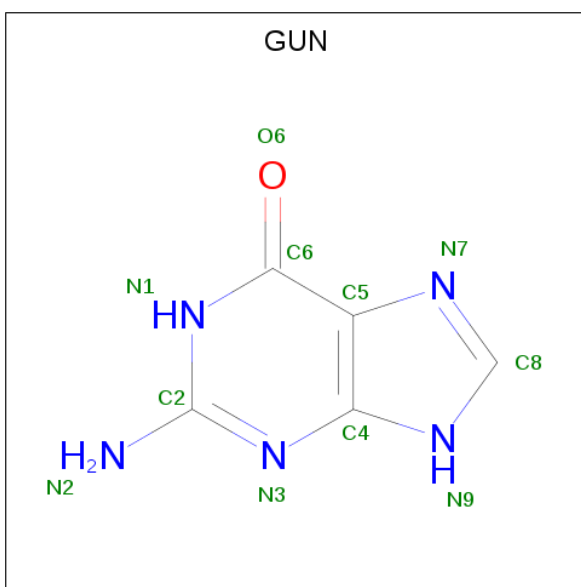
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
65	DA	1	Total	C	O	0	0
			16	10	6		
65	DA	1	Total	C	O	0	0
			16	10	6		

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



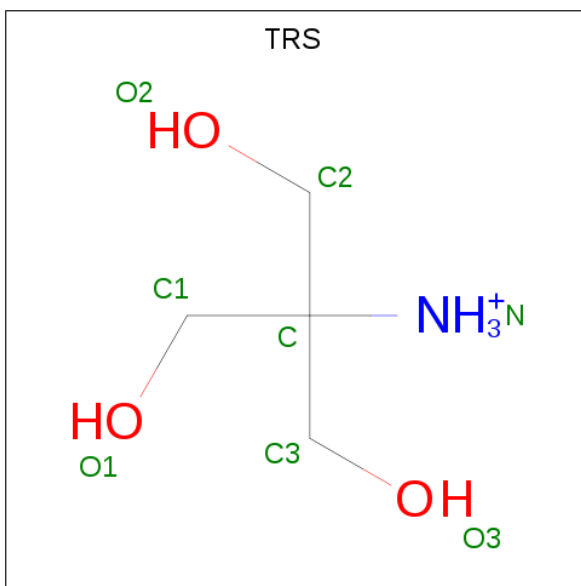
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		

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



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

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



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

- Molecule 69 is water.

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

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

Continued on next page...

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

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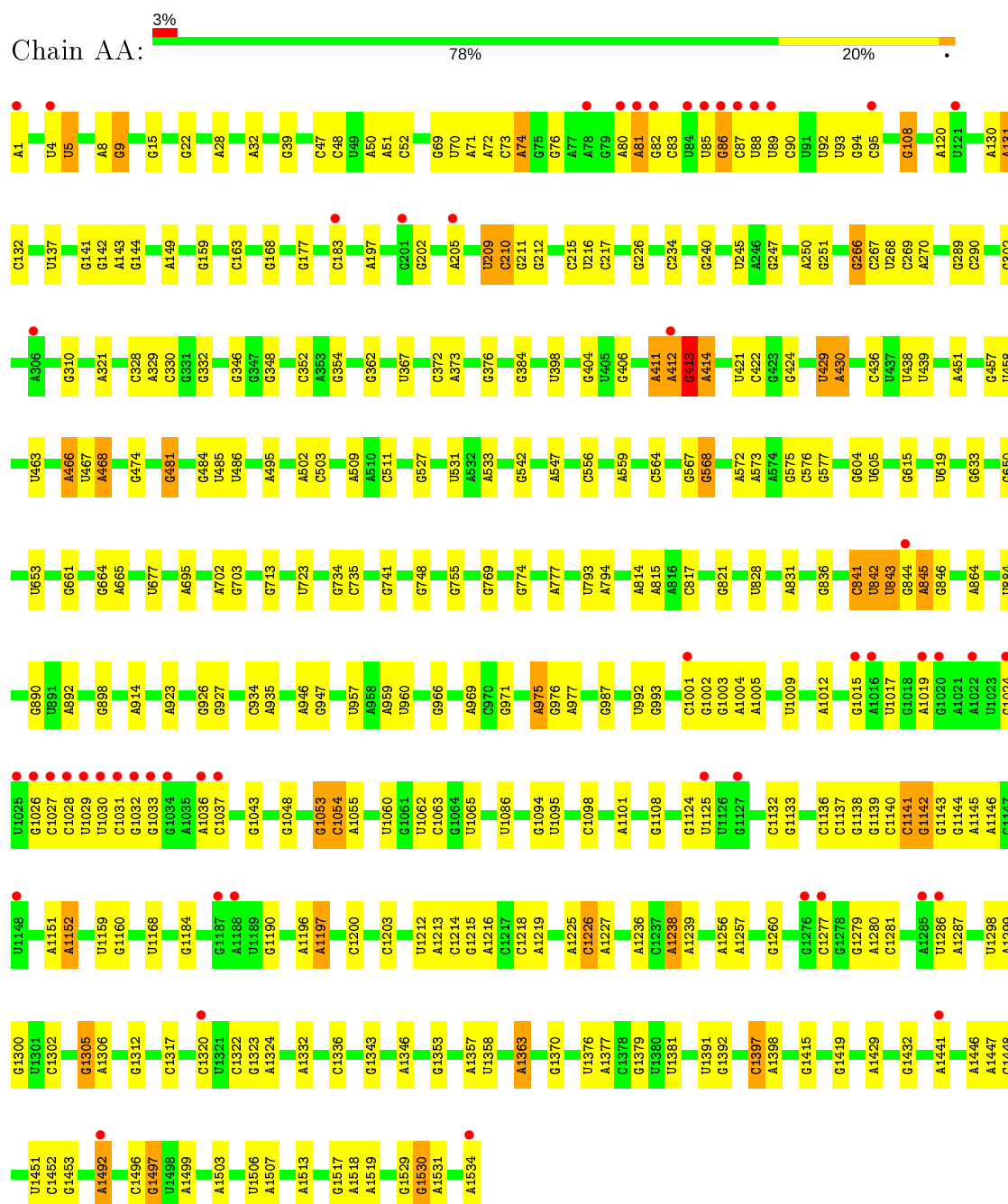
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DS	51	Total 51	O 51	0	0
69	DT	69	Total 69	O 69	0	0
69	DU	17	Total 17	O 17	0	0
69	DV	19	Total 19	O 19	0	0
69	DW	31	Total 31	O 31	0	0
69	DX	30	Total 30	O 30	0	0
69	DY	9	Total 9	O 9	0	0
69	DZ	7	Total 7	O 7	0	0
69	DB	212	Total 212	O 212	0	0
69	DA	4834	Total 4834	O 4834	0	0

3 Residue-property plots [i](#)

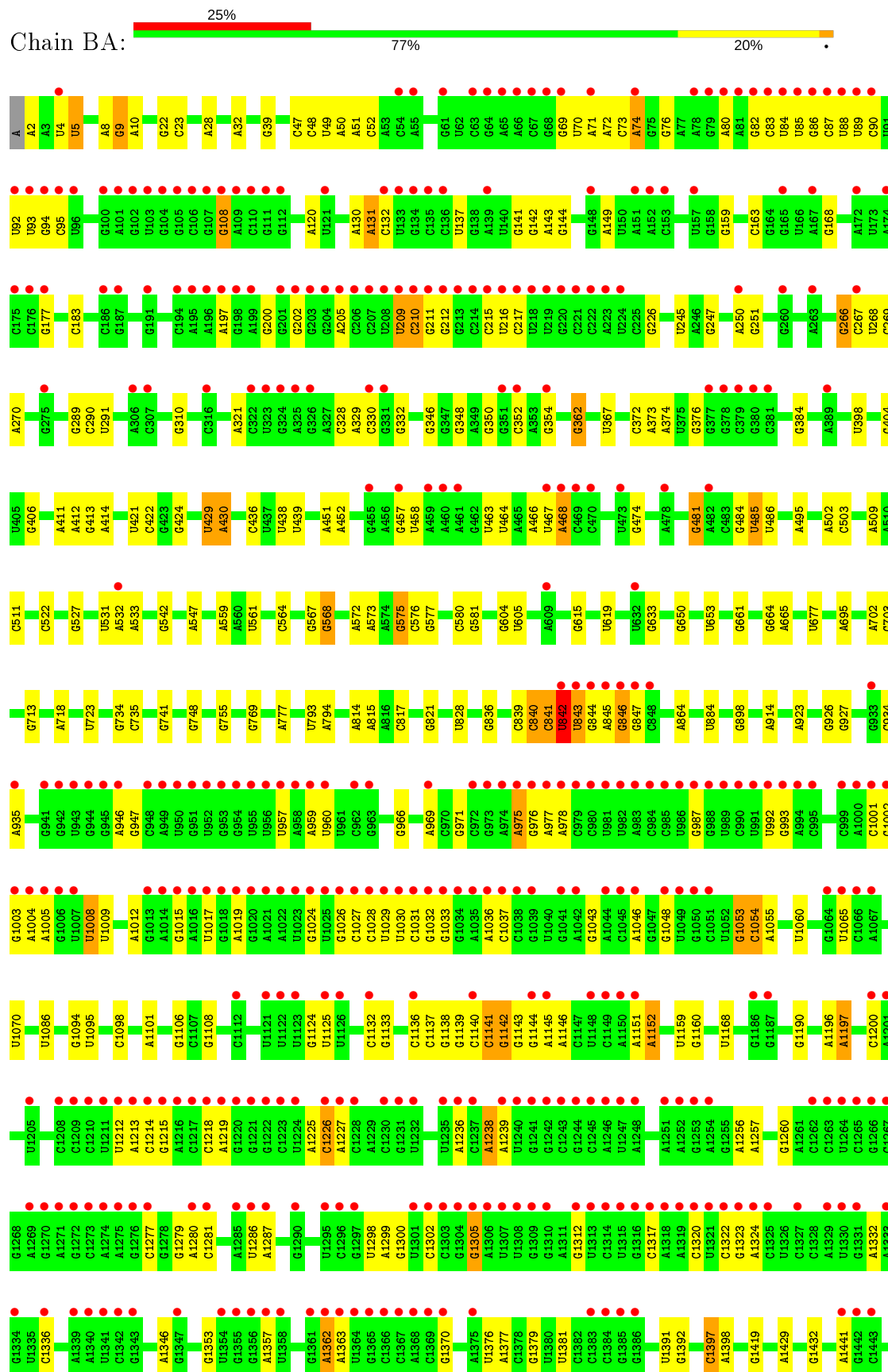
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 16S rRNA



• Molecule 1: 16S rRNA

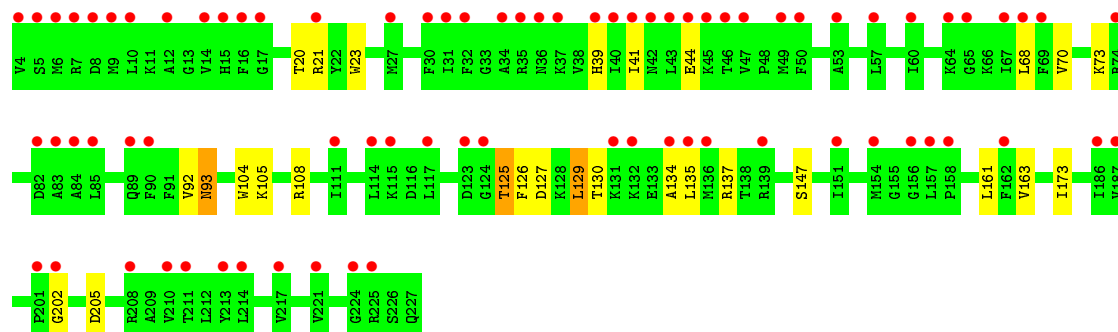
Chain BA:





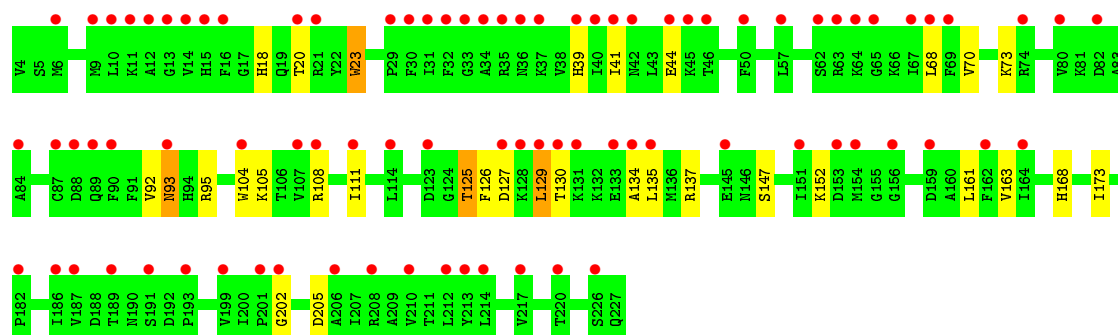
- Molecule 2: 30S ribosomal protein S2

Chain AB: 35% 88% 11%



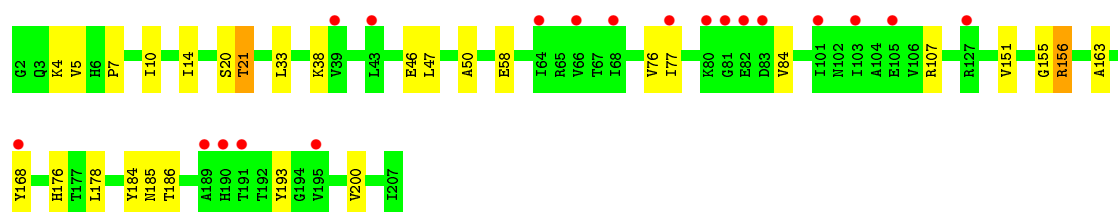
- Molecule 2: 30S ribosomal protein S2

Chain BB: 38% 86% 13%



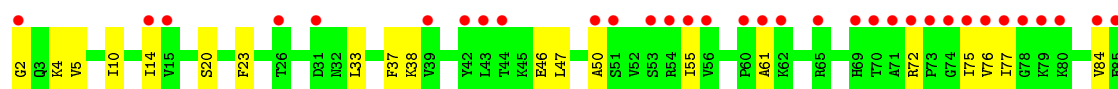
- Molecule 3: 30S ribosomal protein S3

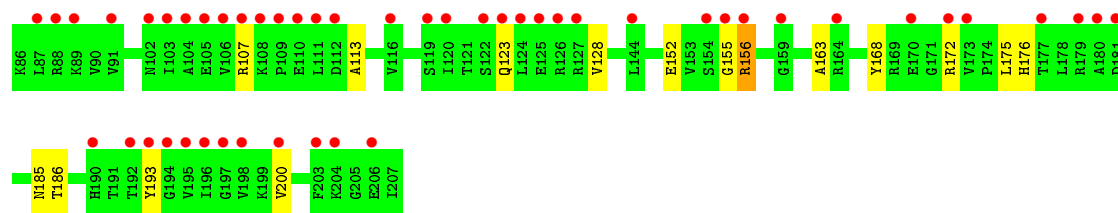
Chain AC: 9% 86% 13%



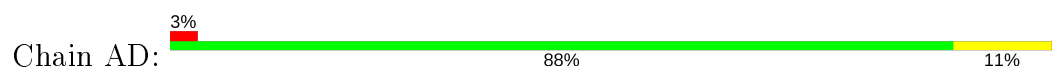
- Molecule 3: 30S ribosomal protein S3

Chain BC: 40% 83% 17%

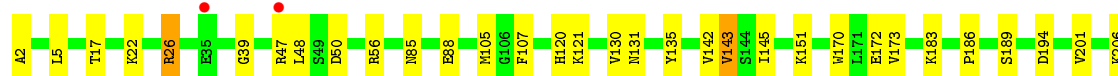
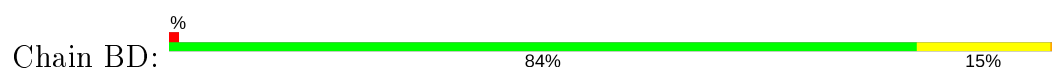




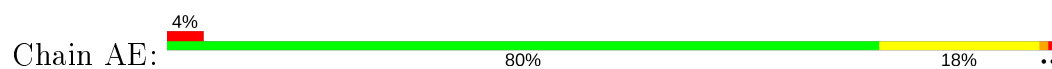
- Molecule 4: 30S ribosomal protein S4



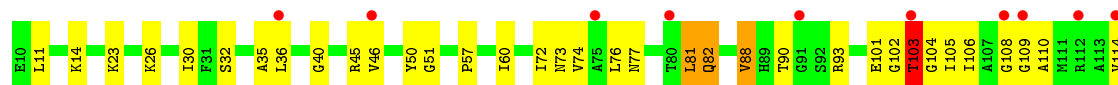
- Molecule 4: 30S ribosomal protein S4



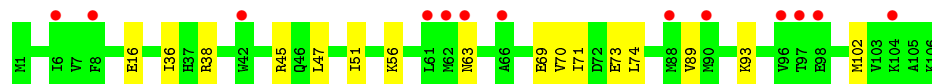
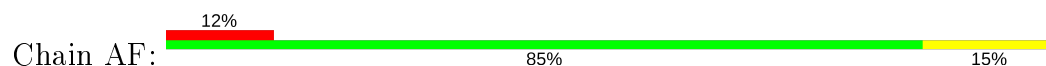
- Molecule 5: 30S ribosomal protein S5

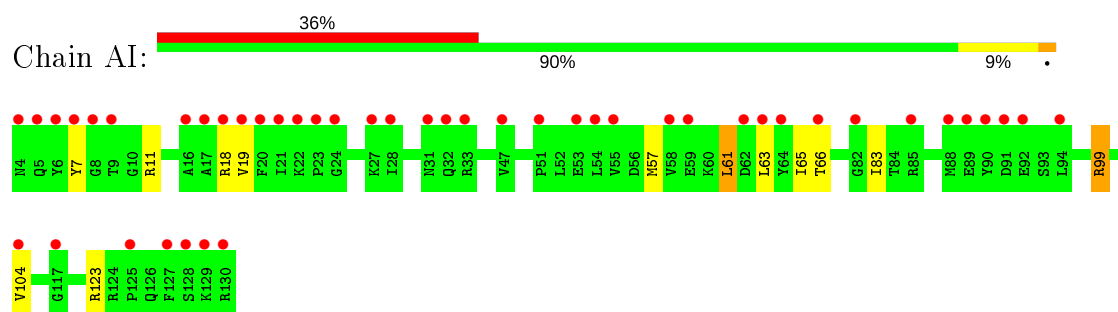


- Molecule 5: 30S ribosomal protein S5

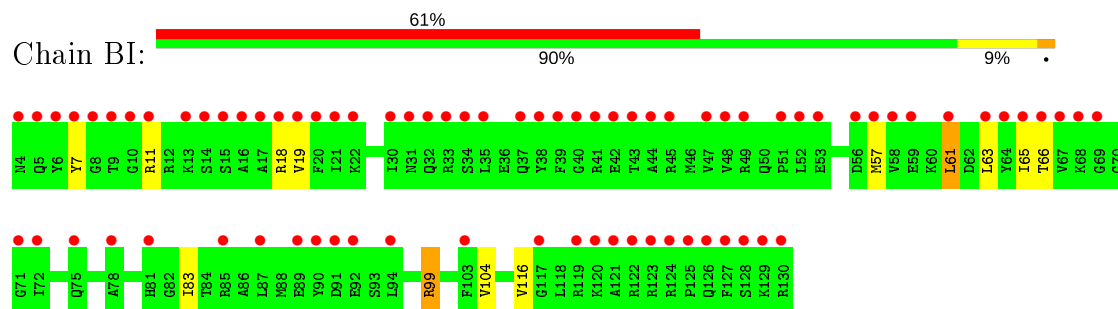


- Molecule 6: 30S ribosomal protein S6

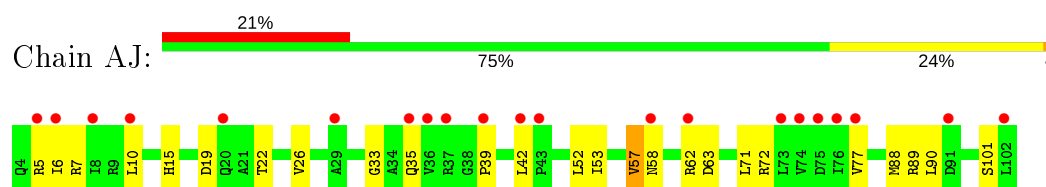




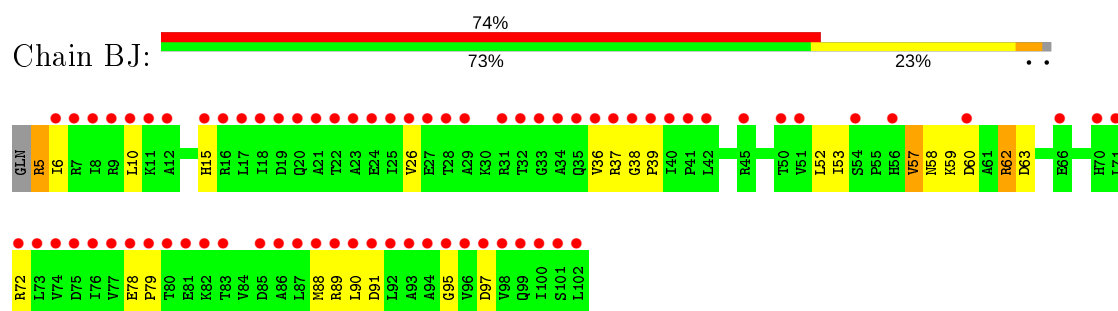
- Molecule 9: 30S ribosomal protein S9



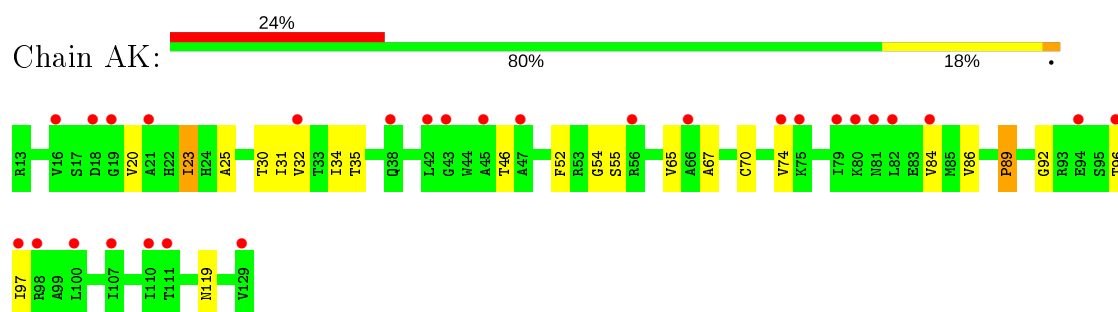
- Molecule 10: 30S ribosomal protein S10



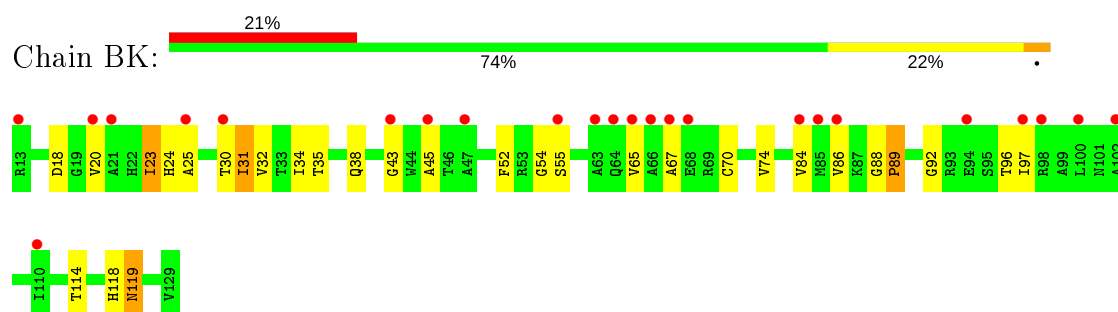
- Molecule 10: 30S ribosomal protein S10



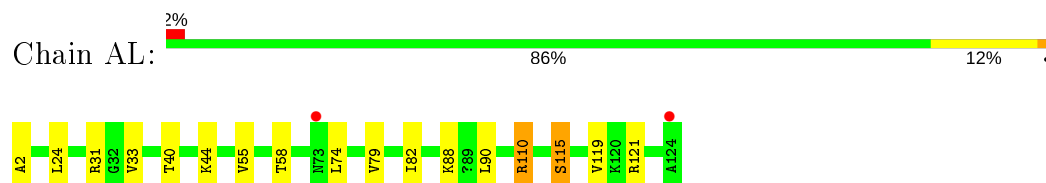
- Molecule 11: 30S ribosomal protein S11



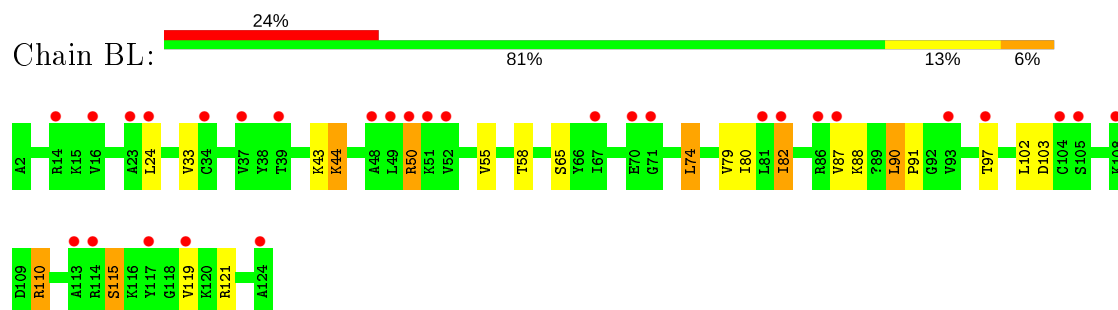
- Molecule 11: 30S ribosomal protein S11



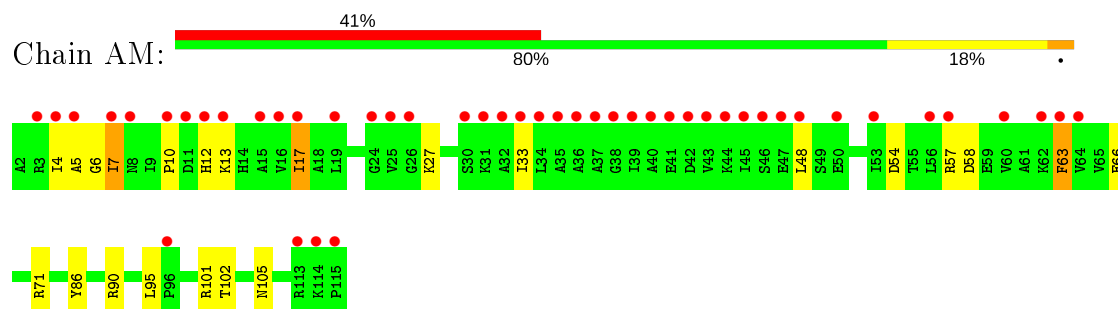
- Molecule 12: 30S ribosomal protein S12



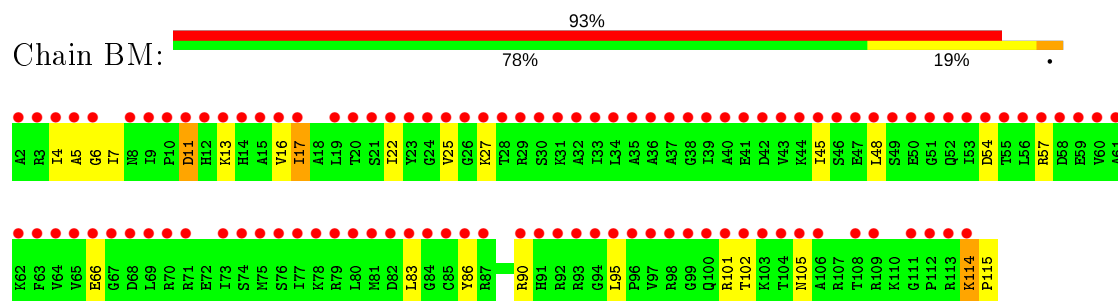
- Molecule 12: 30S ribosomal protein S12



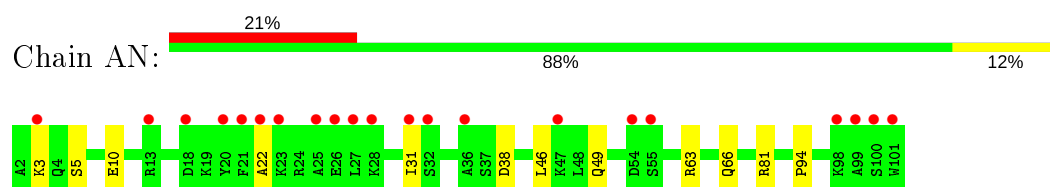
- Molecule 13: 30S ribosomal protein S13



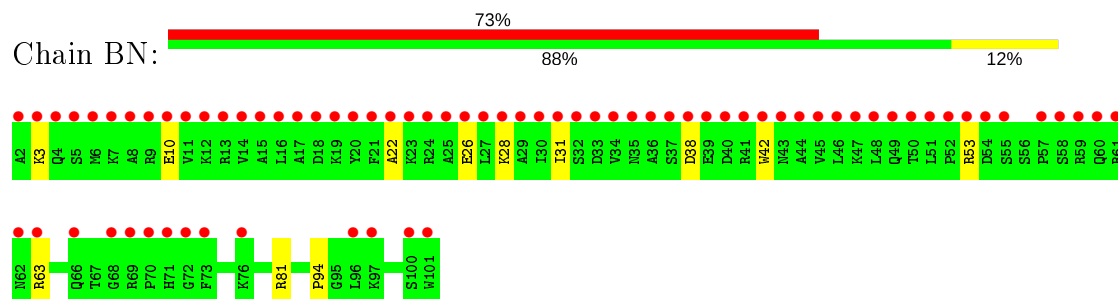
- Molecule 13: 30S ribosomal protein S13



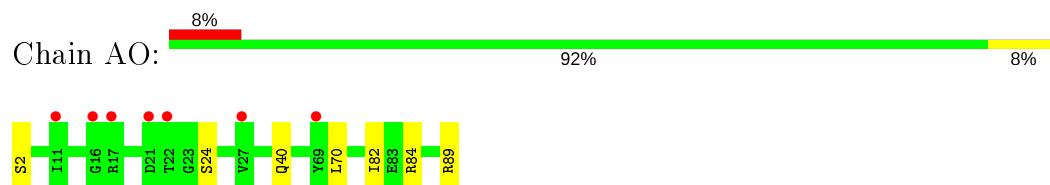
- Molecule 14: 30S ribosomal protein S14



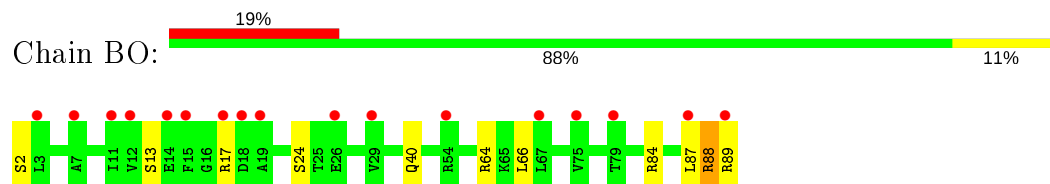
- Molecule 14: 30S ribosomal protein S14



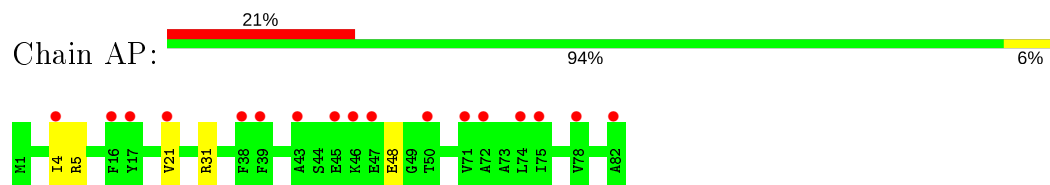
- Molecule 15: 30S ribosomal protein S15



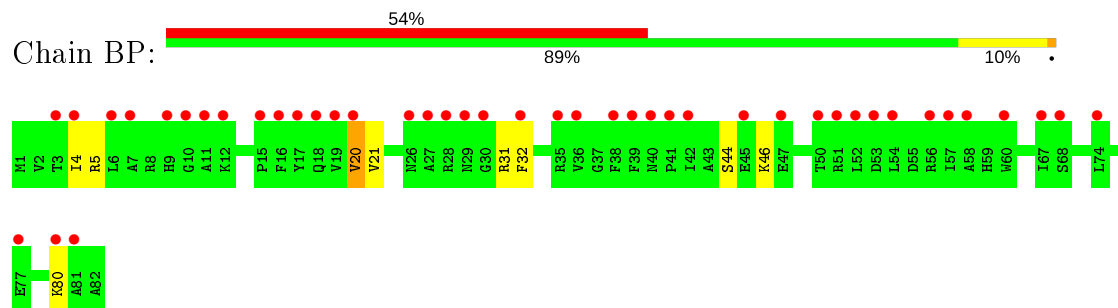
- Molecule 15: 30S ribosomal protein S15



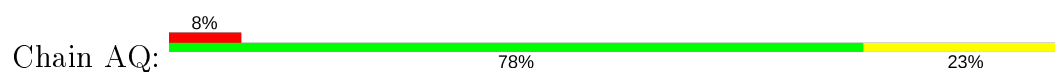
- Molecule 16: 30S ribosomal protein S16



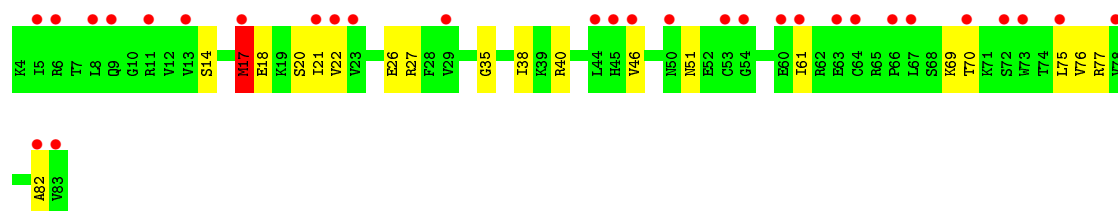
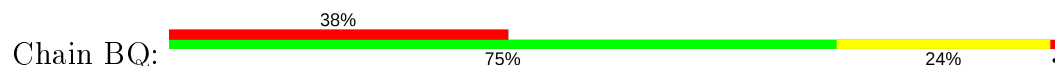
- Molecule 16: 30S ribosomal protein S16



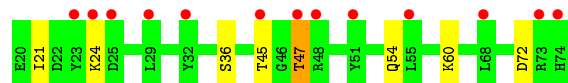
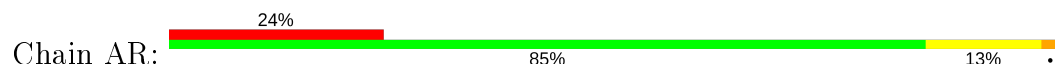
- Molecule 17: 30S ribosomal protein S17



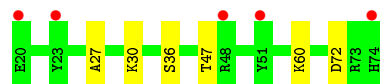
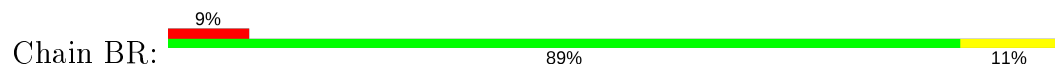
- Molecule 17: 30S ribosomal protein S17



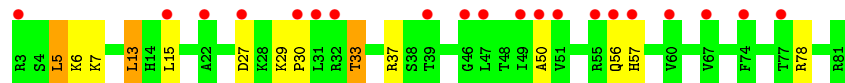
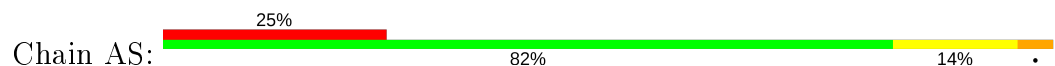
- Molecule 18: 30S ribosomal protein S18



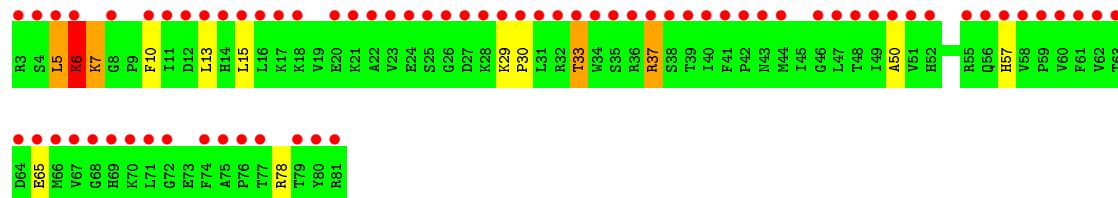
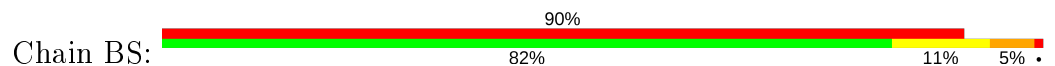
- Molecule 18: 30S ribosomal protein S18



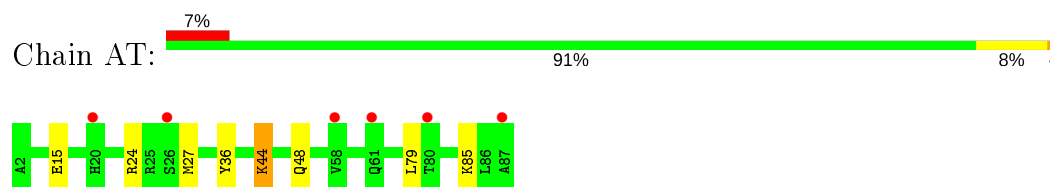
- Molecule 19: 30S ribosomal protein S19



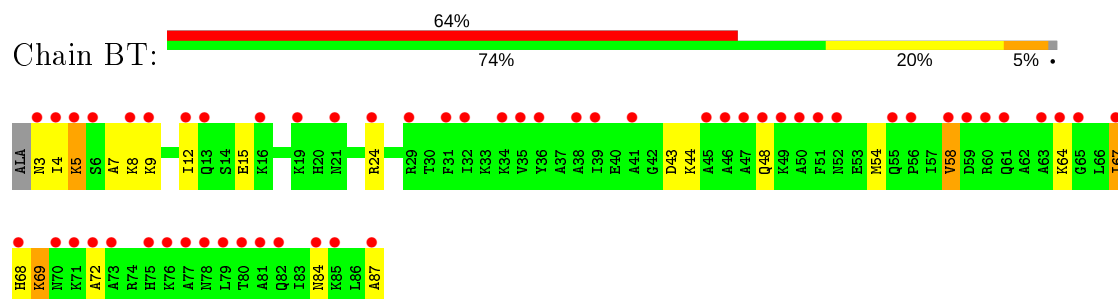
- Molecule 19: 30S ribosomal protein S19



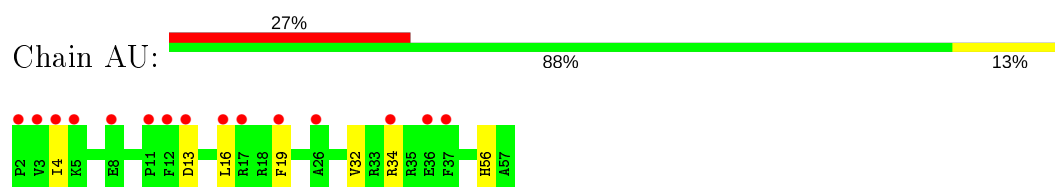
- Molecule 20: 30S ribosomal protein S20



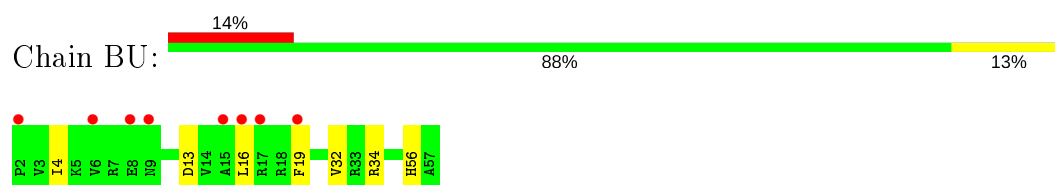
- Molecule 20: 30S ribosomal protein S20



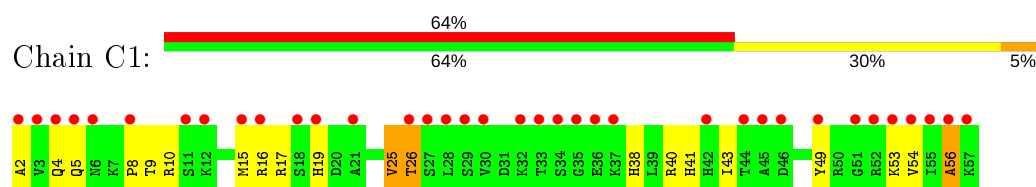
- Molecule 21: 30S ribosomal protein S21



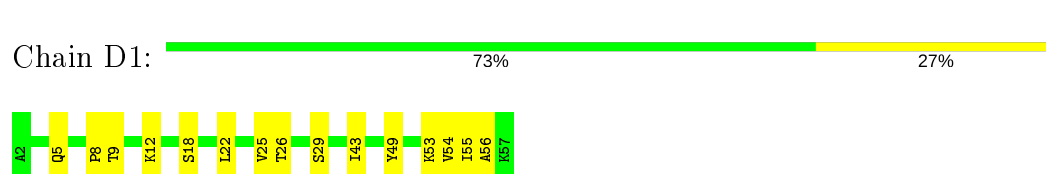
- Molecule 21: 30S ribosomal protein S21



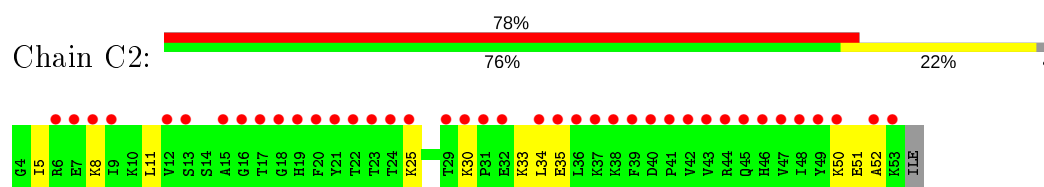
- Molecule 22: 50S ribosomal protein L32



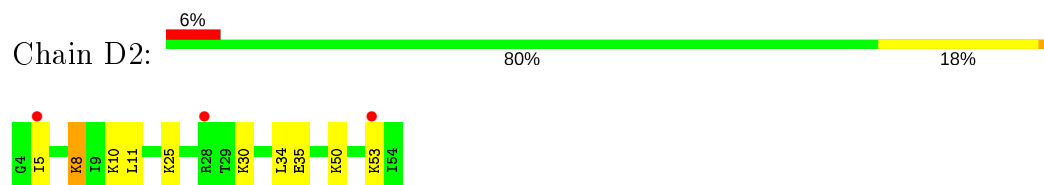
- Molecule 22: 50S ribosomal protein L32



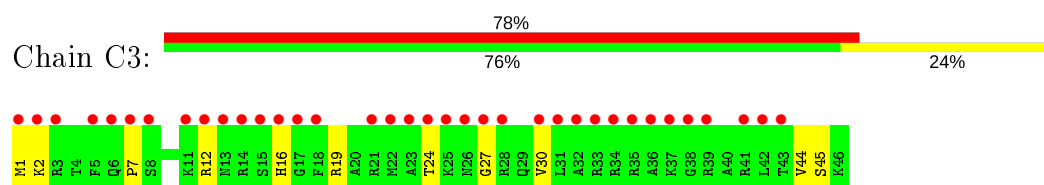
- Molecule 23: 50S ribosomal protein L33



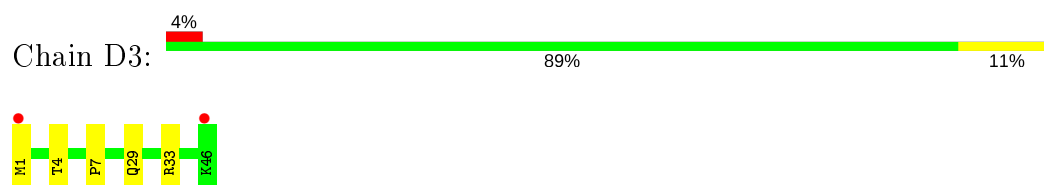
- Molecule 23: 50S ribosomal protein L33



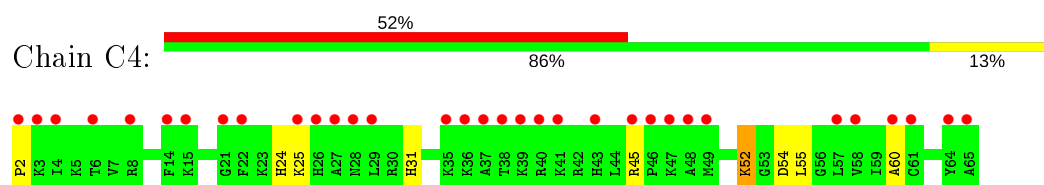
- Molecule 24: 50S ribosomal protein L34



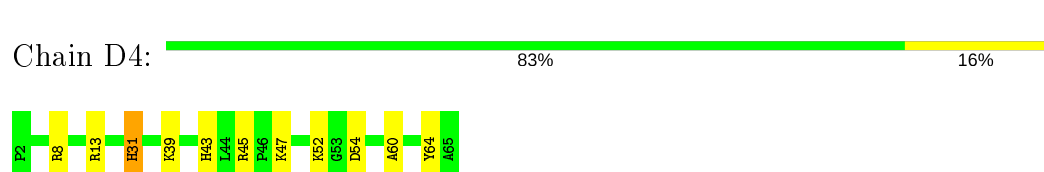
- Molecule 24: 50S ribosomal protein L34



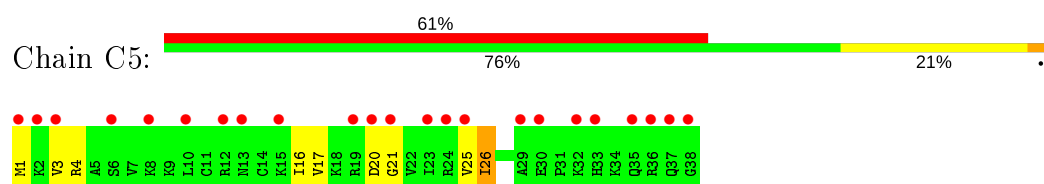
- Molecule 25: 50S ribosomal protein L35



- Molecule 25: 50S ribosomal protein L35



- Molecule 26: 50S ribosomal protein L36




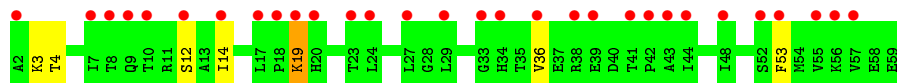
- Molecule 26: 50S ribosomal protein L36

Chain D5:  95% 5%



- Molecule 27: 50S ribosomal protein L30

Chain C0:  52% 88% 10%




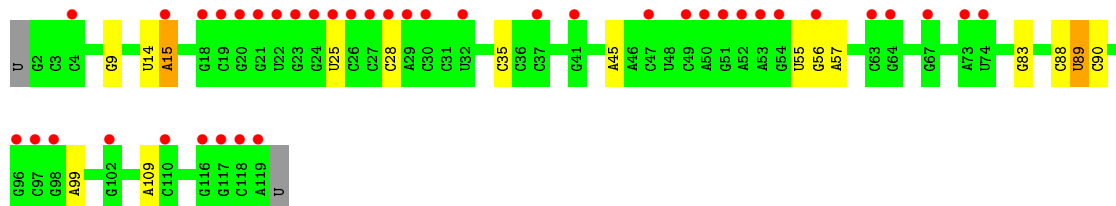
- Molecule 27: 50S ribosomal protein L30

Chain D0:  91% 9%



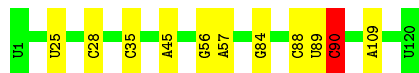
- Molecule 28: 5S rRNA

Chain CB:  33% 85% 12%




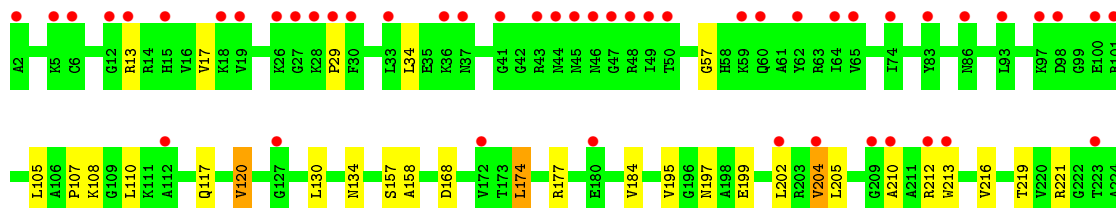
- Molecule 28: 5S rRNA

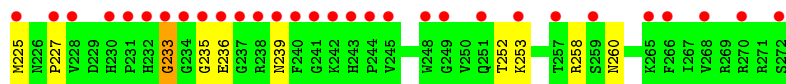
Chain DB:  91% 8%



- Molecule 29: 50S ribosomal protein L2

Chain CC:  29% 85% 14%





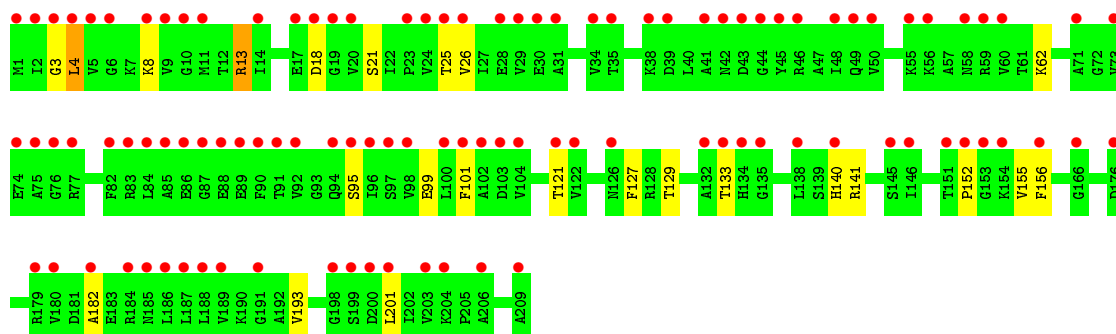
- Molecule 29: 50S ribosomal protein L2

Chain DC: 91% 8% .



- Molecule 30: 50S ribosomal protein L3

Chain CD: 50% 89% 11% .



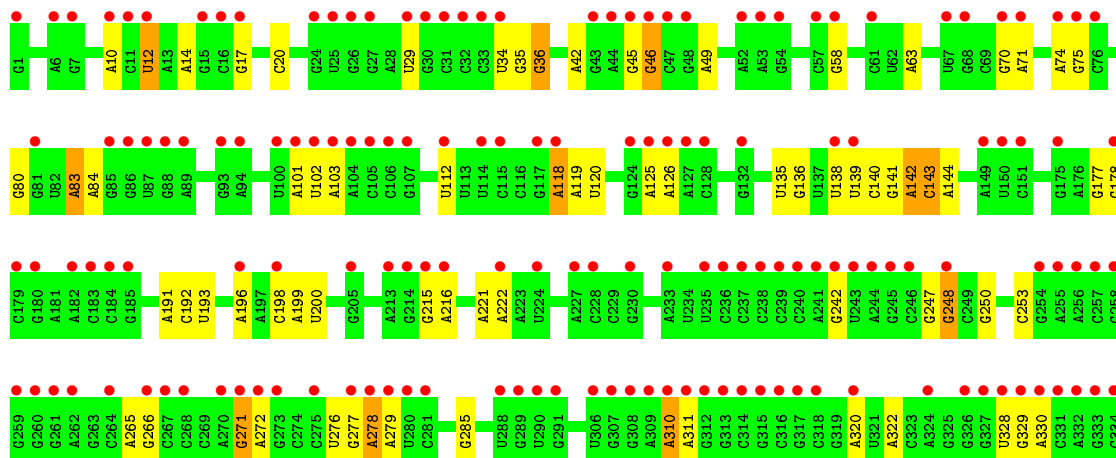
- Molecule 30: 50S ribosomal protein L3

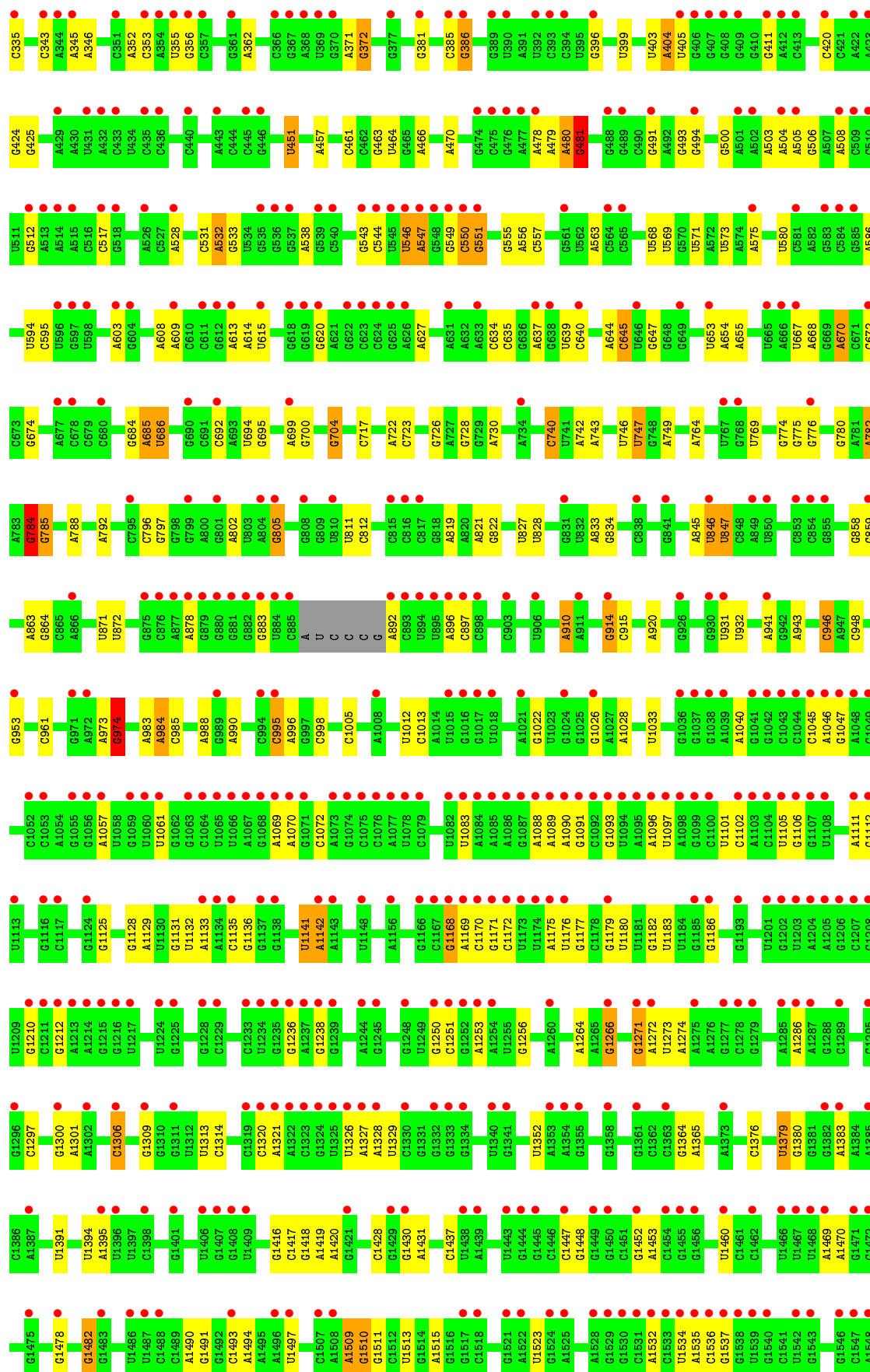
Chain DD: 89% 11% .

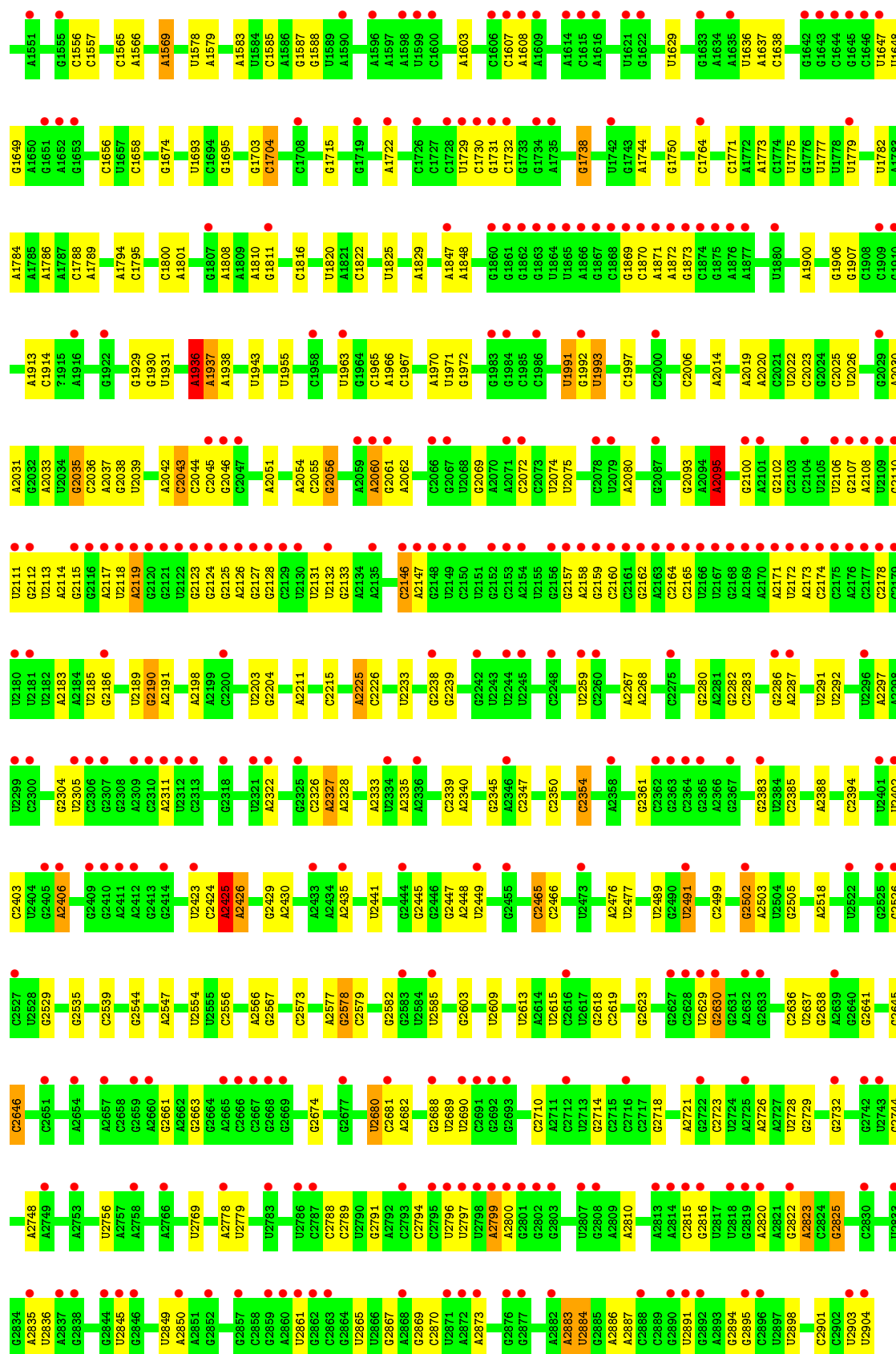


- Molecule 31: 23S rRNA

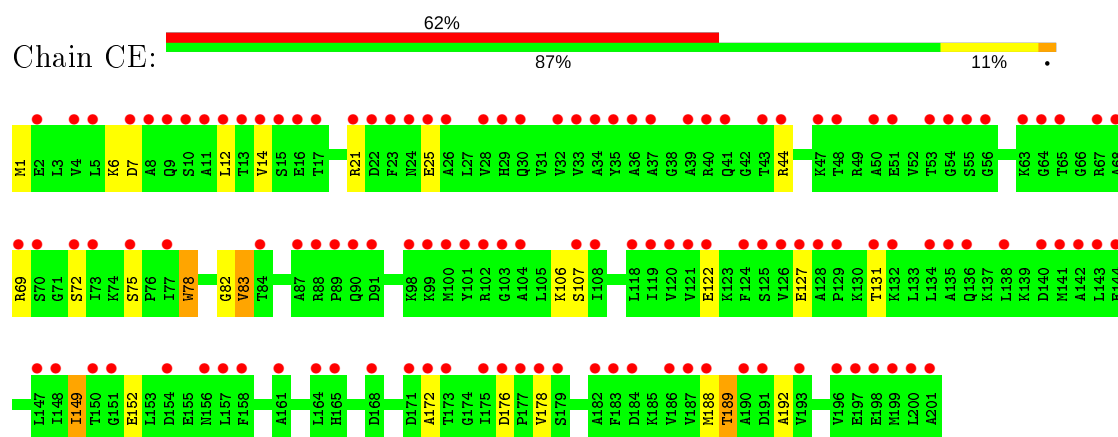
Chain CA: 31% 76% 21% .



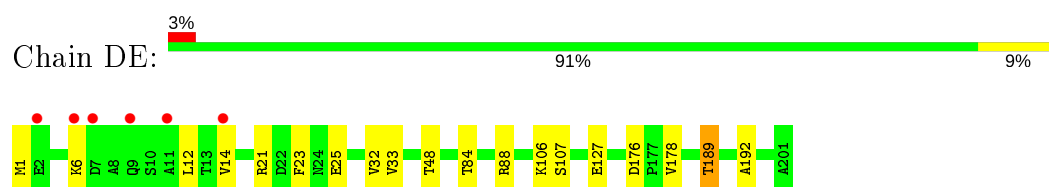




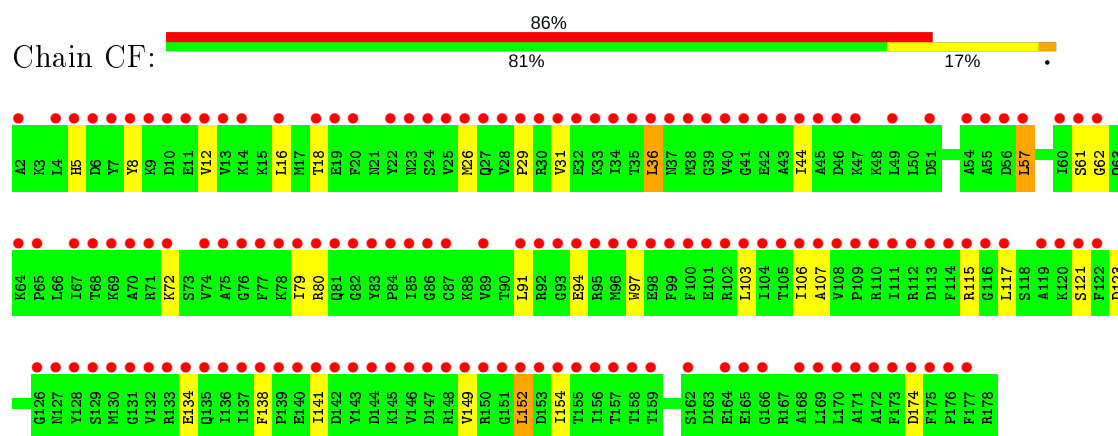
- Molecule 32: 50S ribosomal protein L4



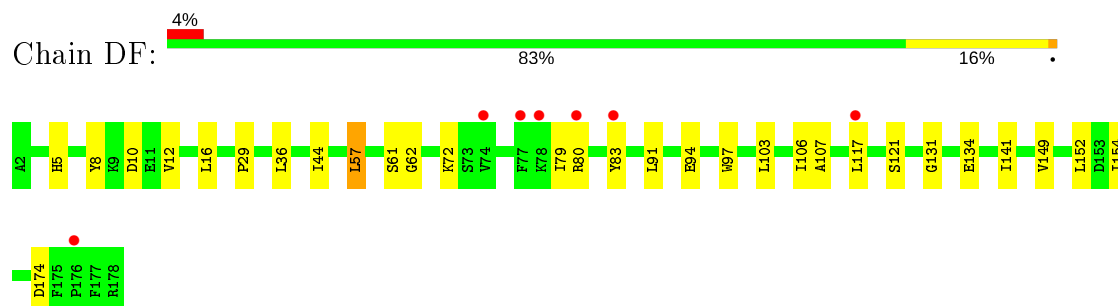
- Molecule 32: 50S ribosomal protein L4



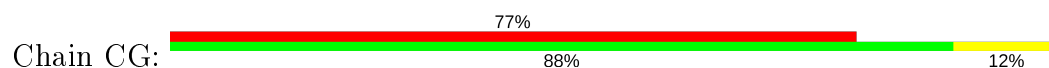
- Molecule 33: 50S ribosomal protein L5

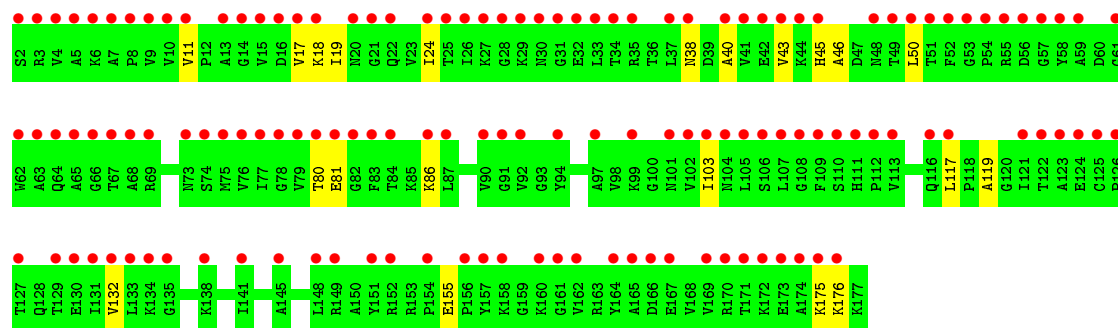


- Molecule 33: 50S ribosomal protein L5

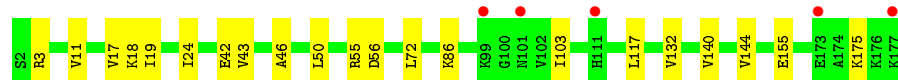
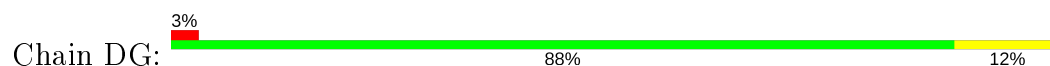


- Molecule 34: 50S ribosomal protein L6

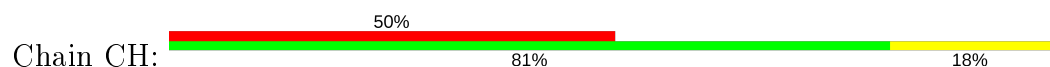




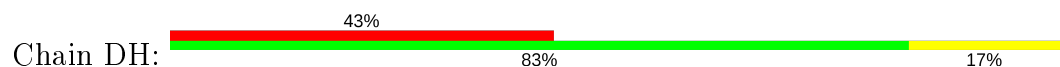
• Molecule 34: 50S ribosomal protein L6



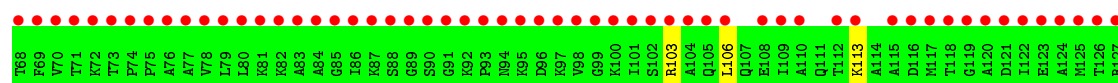
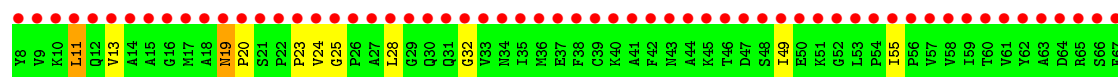
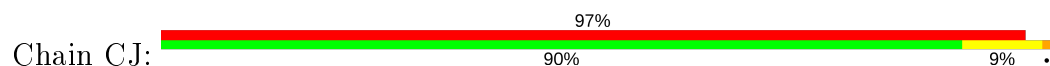
• Molecule 35: 50S ribosomal protein L9

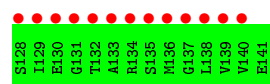


• Molecule 35: 50S ribosomal protein L9

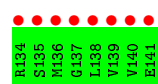
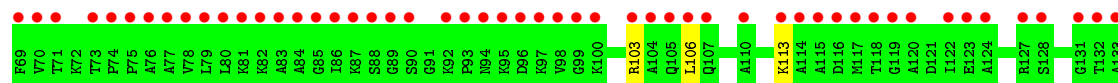
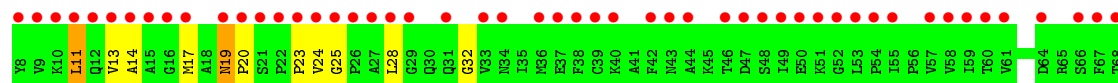
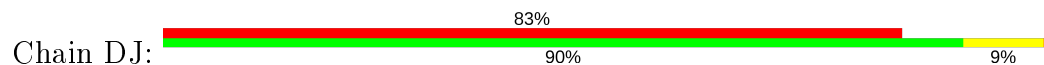


• Molecule 36: 50S ribosomal protein L11

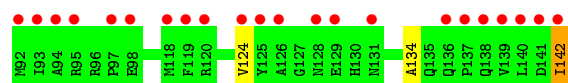
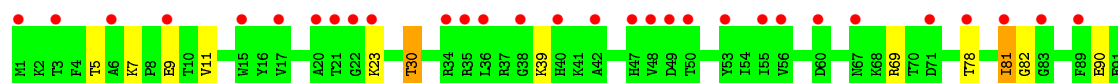
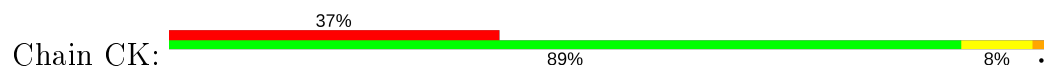




- Molecule 36: 50S ribosomal protein L11



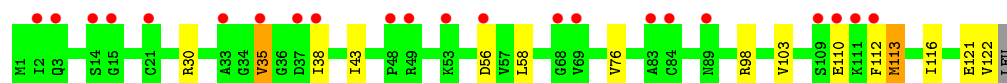
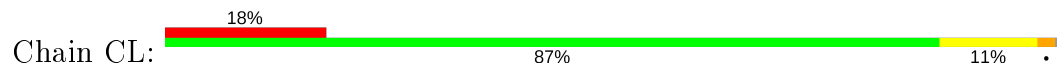
- Molecule 37: 50S ribosomal protein L13



- Molecule 37: 50S ribosomal protein L13



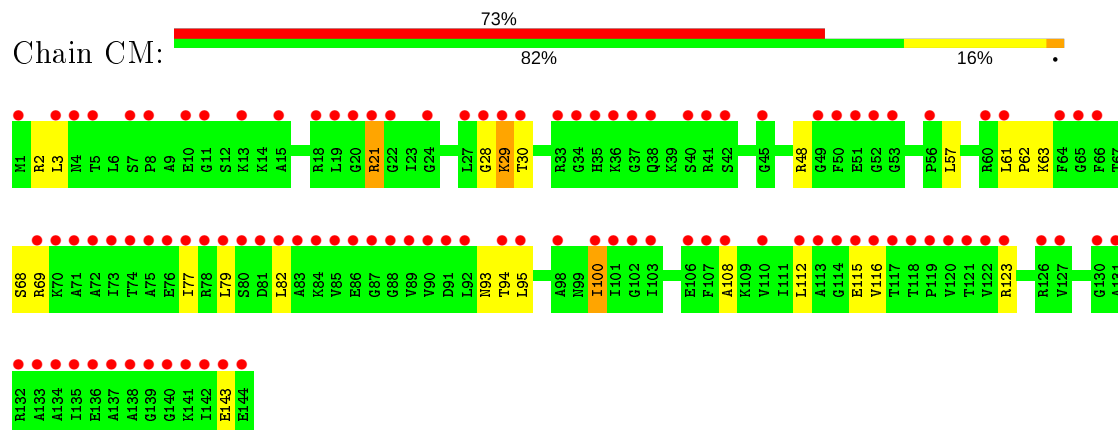
- Molecule 38: 50S ribosomal protein L14



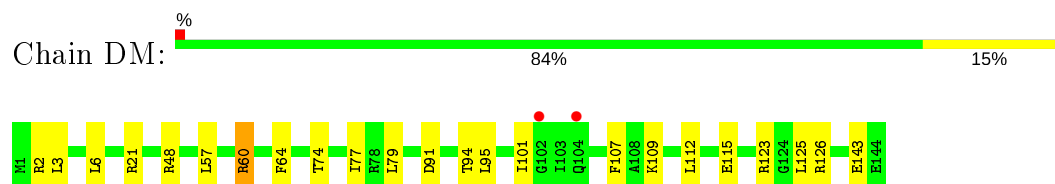
- Molecule 38: 50S ribosomal protein L14



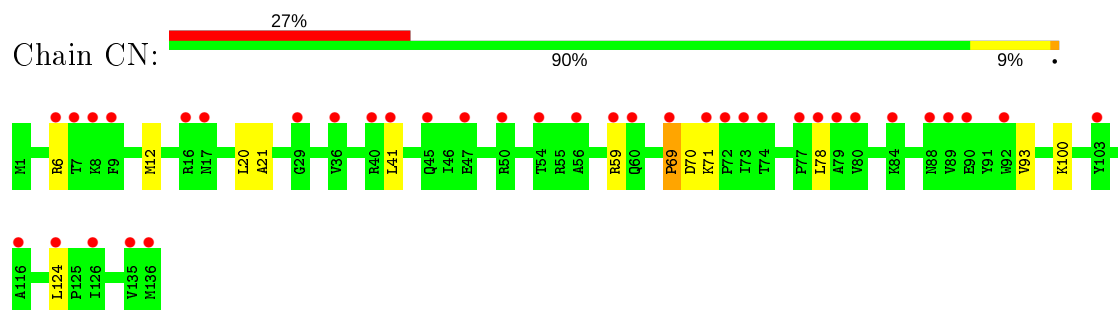
- Molecule 39: 50S ribosomal protein L15



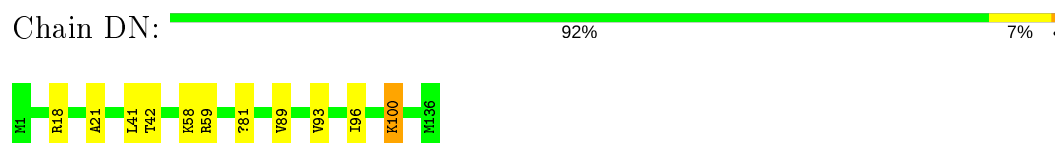
- Molecule 39: 50S ribosomal protein L15



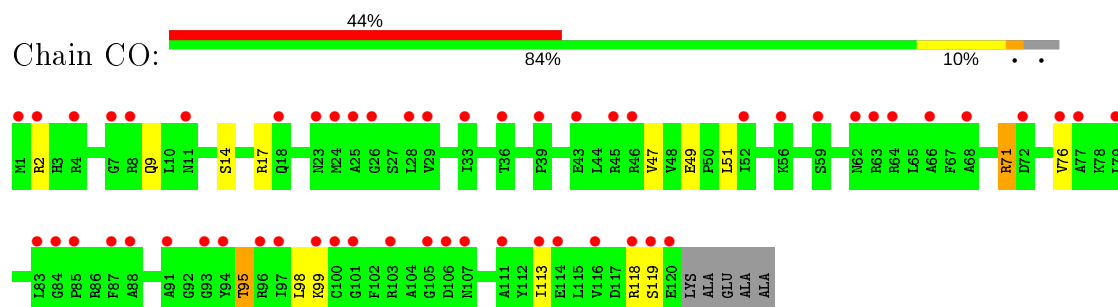
- Molecule 40: 50S ribosomal protein L16



- Molecule 40: 50S ribosomal protein L16



- Molecule 41: 50S ribosomal protein L17




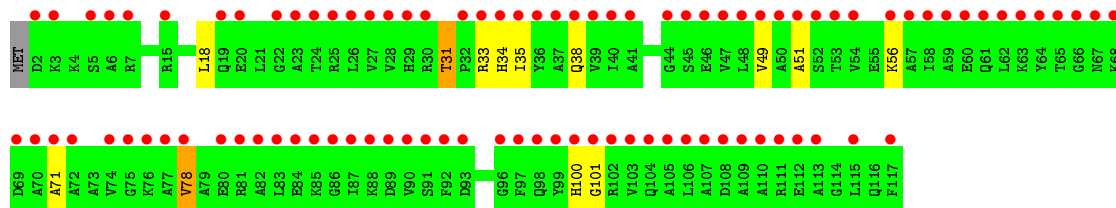
- Molecule 41: 50S ribosomal protein L17

Chain DO:  93% 7%



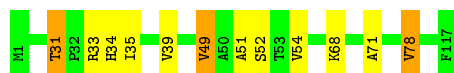
- Molecule 42: 50S ribosomal protein L18

Chain CP:  80% 88% 9% ..

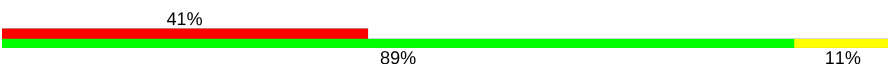


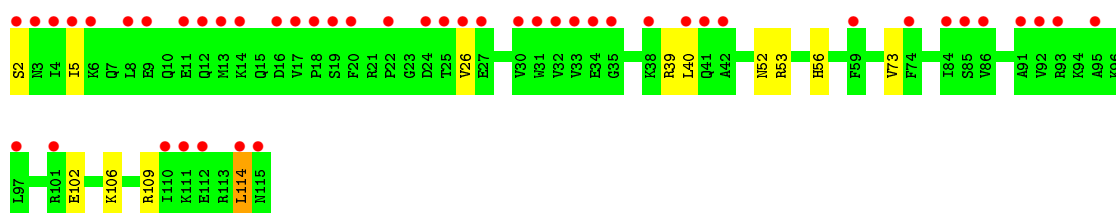
- Molecule 42: 50S ribosomal protein L18

Chain DP:  90% 8% .

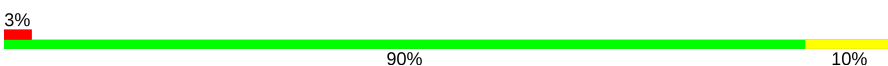


- Molecule 43: 50S ribosomal protein L19

Chain CQ:  41% 89% 11% .



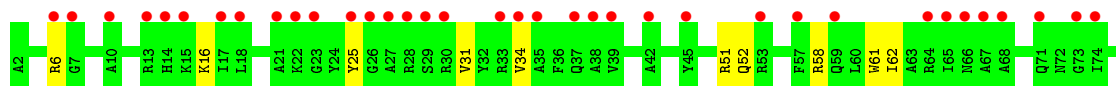
- Molecule 43: 50S ribosomal protein L19

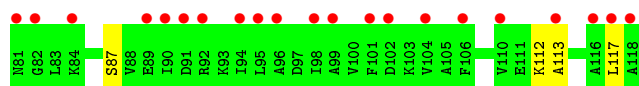
Chain DQ:  3% 90% 10%



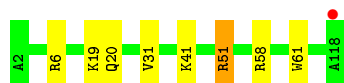
- Molecule 44: 50S ribosomal protein L20

Chain CR:  49% 88% 12%

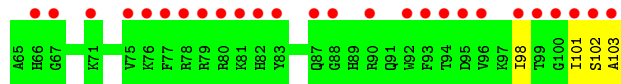
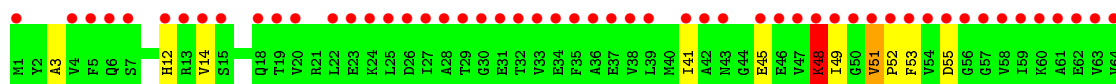
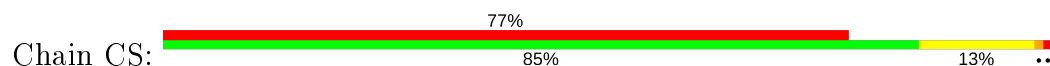




- Molecule 44: 50S ribosomal protein L20



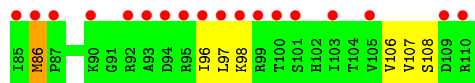
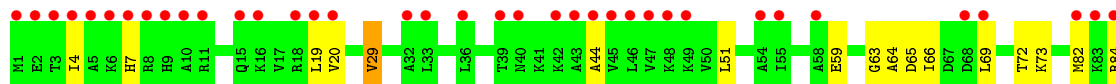
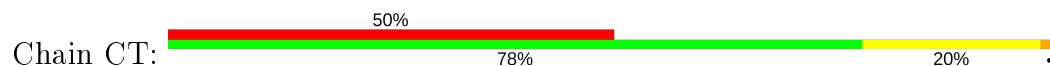
- Molecule 45: 50S ribosomal protein L21



- Molecule 45: 50S ribosomal protein L21



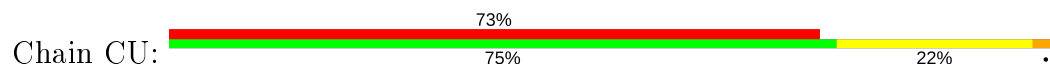
- Molecule 46: 50S ribosomal protein L22

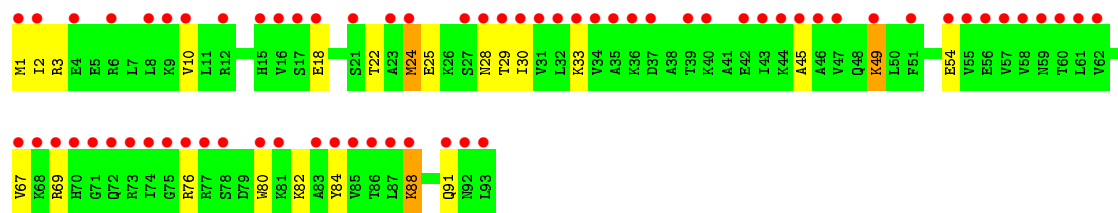


- Molecule 46: 50S ribosomal protein L22



- Molecule 47: 50S ribosomal protein L23

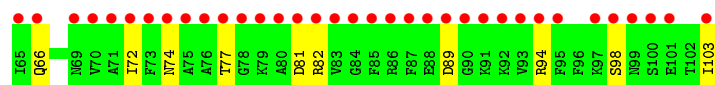
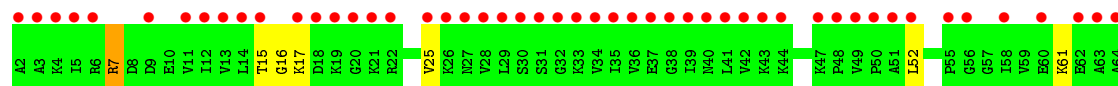
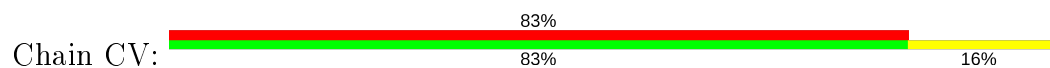




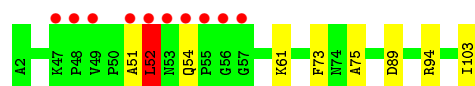
- Molecule 47: 50S ribosomal protein L23



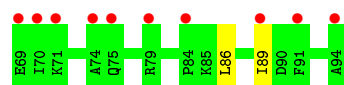
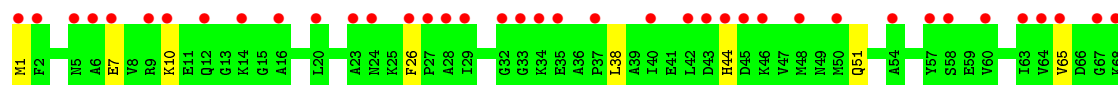
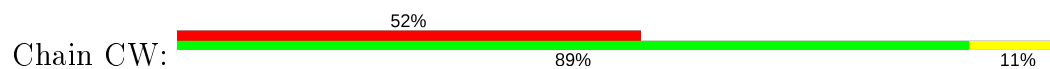
- Molecule 48: 50S ribosomal protein L24



- Molecule 48: 50S ribosomal protein L24



- Molecule 49: 50S ribosomal protein L25

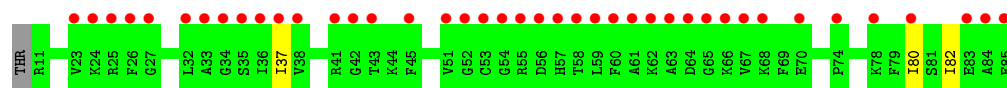


- Molecule 49: 50S ribosomal protein L25



- Molecule 50: 50S ribosomal protein L27

Chain CX: 




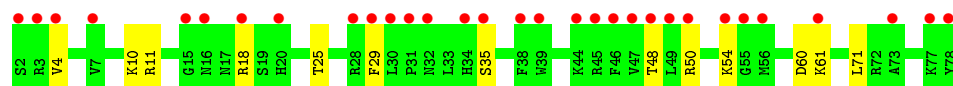
- Molecule 50: 50S ribosomal protein L27

Chain DX: 




- Molecule 51: 50S ribosomal protein L28

Chain CY: 

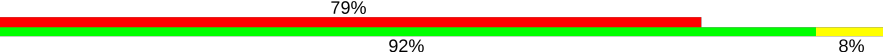


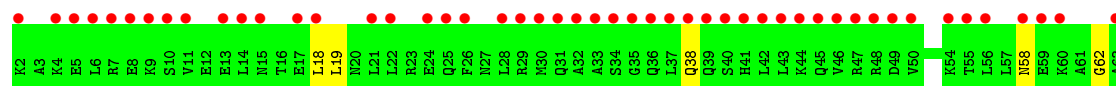
- Molecule 51: 50S ribosomal protein L28

Chain DY: 



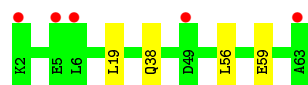
- Molecule 52: 50S ribosomal protein L29

Chain CZ: 



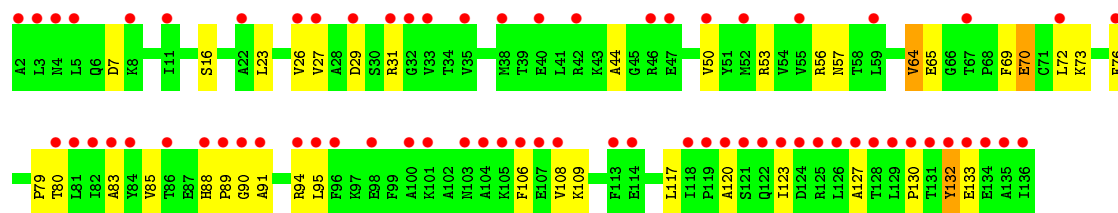
- Molecule 52: 50S ribosomal protein L29

Chain DZ: 

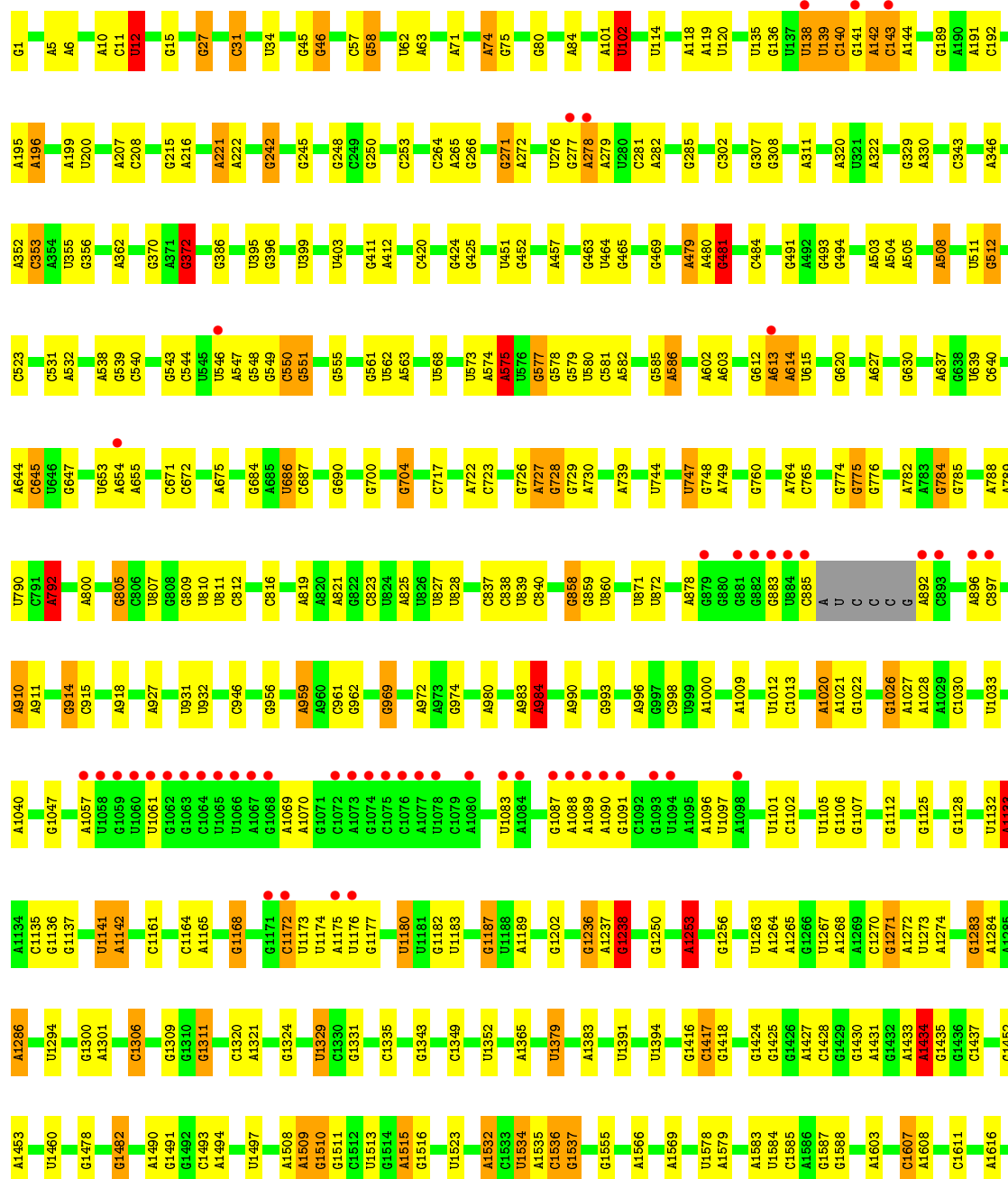


- Molecule 53: 50S ribosomal protein L10

Chain DI: 



• Molecule 54: 23S rRNA



C2730	C2573	C2424	G2286	G2162	G2087	U1971	U1779	G1631
G2731	C2574	A2425	A2287	A2163	A2097	G1972	U1779	A1635
G2732	C2575	A2426	A2288	C2164	A2097	G1975	U1782	U1636
G2744	C2576	C2427	U2291	C2165	G2100	U1991	U1787	A1637
A2748	A2577	U2431	U2292	U2166	A2101	U1991	A1794	C1644
U2756	C2578	A2435	A2297	C2168	G2102	U1992	C1795	G1645
A2765	G2581	U2441	C2301	A2170	U2105	C1987	A1808	C1646
A2766	G2582	U2444	C2304	A2171	U2106	C1987	C1800	U1647
A2778	U2585	G2444	U2305	A2172	A2107	C1999	A1801	G1649
C2788	G2586	G2445	U2308	A2173	A2108	A2014	A1802	A1652
C2789	U2597	G2446	A2309	C2174	U2109	U2017	C1816	G1653
U2790	G2603	A2448	C2310	C2175	G2110	A2020	U1820	G1660
G2791	U2609	U2449	A2311	A2176	U2111	C2023	A1829	A1664
U2796	U2613	G2455	U2312	C2177	G2112	G2029	C1830	A1665
U2797	G2623	A2468	U2324	C2178	U2113	G2030	G1831	G1666
U2798	U2628	A2471	G2325	C2179	A2114	G2031	A1847	G1667
A2799	G2630	U2476	A2326	C2180	G2115	A2032	A1848	A1672
A2800	U2636	G2481	U2327	U2181	G2116	A2033	A1853	G1673
G2811	U2637	U2489	A2333	U2182	A2117	C2036	G1906	G1674
A2820	U2638	U2491	U2334	A2183	U2118	G2043	G1907	G1715
G2821	U2639	C2496	A2335	A2184	A2119	C2044	A1913	C1727
G2822	U2645	A2497	C2339	U2185	G2120	A2051	C1920	C1728
G2823	U2661	C2498	A2340	G2190	U2122	G2053	G1930	U1729
A2826	A2662	G2501	C2347	A2198	G2123	A2055	G1931	G1731
U2836	G2663	G2502	C2354	G2204	G2125	G2056	U1932	C1732
U2845	G2674	G2505	U2360	A2211	A2126	A2060	A1933	G1733
G2848	U2674	U2516	G2375	A2225	G2127	A2062	A1739	A1744
U2849	C2681	C2517	G2382	A2234	G2128	G2069	A1936	G1753
G2867	U2684	A2518	U2383	G2238	U2131	A2070	A1937	C1761
A2868	G2688	U2519	C2385	G2239	G2132	C2072	U1955	C1764
A2873	U2689	C2520	A2386	G2262	A2133	U2074	C1965	A1773
G2885	U2690	C2521	U2387	U2262	A2134	A2077	A1866	C1967
A2886	C2691	G2529	C2394	A2266	G2140	C2078	C1967	G1776
U2891	G2692	G2535	U2402	A2267	G2141	U2086		
G2895	G2708	U2535	C2403	A2268	A2142			
C2901	G2714	A2547	U2404	A2273	A2143			
U2902	C2717	C2556	A2405	A2274	G2144			
U2903	A2726	A2564	A2406	G2280	C2145			
U	A2727	A2565	A2407	A2281	G2146			
		G2567	C2420	C2282	A2147			
			U2423	C2283	G2148			
					G2152			
					C2153			
					A2154			
					U2155			
					G2156			
					A2158			
					C2159			
					C2160			
					C2161			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.31Å 434.58Å 624.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.16 – 2.80 48.14 – 2.80	Depositor EDS
% Data completeness (in resolution range)	85.7 (48.16-2.80) 85.7 (48.14-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	19.79 (at 2.81Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, R_{free}	0.209 , 0.219 0.233 , 0.243	Depositor DCC
R_{free} test set	4734 reflections (0.39%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 80.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	295188	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

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

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

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

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

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

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

All (216) bond length outliers are listed below:

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

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

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

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

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

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

All (59) bond angle outliers are listed below:

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

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

There are no chirality outliers.

All (110) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1432	G	Sidechain

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

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

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

5.2 Too-close contacts ⓘ

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

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

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	DU	739	0	807	4	0
48	CV	780	0	831	6	0
48	DV	780	0	831	4	0
49	CW	753	0	780	5	0
49	DW	753	0	780	3	0
50	CX	569	0	581	1	0
50	DX	591	0	606	7	0
51	CY	625	0	652	7	0
51	DY	625	0	652	4	0
52	CZ	501	0	531	0	0
52	DZ	501	0	531	1	0
53	DI	1023	0	1052	19	0
54	DA	62423	0	31411	171	0
55	AA	71	0	0	0	0
55	BA	43	0	0	0	0
55	C3	1	0	0	0	0
55	CA	155	0	0	0	0
55	CB	3	0	0	0	0
55	DA	182	0	0	0	0
55	DB	9	0	0	0	0
55	DD	2	0	0	0	0
55	DM	1	0	0	0	0
55	DR	2	0	0	0	0
56	AA	13	0	18	1	0
56	BA	13	0	18	0	0
56	DA	26	0	36	2	0
56	DQ	13	0	18	0	0
56	DR	13	0	18	5	0
56	DS	13	0	18	1	0
57	AA	16	0	28	0	0
57	DA	40	0	70	5	0
57	DE	16	0	28	0	0
57	DK	8	0	14	0	0
57	DN	8	0	14	1	0
57	DS	8	0	14	0	0
57	DT	16	0	28	0	0
58	AA	24	0	48	0	0
58	DA	72	0	144	10	0
59	AA	32	0	21	1	0
59	BA	32	0	21	1	0
60	AB	1	0	0	0	0
60	C5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	D5	1	0	0	0	0
61	AL	7	0	10	0	0
61	D1	7	0	10	1	0
61	D3	7	0	10	2	0
61	DA	35	0	50	1	0
61	DL	7	0	10	0	0
61	DP	7	0	10	1	0
61	DQ	7	0	10	0	0
62	D1	4	0	6	0	0
62	DA	36	0	54	2	0
62	DB	8	0	12	1	0
63	D1	10	0	14	2	0
63	D3	10	0	14	0	0
63	DA	40	0	56	5	0
63	DD	10	0	14	2	0
63	DS	10	0	14	0	0
63	DU	10	0	14	1	0
64	DA	40	0	76	4	0
65	DA	32	0	44	0	0
66	DA	12	0	11	0	0
67	DA	11	0	5	0	0
68	DA	8	0	12	1	0
69	AA	507	0	0	0	0
69	AC	4	0	0	0	0
69	AD	2	0	0	0	0
69	AE	4	0	0	0	0
69	AF	1	0	0	0	0
69	AG	1	0	0	0	0
69	AH	1	0	0	0	0
69	AJ	2	0	0	0	0
69	AK	5	0	0	0	0
69	AL	8	0	0	0	0
69	AM	4	0	0	1	0
69	AN	5	0	0	1	0
69	AO	2	0	0	0	0
69	AP	2	0	0	0	0
69	AR	1	0	0	0	0
69	AS	1	0	0	0	0
69	AT	2	0	0	0	0
69	AU	3	0	0	0	0
69	BA	287	0	0	1	0
69	BD	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	BE	1	0	0	0	0
69	BF	1	0	0	0	0
69	BK	1	0	0	0	0
69	BL	3	0	0	0	0
69	BN	2	0	0	0	0
69	BO	1	0	0	0	0
69	BP	3	0	0	0	0
69	BR	1	0	0	0	0
69	BT	4	0	0	0	0
69	BU	2	0	0	0	0
69	C3	3	0	0	1	0
69	C4	2	0	0	0	0
69	CA	692	0	0	1	0
69	CB	13	0	0	0	0
69	CC	10	0	0	0	0
69	CD	5	0	0	0	0
69	CE	7	0	0	0	0
69	CL	1	0	0	0	0
69	CM	3	0	0	0	0
69	CO	1	0	0	0	0
69	CU	3	0	0	0	0
69	CV	1	0	0	0	0
69	CW	1	0	0	0	0
69	CY	1	0	0	0	0
69	D0	27	0	0	0	0
69	D1	42	0	0	0	0
69	D2	7	0	0	0	0
69	D3	24	0	0	0	0
69	D4	33	0	0	1	0
69	D5	13	0	0	0	0
69	DA	4834	0	0	7	0
69	DB	212	0	0	0	0
69	DC	102	0	0	0	0
69	DD	105	0	0	1	0
69	DE	63	0	0	0	0
69	DF	14	0	0	0	0
69	DG	6	0	0	0	0
69	DH	2	0	0	0	0
69	DK	58	0	0	0	0
69	DL	51	0	0	0	0
69	DM	62	0	0	0	0
69	DN	71	0	0	0	0

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (1182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2898:U:O2	37:CK:134:ALA:HB1	2.20	0.41
31:CA:910:A:H62	40:CN:12:MET:HA	1.85	0.41
54:DA:1020:A:C2	54:DA:1141:U:C2	3.08	0.41
54:DA:2324:U:H3'	54:DA:2325:G:H5''	2.03	0.41
50:DX:41[A]:ARG:HD2	54:DA:2387:U:H1'	2.03	0.41
35:DH:68:ARG:HB3	35:DH:134:VAL:HG21	2.03	0.41
50:DX:41[B]:ARG:HA	50:DX:41[B]:ARG:HD3	1.94	0.41
9:AI:19:VAL:HG11	9:AI:83:ILE:HA	2.03	0.41
1:BA:841:C:H3'	1:BA:842:U:C4'	2.51	0.41
19:BS:30:PRO:HB2	19:BS:50:ALA:HB2	2.03	0.41
31:CA:2038:G:H2'	31:CA:2039:U:O4'	2.21	0.41
31:CA:547:A:H2'	31:CA:547:A:N3	2.36	0.41
31:CA:2641:G:H5''	37:CK:78:THR:HB	2.03	0.41
54:DA:2133:G:H21	54:DA:2158:A:N6	2.18	0.41
32:DE:178:VAL:HG23	39:DM:3:LEU:HD21	2.01	0.41
32:DE:23:PHE:HE2	32:DE:25:GLU:HG3	1.86	0.41
50:DX:38:VAL:HG12	50:DX:59:LEU:HB2	2.02	0.41
5:AE:157:ARG:CD	8:AH:43:GLU:O	2.69	0.41
11:AK:20:VAL:HB	11:AK:35:THR:HG23	2.03	0.41
1:BA:567:G:H2'	1:BA:568:G:O4'	2.20	0.41
11:BK:34:ILE:HG12	11:BK:70:CYS:SG	2.60	0.41
25:C4:24:HIS:CG	39:CM:61:LEU:HD13	2.56	0.41
31:CA:1636:U:H2'	31:CA:1637:A:C8	2.55	0.41
34:CG:38:ASN:HD22	34:CG:40:ALA:HB3	1.86	0.41
36:CJ:49:ILE:HG13	36:CJ:55:ILE:HD13	2.03	0.41
53:DI:132:TYR:N	53:DI:133:GLU:HB2	2.35	0.41
30:DD:13:ARG:HH11	43:DQ:56:HIS:HA	1.86	0.41
10:AJ:19:ASP:HA	10:AJ:22:THR:HB	2.03	0.41
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.85	0.41
1:BA:216:U:H4'	1:BA:464:U:H4'	2.02	0.41
1:BA:439:U:H5''	4:BD:121:LYS:HD2	2.02	0.41
26:C5:4:ARG:HB2	31:CA:2466:C:OP1	2.21	0.41
31:CA:29:U:O5'	31:CA:29:U:H6	2.02	0.41
31:CA:780:G:H2'	31:CA:782:A:N7	2.36	0.41
29:CC:107:PRO:HD2	29:CC:110:LEU:HD22	2.03	0.41
54:DA:1306:C:H5''	54:DA:1306:C:H6	1.85	0.41
54:DA:207:A:H2'	54:DA:208:C:O4'	2.20	0.41
53:DI:29:ASP:HB3	53:DI:106:PHE:HB2	2.02	0.41
36:DJ:14:ALA:HB3	36:DJ:17:MET:HB2	2.03	0.41
39:DM:74:THR:HG23	39:DM:107:PHE:HB2	2.02	0.41
40:DN:89:VAL:CG1	57:DN:201:MPD:HM3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:DT:84:ARG:HB2	46:DT:96:ILE:HB	2.02	0.41
51:DY:29:PHE:HB3	54:DA:396:G:H1'	2.03	0.41
1:AA:1141:C:O2'	1:AA:1142:G:H8	2.03	0.40
1:AA:1216:A:H5''	14:AN:5:SER:HB3	2.02	0.40
1:AA:568:G:O6	12:AL:2:ALA:HB2	2.21	0.40
6:BF:22:ILE:HG23	6:BF:39:LEU:HD11	2.02	0.40
10:BJ:59:LYS:HD2	10:BJ:60:ASP:OD1	2.21	0.40
20:BT:69:LYS:H	20:BT:69:LYS:HG3	1.60	0.40
54:DA:281:C:H2'	54:DA:282:A:C8	2.56	0.40
54:DA:839:U:H2'	54:DA:840:C:C6	2.56	0.40
30:DD:26:VAL:HG21	43:DQ:5:ILE:HG12	2.03	0.40
34:DG:50:LEU:HD13	34:DG:72:LEU:HD23	2.02	0.40
53:DI:23:LEU:HD13	53:DI:89:PRO:HD3	2.03	0.40
39:DM:123:ARG:HG3	39:DM:143:GLU:HG3	2.03	0.40
50:DX:41[A]:ARG:HH12	54:DA:2262:U:H5''	1.85	0.40
1:AA:831:A:H5''	2:AB:21:ARG:HD3	2.03	0.40
14:AN:46:LEU:HD22	19:AS:13:LEU:HG	2.02	0.40
1:BA:1197:A:H5''	59:BA:1602:TAC:O12	2.21	0.40
1:BA:268:U:H2'	1:BA:269:C:C6	2.56	0.40
1:BA:718:A:H5'	11:BK:119:ASN:HB2	2.04	0.40
1:BA:1108:G:H5''	3:BC:176:HIS:ND1	2.36	0.40
9:BI:116:VAL:HG21	10:BJ:62:ARG:HD3	2.04	0.40
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.56	0.40
54:DA:2273:A:H2'	54:DA:2274:A:C8	2.55	0.40
53:DI:120:ALA:HA	53:DI:123:ILE:HD11	2.03	0.40
53:DI:65:GLU:HA	53:DI:70:GLU:HG3	2.02	0.40
52:DZ:56:LEU:HA	52:DZ:59:GLU:HG2	2.03	0.40
1:AA:268:U:H2'	1:AA:269:C:C6	2.56	0.40
11:AK:31:ILE:HG12	11:AK:46:THR:CG2	2.51	0.40
25:C4:52:LYS:HA	25:C4:55:LEU:HD12	2.03	0.40
31:CA:1306:C:H5''	31:CA:1306:C:H6	1.86	0.40
31:CA:1418:G:H2'	31:CA:1579:A:N6	2.36	0.40
54:DA:1532:A:H5''	54:DA:1532:A:H8	1.86	0.40
54:DA:2339:C:H2'	54:DA:2340:A:C8	2.57	0.40
39:DM:77:ILE:CD1	39:DM:101:ILE:CG2	2.97	0.40
39:DM:95:LEU:HD11	39:DM:125:LEU:HD21	2.03	0.40
46:DT:72:THR:CG2	46:DT:108:SER:HB3	2.52	0.40
1:AA:234:C:H4'	17:AQ:66:PRO:HG3	2.03	0.40
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	2.04	0.40
12:BL:74:LEU:HD21	12:BL:80:ILE:HG21	2.03	0.40
1:BA:1322:C:P	19:BS:78:ARG:HH22	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1509:A:HO2'	31:CA:1510:G:H8	1.70	0.40
31:CA:2327:A:H2'	31:CA:2328:A:C8	2.56	0.40
31:CA:644:A:H2'	31:CA:645:C:O4'	2.22	0.40
36:CJ:19:ASN:N	36:CJ:20:PRO:HD2	2.37	0.40
44:CR:58:ARG:HH11	44:CR:62:ILE:HD11	1.86	0.40
22:D1:12:LYS:HD2	22:D1:12:LYS:HA	1.86	0.40
22:D1:8:PRO:HD2	54:DA:1263:U:O2'	2.22	0.40
54:DA:2788:C:H2'	54:DA:2789:C:C6	2.57	0.40
38:DL:113:MET:O	38:DL:116:ILE:HG13	2.19	0.40
1:AA:567:G:H2'	1:AA:568:G:O4'	2.21	0.40
1:BA:580:C:H2'	1:BA:581:G:O4'	2.22	0.40
19:BS:5:LEU:CD2	19:BS:10:PHE:HB2	2.51	0.40
31:CA:1072:C:H2'	31:CA:1093:G:O6	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	210 (95%)	9 (4%)	3 (1%)	11	34
2	BB	222/224 (99%)	211 (95%)	7 (3%)	4 (2%)	8	28
3	AC	204/206 (99%)	192 (94%)	11 (5%)	1 (0%)	29	61
3	BC	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	15	44
4	AD	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
4	BD	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
5	AE	153/155 (99%)	147 (96%)	5 (3%)	1 (1%)	22	53
5	BE	148/155 (96%)	132 (89%)	12 (8%)	4 (3%)	5	17
6	AF	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
6	BF	98/106 (92%)	91 (93%)	5 (5%)	2 (2%)	7	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	149/151 (99%)	137 (92%)	11 (7%)	1 (1%)	22	53
7	BG	149/151 (99%)	140 (94%)	9 (6%)	0	100	100
8	AH	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
8	BH	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
9	AI	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
9	BI	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
10	AJ	97/99 (98%)	88 (91%)	7 (7%)	2 (2%)	7	23
10	BJ	96/99 (97%)	77 (80%)	14 (15%)	5 (5%)	2	6
11	AK	115/117 (98%)	107 (93%)	6 (5%)	2 (2%)	9	29
11	BK	115/117 (98%)	104 (90%)	9 (8%)	2 (2%)	9	29
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
12	BL	120/123 (98%)	114 (95%)	5 (4%)	1 (1%)	19	49
13	AM	112/114 (98%)	103 (92%)	6 (5%)	3 (3%)	5	17
13	BM	112/114 (98%)	102 (91%)	5 (4%)	5 (4%)	2	8
14	AN	98/100 (98%)	88 (90%)	8 (8%)	2 (2%)	7	24
14	BN	98/100 (98%)	90 (92%)	6 (6%)	2 (2%)	7	24
15	AO	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
15	BO	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	13	39
16	AP	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
16	BP	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	5	19
17	AQ	78/80 (98%)	70 (90%)	7 (9%)	1 (1%)	12	36
17	BQ	78/80 (98%)	68 (87%)	5 (6%)	5 (6%)	1	3
18	AR	53/55 (96%)	53 (100%)	0	0	100	100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	12	36
19	BS	77/79 (98%)	68 (88%)	7 (9%)	2 (3%)	5	18
20	AT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
20	BT	83/86 (96%)	79 (95%)	3 (4%)	1 (1%)	13	39
21	AU	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
21	BU	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
22	C1	54/56 (96%)	47 (87%)	4 (7%)	3 (6%)	2	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	D1	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	3	9
23	D2	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
24	C3	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	6	21
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	C4	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
25	D4	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
26	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	5	17
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	54 (96%)	0	2 (4%)	3	11
27	D0	57/58 (98%)	56 (98%)	1 (2%)	0	100	100
29	CC	269/271 (99%)	252 (94%)	12 (4%)	5 (2%)	8	26
29	DC	269/271 (99%)	257 (96%)	10 (4%)	2 (1%)	22	53
30	CD	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
30	DD	206/209 (99%)	202 (98%)	4 (2%)	0	100	100
32	CE	199/201 (99%)	191 (96%)	5 (2%)	3 (2%)	10	33
32	DE	199/201 (99%)	194 (98%)	4 (2%)	1 (0%)	29	61
33	CF	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	56
33	DF	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25	56
34	CG	174/176 (99%)	162 (93%)	7 (4%)	5 (3%)	4	15
34	DG	174/176 (99%)	165 (95%)	8 (5%)	1 (1%)	25	56
35	CH	147/149 (99%)	136 (92%)	6 (4%)	5 (3%)	3	13
35	DH	147/149 (99%)	138 (94%)	6 (4%)	3 (2%)	7	24
36	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	4	15
36	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	4	15
37	CK	140/142 (99%)	135 (96%)	4 (3%)	1 (1%)	22	53
37	DK	140/142 (99%)	137 (98%)	2 (1%)	1 (1%)	22	53
38	CL	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	9	29
38	DL	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	19	49
39	CM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	7	23
39	DM	142/144 (99%)	136 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	CN	133/136 (98%)	125 (94%)	7 (5%)	1 (1%)	19	49
40	DN	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
41	CO	118/125 (94%)	111 (94%)	5 (4%)	2 (2%)	9	29
41	DO	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
42	CP	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
42	DP	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
43	CQ	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
43	DQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	17	46
44	CR	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
44	DR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
45	CS	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	4	15
45	DS	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	15	44
46	CT	108/110 (98%)	101 (94%)	5 (5%)	2 (2%)	8	26
46	DT	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
47	CU	91/93 (98%)	86 (94%)	4 (4%)	1 (1%)	14	41
47	DU	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
48	CV	100/102 (98%)	91 (91%)	4 (4%)	5 (5%)	2	6
48	DV	100/102 (98%)	96 (96%)	2 (2%)	2 (2%)	7	24
49	CW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
49	DW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
50	CX	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
50	DX	75/76 (99%)	74 (99%)	1 (1%)	0	100	100
51	CY	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
51	DY	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
52	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	29
52	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
53	DI	133/135 (98%)	114 (86%)	13 (10%)	6 (4%)	2	8
All	All	11406/11629 (98%)	10790 (95%)	484 (4%)	132 (1%)	13	39

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE

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

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

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

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/186 (100%)	173 (93%)	13 (7%)	15	40
2	BB	186/186 (100%)	173 (93%)	13 (7%)	15	40
3	AC	170/170 (100%)	159 (94%)	11 (6%)	17	44
3	BC	170/170 (100%)	156 (92%)	14 (8%)	11	33
4	AD	172/172 (100%)	163 (95%)	9 (5%)	23	55
4	BD	172/172 (100%)	160 (93%)	12 (7%)	15	40
5	AE	118/118 (100%)	106 (90%)	12 (10%)	7	22
5	BE	113/118 (96%)	95 (84%)	18 (16%)	2	7
6	AF	92/92 (100%)	86 (94%)	6 (6%)	17	44
6	BF	87/92 (95%)	77 (88%)	10 (12%)	5	17
7	AG	124/124 (100%)	115 (93%)	9 (7%)	14	38
7	BG	124/124 (100%)	109 (88%)	15 (12%)	5	15
8	AH	104/104 (100%)	93 (89%)	11 (11%)	6	20
8	BH	104/104 (100%)	93 (89%)	11 (11%)	6	20
9	AI	105/105 (100%)	100 (95%)	5 (5%)	25	58
9	BI	105/105 (100%)	100 (95%)	5 (5%)	25	58
10	AJ	87/87 (100%)	81 (93%)	6 (7%)	15	41
10	BJ	86/87 (99%)	78 (91%)	8 (9%)	9	26
11	AK	90/90 (100%)	87 (97%)	3 (3%)	38	72
11	BK	90/90 (100%)	83 (92%)	7 (8%)	12	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	102/102 (100%)	92 (90%)	10 (10%)	8	24
12	BL	102/102 (100%)	90 (88%)	12 (12%)	5	16
13	AM	92/92 (100%)	83 (90%)	9 (10%)	8	24
13	BM	92/92 (100%)	85 (92%)	7 (8%)	13	36
14	AN	83/83 (100%)	82 (99%)	1 (1%)	71	92
14	BN	83/83 (100%)	82 (99%)	1 (1%)	71	92
15	AO	76/76 (100%)	71 (93%)	5 (7%)	16	44
15	BO	76/76 (100%)	65 (86%)	11 (14%)	3	9
16	AP	65/65 (100%)	64 (98%)	1 (2%)	65	89
16	BP	65/65 (100%)	63 (97%)	2 (3%)	40	74
17	AQ	74/74 (100%)	67 (90%)	7 (10%)	8	25
17	BQ	74/74 (100%)	66 (89%)	8 (11%)	6	19
18	AR	48/48 (100%)	47 (98%)	1 (2%)	53	84
18	BR	48/48 (100%)	47 (98%)	1 (2%)	53	84
19	AS	70/70 (100%)	63 (90%)	7 (10%)	7	22
19	BS	70/70 (100%)	65 (93%)	5 (7%)	14	39
20	AT	65/65 (100%)	59 (91%)	6 (9%)	9	27
20	BT	65/65 (100%)	55 (85%)	10 (15%)	2	8
21	AU	48/48 (100%)	44 (92%)	4 (8%)	11	32
21	BU	48/48 (100%)	44 (92%)	4 (8%)	11	32
22	C1	47/47 (100%)	45 (96%)	2 (4%)	29	62
22	D1	47/47 (100%)	44 (94%)	3 (6%)	17	45
23	C2	45/46 (98%)	44 (98%)	1 (2%)	52	83
23	D2	45/46 (98%)	43 (96%)	2 (4%)	28	61
24	C3	38/38 (100%)	37 (97%)	1 (3%)	46	79
24	D3	38/38 (100%)	37 (97%)	1 (3%)	46	79
25	C4	51/51 (100%)	48 (94%)	3 (6%)	19	49
25	D4	51/51 (100%)	48 (94%)	3 (6%)	19	49
26	C5	34/34 (100%)	32 (94%)	2 (6%)	19	49
26	D5	34/34 (100%)	34 (100%)	0	100	100
27	C0	48/48 (100%)	45 (94%)	3 (6%)	18	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	D0	49/48 (102%)	45 (92%)	4 (8%)	11	33
29	CC	216/216 (100%)	203 (94%)	13 (6%)	19	48
29	DC	216/216 (100%)	210 (97%)	6 (3%)	43	77
30	CD	163/163 (100%)	159 (98%)	4 (2%)	47	80
30	DD	163/163 (100%)	160 (98%)	3 (2%)	59	86
32	CE	165/165 (100%)	152 (92%)	13 (8%)	12	34
32	DE	165/165 (100%)	161 (98%)	4 (2%)	49	81
33	CF	148/148 (100%)	133 (90%)	15 (10%)	7	22
33	DF	148/148 (100%)	137 (93%)	11 (7%)	13	37
34	CG	137/137 (100%)	134 (98%)	3 (2%)	52	83
34	DG	137/137 (100%)	132 (96%)	5 (4%)	35	69
35	CH	114/114 (100%)	101 (89%)	13 (11%)	5	18
35	DH	114/114 (100%)	101 (89%)	13 (11%)	5	18
36	CJ	104/104 (100%)	100 (96%)	4 (4%)	33	67
36	DJ	104/104 (100%)	100 (96%)	4 (4%)	33	67
37	CK	116/116 (100%)	110 (95%)	6 (5%)	23	55
37	DK	116/116 (100%)	114 (98%)	2 (2%)	60	87
38	CL	103/104 (99%)	99 (96%)	4 (4%)	32	66
38	DL	104/104 (100%)	99 (95%)	5 (5%)	25	58
39	CM	103/103 (100%)	97 (94%)	6 (6%)	20	50
39	DM	103/103 (100%)	99 (96%)	4 (4%)	32	66
40	CN	108/108 (100%)	104 (96%)	4 (4%)	34	68
40	DN	109/108 (101%)	106 (97%)	3 (3%)	43	77
41	CO	100/102 (98%)	95 (95%)	5 (5%)	24	56
41	DO	102/102 (100%)	99 (97%)	3 (3%)	42	76
42	CP	86/87 (99%)	80 (93%)	6 (7%)	15	40
42	DP	87/87 (100%)	84 (97%)	3 (3%)	37	71
43	CQ	99/99 (100%)	93 (94%)	6 (6%)	18	48
43	DQ	99/99 (100%)	97 (98%)	2 (2%)	55	84
44	CR	89/89 (100%)	86 (97%)	3 (3%)	37	71
44	DR	89/89 (100%)	87 (98%)	2 (2%)	52	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	CS	84/84 (100%)	79 (94%)	5 (6%)	19	48
45	DS	84/84 (100%)	83 (99%)	1 (1%)	71	92
46	CT	93/93 (100%)	88 (95%)	5 (5%)	22	53
46	DT	93/93 (100%)	92 (99%)	1 (1%)	73	92
47	CU	80/80 (100%)	72 (90%)	8 (10%)	7	22
47	DU	80/80 (100%)	77 (96%)	3 (4%)	33	67
48	CV	83/83 (100%)	79 (95%)	4 (5%)	25	58
48	DV	83/83 (100%)	81 (98%)	2 (2%)	49	81
49	CW	78/78 (100%)	75 (96%)	3 (4%)	33	67
49	DW	78/78 (100%)	76 (97%)	2 (3%)	46	79
50	CX	56/58 (97%)	55 (98%)	1 (2%)	59	86
50	DX	58/58 (100%)	57 (98%)	1 (2%)	60	87
51	CY	67/67 (100%)	63 (94%)	4 (6%)	19	48
51	DY	67/67 (100%)	65 (97%)	2 (3%)	41	75
52	CZ	54/54 (100%)	50 (93%)	4 (7%)	13	37
52	DZ	54/54 (100%)	52 (96%)	2 (4%)	34	68
53	DI	103/103 (100%)	98 (95%)	5 (5%)	25	57
All	All	9460/9477 (100%)	8897 (94%)	563 (6%)	19	48

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

5.3.3 RNA ⓘ

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

All (1297) RNA backbone outliers are listed below:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Res	Type
31	CA	1972	G
31	CA	1991	U
31	CA	1993	U
31	CA	1997	C
31	CA	2022	U
31	CA	2023	C
31	CA	2031	A
31	CA	2033	A
31	CA	2036	C
31	CA	2043	C
31	CA	2055	C
31	CA	2056	G
31	CA	2060	A
31	CA	2061	G
31	CA	2062	A
31	CA	2069	G7M
31	CA	2072	C
31	CA	2080	A
31	CA	2093	G
31	CA	2095	A
31	CA	2100	G
31	CA	2102	G
31	CA	2108	A
31	CA	2110	G
31	CA	2111	U
31	CA	2112	G
31	CA	2113	U
31	CA	2115	G
31	CA	2117	A
31	CA	2118	U
31	CA	2119	A
31	CA	2123	G
31	CA	2124	G
31	CA	2125	G
31	CA	2126	A
31	CA	2127	G
31	CA	2128	G
31	CA	2131	U
31	CA	2132	U
31	CA	2133	G
31	CA	2146	C
31	CA	2147	A

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

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

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

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Mol	Chain	Res	Type
54	DA	101	A
54	DA	102	U
54	DA	118	A
54	DA	119	A
54	DA	120	U
54	DA	138	U
54	DA	139	U
54	DA	140	C
54	DA	141	G
54	DA	142	A
54	DA	143	C
54	DA	196	A
54	DA	199	A
54	DA	200	U
54	DA	215	G
54	DA	216	A
54	DA	221	A
54	DA	222	A
54	DA	248	G
54	DA	265	A
54	DA	266	G
54	DA	272	A
54	DA	276	U
54	DA	277	G
54	DA	278	A
54	DA	279	A
54	DA	285	G
54	DA	302	C
54	DA	311	A
54	DA	329	G
54	DA	330	A
54	DA	343	C
54	DA	346	A
54	DA	352	A
54	DA	353	C
54	DA	362	A
54	DA	370	G
54	DA	372	G
54	DA	386	G
54	DA	399	U
54	DA	411	G
54	DA	412	A

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Mol	Chain	Res	Type
54	DA	420	C
54	DA	424	G
54	DA	425	G
54	DA	451	U
54	DA	480	A
54	DA	481	G
54	DA	491	G
54	DA	504	A
54	DA	505	A
54	DA	508	A
54	DA	531	C
54	DA	532	A
54	DA	543	G
54	DA	544	C
54	DA	546	U
54	DA	547	A
54	DA	548	G
54	DA	549	G
54	DA	550	C
54	DA	551	G
54	DA	563	A
54	DA	573	U
54	DA	575	A
54	DA	586	A
54	DA	603	A
54	DA	613	A
54	DA	614	A
54	DA	615	U
54	DA	627	A
54	DA	637	A
54	DA	645	C
54	DA	647	G
54	DA	654	A
54	DA	655	A
54	DA	686	U
54	DA	717	C
54	DA	730	A
54	DA	747	5MU
54	DA	764	A
54	DA	765	C
54	DA	775	G
54	DA	776	G

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Mol	Chain	Res	Type
54	DA	782	A
54	DA	784	G
54	DA	785	G
54	DA	790	U
54	DA	792	A
54	DA	805	G
54	DA	812	C
54	DA	827	U
54	DA	828	U
54	DA	858	G
54	DA	859	G
54	DA	860	U
54	DA	878	A
54	DA	883	G
54	DA	885	C
54	DA	896	A
54	DA	897	C
54	DA	910	A
54	DA	914	G
54	DA	915	C
54	DA	927	A
54	DA	931	U
54	DA	932	U
54	DA	946	C
54	DA	961	C
54	DA	974	G
54	DA	983	A
54	DA	996	A
54	DA	1012	U
54	DA	1013	C
54	DA	1022	G
54	DA	1026	G
54	DA	1033	U
54	DA	1040	A
54	DA	1047	G
54	DA	1057	A
54	DA	1061	U
54	DA	1070	A
54	DA	1083	U
54	DA	1088	A
54	DA	1089	A
54	DA	1090	A

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Mol	Chain	Res	Type
54	DA	1091	G
54	DA	1096	A
54	DA	1097	U
54	DA	1112	G
54	DA	1132	U
54	DA	1133	A
54	DA	1135	C
54	DA	1136	G
54	DA	1142	A
54	DA	1168	G
54	DA	1172	C
54	DA	1174	U
54	DA	1175	A
54	DA	1176	U
54	DA	1177	G
54	DA	1180	U
54	DA	1187	G
54	DA	1237	A
54	DA	1238	G
54	DA	1253	A
54	DA	1256	G
54	DA	1271	G
54	DA	1272	A
54	DA	1273	U
54	DA	1300	G
54	DA	1301	A
54	DA	1329	U
54	DA	1352	U
54	DA	1365	A
54	DA	1379	U
54	DA	1383	A
54	DA	1391	U
54	DA	1416	G
54	DA	1417	C
54	DA	1427	A
54	DA	1428	C
54	DA	1434	A
54	DA	1435	G
54	DA	1452	G
54	DA	1453	A
54	DA	1460	U
54	DA	1482	G

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Mol	Chain	Res	Type
54	DA	1490	A
54	DA	1491	G
54	DA	1493	C
54	DA	1494	A
54	DA	1497	U
54	DA	1508	A
54	DA	1509	A
54	DA	1510	G
54	DA	1515	A
54	DA	1523	U
54	DA	1532	A
54	DA	1534	U
54	DA	1535	A
54	DA	1536	C
54	DA	1537	G
54	DA	1566	A
54	DA	1569	A
54	DA	1578	U
54	DA	1583	A
54	DA	1585	C
54	DA	1607	C
54	DA	1608	A
54	DA	1616	A
54	DA	1647	U
54	DA	1648	U
54	DA	1649	G
54	DA	1674	G
54	DA	1715	G
54	DA	1729	U
54	DA	1730	C
54	DA	1731	G
54	DA	1732	C
54	DA	1738	G
54	DA	1744	A
54	DA	1764	C
54	DA	1773	A
54	DA	1782	U
54	DA	1800	C
54	DA	1801	A
54	DA	1808	A
54	DA	1816	C
54	DA	1829	A

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Mol	Chain	Res	Type
54	DA	1869	G
54	DA	1870	C
54	DA	1871	A
54	DA	1872	A
54	DA	1873	G
54	DA	1906	G
54	DA	1907	G
54	DA	1913	A
54	DA	1914	C
54	DA	1929	G
54	DA	1930	G
54	DA	1931	U
54	DA	1937	A
54	DA	1938	A
54	DA	1955	U
54	DA	1965	C
54	DA	1967	C
54	DA	1970	A
54	DA	1972	G
54	DA	1991	U
54	DA	1993	U
54	DA	1997	C
54	DA	2023	C
54	DA	2031	A
54	DA	2033	A
54	DA	2043	C
54	DA	2055	C
54	DA	2056	G
54	DA	2060	A
54	DA	2061	G
54	DA	2062	A
54	DA	2069	G7M
54	DA	2097	A
54	DA	2100	G
54	DA	2102	G
54	DA	2105	U
54	DA	2111	U
54	DA	2112	G
54	DA	2113	U
54	DA	2116	G
54	DA	2117	A
54	DA	2118	U

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Mol	Chain	Res	Type
54	DA	2119	A
54	DA	2120	G
54	DA	2123	G
54	DA	2125	G
54	DA	2126	A
54	DA	2128	G
54	DA	2131	U
54	DA	2132	U
54	DA	2133	G
54	DA	2134	A
54	DA	2135	A
54	DA	2145	C
54	DA	2146	C
54	DA	2148	G
54	DA	2158	A
54	DA	2159	G
54	DA	2160	C
54	DA	2161	C
54	DA	2162	G
54	DA	2163	A
54	DA	2164	C
54	DA	2165	C
54	DA	2167	U
54	DA	2168	G
54	DA	2169	A
54	DA	2170	A
54	DA	2171	A
54	DA	2172	U
54	DA	2173	A
54	DA	2177	C
54	DA	2178	C
54	DA	2179	C
54	DA	2181	U
54	DA	2183	A
54	DA	2185	U
54	DA	2190	G
54	DA	2198	A
54	DA	2204	G
54	DA	2211	A
54	DA	2225	A
54	DA	2238	G
54	DA	2239	G

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Mol	Chain	Res	Type
54	DA	2268	A
54	DA	2283	C
54	DA	2286	G
54	DA	2287	A
54	DA	2305	U
54	DA	2308	G
54	DA	2312	U
54	DA	2324	U
54	DA	2325	G
54	DA	2333	A
54	DA	2335	A
54	DA	2347	C
54	DA	2383	G
54	DA	2385	C
54	DA	2402	U
54	DA	2403	C
54	DA	2406	A
54	DA	2407	A
54	DA	2423	U
54	DA	2424	C
54	DA	2425	A
54	DA	2431	U
54	DA	2435	A
54	DA	2441	U
54	DA	2448	A
54	DA	2476	A
54	DA	2491	U
54	DA	2502	G
54	DA	2505	G
54	DA	2518	A
54	DA	2529	G
54	DA	2535	G
54	DA	2547	A
54	DA	2556	C
54	DA	2566	A
54	DA	2567	G
54	DA	2573	C
54	DA	2574	G
54	DA	2585	U
54	DA	2603	G
54	DA	2609	U
54	DA	2613	U

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Mol	Chain	Res	Type
54	DA	2629	U
54	DA	2630	G
54	DA	2661	G
54	DA	2663	G
54	DA	2689	U
54	DA	2690	U
54	DA	2714	G
54	DA	2726	A
54	DA	2744	G
54	DA	2748	A
54	DA	2765	A
54	DA	2778	A
54	DA	2791	G
54	DA	2798	U
54	DA	2799	A
54	DA	2811	G
54	DA	2820	A
54	DA	2821	A
54	DA	2836	U
54	DA	2867	G
54	DA	2891	U

All (184) RNA pucker outliers are listed below:

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

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

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

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

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Mol	Chain	Res	Type
54	DA	1070	A
54	DA	1087	G
54	DA	1088	A
54	DA	1089	A
54	DA	1128	G
54	DA	1141	U
54	DA	1142	A
54	DA	1175	A
54	DA	1253	A
54	DA	1286	A
54	DA	1300	G
54	DA	1320	C
54	DA	1490	A
54	DA	1497	U
54	DA	1509	A
54	DA	1535	A
54	DA	1607	C
54	DA	1647	U
54	DA	1730	C
54	DA	1870	C
54	DA	1871	A
54	DA	1936	A
54	DA	2097	A
54	DA	2119	A
54	DA	2127	G
54	DA	2146	C
54	DA	2157	G
54	DA	2158	A
54	DA	2164	C
54	DA	2172	U
54	DA	2286	G
54	DA	2311	A
54	DA	2324	U
54	DA	2406	A
54	DA	2423	U
54	DA	2501	C
54	DA	2585	U
54	DA	2681	C
54	DA	2797	U
54	DA	2798	U
54	DA	2873	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
31	OMG	CA	2251	31	18,26,27	1.25	2 (11%)	20,38,41	2.53	4 (20%)
54	5MU	DA	747	54	15,22,23	1.24	1 (6%)	16,32,35	3.62	2 (12%)
31	PSU	CA	2605	31	17,21,22	1.17	2 (11%)	20,30,33	5.32	5 (25%)
1	2MG	BA	1516	1	19,26,27	1.28	2 (10%)	21,38,41	2.37	4 (19%)
1	5MC	BA	967	1	15,22,23	0.81	0	19,32,35	1.14	2 (10%)
31	2MG	CA	1835	31	19,26,27	1.19	2 (10%)	21,38,41	2.31	4 (19%)
31	2MA	CA	2503	31	17,25,26	0.85	0	19,37,40	2.07	3 (15%)
54	OMG	DA	2251	54	18,26,27	1.06	1 (5%)	20,38,41	2.47	5 (25%)
54	PSU	DA	746	55,54	17,21,22	1.65	4 (23%)	20,30,33	5.31	4 (20%)
31	5MC	CA	1962	31	15,22,23	0.80	0	19,32,35	1.11	1 (5%)
31	PSU	CA	1917	31	17,21,22	1.22	2 (11%)	20,30,33	5.35	4 (20%)
1	PSU	BA	516	1	17,21,22	1.24	3 (17%)	20,30,33	5.32	4 (20%)
31	5MU	CA	747	31	15,22,23	1.17	1 (6%)	16,32,35	3.69	2 (12%)
54	PSU	DA	1917	54	17,21,22	1.30	3 (17%)	20,30,33	5.33	4 (20%)
54	5MC	DA	1962	54	15,22,23	0.91	0	19,32,35	1.13	1 (5%)
1	5MC	AA	1407	1	15,22,23	0.86	0	19,32,35	1.20	2 (10%)
31	PSU	CA	746	55,31	17,21,22	1.40	3 (17%)	20,30,33	5.32	4 (20%)
54	H2U	DA	2449	54	18,21,22	0.47	0	21,30,33	0.50	0
54	6MZ	DA	1618	54	18,25,26	0.91	0	16,36,39	1.79	2 (12%)
1	2MG	AA	1516	1	19,26,27	1.39	2 (10%)	21,38,41	2.35	4 (19%)
54	PSU	DA	2605	54	17,21,22	1.18	2 (11%)	20,30,33	5.31	5 (25%)
40	4D4	DN	81[B]	-	9,11,12	1.41	1 (11%)	8,13,15	2.41	2 (25%)
1	MA6	AA	1518	1	19,26,27	0.84	0	18,38,41	0.92	1 (5%)
12	D2T	BL	89	12	4,9,10	0.58	0	3,11,13	0.87	0
31	2MG	CA	2445	31	19,26,27	1.42	2 (10%)	21,38,41	2.38	4 (19%)
40	4D4	DN	81[A]	-	9,11,12	2.14	2 (22%)	8,13,15	2.17	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	6MZ	CA	1618	31	18,25,26	0.84	0	16,36,39	1.11	2 (12%)
1	MA6	BA	1519	1	19,26,27	0.72	0	18,38,41	1.30	1 (5%)
1	UR3	BA	1498	1	14,22,23	1.14	2 (14%)	15,32,35	0.48	0
1	G7M	AA	527	1	20,26,27	1.21	2 (10%)	20,39,42	3.10	6 (30%)
1	MA6	BA	1518	1	19,26,27	0.86	0	18,38,41	0.97	1 (5%)
1	4OC	BA	1402	1	16,23,24	0.87	0	17,32,35	0.90	1 (5%)
31	3TD	CA	1915	31	17,22,23	1.26	3 (17%)	19,32,35	1.50	2 (10%)
1	PSU	AA	516	1,55	17,21,22	1.21	2 (11%)	20,30,33	5.31	4 (20%)
31	G7M	CA	2069	31	20,26,27	0.97	1 (5%)	20,39,42	2.88	5 (25%)
31	OMU	CA	2552	31	14,22,23	1.24	2 (14%)	14,31,34	1.09	1 (7%)
1	5MC	AA	967	1	15,22,23	0.82	0	19,32,35	1.14	2 (10%)
31	PSU	CA	2457	31	17,21,22	1.26	3 (17%)	20,30,33	5.27	4 (20%)
54	2MG	DA	2445	54	19,26,27	1.25	3 (15%)	21,38,41	2.55	4 (19%)
31	6MZ	CA	2030	31	18,25,26	0.84	0	16,36,39	0.94	2 (12%)
31	PSU	CA	1911	31	17,21,22	1.21	2 (11%)	20,30,33	5.28	4 (20%)
54	OMC	DA	2498	55,54	15,22,23	0.88	1 (6%)	17,31,34	1.30	1 (5%)
30	MEQ	DD	150[A]	30	8,9,10	0.57	0	5,10,12	0.45	0
54	PSU	DA	2604	54	17,21,22	1.33	2 (11%)	20,30,33	5.31	4 (20%)
1	2MG	AA	966	1	19,26,27	1.26	2 (10%)	21,38,41	2.34	3 (14%)
30	MEQ	CD	150	30	7,8,10	0.40	0	4,9,12	0.39	0
31	PSU	CA	2504	31	17,21,22	1.22	3 (17%)	20,30,33	5.28	4 (20%)
31	PSU	CA	955	31	17,21,22	1.21	2 (11%)	20,30,33	5.32	4 (20%)
1	2MG	AA	1207	1	19,26,27	1.17	2 (10%)	21,38,41	2.41	4 (19%)
54	PSU	DA	955	54	17,21,22	1.45	4 (23%)	20,30,33	5.31	4 (20%)
31	5MU	CA	1939	31	15,22,23	1.26	1 (6%)	16,32,35	3.70	2 (12%)
1	G7M	BA	527	1	20,26,27	1.24	2 (10%)	20,39,42	3.16	5 (25%)
54	PSU	DA	2504	54	17,21,22	1.35	3 (17%)	20,30,33	5.34	4 (20%)
54	6MZ	DA	2030	54	18,25,26	0.89	1 (5%)	16,36,39	0.89	1 (6%)
54	2MG	DA	1835	54	19,26,27	1.12	2 (10%)	21,38,41	2.35	4 (19%)
54	G7M	DA	2069	54	20,26,27	1.05	1 (5%)	20,39,42	2.86	4 (20%)
1	UR3	AA	1498	1	14,22,23	0.84	0	15,32,35	0.53	0
31	OMC	CA	2498	55,31	15,22,23	0.98	1 (6%)	17,31,34	1.18	1 (5%)
54	2MA	DA	2503	55,54	17,25,26	0.81	0	19,37,40	1.99	3 (15%)
54	PSU	DA	2457	54	17,21,22	1.14	3 (17%)	20,30,33	5.28	4 (20%)
54	3TD	DA	1915	54	17,22,23	1.32	3 (17%)	19,32,35	1.52	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	OMU	DA	2552	54	14,22,23	1.19	2 (14%)	14,31,34	1.12	1 (7%)
1	MA6	AA	1519	1	19,26,27	0.73	0	18,38,41	1.34	1 (5%)
1	2MG	BA	1207	1	19,26,27	1.25	2 (10%)	21,38,41	2.39	4 (19%)
30	MEQ	DD	150[B]	30	8,9,10	2.21	1 (12%)	5,10,12	1.71	1 (20%)
31	PSU	CA	2580	31	17,21,22	1.32	2 (11%)	20,30,33	5.32	5 (25%)
1	2MG	BA	966	1,55	19,26,27	1.16	2 (10%)	21,38,41	2.36	4 (19%)
54	PSU	DA	2580	54	17,21,22	1.49	4 (23%)	20,30,33	5.33	4 (20%)
1	4OC	AA	1402	1	16,23,24	0.82	0	17,32,35	0.91	1 (5%)
54	1MG	DA	745	54	18,26,27	1.45	3 (16%)	19,39,42	1.29	3 (15%)
54	5MU	DA	1939	54	15,22,23	1.21	1 (6%)	16,32,35	3.68	1 (6%)
12	D2T	AL	89	12	4,9,10	0.51	0	3,11,13	0.87	0
31	1MG	CA	745	31	18,26,27	1.34	1 (5%)	19,39,42	1.23	2 (10%)
1	5MC	BA	1407	1	15,22,23	0.85	0	19,32,35	1.18	2 (10%)
54	PSU	DA	1911	54	17,21,22	1.19	3 (17%)	20,30,33	5.27	4 (20%)
40	4D4	CN	81	40	9,11,12	2.01	2 (22%)	8,13,15	2.39	2 (25%)

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
31	OMG	CA	2251	31	-	1/5/27/28	0/3/3/3
54	5MU	DA	747	54	-	0/5/25/26	0/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
1	5MC	BA	967	1	-	0/5/25/26	0/2/2/2
31	2MG	CA	1835	31	-	2/5/27/28	0/3/3/3
31	2MA	CA	2503	31	-	2/3/25/26	0/3/3/3
54	OMG	DA	2251	54	-	1/5/27/28	0/3/3/3
54	PSU	DA	746	55,54	-	3/7/25/26	0/2/2/2
31	5MC	CA	1962	31	-	2/5/25/26	0/2/2/2
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
31	5MU	CA	747	31	-	0/5/25/26	0/2/2/2
54	PSU	DA	1917	54	-	0/7/25/26	0/2/2/2
54	5MC	DA	1962	54	-	2/5/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PSU	CA	746	55,31	-	3/7/25/26	0/2/2/2
54	H2U	DA	2449	54	-	1/7/38/39	0/2/2/2
54	6MZ	DA	1618	54	-	0/5/27/28	0/3/3/3
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
54	PSU	DA	2605	54	-	0/7/25/26	0/2/2/2
40	4D4	DN	81[B]	-	-	2/11/12/14	-
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
12	D2T	BL	89	12	-	1/3/12/14	-
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3
40	4D4	DN	81[A]	-	-	0/11/12/14	-
31	6MZ	CA	1618	31	-	0/5/27/28	0/3/3/3
1	MA6	BA	1519	1	-	1/7/29/30	0/3/3/3
1	UR3	BA	1498	1	-	0/5/25/26	0/2/2/2
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3
1	MA6	BA	1518	1	-	0/7/29/30	0/3/3/3
1	4OC	BA	1402	1	-	0/9/29/30	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	1,55	-	0/7/25/26	0/2/2/2
31	G7M	CA	2069	31	-	2/3/25/26	0/3/3/3
31	OMU	CA	2552	31	-	1/7/27/28	0/2/2/2
1	5MC	AA	967	1	-	0/5/25/26	0/2/2/2
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
54	2MG	DA	2445	54	-	0/5/27/28	0/3/3/3
31	6MZ	CA	2030	31	-	1/5/27/28	0/3/3/3
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
54	OMC	DA	2498	55,54	-	0/7/27/28	0/2/2/2
30	MEQ	DD	150[A]	30	-	3/8/9/11	-
54	PSU	DA	2604	54	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
30	MEQ	CD	150	30	-	2/6/7/11	-
31	PSU	CA	2504	31	-	1/7/25/26	0/2/2/2
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
54	PSU	DA	955	54	-	0/7/25/26	0/2/2/2
31	5MU	CA	1939	31	-	0/5/25/26	0/2/2/2
1	G7M	BA	527	1	-	2/3/25/26	0/3/3/3
54	PSU	DA	2504	54	-	1/7/25/26	0/2/2/2
54	6MZ	DA	2030	54	-	2/5/27/28	0/3/3/3
54	2MG	DA	1835	54	-	2/5/27/28	0/3/3/3
54	G7M	DA	2069	54	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	AA	1498	1	-	0/5/25/26	0/2/2/2
31	OMC	CA	2498	55,31	-	0/7/27/28	0/2/2/2
54	2MA	DA	2503	55,54	-	2/3/25/26	0/3/3/3
54	PSU	DA	2457	54	-	0/7/25/26	0/2/2/2
54	3TD	DA	1915	54	-	0/7/25/26	0/2/2/2
54	OMU	DA	2552	54	-	1/7/27/28	0/2/2/2
1	MA6	AA	1519	1	-	1/7/29/30	0/3/3/3
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
30	MEQ	DD	150[B]	30	-	4/8/9/11	-
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
1	2MG	BA	966	1,55	-	0/5/27/28	0/3/3/3
54	PSU	DA	2580	54	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
54	1MG	DA	745	54	-	0/3/25/26	0/3/3/3
54	5MU	DA	1939	54	-	0/5/25/26	0/2/2/2
12	D2T	AL	89	12	-	1/3/12/14	-
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
1	5MC	BA	1407	1	-	0/5/25/26	0/2/2/2
54	PSU	DA	1911	54	-	0/7/25/26	0/2/2/2
40	4D4	CN	81	40	-	1/11/12/14	-

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	DD	150[B]	MEQ	CB-CA	6.09	1.61	1.53
40	DN	81[A]	4D4	CZ-NE	5.93	1.45	1.33
40	CN	81	4D4	CZ-NE	5.49	1.44	1.33
31	CA	745	1MG	C6-C5	4.49	1.48	1.41
54	DA	1915	3TD	C4-C5	3.91	1.49	1.41
54	DA	745	1MG	C6-C5	3.85	1.47	1.41
40	DN	81[B]	4D4	CZ-NE	3.75	1.40	1.33
1	AA	1516	2MG	C6-C5	3.71	1.47	1.41
31	CA	2445	2MG	C6-C5	3.56	1.47	1.41
1	AA	1516	2MG	C6-N1	3.55	1.39	1.33
31	CA	2445	2MG	C6-N1	3.55	1.39	1.33
1	AA	966	2MG	C6-N1	3.55	1.39	1.33
31	CA	2251	OMG	C6-N1	3.55	1.39	1.33
31	CA	1939	5MU	C4-N3	3.54	1.39	1.33
1	BA	1516	2MG	C6-N1	3.52	1.39	1.33
1	BA	1207	2MG	C6-N1	3.52	1.39	1.33
54	DA	2251	OMG	C6-N1	3.51	1.39	1.33
31	CA	1911	PSU	C4-N3	3.51	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	1835	2MG	C6-N1	3.45	1.39	1.33
1	AA	1207	2MG	C6-N1	3.45	1.39	1.33
1	AA	516	PSU	C4-N3	3.45	1.39	1.33
31	CA	746	PSU	C4-N3	3.45	1.39	1.33
31	CA	955	PSU	C4-N3	3.44	1.39	1.33
54	DA	955	PSU	C4-N3	3.44	1.39	1.33
31	CA	2580	PSU	C4-N3	3.43	1.39	1.33
54	DA	2069	G7M	C6-N1	3.41	1.39	1.33
31	CA	1917	PSU	C4-N3	3.41	1.39	1.33
31	CA	2457	PSU	C4-N3	3.40	1.39	1.33
1	BA	966	2MG	C6-N1	3.40	1.38	1.33
31	CA	747	5MU	C4-N3	3.40	1.38	1.33
31	CA	1915	3TD	C4-C5	3.39	1.48	1.41
54	DA	2504	PSU	C4-N3	3.38	1.38	1.33
54	DA	1911	PSU	C4-N3	3.35	1.38	1.33
31	CA	2605	PSU	C4-N3	3.33	1.38	1.33
1	BA	516	PSU	C4-N3	3.32	1.38	1.33
54	DA	1917	PSU	C4-N3	3.31	1.38	1.33
54	DA	2552	OMU	C4-N3	3.28	1.38	1.33
54	DA	2605	PSU	C4-N3	3.27	1.38	1.33
54	DA	746	PSU	C2'-C1'	-3.27	1.50	1.54
31	CA	2504	PSU	C4-N3	3.26	1.38	1.33
31	CA	2552	OMU	C4-N3	3.25	1.38	1.33
54	DA	747	5MU	C4-N3	3.24	1.38	1.33
31	CA	2069	G7M	C6-N1	3.24	1.38	1.33
54	DA	1939	5MU	C4-N3	3.20	1.38	1.33
1	AA	527	G7M	C6-N1	3.19	1.38	1.33
54	DA	1835	2MG	C6-N1	3.17	1.38	1.33
1	AA	966	2MG	C6-C5	3.15	1.46	1.41
54	DA	746	PSU	C4-N3	3.15	1.38	1.33
1	BA	1516	2MG	C6-C5	3.15	1.46	1.41
1	BA	527	G7M	C6-N1	3.10	1.38	1.33
54	DA	2445	2MG	C6-N1	3.10	1.38	1.33
54	DA	746	PSU	O4'-C1'	-3.08	1.40	1.44
1	BA	1207	2MG	C6-C5	3.03	1.46	1.41
54	DA	2604	PSU	C4-N3	2.97	1.38	1.33
54	DA	2445	2MG	C6-C5	2.89	1.46	1.41
54	DA	2457	PSU	C4-N3	2.87	1.38	1.33
54	DA	2580	PSU	O4'-C1'	-2.83	1.40	1.44
54	DA	2580	PSU	C4-N3	2.75	1.37	1.33
1	BA	1498	UR3	C4-N3	2.73	1.42	1.38
31	CA	746	PSU	O4'-C1'	-2.70	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	DA	955	PSU	C2'-C1'	-2.69	1.50	1.54
1	BA	966	2MG	C6-C5	2.60	1.45	1.41
1	AA	1207	2MG	C6-C5	2.59	1.45	1.41
31	CA	2251	OMG	C6-C5	2.56	1.45	1.41
31	CA	2552	OMU	C6-N1	2.50	1.38	1.35
54	DA	745	1MG	C8-N7	-2.48	1.30	1.34
54	DA	2580	PSU	C6-C5	-2.41	1.35	1.38
54	DA	745	1MG	C6-N1	2.41	1.41	1.38
54	DA	2580	PSU	C5-C1'	-2.35	1.50	1.52
31	CA	1915	3TD	C4-N3	2.31	1.41	1.38
31	CA	2498	OMC	C6-N1	2.28	1.38	1.35
1	BA	1498	UR3	C6-N1	2.24	1.38	1.35
1	BA	527	G7M	C6-C5	2.23	1.45	1.41
54	DA	2457	PSU	C6-C5	-2.23	1.35	1.38
54	DA	2604	PSU	C6-C5	-2.22	1.35	1.38
1	AA	527	G7M	C6-C5	2.19	1.45	1.41
54	DA	1915	3TD	C4-N3	2.19	1.41	1.38
54	DA	2552	OMU	C6-N1	2.18	1.38	1.35
40	DN	81[A]	4D4	CZ-NH1	2.18	1.43	1.34
31	CA	1915	3TD	C6-C5	-2.18	1.35	1.38
54	DA	1835	2MG	C6-C5	2.18	1.45	1.41
54	DA	1915	3TD	C6-C5	-2.16	1.35	1.38
54	DA	746	PSU	C6-C5	-2.14	1.35	1.38
54	DA	2504	PSU	C6-C5	-2.14	1.35	1.38
1	BA	516	PSU	C6-C5	-2.14	1.35	1.38
31	CA	2580	PSU	C6-C5	-2.14	1.35	1.38
54	DA	2498	OMC	O4'-C1'	2.14	1.44	1.41
54	DA	1911	PSU	C6-C5	-2.13	1.35	1.38
40	CN	81	4D4	CZ-NH1	2.13	1.43	1.34
54	DA	2030	6MZ	O5'-C5'	-2.13	1.39	1.44
31	CA	2504	PSU	C4-C5	2.12	1.46	1.41
31	CA	2457	PSU	C6-C5	-2.11	1.35	1.38
31	CA	2504	PSU	C6-C5	-2.10	1.35	1.38
31	CA	955	PSU	C6-C5	-2.09	1.35	1.38
54	DA	2605	PSU	C6-C5	-2.09	1.35	1.38
54	DA	1917	PSU	C4-C5	2.09	1.46	1.41
54	DA	2445	2MG	O3'-C3'	-2.09	1.38	1.43
54	DA	955	PSU	C5-C1'	-2.07	1.50	1.52
54	DA	955	PSU	C6-C5	-2.07	1.35	1.38
31	CA	1835	2MG	C6-C5	2.07	1.44	1.41
1	AA	516	PSU	C6-C5	-2.07	1.35	1.38
31	CA	2605	PSU	C6-C5	-2.06	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2457	PSU	C4-C5	2.06	1.45	1.41
31	CA	1911	PSU	C6-C5	-2.05	1.35	1.38
54	DA	1911	PSU	C4-C5	2.04	1.45	1.41
54	DA	1917	PSU	C6-C5	-2.04	1.35	1.38
31	CA	1917	PSU	C6-C5	-2.03	1.35	1.38
31	CA	746	PSU	C6-C5	-2.02	1.35	1.38
1	BA	516	PSU	C4-C5	2.02	1.45	1.41
54	DA	2457	PSU	C4-C5	2.02	1.45	1.41
54	DA	2504	PSU	C4-C5	2.02	1.45	1.41

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DA	2504	PSU	N1-C2-N3	-17.23	114.73	128.43
31	CA	1917	PSU	N1-C2-N3	-17.18	114.77	128.43
1	BA	516	PSU	N1-C2-N3	-17.17	114.78	128.43
31	CA	746	PSU	N1-C2-N3	-17.16	114.78	128.43
54	DA	1917	PSU	N1-C2-N3	-17.11	114.82	128.43
1	AA	516	PSU	N1-C2-N3	-17.10	114.83	128.43
31	CA	955	PSU	N1-C2-N3	-17.09	114.84	128.43
31	CA	2605	PSU	N1-C2-N3	-17.08	114.85	128.43
31	CA	2580	PSU	N1-C2-N3	-17.08	114.85	128.43
54	DA	1911	PSU	N1-C2-N3	-17.06	114.86	128.43
54	DA	2580	PSU	N1-C2-N3	-17.05	114.87	128.43
54	DA	746	PSU	N1-C2-N3	-17.04	114.88	128.43
31	CA	2504	PSU	N1-C2-N3	-17.04	114.89	128.43
31	CA	1911	PSU	N1-C2-N3	-17.02	114.90	128.43
54	DA	2457	PSU	N1-C2-N3	-17.01	114.91	128.43
54	DA	955	PSU	N1-C2-N3	-16.99	114.92	128.43
54	DA	2605	PSU	N1-C2-N3	-16.98	114.93	128.43
31	CA	2457	PSU	N1-C2-N3	-16.94	114.96	128.43
54	DA	2604	PSU	N1-C2-N3	-16.93	114.97	128.43
31	CA	1939	5MU	C4-N3-C2	14.39	127.30	115.14
31	CA	747	5MU	C4-N3-C2	14.35	127.26	115.14
54	DA	1939	5MU	C4-N3-C2	14.30	127.22	115.14
54	DA	747	5MU	C4-N3-C2	14.09	127.03	115.14
31	CA	1917	PSU	C4-N3-C2	13.62	126.64	115.14
1	BA	516	PSU	C4-N3-C2	13.52	126.56	115.14
54	DA	2504	PSU	C4-N3-C2	13.52	126.56	115.14
54	DA	746	PSU	C4-N3-C2	13.50	126.54	115.14
54	DA	2457	PSU	C4-N3-C2	13.50	126.54	115.14
54	DA	1917	PSU	C4-N3-C2	13.48	126.52	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	516	PSU	C4-N3-C2	13.46	126.50	115.14
54	DA	2580	PSU	C4-N3-C2	13.46	126.50	115.14
54	DA	2605	PSU	C4-N3-C2	13.44	126.49	115.14
31	CA	955	PSU	C4-N3-C2	13.44	126.48	115.14
31	CA	746	PSU	C4-N3-C2	13.43	126.48	115.14
31	CA	2605	PSU	C4-N3-C2	13.41	126.46	115.14
31	CA	2457	PSU	C4-N3-C2	13.40	126.46	115.14
54	DA	2604	PSU	C4-N3-C2	13.40	126.46	115.14
31	CA	2504	PSU	C4-N3-C2	13.40	126.46	115.14
31	CA	1911	PSU	C4-N3-C2	13.39	126.45	115.14
31	CA	2580	PSU	C4-N3-C2	13.38	126.44	115.14
54	DA	1911	PSU	C4-N3-C2	13.36	126.42	115.14
54	DA	955	PSU	C4-N3-C2	13.34	126.41	115.14
31	CA	2069	G7M	C5-C6-N1	-9.44	110.52	123.43
1	AA	527	G7M	C5-C6-N1	-9.44	110.52	123.43
54	DA	2069	G7M	C5-C6-N1	-9.34	110.66	123.43
1	BA	527	G7M	C5-C6-N1	-9.29	110.72	123.43
54	DA	2445	2MG	C5-C6-N1	-8.60	111.67	123.43
31	CA	2445	2MG	C5-C6-N1	-8.25	112.14	123.43
1	AA	1207	2MG	C5-C6-N1	-8.24	112.16	123.43
31	CA	2503	2MA	C5-C6-N1	-8.22	114.44	123.06
1	AA	966	2MG	C5-C6-N1	-8.16	112.26	123.43
31	CA	2251	OMG	C5-C6-N1	-8.06	112.40	123.43
1	BA	966	2MG	C5-C6-N1	-8.03	112.44	123.43
54	DA	746	PSU	C5-C4-N3	-7.96	115.10	125.36
1	BA	1207	2MG	C5-C6-N1	-7.95	112.56	123.43
1	AA	516	PSU	C5-C4-N3	-7.94	115.13	125.36
31	CA	2457	PSU	C5-C4-N3	-7.90	115.18	125.36
54	DA	2580	PSU	C5-C4-N3	-7.90	115.18	125.36
31	CA	1917	PSU	C5-C4-N3	-7.90	115.18	125.36
31	CA	1911	PSU	C5-C4-N3	-7.88	115.20	125.36
1	BA	516	PSU	C5-C4-N3	-7.88	115.21	125.36
31	CA	746	PSU	C5-C4-N3	-7.87	115.22	125.36
54	DA	1917	PSU	C5-C4-N3	-7.87	115.22	125.36
31	CA	955	PSU	C5-C4-N3	-7.86	115.23	125.36
54	DA	955	PSU	C5-C4-N3	-7.86	115.23	125.36
31	CA	1835	2MG	C5-C6-N1	-7.84	112.70	123.43
31	CA	2580	PSU	C5-C4-N3	-7.84	115.26	125.36
54	DA	2504	PSU	C5-C4-N3	-7.83	115.27	125.36
54	DA	1835	2MG	C5-C6-N1	-7.82	112.74	123.43
1	BA	1516	2MG	C5-C6-N1	-7.81	112.75	123.43
54	DA	2604	PSU	C5-C4-N3	-7.81	115.30	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2605	PSU	C5-C4-N3	-7.79	115.33	125.36
31	CA	2504	PSU	C5-C4-N3	-7.77	115.34	125.36
54	DA	2457	PSU	C5-C4-N3	-7.76	115.37	125.36
54	DA	2605	PSU	C5-C4-N3	-7.74	115.38	125.36
54	DA	1911	PSU	C5-C4-N3	-7.74	115.39	125.36
54	DA	2503	2MA	C5-C6-N1	-7.68	115.01	123.06
1	AA	1516	2MG	C5-C6-N1	-7.67	112.95	123.43
54	DA	2251	OMG	C5-C6-N1	-7.64	112.98	123.43
1	BA	527	G7M	C6-C5-C4	-7.50	113.64	120.80
1	AA	527	G7M	C6-C5-C4	-6.73	114.37	120.80
54	DA	1618	6MZ	C9-N6-C6	6.51	128.48	122.87
54	DA	2445	2MG	C6-N1-C2	5.98	125.89	115.18
31	CA	2251	OMG	C6-N1-C2	5.91	125.33	115.93
54	DA	2251	OMG	C6-N1-C2	5.65	124.90	115.93
40	CN	81	4D4	NE-CZ-NH2	5.62	130.58	120.70
40	DN	81[B]	4D4	NE-CZ-NH2	5.51	130.39	120.70
1	BA	527	G7M	C6-N1-C2	5.47	124.61	115.93
31	CA	2069	G7M	C6-N1-C2	5.44	124.57	115.93
1	AA	1207	2MG	C6-N1-C2	5.37	124.79	115.18
54	DA	2069	G7M	C6-N1-C2	5.29	124.34	115.93
1	BA	1207	2MG	C6-N1-C2	5.28	124.63	115.18
31	CA	2069	G7M	C6-C5-C4	-5.24	115.79	120.80
54	DA	1835	2MG	C6-N1-C2	5.24	124.56	115.18
31	CA	1915	3TD	C6-N1-C2	5.23	123.99	115.36
1	BA	966	2MG	C6-N1-C2	5.23	124.54	115.18
31	CA	2445	2MG	C6-N1-C2	5.23	124.54	115.18
1	AA	966	2MG	C6-N1-C2	5.21	124.51	115.18
54	DA	1915	3TD	C6-N1-C2	5.21	123.95	115.36
1	AA	527	G7M	C6-N1-C2	5.19	124.18	115.93
1	BA	1516	2MG	C6-N1-C2	5.19	124.47	115.18
31	CA	1835	2MG	C6-N1-C2	5.09	124.30	115.18
40	DN	81[A]	4D4	NE-CZ-NH2	5.09	129.64	120.70
1	AA	1516	2MG	C6-N1-C2	5.04	124.20	115.18
54	DA	2069	G7M	C6-C5-C4	-5.04	115.99	120.80
1	AA	1519	MA6	N1-C6-N6	-4.75	112.06	117.06
1	BA	1519	MA6	N1-C6-N6	-4.58	112.24	117.06
54	DA	2504	PSU	C6-N1-C2	4.53	122.84	115.36
54	DA	2498	OMC	C2-N3-C4	4.51	120.91	116.34
54	DA	1917	PSU	C6-N1-C2	4.49	122.76	115.36
54	DA	2580	PSU	C6-N1-C2	4.48	122.76	115.36
54	DA	746	PSU	C6-N1-C2	4.48	122.75	115.36
54	DA	2457	PSU	C6-N1-C2	4.47	122.74	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DA	1911	PSU	C6-N1-C2	4.47	122.74	115.36
31	CA	2580	PSU	C6-N1-C2	4.47	122.73	115.36
31	CA	746	PSU	C6-N1-C2	4.46	122.72	115.36
1	AA	516	PSU	C6-N1-C2	4.46	122.72	115.36
31	CA	2605	PSU	C6-N1-C2	4.45	122.70	115.36
31	CA	955	PSU	C6-N1-C2	4.45	122.70	115.36
31	CA	1911	PSU	C6-N1-C2	4.45	122.70	115.36
31	CA	1917	PSU	C6-N1-C2	4.44	122.69	115.36
54	DA	955	PSU	C6-N1-C2	4.44	122.68	115.36
1	BA	516	PSU	C6-N1-C2	4.43	122.67	115.36
31	CA	2457	PSU	C6-N1-C2	4.42	122.65	115.36
54	DA	2605	PSU	C6-N1-C2	4.42	122.65	115.36
31	CA	2504	PSU	C6-N1-C2	4.42	122.64	115.36
54	DA	2604	PSU	C6-N1-C2	4.39	122.60	115.36
31	CA	2498	OMC	C2-N3-C4	4.31	120.71	116.34
1	BA	967	5MC	C2-N3-C4	4.14	121.02	116.02
1	AA	1407	5MC	C2-N3-C4	4.10	120.97	116.02
1	AA	967	5MC	C2-N3-C4	4.09	120.95	116.02
1	BA	1407	5MC	C2-N3-C4	4.07	120.94	116.02
54	DA	1962	5MC	C2-N3-C4	4.07	120.93	116.02
31	CA	1962	5MC	C2-N3-C4	4.03	120.88	116.02
31	CA	745	1MG	C6-C5-C4	-3.87	117.48	119.96
1	AA	1516	2MG	C6-C5-C4	-3.85	117.12	120.80
54	DA	2552	OMU	C5-C4-N3	-3.85	114.85	123.31
31	CA	2552	OMU	C5-C4-N3	-3.83	114.88	123.31
30	DD	150[B]	MEQ	CB-CG-CD	3.81	121.55	113.04
54	DA	2069	G7M	N3-C2-N1	-3.72	122.27	127.22
1	BA	1516	2MG	C6-C5-C4	-3.70	117.26	120.80
40	DN	81[B]	4D4	NH1-CZ-NE	-3.68	110.70	119.19
1	AA	527	G7M	N3-C2-N1	-3.55	122.49	127.22
1	BA	1207	2MG	C6-C5-C4	-3.50	117.45	120.80
54	DA	2445	2MG	C6-C5-C4	-3.46	117.50	120.80
1	BA	527	G7M	N3-C2-N1	-3.43	122.65	127.22
31	CA	2069	G7M	N3-C2-N1	-3.38	122.71	127.22
54	DA	745	1MG	C6-C5-C4	-3.37	117.80	119.96
31	CA	2445	2MG	C6-C5-C4	-3.36	117.58	120.80
1	AA	966	2MG	C6-C5-C4	-3.29	117.66	120.80
40	CN	81	4D4	NH1-CZ-NE	-3.28	111.61	119.19
54	DA	1835	2MG	C6-C5-C4	-3.27	117.67	120.80
31	CA	1618	6MZ	C9-N6-C6	3.23	125.66	122.87
1	AA	1402	4OC	CM4-N4-C4	3.20	125.71	122.97
31	CA	2251	OMG	C6-C5-C4	-3.16	117.78	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	966	2MG	C6-C5-C4	-3.14	117.80	120.80
1	AA	1207	2MG	C6-C5-C4	-3.14	117.80	120.80
54	DA	1915	3TD	C5-C4-N3	-3.13	116.13	118.66
54	DA	745	1MG	C5-C6-N1	-3.12	114.88	118.20
1	BA	1402	4OC	CM4-N4-C4	3.07	125.60	122.97
31	CA	1915	3TD	C5-C4-N3	-3.06	116.18	118.66
54	DA	2251	OMG	N3-C2-N1	-3.06	123.14	127.22
31	CA	1835	2MG	C6-C5-C4	-2.96	117.97	120.80
1	BA	1207	2MG	N2-C2-N3	2.96	119.80	116.96
31	CA	745	1MG	C5-C6-N1	-2.95	115.05	118.20
1	BA	966	2MG	N2-C2-N3	2.94	119.78	116.96
54	DA	1835	2MG	N2-C2-N3	2.88	119.73	116.96
31	CA	1835	2MG	N2-C2-N3	2.84	119.69	116.96
54	DA	2251	OMG	C6-C5-C4	-2.83	118.10	120.80
31	CA	2251	OMG	N3-C2-N1	-2.81	123.47	127.22
1	AA	1207	2MG	N2-C2-N3	2.78	119.63	116.96
40	DN	81[A]	4D4	NH1-CZ-NE	-2.74	112.87	119.19
1	AA	1516	2MG	N2-C2-N3	2.74	119.59	116.96
1	BA	1516	2MG	N2-C2-N3	2.66	119.52	116.96
1	BA	1518	MA6	N1-C6-N6	-2.61	114.31	117.06
54	DA	2445	2MG	N2-C2-N3	2.46	119.33	116.96
31	CA	2445	2MG	N2-C2-N3	2.46	119.32	116.96
31	CA	1618	6MZ	C2-N1-C6	2.40	118.64	116.59
1	AA	527	G7M	O4'-C1'-C2'	-2.36	103.47	106.93
31	CA	2030	6MZ	C2-N1-C6	2.32	118.58	116.59
31	CA	2030	6MZ	C9-N6-C6	2.30	124.85	122.87
54	DA	2030	6MZ	C2-N1-C6	2.25	118.52	116.59
54	DA	2503	2MA	CM2-C2-N3	2.25	120.66	117.16
54	DA	1618	6MZ	C2-N1-C6	2.23	118.50	116.59
54	DA	2251	OMG	C2-N3-C4	-2.21	112.84	115.36
1	AA	527	G7M	C2-N3-C4	-2.19	112.86	115.36
31	CA	2605	PSU	C4-C5-C1'	-2.19	117.00	121.12
1	BA	527	G7M	C2-N3-C4	-2.17	112.88	115.36
1	AA	1518	MA6	N1-C6-N6	-2.16	114.78	117.06
54	DA	2503	2MA	N3-C2-N1	-2.16	121.74	125.72
1	AA	967	5MC	CM5-C5-C6	2.11	123.12	118.68
31	CA	2580	PSU	O4'-C1'-C2'	2.09	108.04	104.66
31	CA	747	5MU	C5M-C5-C6	2.09	123.09	118.68
31	CA	2503	2MA	N3-C2-N1	-2.08	121.89	125.72
1	BA	1407	5MC	CM5-C5-C6	2.08	123.08	118.68
54	DA	745	1MG	O4'-C4'-C3'	-2.08	100.99	105.11
1	BA	967	5MC	CM5-C5-C6	2.06	123.03	118.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1407	5MC	CM5-C5-C6	2.06	123.02	118.68
31	CA	2069	G7M	C2-N3-C4	-2.05	113.01	115.36
31	CA	1939	5MU	C5M-C5-C6	2.05	123.01	118.68
54	DA	2605	PSU	C4-C5-C1'	-2.03	117.30	121.12
54	DA	747	5MU	C5M-C5-C6	2.02	122.95	118.68
31	CA	2503	2MA	CM2-C2-N3	2.00	120.27	117.16

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	CA	2251	OMG	C1'-C2'-O2'-CM2
54	DA	746	PSU	O4'-C1'-C5-C6
31	CA	1962	5MC	O4'-C1'-N1-C6
31	CA	1962	5MC	C2'-C1'-N1-C6
54	DA	1962	5MC	O4'-C1'-N1-C6
54	DA	1962	5MC	C2'-C1'-N1-C6
31	CA	746	PSU	O4'-C1'-C5-C6
40	DN	81[B]	4D4	CA-CB-CG-CD
12	BL	89	D2T	CG-CB-SB-CB1
1	AA	527	G7M	O4'-C4'-C5'-O5'
1	AA	527	G7M	C3'-C4'-C5'-O5'
30	CD	150	MEQ	C-CA-CB-CG
1	BA	527	G7M	O4'-C4'-C5'-O5'
1	BA	527	G7M	C3'-C4'-C5'-O5'
54	DA	2030	6MZ	O4'-C4'-C5'-O5'
30	DD	150[B]	MEQ	N-CA-CB-CG
12	AL	89	D2T	CG-CB-SB-CB1
30	DD	150[A]	MEQ	OE1-CD-CG-CB
30	DD	150[A]	MEQ	NE2-CD-CG-CB
54	DA	2030	6MZ	C3'-C4'-C5'-O5'
30	CD	150	MEQ	CA-CB-CG-CD
40	DN	81[B]	4D4	OB-CB-CG-CD
30	DD	150[A]	MEQ	CA-CB-CG-CD
30	DD	150[B]	MEQ	C-CA-CB-CG
54	DA	746	PSU	C2'-C1'-C5-C6
31	CA	1835	2MG	O4'-C4'-C5'-O5'
54	DA	2069	G7M	C4'-C5'-O5'-P
31	CA	2030	6MZ	O4'-C4'-C5'-O5'
54	DA	1835	2MG	O4'-C4'-C5'-O5'
31	CA	746	PSU	C2'-C1'-C5-C6
1	BA	1519	MA6	C5-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
1	AA	1519	MA6	C5-C6-N6-C9
31	CA	1835	2MG	C3'-C4'-C5'-O5'
30	DD	150[B]	MEQ	CA-CB-CG-CD
31	CA	2069	G7M	C4'-C5'-O5'-P
54	DA	2503	2MA	C4'-C5'-O5'-P
54	DA	1835	2MG	C3'-C4'-C5'-O5'
30	DD	150[B]	MEQ	OE1-CD-NE2-CE
31	CA	2503	2MA	C4'-C5'-O5'-P
40	CN	81	4D4	CG-CD-NE-CZ
54	DA	746	PSU	O4'-C1'-C5-C4
31	CA	746	PSU	O4'-C1'-C5-C4
31	CA	2504	PSU	O4'-C4'-C5'-O5'
54	DA	2251	OMG	C1'-C2'-O2'-CM2
31	CA	2552	OMU	C3'-C2'-O2'-CM2
54	DA	2069	G7M	O4'-C4'-C5'-O5'
54	DA	2552	OMU	C3'-C2'-O2'-CM2
31	CA	2503	2MA	O4'-C4'-C5'-O5'
31	CA	2069	G7M	O4'-C4'-C5'-O5'
54	DA	2504	PSU	O4'-C4'-C5'-O5'
54	DA	2503	2MA	O4'-C4'-C5'-O5'
54	DA	2449	H2U	C4'-C5'-O5'-P

There are no ring outliers.

15 monomers are involved in 13 short contacts:

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	PUT	AA	1674	-	5,5,5	0.16	0	4,4,4	0.15	0
57	MPD	DT	202	-	7,7,7	0.85	1 (14%)	9,10,10	0.43	0
56	PG4	DA	3215	-	12,12,12	0.17	0	11,11,11	0.13	0
61	PEG	DA	3226	-	6,6,6	0.42	0	5,5,5	0.28	0
59	TAC	BA	1602	55	33,35,35	0.37	0	42,58,58	0.74	1 (2%)
63	PGE	D3	101	-	9,9,9	0.29	0	8,8,8	0.23	0
57	MPD	DA	3203	-	7,7,7	0.92	1 (14%)	9,10,10	0.66	0
57	MPD	DA	3206	-	7,7,7	1.05	1 (14%)	9,10,10	0.54	0
62	EDO	D1	101	-	3,3,3	0.68	0	2,2,2	0.15	0
63	PGE	D1	102	-	9,9,9	0.29	0	8,8,8	0.30	0
57	MPD	DE	301	-	7,7,7	0.88	0	9,10,10	0.78	0
62	EDO	DA	3208	-	3,3,3	0.60	0	2,2,2	0.30	0
58	PUT	DA	3002	-	5,5,5	0.19	0	4,4,4	0.09	0
61	PEG	DA	3199	-	6,6,6	0.30	0	5,5,5	0.20	0
66	ACY	DA	3201	-	1,3,3	2.00	0	0,3,3	0.00	-
56	PG4	DQ	202	-	12,12,12	0.15	0	11,11,11	0.16	0
56	PG4	DR	202	-	12,12,12	0.43	0	11,11,11	0.55	0
61	PEG	DP	201	-	6,6,6	0.29	0	5,5,5	0.16	0
62	EDO	DA	3207	-	3,3,3	0.72	0	2,2,2	0.16	0
58	PUT	DA	3188	-	5,5,5	0.44	0	4,4,4	0.27	0
62	EDO	DA	3198	-	3,3,3	0.69	0	2,2,2	0.38	0
63	PGE	DU	101	-	9,9,9	0.26	0	8,8,8	0.37	0
66	ACY	DA	3196	-	1,3,3	3.07	1 (100%)	0,3,3	0.00	-
58	PUT	DA	3220	-	5,5,5	0.19	0	4,4,4	0.13	0
63	PGE	DS	201	-	9,9,9	0.48	0	8,8,8	0.48	0
58	PUT	AA	1672	-	5,5,5	0.23	0	4,4,4	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PG4	DA	3193	-	12,12,12	0.30	0	11,11,11	0.43	0
62	EDO	DA	3197	-	3,3,3	0.64	0	2,2,2	0.22	0
58	PUT	DA	3221	-	5,5,5	0.46	0	4,4,4	0.61	0
58	PUT	DA	3211	-	5,5,5	0.31	0	4,4,4	0.16	0
57	MPD	DS	203	-	7,7,7	0.42	0	9,10,10	0.69	0
57	MPD	DT	201	-	7,7,7	0.63	0	9,10,10	0.21	0
56	PG4	BA	1601	-	12,12,12	0.21	0	11,11,11	0.22	0
63	PGE	DD	301	-	9,9,9	0.29	0	8,8,8	0.32	0
58	PUT	AA	1673	-	5,5,5	0.16	0	4,4,4	0.15	0
61	PEG	D1	103	-	6,6,6	0.42	0	5,5,5	0.16	0
58	PUT	DA	3195	-	5,5,5	0.32	0	4,4,4	0.51	0
63	PGE	DA	3216	-	9,9,9	0.14	0	8,8,8	0.25	0
58	PUT	DA	3184	-	5,5,5	0.24	0	4,4,4	0.16	0
61	PEG	D3	102	-	6,6,6	0.33	0	5,5,5	0.25	0
62	EDO	DA	3003	-	3,3,3	0.77	0	2,2,2	0.11	0
64	SPD	DA	3205	-	9,9,9	0.24	0	8,8,8	0.17	0
61	PEG	DQ	201	-	6,6,6	0.20	0	5,5,5	0.15	0
61	PEG	DL	201	-	6,6,6	0.13	0	5,5,5	0.12	0
66	ACY	DA	3191	-	1,3,3	2.16	1 (100%)	0,3,3	0.00	-
63	PGE	DA	3186	-	9,9,9	0.35	0	8,8,8	0.56	0
57	MPD	DK	201	-	7,7,7	0.76	0	9,10,10	0.26	0
58	PUT	DA	3222	-	5,5,5	0.29	0	4,4,4	0.30	0
58	PUT	AA	1675	-	5,5,5	0.21	0	4,4,4	0.22	0
57	MPD	DA	3209	-	7,7,7	0.73	0	9,10,10	0.39	0
62	EDO	DA	3004	-	3,3,3	0.74	0	2,2,2	0.13	0
62	EDO	DA	3001	-	3,3,3	0.85	0	2,2,2	0.10	0
56	PG4	DS	202	-	12,12,12	0.48	0	11,11,11	0.43	0
57	MPD	DA	3192	-	7,7,7	0.71	0	9,10,10	0.80	0
58	PUT	DA	3189	-	5,5,5	0.47	0	4,4,4	0.42	0
62	EDO	DB	211	-	3,3,3	0.60	0	2,2,2	0.17	0
57	MPD	AA	1671	-	7,7,7	0.73	0	9,10,10	0.45	0
59	TAC	AA	1678	55	33,35,35	0.48	0	42,58,58	0.68	1 (2%)
62	EDO	DA	3214	-	3,3,3	0.67	0	2,2,2	0.23	0
57	MPD	AA	1676	-	7,7,7	0.62	0	9,10,10	0.42	0
56	PG4	AA	1670	-	12,12,12	0.27	0	11,11,11	0.41	0
57	MPD	DA	3190	-	7,7,7	0.49	0	9,10,10	0.47	0
57	MPD	DE	302	-	7,7,7	0.92	1 (14%)	9,10,10	0.48	0
67	GUN	DA	3210	-	9,12,12	2.26	2 (22%)	8,17,17	3.98	4 (50%)
64	SPD	DA	3223	-	9,9,9	0.18	0	8,8,8	0.67	0
64	SPD	DA	3187	-	9,9,9	0.16	0	8,8,8	0.41	0
58	PUT	DA	3218	-	5,5,5	0.13	0	4,4,4	0.12	0
61	PEG	AL	201	-	6,6,6	0.25	0	5,5,5	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
64	SPD	DA	3183	-	9,9,9	0.13	0	8,8,8	0.19	0
57	MPD	DN	201	-	7,7,7	1.12	1 (14%)	9,10,10	0.61	0
61	PEG	DA	3200	-	6,6,6	0.51	0	5,5,5	0.29	0
65	1PE	DA	3202	-	15,15,15	0.36	0	14,14,14	0.39	0
61	PEG	DA	3225	-	6,6,6	0.49	0	5,5,5	0.27	0
61	PEG	DA	3217	-	6,6,6	0.29	0	5,5,5	0.09	0
68	TRS	DA	3219	-	7,7,7	0.29	0	9,9,9	0.29	0
62	EDO	DB	210	-	3,3,3	0.61	0	2,2,2	0.22	0
63	PGE	DA	3224	-	9,9,9	0.25	0	8,8,8	0.17	0
58	PUT	DA	3212	-	5,5,5	0.37	0	4,4,4	0.30	0
58	PUT	DA	3204	-	5,5,5	0.35	0	4,4,4	0.28	0
65	1PE	DA	3185	-	15,15,15	0.16	0	14,14,14	0.16	0
63	PGE	DA	3213	-	9,9,9	0.17	0	8,8,8	0.18	0
62	EDO	DA	3194	-	3,3,3	0.65	0	2,2,2	0.06	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
58	PUT	AA	1674	-	-	0/3/3/3	-
57	MPD	DT	202	-	-	2/5/5/5	-
57	MPD	DA	3209	-	-	1/5/5/5	-
61	PEG	DA	3226	-	-	0/4/4/4	-
59	TAC	BA	1602	55	-	6/8/74/74	0/4/4/4
63	PGE	D3	101	-	-	2/7/7/7	-
57	MPD	DA	3203	-	-	1/5/5/5	-
57	MPD	DA	3206	-	-	1/5/5/5	-
62	EDO	D1	101	-	-	0/1/1/1	-
63	PGE	D1	102	-	-	4/7/7/7	-
57	MPD	DE	301	-	-	5/5/5/5	-
62	EDO	DA	3208	-	-	0/1/1/1	-
58	PUT	DA	3002	-	-	0/3/3/3	-
61	PEG	DA	3199	-	-	3/4/4/4	-
56	PG4	DA	3215	-	-	4/10/10/10	-
56	PG4	DQ	202	-	-	1/10/10/10	-
56	PG4	DR	202	-	-	6/10/10/10	-
62	EDO	DA	3207	-	-	0/1/1/1	-
58	PUT	DA	3188	-	-	0/3/3/3	-
62	EDO	DA	3198	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PGE	DU	101	-	-	4/7/7/7	-
58	PUT	DA	3220	-	-	0/3/3/3	-
61	PEG	DA	3217	-	-	3/4/4/4	-
63	PGE	DS	201	-	-	3/7/7/7	-
58	PUT	AA	1672	-	-	0/3/3/3	-
56	PG4	DA	3193	-	-	8/10/10/10	-
62	EDO	DA	3197	-	-	0/1/1/1	-
58	PUT	DA	3221	-	-	1/3/3/3	-
58	PUT	DA	3211	-	-	0/3/3/3	-
57	MPD	DS	203	-	-	0/5/5/5	-
57	MPD	DT	201	-	-	2/5/5/5	-
56	PG4	BA	1601	-	-	0/10/10/10	-
63	PGE	DD	301	-	-	4/7/7/7	-
58	PUT	AA	1673	-	-	0/3/3/3	-
61	PEG	D1	103	-	-	1/4/4/4	-
58	PUT	DA	3195	-	-	1/3/3/3	-
63	PGE	DA	3216	-	-	4/7/7/7	-
58	PUT	DA	3184	-	-	0/3/3/3	-
61	PEG	D3	102	-	-	2/4/4/4	-
62	EDO	DA	3003	-	-	0/1/1/1	-
64	SPD	DA	3205	-	-	5/7/7/7	-
61	PEG	DQ	201	-	-	2/4/4/4	-
61	PEG	DL	201	-	-	2/4/4/4	-
63	PGE	DA	3186	-	-	4/7/7/7	-
57	MPD	DK	201	-	-	2/5/5/5	-
58	PUT	DA	3222	-	-	1/3/3/3	-
58	PUT	AA	1675	-	-	1/3/3/3	-
58	PUT	DA	3204	-	-	1/3/3/3	-
62	EDO	DA	3004	-	-	0/1/1/1	-
62	EDO	DA	3001	-	-	1/1/1/1	-
57	MPD	DA	3192	-	-	2/5/5/5	-
58	PUT	DA	3189	-	-	0/3/3/3	-
62	EDO	DB	211	-	-	0/1/1/1	-
57	MPD	AA	1671	-	-	1/5/5/5	-
59	TAC	AA	1678	55	-	4/8/74/74	0/4/4/4
62	EDO	DA	3214	-	-	0/1/1/1	-
57	MPD	AA	1676	-	-	2/5/5/5	-
56	PG4	AA	1670	-	-	4/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	MPD	DA	3190	-	-	2/5/5/5	-
57	MPD	DE	302	-	-	2/5/5/5	-
67	GUN	DA	3210	-	-	-	0/2/2/2
64	SPD	DA	3223	-	-	4/7/7/7	-
64	SPD	DA	3187	-	-	0/7/7/7	-
58	PUT	DA	3218	-	-	0/3/3/3	-
61	PEG	AL	201	-	-	2/4/4/4	-
64	SPD	DA	3183	-	-	1/7/7/7	-
57	MPD	DN	201	-	-	4/5/5/5	-
61	PEG	DA	3200	-	-	3/4/4/4	-
61	PEG	DP	201	-	-	2/4/4/4	-
61	PEG	DA	3225	-	-	2/4/4/4	-
65	1PE	DA	3202	-	-	8/13/13/13	-
68	TRS	DA	3219	-	-	0/9/9/9	-
62	EDO	DB	210	-	-	0/1/1/1	-
63	PGE	DA	3224	-	-	4/7/7/7	-
58	PUT	DA	3212	-	-	1/3/3/3	-
56	PG4	DS	202	-	-	2/10/10/10	-
65	1PE	DA	3185	-	-	5/13/13/13	-
63	PGE	DA	3213	-	-	2/7/7/7	-
62	EDO	DA	3194	-	-	1/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	DA	3210	GUN	C6-C5	5.29	1.50	1.41
67	DA	3210	GUN	C6-N1	3.41	1.39	1.33
66	DA	3196	ACY	CH3-C	3.07	1.52	1.48
57	DN	201	MPD	C3-C2	2.58	1.60	1.53
57	DA	3206	MPD	C3-C2	2.43	1.60	1.53
57	DE	302	MPD	C3-C2	2.17	1.59	1.53
66	DA	3191	ACY	CH3-C	2.16	1.51	1.48
57	DT	202	MPD	C3-C2	2.02	1.59	1.53
57	DA	3203	MPD	C3-C2	2.01	1.59	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	DA	3210	GUN	C5-C6-N1	-8.35	112.02	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	DA	3210	GUN	C6-N1-C2	5.80	125.14	115.93
67	DA	3210	GUN	C6-C5-C4	-3.54	117.42	120.80
59	BA	1602	TAC	O3-C3-C2	-2.50	118.57	122.96
67	DA	3210	GUN	N3-C2-N1	-2.42	123.99	127.22
59	AA	1678	TAC	O3-C3-C2	-2.33	118.88	122.96

There are no chirality outliers.

All (147) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	BA	1602	TAC	C1-C2-C21-O21
59	BA	1602	TAC	C1-C2-C21-N21
59	BA	1602	TAC	C3-C2-C21-O21
59	BA	1602	TAC	C3-C2-C21-N21
59	BA	1602	TAC	C41-C4-N4-C42
57	DA	3190	MPD	C2-C3-C4-O4
57	DA	3190	MPD	C2-C3-C4-C5
59	AA	1678	TAC	C3-C4-N4-C42
59	AA	1678	TAC	C3-C4-N4-C43
59	AA	1678	TAC	C41-C4-N4-C42
57	AA	1676	MPD	C2-C3-C4-O4
57	DT	202	MPD	C2-C3-C4-C5
57	DE	301	MPD	C1-C2-C3-C4
57	DE	301	MPD	O2-C2-C3-C4
57	DE	301	MPD	C2-C3-C4-O4
57	DN	201	MPD	CM-C2-C3-C4
56	DR	202	PG4	O3-C5-C6-O4
65	DA	3202	1PE	OH6-C15-C25-OH5
63	DA	3213	PGE	O2-C3-C4-O3
64	DA	3205	SPD	C3-C4-C5-N6
56	DA	3193	PG4	O3-C5-C6-O4
56	DR	202	PG4	O2-C3-C4-O3
65	DA	3202	1PE	OH4-C13-C23-OH3
65	DA	3185	1PE	OH2-C12-C22-OH3
63	DA	3186	PGE	O3-C5-C6-O4
56	DS	202	PG4	O4-C7-C8-O5
63	DU	101	PGE	O3-C5-C6-O4
56	DQ	202	PG4	O1-C1-C2-O2
58	DA	3195	PUT	C1-C2-C3-C4
63	DS	201	PGE	O3-C5-C6-O4
62	DA	3194	EDO	O1-C1-C2-O2
64	DA	3205	SPD	C4-C5-N6-C7

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Mol	Chain	Res	Type	Atoms
64	DA	3205	SPD	C8-C7-N6-C5
61	DL	201	PEG	O2-C3-C4-O4
61	D1	103	PEG	O2-C3-C4-O4
61	DA	3199	PEG	O2-C3-C4-O4
63	DA	3224	PGE	O3-C5-C6-O4
65	DA	3202	1PE	OH2-C12-C22-OH3
63	DA	3186	PGE	O1-C1-C2-O2
61	DA	3200	PEG	O2-C3-C4-O4
64	DA	3205	SPD	C2-C3-C4-C5
58	DA	3204	PUT	C1-C2-C3-C4
63	DD	301	PGE	O2-C3-C4-O3
63	DA	3224	PGE	O1-C1-C2-O2
58	DA	3222	PUT	C1-C2-C3-C4
56	DR	202	PG4	C5-C6-O4-C7
61	DA	3217	PEG	O2-C3-C4-O4
58	DA	3212	PUT	C1-C2-C3-C4
63	DU	101	PGE	O1-C1-C2-O2
57	DN	201	MPD	O2-C2-C3-C4
64	DA	3223	SPD	C4-C5-N6-C7
61	DA	3199	PEG	O1-C1-C2-O2
63	DD	301	PGE	O3-C5-C6-O4
56	DR	202	PG4	C6-C5-O3-C4
61	DL	201	PEG	C4-C3-O2-C2
61	DP	201	PEG	C1-C2-O2-C3
56	DA	3193	PG4	C1-C2-O2-C3
56	AA	1670	PG4	C4-C3-O2-C2
63	D3	101	PGE	C3-C4-O3-C5
65	DA	3185	1PE	C12-C22-OH3-C23
56	DA	3215	PG4	C3-C4-O3-C5
61	AL	201	PEG	C1-C2-O2-C3
56	DA	3215	PG4	C1-C2-O2-C3
63	DA	3213	PGE	C4-C3-O2-C2
61	DA	3199	PEG	C1-C2-O2-C3
56	AA	1670	PG4	C3-C4-O3-C5
65	DA	3202	1PE	C16-C26-OH6-C15
61	DA	3200	PEG	C1-C2-O2-C3
56	DA	3193	PG4	C4-C3-O2-C2
61	DA	3225	PEG	C1-C2-O2-C3
61	DA	3225	PEG	C4-C3-O2-C2
61	DA	3217	PEG	O1-C1-C2-O2
65	DA	3185	1PE	C16-C26-OH6-C15
65	DA	3202	1PE	C12-C22-OH3-C23

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Mol	Chain	Res	Type	Atoms
56	DA	3215	PG4	C8-C7-O4-C6
56	AA	1670	PG4	C5-C6-O4-C7
63	DD	301	PGE	C4-C3-O2-C2
61	DP	201	PEG	C4-C3-O2-C2
56	DR	202	PG4	C4-C3-O2-C2
59	BA	1602	TAC	C3-C4-N4-C43
59	AA	1678	TAC	C41-C4-N4-C43
57	DA	3192	MPD	C2-C3-C4-C5
65	DA	3185	1PE	C24-C14-OH5-C25
56	AA	1670	PG4	O1-C1-C2-O2
62	DA	3001	EDO	O1-C1-C2-O2
61	DA	3200	PEG	C4-C3-O2-C2
63	DA	3216	PGE	C3-C4-O3-C5
61	DA	3217	PEG	C1-C2-O2-C3
57	DE	302	MPD	C2-C3-C4-O4
57	DA	3192	MPD	C2-C3-C4-O4
63	DA	3224	PGE	C1-C2-O2-C3
57	DT	201	MPD	C1-C2-C3-C4
57	DE	301	MPD	CM-C2-C3-C4
57	DN	201	MPD	C1-C2-C3-C4
63	DA	3216	PGE	C4-C3-O2-C2
58	AA	1675	PUT	C1-C2-C3-C4
63	DA	3224	PGE	C3-C4-O3-C5
64	DA	3223	SPD	C3-C4-C5-N6
56	DA	3193	PG4	C3-C4-O3-C5
64	DA	3205	SPD	N6-C7-C8-C9
58	DA	3221	PUT	C1-C2-C3-C4
56	DR	202	PG4	C3-C4-O3-C5
61	AL	201	PEG	C4-C3-O2-C2
63	D1	102	PGE	O3-C5-C6-O4
62	DA	3198	EDO	O1-C1-C2-O2
63	DA	3186	PGE	C3-C4-O3-C5
65	DA	3202	1PE	C15-C25-OH5-C14
63	D1	102	PGE	C3-C4-O3-C5
63	D1	102	PGE	C4-C3-O2-C2
56	DA	3193	PG4	C6-C5-O3-C4
63	DS	201	PGE	C6-C5-O3-C4
63	DU	101	PGE	C6-C5-O3-C4
63	DA	3186	PGE	C4-C3-O2-C2
56	DS	202	PG4	O2-C3-C4-O3
56	DA	3193	PG4	C8-C7-O4-C6
63	DA	3216	PGE	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
63	DD	301	PGE	C3-C4-O3-C5
61	D3	102	PEG	C1-C2-O2-C3
57	DT	201	MPD	O2-C2-C3-C4
56	DA	3193	PG4	O4-C7-C8-O5
63	DU	101	PGE	O2-C3-C4-O3
64	DA	3183	SPD	C8-C7-N6-C5
65	DA	3185	1PE	C13-C23-OH3-C22
56	DA	3193	PG4	O2-C3-C4-O3
64	DA	3223	SPD	C8-C7-N6-C5
63	DA	3216	PGE	O2-C3-C4-O3
63	D3	101	PGE	C4-C3-O2-C2
64	DA	3223	SPD	C7-C8-C9-N10
56	DA	3215	PG4	O1-C1-C2-O2
61	DQ	201	PEG	O1-C1-C2-O2
63	DS	201	PGE	O2-C3-C4-O3
63	D1	102	PGE	O2-C3-C4-O3
57	DA	3206	MPD	C2-C3-C4-C5
57	AA	1676	MPD	C2-C3-C4-C5
57	DK	201	MPD	C2-C3-C4-C5
57	DE	302	MPD	C2-C3-C4-C5
57	DA	3203	MPD	C2-C3-C4-C5
57	DE	301	MPD	C2-C3-C4-C5
65	DA	3202	1PE	OH5-C14-C24-OH4
61	D3	102	PEG	O1-C1-C2-O2
61	DQ	201	PEG	C1-C2-O2-C3
57	DA	3209	MPD	C2-C3-C4-O4
57	DK	201	MPD	C2-C3-C4-O4
57	AA	1671	MPD	C2-C3-C4-O4
57	DT	202	MPD	C2-C3-C4-O4
57	DN	201	MPD	C2-C3-C4-O4
65	DA	3202	1PE	C14-C24-OH4-C13

There are no ring outliers.

32 monomers are involved in 50 short contacts:

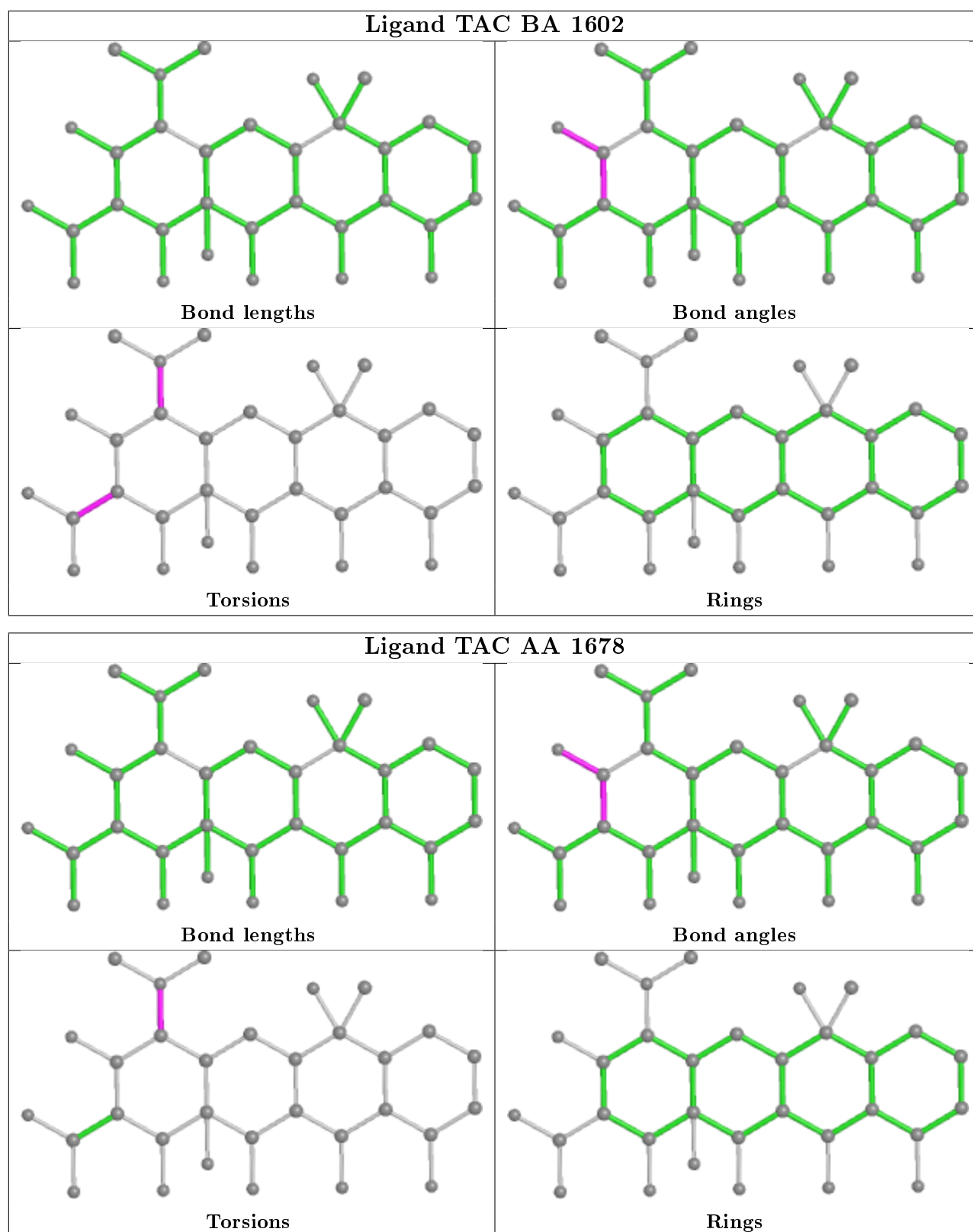
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	DA	3215	PG4	1	0
59	BA	1602	TAC	1	0
57	DA	3203	MPD	2	0
63	D1	102	PGE	2	0
56	DR	202	PG4	5	0
61	DP	201	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	DU	101	PGE	1	0
56	DA	3193	PG4	1	0
62	DA	3197	EDO	1	0
58	DA	3221	PUT	3	0
63	DD	301	PGE	2	0
61	D1	103	PEG	1	0
58	DA	3195	PUT	3	0
63	DA	3216	PGE	1	0
61	D3	102	PEG	2	0
58	DA	3222	PUT	1	0
56	DS	202	PG4	1	0
57	DA	3192	MPD	2	0
58	DA	3189	PUT	1	0
62	DB	211	EDO	1	0
59	AA	1678	TAC	1	0
56	AA	1670	PG4	1	0
57	DA	3190	MPD	1	0
64	DA	3223	SPD	4	0
58	DA	3218	PUT	1	0
57	DN	201	MPD	1	0
61	DA	3200	PEG	1	0
68	DA	3219	TRS	1	0
63	DA	3224	PGE	3	0
58	DA	3212	PUT	1	0
63	DA	3213	PGE	1	0
62	DA	3194	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1523/1534 (99%)	0.42	52 (3%) 45 35	43, 97, 239, 285	0
1	BA	1522/1534 (99%)	1.36	387 (25%) 0 0	52, 139, 267, 278	0
2	AB	224/224 (100%)	1.57	78 (34%) 0 0	78, 123, 207, 275	0
2	BB	224/224 (100%)	1.90	85 (37%) 0 0	93, 139, 208, 261	0
3	AC	206/206 (100%)	0.57	19 (9%) 9 5	73, 101, 135, 157	0
3	BC	206/206 (100%)	1.95	82 (39%) 0 0	103, 141, 180, 219	0
4	AD	205/205 (100%)	0.29	6 (2%) 51 41	53, 96, 127, 158	0
4	BD	205/205 (100%)	0.09	2 (0%) 82 77	53, 77, 106, 135	0
5	AE	155/155 (100%)	0.45	6 (3%) 39 29	60, 87, 139, 174	0
5	BE	150/155 (96%)	0.73	19 (12%) 3 2	71, 91, 142, 229	0
6	AF	106/106 (100%)	0.55	13 (12%) 4 2	72, 97, 120, 134	0
6	BF	100/106 (94%)	0.86	9 (9%) 9 5	79, 112, 139, 147	0
7	AG	151/151 (100%)	1.46	42 (27%) 0 0	99, 128, 157, 169	0
7	BG	151/151 (100%)	3.74	108 (71%) 0 0	139, 193, 209, 220	0
8	AH	129/129 (100%)	0.41	6 (4%) 31 22	66, 85, 113, 128	0
8	BH	129/129 (100%)	0.83	18 (13%) 2 1	86, 110, 145, 164	0
9	AI	127/127 (100%)	1.83	46 (36%) 0 0	85, 123, 161, 188	0
9	BI	127/127 (100%)	3.74	77 (60%) 0 0	130, 168, 201, 223	0
10	AJ	99/99 (100%)	1.38	21 (21%) 0 0	85, 111, 142, 157	0
10	BJ	98/99 (98%)	4.87	73 (74%) 0 0	132, 163, 188, 200	0
11	AK	117/117 (100%)	1.24	28 (23%) 0 0	52, 102, 138, 153	0
11	BK	117/117 (100%)	1.04	24 (20%) 1 0	73, 109, 139, 160	0
12	AL	122/123 (99%)	0.32	2 (1%) 72 66	48, 66, 99, 126	0
12	BL	122/123 (99%)	1.20	29 (23%) 0 0	75, 91, 112, 133	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	1.92	47 (41%) 0 0	90, 118, 167, 184	0
13	BM	114/114 (100%)	5.82	106 (92%) 0 0	195, 228, 237, 241	0
14	AN	100/100 (100%)	1.39	21 (21%) 1 0	82, 108, 198, 210	0
14	BN	100/100 (100%)	4.08	73 (73%) 0 0	125, 173, 232, 242	0
15	AO	88/88 (100%)	0.55	7 (7%) 12 6	63, 87, 108, 128	0
15	BO	88/88 (100%)	1.08	17 (19%) 1 0	75, 105, 125, 144	0
16	AP	82/82 (100%)	1.17	17 (20%) 1 0	60, 79, 114, 133	0
16	BP	82/82 (100%)	2.47	44 (53%) 0 0	89, 105, 151, 161	0
17	AQ	80/80 (100%)	0.61	6 (7%) 14 8	63, 79, 114, 136	0
17	BQ	80/80 (100%)	1.98	30 (37%) 0 0	94, 119, 143, 147	0
18	AR	55/55 (100%)	1.09	13 (23%) 0 0	68, 91, 126, 154	0
18	BR	55/55 (100%)	0.81	5 (9%) 9 5	71, 89, 123, 150	0
19	AS	79/79 (100%)	1.37	20 (25%) 0 0	94, 109, 146, 153	0
19	BS	79/79 (100%)	5.37	71 (89%) 0 0	206, 223, 234, 242	0
20	AT	86/86 (100%)	0.67	6 (6%) 16 9	67, 79, 116, 132	0
20	BT	85/86 (98%)	2.93	55 (64%) 0 0	101, 121, 164, 175	0
21	AU	56/56 (100%)	1.50	15 (26%) 0 0	80, 118, 156, 170	0
21	BU	56/56 (100%)	0.77	8 (14%) 2 1	75, 100, 143, 156	0
22	C1	56/56 (100%)	2.88	36 (64%) 0 0	94, 138, 164, 182	0
22	D1	56/56 (100%)	0.32	0 100 100	20, 41, 64, 95	0
23	C2	50/51 (98%)	4.06	40 (80%) 0 0	126, 141, 153, 175	0
23	D2	51/51 (100%)	0.32	3 (5%) 22 14	49, 63, 89, 104	0
24	C3	46/46 (100%)	3.68	36 (78%) 0 0	99, 109, 119, 131	0
24	D3	46/46 (100%)	0.37	2 (4%) 35 25	30, 42, 56, 99	0
25	C4	64/64 (100%)	2.51	33 (51%) 0 0	105, 121, 134, 140	0
25	D4	64/64 (100%)	0.36	0 100 100	34, 41, 52, 63	0
26	C5	38/38 (100%)	2.73	23 (60%) 0 0	100, 114, 124, 134	0
26	D5	38/38 (100%)	0.38	0 100 100	31, 46, 62, 82	0
27	C0	58/58 (100%)	2.44	30 (51%) 0 0	98, 113, 132, 135	0
27	D0	58/58 (100%)	0.25	0 100 100	28, 35, 54, 72	0
28	CB	118/120 (98%)	1.77	40 (33%) 0 0	132, 189, 251, 254	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	120/120 (100%)	0.14	0 100 100	29, 56, 101, 148	0
29	CC	271/271 (100%)	1.36	79 (29%) 0 0	80, 112, 146, 165	0
29	DC	271/271 (100%)	0.09	1 (0%) 92 91	28, 56, 84, 100	0
30	CD	208/209 (99%)	2.21	104 (50%) 0 0	86, 121, 156, 181	0
30	DD	208/209 (99%)	0.01	0 100 100	18, 39, 67, 88	0
31	CA	2876/2904 (99%)	1.74	891 (30%) 0 0	71, 170, 260, 285	0
32	CE	201/201 (100%)	2.99	125 (62%) 0 0	112, 159, 194, 210	0
32	DE	201/201 (100%)	0.15	6 (2%) 50 40	24, 55, 100, 139	0
33	CF	177/177 (100%)	4.98	153 (86%) 0 0	198, 211, 219, 226	0
33	DF	177/177 (100%)	0.48	7 (3%) 38 28	50, 79, 125, 137	0
34	CG	176/176 (100%)	3.79	135 (76%) 0 0	130, 170, 205, 215	0
34	DG	176/176 (100%)	0.24	5 (2%) 53 43	42, 70, 97, 139	0
35	CH	149/149 (100%)	2.24	74 (49%) 0 0	84, 151, 170, 180	0
35	DH	149/149 (100%)	1.87	64 (42%) 0 0	74, 150, 187, 199	0
36	CJ	134/134 (100%)	8.40	130 (97%) 0 0	227, 245, 255, 263	0
36	DJ	134/134 (100%)	5.70	111 (82%) 0 0	196, 220, 229, 237	0
37	CK	142/142 (100%)	1.66	52 (36%) 0 0	95, 117, 152, 194	0
37	DK	142/142 (100%)	-0.03	0 100 100	19, 34, 58, 72	0
38	CL	122/123 (99%)	1.14	22 (18%) 1 1	90, 109, 141, 158	0
38	DL	123/123 (100%)	-0.07	0 100 100	28, 43, 70, 106	0
39	CM	144/144 (100%)	3.62	105 (72%) 0 0	104, 151, 201, 235	0
39	DM	144/144 (100%)	0.18	2 (1%) 75 70	18, 55, 84, 116	0
40	CN	135/136 (99%)	1.35	37 (27%) 0 0	92, 112, 142, 180	0
40	DN	135/136 (99%)	-0.19	0 100 100	25, 39, 67, 86	0
41	CO	120/125 (96%)	2.26	55 (45%) 0 0	101, 123, 143, 177	0
41	DO	125/125 (100%)	0.01	0 100 100	24, 36, 65, 108	0
42	CP	116/117 (99%)	3.70	94 (81%) 0 0	139, 162, 177, 181	0
42	DP	117/117 (100%)	0.17	0 100 100	36, 56, 84, 93	0
43	CQ	114/114 (100%)	2.11	47 (41%) 0 0	100, 117, 149, 164	0
43	DQ	114/114 (100%)	-0.01	3 (2%) 56 46	30, 49, 77, 109	0
44	CR	117/117 (100%)	2.33	57 (48%) 0 0	89, 122, 157, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DR	117/117 (100%)	0.13	1 (0%) 84 80	18, 29, 48, 72	0
45	CS	103/103 (100%)	3.83	79 (76%) 0 0	107, 133, 172, 185	0
45	DS	103/103 (100%)	-0.16	0 100 100	19, 41, 69, 91	0
46	CT	110/110 (100%)	2.29	55 (50%) 0 0	99, 127, 167, 182	0
46	DT	110/110 (100%)	-0.05	0 100 100	19, 33, 60, 116	0
47	CU	93/93 (100%)	3.54	68 (73%) 0 0	123, 147, 176, 185	0
47	DU	93/93 (100%)	0.57	5 (5%) 25 17	31, 53, 109, 124	0
48	CV	102/102 (100%)	4.69	85 (83%) 0 0	113, 161, 198, 209	0
48	DV	102/102 (100%)	0.44	10 (9%) 7 4	42, 60, 121, 157	0
49	CW	94/94 (100%)	2.41	49 (52%) 0 0	116, 137, 156, 161	0
49	DW	94/94 (100%)	-0.22	0 100 100	31, 51, 76, 86	0
50	CX	75/76 (98%)	3.19	41 (54%) 0 0	103, 126, 140, 170	0
50	DX	76/76 (100%)	-0.05	1 (1%) 77 72	25, 39, 64, 104	0
51	CY	77/77 (100%)	1.86	31 (40%) 0 0	97, 117, 142, 161	0
51	DY	77/77 (100%)	0.09	1 (1%) 77 72	38, 54, 88, 103	0
52	CZ	62/62 (100%)	4.12	49 (79%) 0 0	127, 163, 175, 186	0
52	DZ	62/62 (100%)	0.58	5 (8%) 12 6	48, 70, 103, 126	0
53	DI	135/135 (100%)	2.50	69 (51%) 0 0	78, 150, 197, 207	1 (0%)
54	DA	2873/2904 (98%)	0.46	123 (4%) 35 25	17, 44, 217, 299	0
All	All	20633/20745 (99%)	1.39	5067 (24%) 0 0	17, 108, 239, 299	1 (0%)

All (5067) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	DJ	54	PRO	28.1
36	CJ	69	PHE	27.3
36	CJ	76	ALA	25.6
36	DJ	53	LEU	23.6
36	CJ	14	ALA	23.2
36	CJ	13	VAL	23.1
36	CJ	54	PRO	20.9
36	CJ	55	ILE	20.2
9	BI	128	SER	19.5
36	CJ	57	VAL	18.2
45	CS	50	GLY	18.2

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Mol	Chain	Res	Type	RSRZ
36	CJ	59	ILE	17.9
10	BJ	74	VAL	17.6
33	CF	85	ILE	17.4
33	CF	128	TYR	17.2
36	CJ	11	LEU	17.0
9	BI	31	ASN	17.0
33	CF	40	VAL	16.5
54	DA	2120	G	16.1
39	CM	101	ILE	16.0
13	BM	10	PRO	15.9
36	CJ	12	GLN	15.9
36	CJ	23	PRO	15.8
39	CM	80	SER	15.7
31	CA	1067	A	15.5
36	DJ	76	ALA	15.4
1	BA	211	G	15.3
36	DJ	80	LEU	15.1
36	DJ	96	ASP	15.1
19	BS	48	THR	15.0
36	DJ	67	PHE	14.9
36	DJ	23	PRO	14.9
36	CJ	17	MET	14.8
33	CF	76	GLY	14.5
13	BM	5	ALA	14.5
36	DJ	94	ASN	14.5
20	BT	4	ILE	14.4
36	CJ	56	PRO	14.4
36	CJ	126	THR	14.3
33	CF	156	ILE	14.1
31	CA	2172	U	14.0
31	CA	1068	G	14.0
36	CJ	51	LYS	13.8
39	CM	81	ASP	13.7
10	BJ	8	ILE	13.6
48	CV	20	GLY	13.6
1	BA	209	U	13.4
48	CV	13	VAL	13.4
36	CJ	21	SER	13.3
36	CJ	68	THR	13.3
53	DI	131	THR	13.2
52	CZ	45	GLN	13.2
36	CJ	80	LEU	13.2

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Mol	Chain	Res	Type	RSRZ
36	CJ	87	LYS	13.1
36	DJ	135	SER	13.1
36	DJ	88	SER	13.1
36	CJ	38	PHE	13.1
36	DJ	55	ILE	12.9
36	CJ	22	PRO	12.8
36	CJ	61	VAL	12.7
36	CJ	82	LYS	12.6
54	DA	2110	G	12.6
36	DJ	79	LEU	12.5
36	CJ	8	TYR	12.5
36	CJ	20	PRO	12.5
36	CJ	71	THR	12.5
19	BS	14	HIS	12.5
36	DJ	78	VAL	12.5
9	BI	44	ALA	12.4
34	CG	40	ALA	12.4
9	BI	67	VAL	12.4
50	CX	54	GLY	12.3
19	BS	38	SER	12.3
39	CM	92	LEU	12.2
36	CJ	28	LEU	12.2
45	CS	27	ILE	12.2
39	CM	114	GLY	12.0
53	DI	128	THR	12.0
36	DJ	114	ALA	11.9
54	DA	2163	A	11.9
36	CJ	60	THR	11.9
31	CA	1066	U	11.9
36	CJ	42	PHE	11.9
13	BM	45	ILE	11.9
29	CC	27	GLY	11.9
36	CJ	99	GLY	11.8
10	BJ	73	LEU	11.8
13	BM	23	TYR	11.7
36	DJ	52	GLY	11.7
1	BA	1302	C	11.7
34	CG	32	GLU	11.7
36	CJ	138	LEU	11.6
9	AI	130	ARG	11.6
48	CV	80	ALA	11.6
36	CJ	9	VAL	11.6

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Mol	Chain	Res	Type	RSRZ
47	CU	43	ILE	11.6
54	DA	2111	U	11.5
9	BI	40	GLY	11.5
13	BM	22	ILE	11.4
36	DJ	137	GLY	11.4
36	DJ	20	PRO	11.4
33	CF	157	THR	11.4
33	CF	154	ILE	11.4
39	CM	100	ILE	11.4
1	BA	983	A	11.3
10	BJ	76	ILE	11.3
48	CV	19	LYS	11.3
14	BN	60	GLN	11.3
33	CF	155	THR	11.2
10	BJ	101	SER	11.2
48	CV	36	VAL	11.2
19	BS	12	ASP	11.2
36	DJ	13	VAL	11.2
9	BI	126	GLN	11.1
31	CA	1537	G	11.1
33	CF	106	ILE	11.1
36	CJ	121	ASP	11.1
1	BA	1242	G	11.1
36	DJ	138	LEU	11.0
53	DI	96	PHE	11.0
33	CF	129	SER	11.0
7	BG	8	GLY	10.9
48	CV	78	GLY	10.9
36	CJ	47	ASP	10.9
36	CJ	98	VAL	10.9
43	CQ	85	SER	10.9
14	BN	33	ASP	10.8
10	BJ	87	LEU	10.8
9	BI	16	ALA	10.8
48	CV	89	ASP	10.8
19	BS	5	LEU	10.7
36	CJ	62	TYR	10.7
36	CJ	83	ALA	10.6
33	CF	117	LEU	10.6
52	CZ	32	ALA	10.5
14	AN	21	PHE	10.5
45	CS	96	VAL	10.5

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Mol	Chain	Res	Type	RSRZ
34	CG	62	TRP	10.5
7	BG	43	VAL	10.4
9	BI	127	PHE	10.4
1	BA	1030	U	10.4
36	CJ	75	PRO	10.4
36	CJ	85	GLY	10.4
13	BM	2	ALA	10.4
33	CF	35	THR	10.3
36	DJ	12	GLN	10.3
34	CG	43	VAL	10.3
1	AA	1030	U	10.3
19	BS	29	LYS	10.3
10	BJ	26	VAL	10.3
42	CP	63	LYS	10.3
10	BJ	77	VAL	10.2
36	CJ	33	VAL	10.2
13	BM	95	LEU	10.2
36	CJ	132	THR	10.2
33	CF	86	GLY	10.1
14	BN	49	GLN	10.1
42	CP	64	TYR	10.1
30	CD	26	VAL	10.1
19	BS	24	GLU	10.1
1	BA	1016	A	10.1
36	CJ	139	VAL	10.1
9	BI	130	ARG	10.1
7	BG	116	MET	10.0
19	BS	39	THR	10.0
23	C2	21	TYR	10.0
36	CJ	74	PRO	10.0
36	CJ	130	GLU	9.9
13	BM	32	ALA	9.9
36	CJ	53	LEU	9.9
7	BG	62	PHE	9.9
7	BG	42	ILE	9.9
31	CA	2110	G	9.9
23	C2	47	VAL	9.9
54	DA	2124	G	9.9
36	CJ	129	ILE	9.8
7	BG	4	ARG	9.8
52	CZ	31	GLN	9.8
34	CG	105	LEU	9.8

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Mol	Chain	Res	Type	RSRZ
54	DA	2118	U	9.8
24	C3	1	MET	9.8
36	CJ	67	PHE	9.8
19	BS	66	MET	9.7
54	DA	2125	G	9.7
13	BM	55	THR	9.7
36	DJ	133	ALA	9.7
1	AA	86	G	9.7
23	C2	24	THR	9.7
45	CS	63	VAL	9.6
33	CF	144	ASP	9.6
34	CG	103	ILE	9.6
33	CF	153	ASP	9.6
48	CV	87	PHE	9.6
3	BC	193	TYR	9.5
36	DJ	24	VAL	9.5
1	BA	1032	G	9.5
49	CW	94	ALA	9.5
31	CA	1065	U	9.5
54	DA	2174	C	9.4
32	CE	128	ALA	9.4
36	CJ	120	ALA	9.4
19	BS	63	THR	9.4
19	BS	37	ARG	9.3
33	CF	151	GLY	9.3
13	BM	46	SER	9.3
34	CG	52	PHE	9.3
1	BA	1026	G	9.3
13	BM	19	LEU	9.3
48	CV	31	SER	9.3
10	BJ	41	PRO	9.2
14	BN	36	ALA	9.2
31	CA	1095	A	9.2
36	DJ	22	PRO	9.2
13	BM	33	ILE	9.2
32	CE	119	ILE	9.2
13	BM	56	LEU	9.2
34	CG	33	LEU	9.2
33	CF	147	ASP	9.2
36	CJ	77	ALA	9.2
45	CS	32	THR	9.1
13	BM	39	ILE	9.1

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Mol	Chain	Res	Type	RSRZ
14	BN	27	LEU	9.1
19	BS	31	LEU	9.1
36	CJ	94	ASN	9.1
13	BM	48	LEU	9.1
36	CJ	24	VAL	9.1
10	BJ	22	THR	9.0
1	BA	1024	G	9.0
19	BS	32	ARG	9.0
52	CZ	15	ASN	9.0
36	DJ	131	GLY	9.0
36	CJ	89	GLY	8.9
19	BS	49	ILE	8.9
7	AG	4	ARG	8.9
24	C3	35	ARG	8.9
10	BJ	42	LEU	8.9
24	C3	42	LEU	8.9
9	BI	39	PHE	8.9
2	BB	135	LEU	8.9
7	BG	106	GLU	8.9
50	CX	53	CYS	8.9
36	CJ	96	ASP	8.9
36	CJ	78	VAL	8.8
13	BM	30	SER	8.8
52	CZ	40	SER	8.8
10	BJ	98	VAL	8.8
14	BN	43	ASN	8.8
45	CS	103	ALA	8.8
13	BM	94	GLY	8.8
10	BJ	6	ILE	8.8
36	DJ	84	ALA	8.8
31	CA	75	G	8.8
36	CJ	43	ASN	8.8
13	BM	96	PRO	8.7
31	CA	2402	U	8.7
33	CF	113	ASP	8.7
36	DJ	59	ILE	8.7
36	DJ	134	ARG	8.7
9	BI	17	ALA	8.7
47	CU	55	VAL	8.7
36	CJ	122	ILE	8.7
36	DJ	85	GLY	8.7
14	BN	54	ASP	8.7

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Mol	Chain	Res	Type	RSRZ
48	CV	88	GLU	8.7
52	CZ	42	LEU	8.7
34	CG	157	TYR	8.7
45	CS	35	PHE	8.6
48	CV	26	LYS	8.6
13	BM	29	ARG	8.6
9	BI	38	TYR	8.6
10	BJ	75	ASP	8.6
2	BB	34	ALA	8.6
19	BS	13	LEU	8.6
31	CA	2126	A	8.6
12	AL	124	ALA	8.6
47	CU	60	THR	8.6
32	CE	33	VAL	8.6
54	DA	1172	C	8.6
33	CF	105	THR	8.6
1	BA	942	G	8.6
9	BI	68	LYS	8.6
14	BN	52	PRO	8.6
14	BN	22	ALA	8.6
33	CF	65	PRO	8.5
36	CJ	90	SER	8.5
20	BT	3	ASN	8.5
47	CU	75	GLY	8.5
14	BN	35	ASN	8.5
47	CU	57	VAL	8.5
13	BM	105	ASN	8.5
13	BM	63	PHE	8.5
18	BR	20	GLU	8.5
48	CV	79	LYS	8.5
45	CS	49	ILE	8.5
1	BA	1222	G	8.5
31	CA	2125	G	8.5
26	C5	38	GLY	8.4
39	CM	82	LEU	8.4
7	BG	133	THR	8.4
1	BA	1017	U	8.4
36	CJ	86	ILE	8.4
36	DJ	36	MET	8.4
52	CZ	41	HIS	8.4
23	C2	45	GLN	8.3
39	CM	79	LEU	8.3

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Mol	Chain	Res	Type	RSRZ
34	CG	26	ILE	8.3
9	BI	4	ASN	8.3
36	DJ	66	SER	8.3
1	BA	1307	U	8.3
14	BN	31	ILE	8.3
33	CF	165	GLU	8.2
9	BI	5	GLN	8.2
42	CP	103	VAL	8.2
22	C1	5	GLN	8.2
53	DI	130	PRO	8.2
33	CF	97	TRP	8.2
42	CP	29	HIS	8.2
36	CJ	45	LYS	8.2
36	CJ	84	ALA	8.2
7	BG	49	THR	8.2
33	CF	173	PHE	8.2
54	DA	2127	G	8.2
31	CA	1094	U	8.2
22	C1	3	VAL	8.2
50	CX	56	ASP	8.2
36	CJ	31	GLN	8.2
43	CQ	115	ASN	8.1
33	CF	131	GLY	8.1
7	BG	52	GLN	8.1
24	C3	33	ARG	8.1
39	CM	10	GLU	8.1
39	CM	85	VAL	8.1
21	AU	2	PRO	8.1
13	BM	31	LYS	8.1
48	DV	56	GLY	8.1
34	CG	57	GLY	8.0
30	CD	8	LYS	8.0
10	BJ	72	ARG	8.0
19	BS	11	ILE	8.0
31	CA	613	A	8.0
19	BS	60	VAL	8.0
42	CP	40	ILE	8.0
1	BA	1028	C	8.0
33	CF	152	LEU	8.0
13	BM	40	ALA	8.0
1	BA	1218	C	8.0
14	BN	21	PHE	8.0

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Mol	Chain	Res	Type	RSRZ
1	BA	1020	G	8.0
36	CJ	50	GLU	8.0
14	BN	47	LYS	8.0
48	CV	12	ILE	8.0
1	BA	204	G	7.9
1	BA	958	A	7.9
10	BJ	38	GLY	7.9
13	BM	4	ILE	7.9
50	CX	33	ALA	7.9
22	C1	2	ALA	7.9
1	BA	1243	C	7.9
14	BN	4	GLN	7.9
32	CE	104	ALA	7.9
48	CV	25	VAL	7.9
33	CF	176	PRO	7.9
9	AI	21	ILE	7.9
10	BJ	7	ARG	7.8
10	BJ	90	LEU	7.8
36	CJ	88	SER	7.8
19	BS	41	PHE	7.8
2	BB	67	ILE	7.8
50	CX	63	ALA	7.8
33	CF	143	TYR	7.8
31	CA	1211	C	7.8
39	CM	7	SER	7.8
36	CJ	46	THR	7.8
36	DJ	69	PHE	7.8
1	BA	1296	C	7.8
13	BM	64	VAL	7.8
23	C2	36	LEU	7.8
36	CJ	123	GLU	7.8
48	CV	75	ALA	7.8
34	CG	2	SER	7.8
34	CG	171	THR	7.8
54	DA	2121	G	7.8
31	CA	1175	A	7.8
31	CA	1535	A	7.8
10	BJ	19	ASP	7.7
54	DA	138	U	7.7
16	BP	52	LEU	7.7
19	BS	52	HIS	7.7
31	CA	329	G	7.7

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Mol	Chain	Res	Type	RSRZ
42	CP	24	THR	7.7
14	BN	50	THR	7.7
33	CF	69	LYS	7.7
13	BM	103	LYS	7.7
23	C2	37	LYS	7.7
27	C0	56	LYS	7.7
1	BA	1025	U	7.6
48	CV	33	LYS	7.6
33	CF	31	VAL	7.6
10	BJ	80	THR	7.6
48	CV	50	PRO	7.6
36	CJ	58	VAL	7.6
1	BA	984	C	7.6
36	DJ	19	ASN	7.6
33	CF	110	ARG	7.6
32	CE	150	THR	7.6
31	CA	1069	A	7.6
1	BA	985	C	7.6
29	CC	239	ASN	7.6
48	CV	14	LEU	7.5
1	BA	1274	A	7.5
48	CV	51	ALA	7.5
33	CF	130	MET	7.5
13	BM	6	GLY	7.5
19	BS	76	PRO	7.5
13	BM	13	LYS	7.5
34	CG	172	LYS	7.5
10	BJ	102	LEU	7.5
7	BG	17	LYS	7.5
9	BI	58	VAL	7.5
1	AA	1031	C	7.5
32	CE	47	LYS	7.5
47	CU	87	LEU	7.5
39	CM	78	ARG	7.5
25	C4	61	CYS	7.5
33	CF	107	ALA	7.5
36	DJ	87	LYS	7.5
3	BC	192	THR	7.4
31	CA	1103	A	7.4
53	DI	121	SER	7.4
16	BP	17	TYR	7.4
53	DI	132	TYR	7.4

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Mol	Chain	Res	Type	RSRZ
36	DJ	98	VAL	7.4
7	BG	16	PRO	7.4
45	CS	59	ILE	7.4
13	BM	41	GLU	7.4
39	CM	102	GLY	7.4
1	AA	1032	G	7.4
34	CG	111	HIS	7.3
50	CX	26	PHE	7.3
36	CJ	27	ALA	7.3
42	CP	54	VAL	7.3
54	DA	2172	U	7.3
13	BM	93	ARG	7.3
54	DA	896	A	7.3
24	C3	36	ALA	7.3
40	CN	136	MET	7.3
52	CZ	29	ARG	7.3
1	AA	844	G	7.3
1	BA	1031	C	7.3
9	BI	66	THR	7.3
54	DA	2175	C	7.3
11	BK	47	ALA	7.3
32	CE	143	LEU	7.3
36	CJ	18	ALA	7.3
33	CF	83	TYR	7.2
26	C5	10	LEU	7.2
33	CF	132	VAL	7.2
36	DJ	89	GLY	7.2
7	BG	41	SER	7.2
36	CJ	44	ALA	7.2
33	CF	93	GLY	7.2
25	C4	28	ASN	7.2
48	CV	48	PRO	7.2
36	DJ	99	GLY	7.2
1	BA	208	U	7.2
32	CE	12	LEU	7.2
13	BM	24	GLY	7.2
16	AP	47	GLU	7.2
48	CV	43	LYS	7.2
36	CJ	113	LYS	7.2
45	CS	37	GLU	7.2
33	CF	39	GLY	7.2
54	DA	2116	G	7.2

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Mol	Chain	Res	Type	RSRZ
33	CF	75	ALA	7.2
36	CJ	136	MET	7.2
2	BB	82	ASP	7.2
13	BM	99	GLY	7.1
48	CV	29	LEU	7.1
10	BJ	100	ILE	7.1
31	CA	2174	C	7.1
42	CP	51	ALA	7.1
35	CH	132	PHE	7.1
34	CG	8	PRO	7.1
52	CZ	37	LEU	7.1
2	AB	123	ASP	7.1
19	BS	61	PHE	7.1
47	CU	72	GLN	7.1
13	BM	83	LEU	7.1
31	CA	2666	C	7.1
47	CU	15	HIS	7.1
19	BS	74	PHE	7.1
24	C3	37	LYS	7.1
1	BA	1221	G	7.1
43	CQ	84	ILE	7.1
34	CG	80	THR	7.1
53	DI	129	LEU	7.1
39	CM	8	PRO	7.1
30	CD	25	THR	7.1
13	BM	47	GLU	7.1
13	BM	86	TYR	7.1
10	BJ	95	GLY	7.1
7	BG	137	LYS	7.1
36	CJ	73	THR	7.1
36	CJ	79	LEU	7.0
31	CA	2163	A	7.0
46	CT	43	ALA	7.0
7	BG	111	ARG	7.0
10	BJ	91	ASP	7.0
1	BA	94	G	7.0
31	CA	549	G	7.0
2	BB	12	ALA	7.0
50	CX	60	PHE	7.0
14	BN	34	VAL	7.0
54	DA	1077	A	7.0
34	CG	102	VAL	7.0

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Mol	Chain	Res	Type	RSRZ
9	AI	20	PHE	7.0
48	CV	77	THR	7.0
52	CZ	33	ALA	7.0
23	C2	53	LYS	7.0
13	BM	80	LEU	7.0
31	CA	2127	G	7.0
19	BS	69	HIS	7.0
47	CU	47	VAL	7.0
47	CU	85	VAL	7.0
1	BA	1245	C	7.0
9	BI	71	GLY	7.0
33	CF	136	ILE	7.0
42	CP	62	LEU	7.0
39	CM	20	GLY	7.0
9	BI	32	GLN	6.9
14	BN	30	ILE	6.9
30	CD	10	GLY	6.9
24	C3	30	VAL	6.9
7	BG	5	ARG	6.9
1	BA	80	A	6.9
1	BA	213	G	6.9
33	CF	28	VAL	6.9
34	CG	174	ALA	6.9
19	BS	6	LYS	6.9
34	CG	148	LEU	6.9
13	BM	79	ARG	6.9
31	CA	331	C	6.9
10	BJ	10	LEU	6.9
52	CZ	49	ASP	6.9
10	BJ	35	GLN	6.9
1	BA	203	G	6.9
33	CF	121	SER	6.9
36	CJ	97	LYS	6.9
9	BI	125	PRO	6.9
13	BM	54	ASP	6.9
36	DJ	116	ASP	6.9
36	DJ	117	MET	6.9
1	BA	1271	A	6.9
35	DH	137	GLU	6.9
36	CJ	41	ALA	6.9
44	CR	118	ALA	6.9
31	CA	103	A	6.9

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Mol	Chain	Res	Type	RSRZ
51	CY	78	TYR	6.9
36	DJ	103	ARG	6.8
53	DI	134	GLU	6.8
39	CM	89	VAL	6.8
43	CQ	110	ILE	6.8
31	CA	355	U	6.8
31	CA	1049	C	6.8
33	CF	112	ARG	6.8
33	CF	135	GLN	6.8
14	AN	31	ILE	6.8
1	BA	1021	A	6.8
31	CA	1046	A	6.8
7	BG	75	VAL	6.8
13	BM	109	ARG	6.8
1	BA	1241	G	6.8
19	BS	21	LYS	6.8
50	CX	52	GLY	6.8
7	BG	151	PHE	6.8
14	BN	32	SER	6.8
32	CE	55	SER	6.8
23	C2	15	ALA	6.8
47	CU	59	ASN	6.8
10	BJ	25	ILE	6.8
14	BN	20	TYR	6.8
36	CJ	70	VAL	6.8
35	CH	11	ASN	6.8
9	AI	129	LYS	6.8
35	CH	74	ALA	6.8
45	CS	36	ALA	6.7
52	CZ	17	GLU	6.7
1	BA	989	U	6.7
33	CF	80	ARG	6.7
46	CT	84	ARG	6.7
31	CA	878	A	6.7
34	CG	45	HIS	6.7
41	CO	119	SER	6.7
23	C2	44	ARG	6.7
43	CQ	111	LYS	6.7
45	CS	28	ALA	6.7
1	BA	1022	A	6.7
31	CA	267	C	6.7
32	CE	164	LEU	6.7

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Mol	Chain	Res	Type	RSRZ
9	AI	19	VAL	6.7
14	BN	2	ALA	6.7
7	BG	15	ASP	6.7
1	BA	202	G	6.7
33	CF	60	ILE	6.7
16	BP	41	PRO	6.7
19	BS	30	PRO	6.7
30	CD	4	LEU	6.7
7	BG	54	SER	6.7
2	BB	187	VAL	6.7
13	BM	65	VAL	6.7
13	BM	85	CYS	6.6
17	BQ	70	THR	6.6
1	BA	959	A	6.6
13	BM	61	ALA	6.6
27	C0	2	ALA	6.6
32	CE	172	ALA	6.6
48	CV	81	ASP	6.6
43	CQ	12	GLN	6.6
52	CZ	47	ARG	6.6
1	BA	82	G	6.6
34	CG	169	VAL	6.6
32	CE	131	THR	6.6
33	CF	34	ILE	6.6
9	BI	41	ARG	6.6
33	CF	102	ARG	6.6
29	CC	233	GLY	6.6
1	BA	1219	A	6.6
48	CV	32	GLY	6.6
9	AI	88	MET	6.6
10	BJ	11	LYS	6.6
13	BM	77	ILE	6.6
16	BP	57	ILE	6.6
31	CA	1077	A	6.6
35	CH	136	SER	6.5
14	BN	45	VAL	6.5
45	CS	20	VAL	6.5
7	BG	129	GLU	6.5
13	BM	35	ALA	6.5
23	C2	49	TYR	6.5
23	C2	52	ALA	6.5
24	C3	32	ALA	6.5

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Mol	Chain	Res	Type	RSRZ
9	BI	129	LYS	6.5
14	BN	37	SER	6.5
34	CG	104	ASN	6.5
31	CA	318	C	6.5
1	BA	1275	A	6.5
48	CV	39	ILE	6.5
32	CE	127	GLU	6.5
36	DJ	33	VAL	6.5
36	CJ	81	LYS	6.5
7	BG	73	VAL	6.5
31	CA	1084	A	6.5
39	CM	120	VAL	6.5
54	DA	2176	A	6.5
50	CX	25	ARG	6.5
10	BJ	39	PRO	6.5
46	CT	82	MET	6.5
32	CE	140	ASP	6.5
36	DJ	97	LYS	6.5
7	BG	144	MET	6.5
7	BG	71	PRO	6.5
19	BS	71	LEU	6.5
31	CA	1064	C	6.5
35	CH	107	GLY	6.4
31	CA	1536	C	6.4
7	BG	65	ALA	6.4
1	BA	844	G	6.4
31	CA	877	A	6.4
35	CH	72	ILE	6.4
33	CF	25	VAL	6.4
33	CF	23	ASN	6.4
12	BL	124	ALA	6.4
27	C0	43	ALA	6.4
10	AJ	35	GLN	6.4
10	BJ	99	GLN	6.4
33	CF	116	GLY	6.4
48	CV	35	ILE	6.4
36	DJ	106	LEU	6.4
54	DA	2132	U	6.4
7	BG	134	ALA	6.4
31	CA	183	C	6.4
43	CQ	91	ALA	6.4
3	BC	197	GLY	6.4

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Mol	Chain	Res	Type	RSRZ
9	BI	90	TYR	6.4
31	CA	2797	U	6.4
31	CA	1048	A	6.4
31	CA	1087	G	6.4
10	BJ	27	GLU	6.4
31	CA	356	G	6.4
1	BA	1314	C	6.4
13	BM	25	VAL	6.4
33	CF	95	ARG	6.4
48	CV	42	VAL	6.4
31	CA	931	U	6.4
36	DJ	95	LYS	6.4
9	BI	14	SER	6.4
30	CD	97	SER	6.4
14	BN	28	LYS	6.4
47	CU	37	ASP	6.4
31	CA	1202	G	6.4
45	CS	58	VAL	6.4
22	C1	35	GLY	6.4
7	BG	48	GLU	6.4
2	BB	37	LYS	6.3
25	C4	43	HIS	6.3
2	BB	131	LYS	6.3
31	CA	1238	G	6.3
31	CA	1407	G	6.3
47	CU	83	ALA	6.3
44	CR	106	PHE	6.3
36	CJ	52	GLY	6.3
54	DA	2109	U	6.3
31	CA	892	A	6.3
32	CE	142	ALA	6.3
31	CA	289	G	6.3
8	BH	2	SER	6.3
50	CX	34	GLY	6.3
31	CA	12	U	6.3
36	DJ	68	THR	6.3
33	CF	175	PHE	6.3
34	CG	167	GLU	6.3
42	CP	38	GLN	6.3
42	CP	104	GLN	6.3
37	CK	97	PRO	6.3
13	BM	62	LYS	6.3

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Mol	Chain	Res	Type	RSRZ
23	C2	43	VAL	6.3
31	CA	2128	G	6.3
10	BJ	21	ALA	6.3
14	BN	53	ARG	6.3
32	CE	11	ALA	6.3
42	CP	30	ARG	6.3
1	AA	87	C	6.3
13	AM	33	ILE	6.3
31	CA	1075	C	6.3
41	CO	28	LEU	6.3
31	CA	1086	A	6.3
10	BJ	37	ARG	6.3
13	AM	30	SER	6.2
32	CE	138	LEU	6.2
9	BI	43	THR	6.2
36	CJ	30	GLN	6.2
32	CE	24	ASN	6.2
54	DA	2141	G	6.2
32	CE	124	PHE	6.2
9	AI	17	ALA	6.2
54	DA	2126	A	6.2
9	BI	37	GLN	6.2
30	CD	74	GLU	6.2
41	CO	120	GLU	6.2
54	DA	2147	A	6.2
7	BG	39	ALA	6.2
34	CG	30	ASN	6.2
48	CV	52	LEU	6.2
3	BC	71	ALA	6.2
45	CS	61	ALA	6.2
31	CA	1093	G	6.2
47	CU	10	VAL	6.2
9	BI	18	ARG	6.2
26	C5	32	LYS	6.2
32	CE	8	ALA	6.2
42	CP	32	PRO	6.2
44	CR	29	SER	6.2
25	C4	41	LYS	6.2
1	BA	85	U	6.2
31	CA	846	U	6.2
53	DI	136	ILE	6.2
49	CW	27	PRO	6.1

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Mol	Chain	Res	Type	RSRZ
8	AH	2	SER	6.1
54	DA	2123	G	6.1
31	CA	896	A	6.1
45	CS	22	LEU	6.1
53	DI	104	ALA	6.1
3	BC	79	LYS	6.1
10	BJ	89	ARG	6.1
34	CG	175	LYS	6.1
31	CA	101	A	6.1
33	CF	67	ILE	6.1
49	CW	29	ILE	6.1
45	CS	31	GLU	6.1
1	BA	1321	U	6.1
31	CA	546	U	6.1
31	CA	1870	C	6.1
23	C2	18	GLY	6.1
13	BM	9	ILE	6.1
10	BJ	9	ARG	6.1
36	CJ	29	GLY	6.1
14	BN	24	ARG	6.1
31	CA	885	C	6.1
1	BA	987	G	6.1
13	BM	17	ILE	6.1
36	DJ	11	LEU	6.1
13	BM	28	THR	6.1
31	CA	1083	U	6.1
1	BA	1305	G	6.1
31	CA	180	G	6.1
48	CV	98	SER	6.1
54	DA	2115	G	6.1
47	CU	58	VAL	6.1
9	BI	122	ARG	6.1
53	DI	38	MET	6.1
1	BA	1050	G	6.1
10	BJ	82	LYS	6.0
1	BA	1049	U	6.0
7	BG	66	LEU	6.0
20	BT	46	ALA	6.0
31	CA	1105	U	6.0
2	BB	32	PHE	6.0
36	CJ	32	GLY	6.0
31	CA	548	G	6.0

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Mol	Chain	Res	Type	RSRZ
35	DH	63	ALA	6.0
34	CG	86	LYS	6.0
32	CE	23	PHE	6.0
36	DJ	21	SER	6.0
14	BN	16	LEU	6.0
14	BN	46	LEU	6.0
48	CV	95	PHE	6.0
41	CO	63	ARG	6.0
36	DJ	100	LYS	6.0
36	CJ	135	SER	6.0
42	CP	107	ALA	6.0
10	AJ	74	VAL	6.0
32	CE	193	VAL	6.0
31	CA	228	C	6.0
31	CA	1872	A	6.0
33	CF	32	GLU	6.0
34	CG	82	GLY	6.0
2	AB	135	LEU	6.0
30	CD	201	LEU	6.0
52	CZ	14	LEU	6.0
2	BB	40	ILE	6.0
22	C1	57	LYS	6.0
31	CA	74	A	6.0
31	CA	330	A	6.0
13	BM	104	THR	6.0
1	BA	210	C	6.0
13	BM	11	ASP	6.0
36	DJ	27	ALA	6.0
47	CU	8	LEU	6.0
31	CA	1547	C	5.9
48	CV	3	ALA	5.9
48	CV	76	ALA	5.9
49	CW	57	TYR	5.9
19	BS	28	LYS	5.9
34	CG	27	LYS	5.9
43	CQ	9	GLU	5.9
1	BA	79	G	5.9
32	CE	88	ARG	5.9
10	BJ	71	LEU	5.9
20	BT	79	LEU	5.9
16	BP	20	VAL	5.9
3	BC	43	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
7	BG	112	GLY	5.9
42	CP	117	PHE	5.9
2	AB	42	ASN	5.9
19	BS	72	GLY	5.9
31	CA	2108	A	5.9
2	AB	136	MET	5.9
13	BM	58	ASP	5.9
34	CG	83	PHE	5.9
31	CA	1107	G	5.9
34	CG	17	VAL	5.9
19	BS	68	GLY	5.9
33	CF	92	ARG	5.9
7	BG	132	GLY	5.9
50	CX	59	LEU	5.9
2	BB	201	PRO	5.9
48	CV	6	ARG	5.9
22	C1	6	ASN	5.9
31	CA	1076	C	5.8
38	CL	110	GLU	5.8
31	CA	1174	U	5.8
42	CP	99	TYR	5.8
50	CX	57	HIS	5.8
36	DJ	127	ARG	5.8
14	AN	23	LYS	5.8
42	CP	65	THR	5.8
35	DH	66	ASN	5.8
28	CB	24	G	5.8
11	AK	82	LEU	5.8
31	CA	268	C	5.8
31	CA	1213	A	5.8
54	DA	1067	A	5.8
44	CR	37	GLN	5.8
16	BP	60	TRP	5.8
35	CH	140	ALA	5.8
39	CM	77	ILE	5.8
54	DA	2146	C	5.8
9	BI	124	ARG	5.8
31	CA	2168	G	5.8
9	BI	81	HIS	5.8
10	BJ	94	ALA	5.8
13	BM	36	ALA	5.8
19	BS	80	TYR	5.8

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Mol	Chain	Res	Type	RSRZ
14	BN	61	ARG	5.8
35	CH	110	VAL	5.8
36	CJ	95	LYS	5.8
45	CS	14	VAL	5.8
32	CE	89	PRO	5.8
42	CP	106	LEU	5.8
31	CA	2665	A	5.8
10	BJ	12	ALA	5.8
3	BC	156	ARG	5.8
3	BC	195	VAL	5.8
31	CA	2118	U	5.8
31	CA	2891	U	5.8
32	CE	28	VAL	5.8
13	BM	81	MET	5.7
34	CG	108	GLY	5.7
36	CJ	34	ASN	5.7
24	C3	18	PHE	5.7
7	BG	45	SER	5.7
42	CP	61	GLN	5.7
7	BG	69	VAL	5.7
1	BA	1244	G	5.7
1	BA	948	C	5.7
10	BJ	33	GLY	5.7
36	DJ	132	THR	5.7
45	CS	54	VAL	5.7
13	BM	34	LEU	5.7
42	CP	115	LEU	5.7
2	AB	6	MET	5.7
53	DI	124	ASP	5.7
31	CA	1047	G	5.7
33	CF	126	GLY	5.7
36	CJ	133	ALA	5.7
42	CP	67	ASN	5.7
36	DJ	92	LYS	5.7
42	CP	66	GLY	5.7
34	CG	54	PRO	5.7
34	CG	121	ILE	5.7
7	BG	109	ARG	5.7
50	CX	83	GLU	5.7
52	CZ	24	GLU	5.7
54	DA	2165	C	5.7
2	AB	14	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
25	C4	64	TYR	5.7
31	CA	1215	G	5.7
33	CF	41	GLY	5.7
2	BB	35	ARG	5.7
31	CA	2161	C	5.7
48	CV	21	LYS	5.7
14	BN	9	ARG	5.7
31	CA	2802	G	5.7
36	DJ	93	PRO	5.7
49	CW	6	ALA	5.6
33	CF	12	VAL	5.6
47	CU	16	VAL	5.6
19	BS	3	ARG	5.6
36	DJ	15	ALA	5.6
9	BI	48	VAL	5.6
31	CA	2119	A	5.6
32	CE	54	GLY	5.6
47	CU	71	GLY	5.6
53	DI	84	TYR	5.6
10	BJ	92	LEU	5.6
3	BC	196	ILE	5.6
10	AJ	6	ILE	5.6
23	C2	23	THR	5.6
24	C3	34	ARG	5.6
52	CZ	22	LEU	5.6
45	CS	88	GLY	5.6
1	BA	81	A	5.6
42	CP	41	ALA	5.6
1	BA	1240	U	5.6
22	C1	55	ILE	5.6
31	CA	81	G	5.6
45	CS	55	ASP	5.6
33	CF	141	ILE	5.6
31	CA	214	G	5.6
22	C1	27	SER	5.6
35	DH	87	GLU	5.6
49	CW	67	GLY	5.6
9	BI	64	TYR	5.6
10	BJ	81	GLU	5.6
35	DH	70	GLU	5.6
52	CZ	59	GLU	5.6
33	CF	26	MET	5.6

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Mol	Chain	Res	Type	RSRZ
31	CA	2693	G	5.6
7	BG	46	ALA	5.5
20	BT	47	ALA	5.5
13	AM	43	VAL	5.5
47	CU	24	MET	5.5
13	BM	51	GLY	5.5
17	BQ	21	ILE	5.5
37	CK	93	ILE	5.5
42	CP	87	ILE	5.5
10	BJ	34	ALA	5.5
34	CG	31	GLY	5.5
1	BA	1029	U	5.5
48	CV	5	ILE	5.5
36	DJ	38	PHE	5.5
50	CX	61	ALA	5.5
54	DA	2167	U	5.5
31	CA	312	G	5.5
31	CA	2116	G	5.5
23	C2	31	PRO	5.5
26	C5	1	MET	5.5
34	CG	151	TYR	5.5
14	BN	10	GLU	5.5
1	BA	1217	C	5.5
34	CG	106	SER	5.5
42	CP	52	SER	5.5
54	DA	1065	U	5.5
36	CJ	119	GLY	5.5
47	CU	42	GLU	5.5
3	BC	126	ARG	5.5
16	BP	42	ILE	5.5
46	CT	94	ASP	5.5
33	CF	43	ALA	5.5
50	CX	68	LYS	5.5
34	CG	92	VAL	5.5
34	CG	112	PRO	5.5
47	CU	61	LEU	5.5
50	CX	38	VAL	5.5
1	BA	207	C	5.5
3	BC	103	ILE	5.5
17	BQ	63	GLU	5.5
32	CE	183	PHE	5.5
48	CV	28	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
13	BM	3	ARG	5.5
13	BM	70	ARG	5.5
36	CJ	125	MET	5.5
36	DJ	17	MET	5.5
17	BQ	50	ASN	5.5
50	CX	62	LYS	5.5
13	BM	67	GLY	5.5
36	DJ	77	ALA	5.5
44	CR	90	ILE	5.5
1	BA	1276	G	5.5
19	BS	27	ASP	5.5
33	CF	99	PHE	5.5
7	BG	150	ALA	5.4
31	CA	895	U	5.4
31	CA	2170	A	5.4
17	BQ	78	VAL	5.4
31	CA	1106	G	5.4
1	BA	1247	U	5.4
7	BG	53	ARG	5.4
29	CC	234	GLY	5.4
44	CR	73	GLY	5.4
16	BP	16	PHE	5.4
34	CG	7	ALA	5.4
25	C4	2	PRO	5.4
29	CC	241	GLY	5.4
1	BA	1004	A	5.4
42	CP	33	ARG	5.4
9	BI	117	GLY	5.4
19	BS	77	THR	5.4
34	CG	25	THR	5.4
54	DA	2166	U	5.4
13	BM	74	SER	5.4
36	CJ	124	ALA	5.4
41	CO	118	ARG	5.4
44	CR	33	ARG	5.4
44	CR	26	GLY	5.4
15	BO	89	ARG	5.4
49	CW	1	MET	5.4
48	CV	60	GLU	5.4
20	BT	72	ALA	5.4
31	CA	85	G	5.4
31	CA	1444	G	5.4

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Mol	Chain	Res	Type	RSRZ
27	C0	7	ILE	5.4
31	CA	501	A	5.4
39	CM	142	ILE	5.4
31	CA	1061	U	5.4
39	CM	115	GLU	5.4
36	DJ	43	ASN	5.4
19	BS	75	ALA	5.4
46	CT	97	LEU	5.4
9	AI	55	VAL	5.4
50	CX	23	VAL	5.4
11	AK	19	GLY	5.4
50	CX	42	GLY	5.4
9	BI	21	ILE	5.4
24	C3	43	THR	5.4
34	CG	56	ASP	5.4
7	BG	91	VAL	5.3
14	BN	55	SER	5.3
17	BQ	17	MET	5.3
45	CS	101	ILE	5.3
54	DA	2178	C	5.3
32	CE	147	LEU	5.3
33	CF	55	ALA	5.3
31	CA	88	G	5.3
3	BC	198	VAL	5.3
7	BG	103	TRP	5.3
34	CG	81	GLU	5.3
49	CW	89	ILE	5.3
9	AI	90	TYR	5.3
39	CM	28	GLY	5.3
52	CZ	44	LYS	5.3
33	CF	36	LEU	5.3
42	CP	108	ASP	5.3
33	CF	74	VAL	5.3
1	BA	1027	C	5.3
36	CJ	19	ASN	5.3
31	CA	2123	G	5.3
32	CE	43	THR	5.3
2	AB	49	MET	5.3
48	CV	49	VAL	5.3
41	CO	24	MET	5.3
9	BI	7	TYR	5.3
31	CA	316	C	5.3

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Mol	Chain	Res	Type	RSRZ
47	CU	1	MET	5.3
47	DU	1	MET	5.3
50	CX	55	ARG	5.3
1	BA	1270	G	5.3
31	CA	308	G	5.3
47	CU	56	GLU	5.3
31	CA	1085	A	5.3
20	BT	36	TYR	5.3
9	BI	11	ARG	5.3
13	BM	98	ARG	5.3
14	BN	40	ASP	5.3
31	CA	1078	U	5.3
34	CG	166	ASP	5.3
9	BI	30	ILE	5.2
33	CF	68	THR	5.2
50	CX	32	LEU	5.2
32	CE	37	ALA	5.2
41	CO	29	VAL	5.2
1	AA	81	A	5.2
36	DJ	40	LYS	5.2
24	C3	7	PRO	5.2
13	BM	60	VAL	5.2
42	CP	25	ARG	5.2
42	CP	105	ALA	5.2
33	CF	114	PHE	5.2
34	CG	44	LYS	5.2
1	BA	1018	G	5.2
31	CA	2120	G	5.2
46	CT	98	LYS	5.2
39	CM	107	PHE	5.2
16	BP	9	HIS	5.2
9	AI	5	GLN	5.2
37	CK	136	GLN	5.2
34	CG	161	GLY	5.2
10	BJ	86	ALA	5.2
19	AS	49	ILE	5.2
2	BB	33	GLY	5.2
52	CZ	35	GLY	5.2
31	CA	1045	C	5.2
53	DI	135	ALA	5.2
7	BG	82	GLY	5.2
41	CO	62	ASN	5.2

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Mol	Chain	Res	Type	RSRZ
13	BM	66	GLU	5.2
2	BB	14	VAL	5.2
29	CC	30	PHE	5.2
40	CN	72	PRO	5.2
31	CA	1044	C	5.2
32	CE	90	GLN	5.2
32	CE	118	LEU	5.2
42	CP	26	LEU	5.2
1	BA	982	U	5.2
14	BN	18	ASP	5.2
36	DJ	81	LYS	5.2
54	DA	884	U	5.2
13	BM	90	ARG	5.2
31	CA	44	A	5.2
34	CG	51	THR	5.2
10	BJ	40	ILE	5.2
31	CA	2162	G	5.2
51	CY	35	SER	5.2
9	BI	92	GLU	5.2
36	CJ	92	LYS	5.2
49	CW	34	LYS	5.2
1	AA	85	U	5.2
15	AO	17	ARG	5.2
33	CF	77	PHE	5.2
36	DJ	14	ALA	5.2
42	CP	59	ALA	5.2
7	BG	38	THR	5.1
33	CF	137	ILE	5.1
37	CK	142	ILE	5.1
30	CD	186	LEU	5.1
34	CG	117	LEU	5.1
40	CN	41	LEU	5.1
31	CA	1873	G	5.1
31	CA	2803	G	5.1
30	CD	1	MET	5.1
31	CA	1406	U	5.1
37	CK	22	GLY	5.1
44	CR	98	ILE	5.1
31	CA	1104	C	5.1
17	BQ	73	TRP	5.1
31	CA	879	G	5.1
31	CA	2305	U	5.1

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Mol	Chain	Res	Type	RSRZ
37	CK	119	PHE	5.1
36	CJ	101	ILE	5.1
30	CD	43	ASP	5.1
1	AA	1026	G	5.1
25	C4	40	ARG	5.1
28	CB	37	C	5.1
9	AI	6	TYR	5.1
31	CA	2173	A	5.1
7	BG	148	ASN	5.1
13	BM	50	GLU	5.1
51	CY	3	ARG	5.1
31	CA	476	G	5.1
43	DQ	2	SER	5.1
39	CM	45	GLY	5.1
52	CZ	36	GLN	5.1
1	BA	1034	G	5.1
1	BA	90	C	5.1
7	AG	53	ARG	5.1
9	AI	128	SER	5.1
20	BT	60	ARG	5.1
34	CG	58	TYR	5.1
42	CP	109	ALA	5.1
13	AM	115	PRO	5.1
54	DA	1847	A	5.1
13	AM	48	LEU	5.1
13	BM	69	LEU	5.1
14	BN	41	ARG	5.1
29	CC	48	ARG	5.1
1	BA	1304	G	5.1
31	CA	45	G	5.1
34	CG	75	MET	5.1
20	BT	64	LYS	5.1
31	CA	344	A	5.1
23	C2	39	PHE	5.1
44	CR	6	ARG	5.1
13	BM	43	VAL	5.1
33	CF	149	VAL	5.1
31	CA	2300	C	5.1
31	CA	626	A	5.0
39	CM	84	LYS	5.0
10	BJ	23	ALA	5.0
2	BB	213	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
39	CM	117	THR	5.0
13	AM	56	LEU	5.0
14	BN	51	LEU	5.0
31	CA	2107	G	5.0
31	CA	2121	G	5.0
44	CR	30	ARG	5.0
47	CU	36	LYS	5.0
7	BG	141	VAL	5.0
33	CF	56	ASP	5.0
36	DJ	83	ALA	5.0
10	AJ	76	ILE	5.0
46	CT	101	SER	5.0
1	BA	1303	C	5.0
1	BA	1019	A	5.0
19	BS	34	TRP	5.0
42	CP	49	VAL	5.0
36	CJ	35	ILE	5.0
33	CF	122	PHE	5.0
1	BA	1201	A	5.0
6	AF	61	LEU	5.0
13	AM	19	LEU	5.0
24	C3	27	GLY	5.0
20	BT	76	LYS	5.0
35	CH	130	VAL	5.0
34	CG	63	ALA	5.0
47	CU	46	ALA	5.0
13	BM	75	MET	5.0
1	BA	78	A	5.0
34	CG	24	ILE	5.0
7	AG	50	LEU	5.0
39	CM	3	LEU	5.0
52	CZ	6	LEU	5.0
32	CE	64	GLY	5.0
41	CO	116	VAL	5.0
45	CS	38	VAL	5.0
33	CF	91	LEU	5.0
33	CF	170	LEU	5.0
7	BG	18	PHE	5.0
13	BM	21	SER	5.0
31	CA	2171	A	5.0
10	BJ	93	ALA	5.0
33	DF	80	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
7	BG	58	GLU	5.0
7	BG	9	GLN	5.0
13	BM	84	GLY	4.9
9	BI	91	ASP	4.9
33	CF	172	ALA	4.9
31	CA	1100	C	4.9
31	CA	2667	C	4.9
36	DJ	42	PHE	4.9
19	BS	43	ASN	4.9
32	CE	4	VAL	4.9
31	CA	309	A	4.9
1	BA	63	C	4.9
33	CF	37	ASN	4.9
42	CP	69	ASP	4.9
19	BS	10	PHE	4.9
14	BN	42	TRP	4.9
32	CE	122	GLU	4.9
40	CN	79	ALA	4.9
17	BQ	53	CYS	4.9
31	CA	1169	A	4.9
30	CD	132	ALA	4.9
47	CU	21	SER	4.9
36	CJ	25	GLY	4.9
2	BB	21	ARG	4.9
19	BS	55	ARG	4.9
20	BT	24	ARG	4.9
31	CA	2169	A	4.9
3	BC	206	GLU	4.9
1	BA	68	G	4.9
1	BA	954	G	4.9
9	BI	20	PHE	4.9
31	CA	280	U	4.9
27	C0	8	THR	4.9
30	CD	154	LYS	4.9
13	BM	14	HIS	4.9
34	CG	9	VAL	4.9
35	CH	108	VAL	4.9
33	CF	71	ARG	4.9
36	CJ	116	ASP	4.9
16	AP	4	ILE	4.9
31	CA	1534	U	4.9
48	CV	30	SER	4.9

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Mol	Chain	Res	Type	RSRZ
2	AB	9	MET	4.9
7	BG	87	VAL	4.9
31	CA	876	C	4.9
34	CG	162	VAL	4.9
31	CA	2860	A	4.9
34	CG	78	GLY	4.9
32	CE	157	LEU	4.9
39	CM	70	LYS	4.9
10	BJ	96	VAL	4.8
47	CU	34	VAL	4.8
27	C0	34	HIS	4.8
36	CJ	100	LYS	4.8
10	BJ	24	GLU	4.8
1	BA	1253	G	4.8
7	BG	79	ARG	4.8
13	BM	108	THR	4.8
20	BT	38	ALA	4.8
41	CO	79	LEU	4.8
14	BN	39	GLU	4.8
44	CR	74	ILE	4.8
27	C0	9	GLN	4.8
2	AB	46	THR	4.8
3	BC	155	GLY	4.8
31	CA	2124	G	4.8
35	CH	77	THR	4.8
39	CM	138	ALA	4.8
18	AR	23	TYR	4.8
51	CY	49	LEU	4.8
25	C4	35	LYS	4.8
48	CV	83	VAL	4.8
2	BB	123	ASP	4.8
13	BM	68	ASP	4.8
3	BC	107	ARG	4.8
16	BP	80	LYS	4.8
30	CD	38	LYS	4.8
31	CA	475	C	4.8
26	C5	25	VAL	4.8
30	CD	9	VAL	4.8
10	AJ	73	LEU	4.8
33	CF	174	ASP	4.8
39	CM	108	ALA	4.8
22	C1	15	MET	4.8

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Mol	Chain	Res	Type	RSRZ
32	CE	10	SER	4.8
2	AB	37	LYS	4.8
3	BC	106	VAL	4.8
22	C1	36	GLU	4.8
6	BF	39	LEU	4.8
35	CH	15	LEU	4.8
35	DH	56	ALA	4.8
23	C2	29	THR	4.8
51	CY	34	HIS	4.8
38	CL	111	LYS	4.8
54	DA	1062	G	4.8
14	BN	68	GLY	4.8
36	CJ	91	GLY	4.8
27	C0	53	PHE	4.8
39	CM	113	ALA	4.8
38	CL	48	PRO	4.8
1	BA	4	U	4.8
2	BB	39	HIS	4.8
39	CM	35	HIS	4.8
13	AM	44	LYS	4.8
22	C1	18	SER	4.8
32	CE	186	VAL	4.8
34	CG	10	VAL	4.8
46	CT	47	VAL	4.8
53	DI	27	VAL	4.8
7	AG	7	ILE	4.8
33	CF	158	THR	4.8
36	CJ	16	GLY	4.7
9	AI	104	VAL	4.7
16	BP	53	ASP	4.7
19	BS	22	ALA	4.7
30	CD	56	LYS	4.7
53	DI	72	LEU	4.7
33	CF	111	ILE	4.7
45	CS	98	ILE	4.7
31	CA	369	U	4.7
42	CP	46	GLU	4.7
1	BA	325	A	4.7
31	CA	893	C	4.7
31	CA	1167	C	4.7
34	CG	6	LYS	4.7
20	BT	63	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
37	CK	55	ILE	4.7
34	CG	132	VAL	4.7
14	BN	48	LEU	4.7
31	CA	882	G	4.7
3	BC	91	VAL	4.7
23	C2	12	VAL	4.7
3	BC	159	GLY	4.7
1	BA	1033	G	4.7
2	BB	80	VAL	4.7
36	DJ	73	THR	4.7
43	CQ	27	GLU	4.7
45	CS	62	GLU	4.7
31	CA	1214	A	4.7
35	DH	67	ALA	4.7
36	CJ	26	PRO	4.7
46	CT	99	ARG	4.7
20	BT	34	LYS	4.7
34	CG	160	LYS	4.7
44	DR	118	ALA	4.7
53	DI	133	GLU	4.7
9	AI	22	LYS	4.7
33	CF	177	PHE	4.7
45	CS	33	VAL	4.7
53	DI	106	PHE	4.7
35	DH	105	ALA	4.7
36	DJ	110	ALA	4.7
45	CS	26	ASP	4.7
31	CA	117	G	4.7
31	CA	1074	G	4.7
36	DJ	113	LYS	4.7
7	BG	47	LEU	4.7
35	DH	77	THR	4.7
30	CD	6	GLY	4.7
36	CJ	131	GLY	4.7
42	CP	20	GLU	4.7
31	CA	213	A	4.7
7	AG	6	VAL	4.6
36	CJ	15	ALA	4.6
48	CV	63	ALA	4.6
35	DH	86	ASP	4.6
3	BC	119	SER	4.6
33	CF	38	MET	4.6

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Mol	Chain	Res	Type	RSRZ
45	CS	25	LEU	4.6
7	AG	5	ARG	4.6
9	BI	123	ARG	4.6
22	C1	21	ALA	4.6
29	CC	47	GLY	4.6
36	DJ	86	ILE	4.6
10	BJ	97	ASP	4.6
32	DE	7	ASP	4.6
39	CM	4	ASN	4.6
1	AA	88	U	4.6
19	BS	81	ARG	4.6
20	BT	85	LYS	4.6
25	C4	37	ALA	4.6
32	CE	36	ALA	4.6
13	BM	16	VAL	4.6
1	BA	962	C	4.6
3	BC	124	LEU	4.6
31	CA	1606	C	4.6
20	BT	45	ALA	4.6
30	CD	55	LYS	4.6
9	AI	127	PHE	4.6
39	CM	126	ARG	4.6
7	BG	37	SER	4.6
27	C0	29	LEU	4.6
45	CS	51	VAL	4.6
35	CH	109	GLU	4.6
49	CW	69	GLU	4.6
13	AM	5	ALA	4.6
35	DH	74	ALA	4.6
32	CE	7	ASP	4.6
1	BA	1441	A	4.6
31	CA	1090	A	4.6
30	CD	59	ARG	4.6
2	AB	221	VAL	4.6
32	CE	144	GLU	4.6
22	C1	11	SER	4.6
13	AM	39	ILE	4.6
13	BM	37	ALA	4.6
20	BT	73	ALA	4.6
31	CA	2150	C	4.6
31	CA	2164	C	4.6
10	BJ	85	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
54	DA	2117	A	4.6
31	CA	596	U	4.6
33	CF	42	GLU	4.6
43	CQ	3	ASN	4.6
31	CA	317	G	4.6
39	CM	90	VAL	4.6
41	CO	83	LEU	4.6
54	DA	1068	G	4.6
27	C0	48	ILE	4.6
30	CD	41	ALA	4.6
35	CH	143	ILE	4.6
47	CU	74	ILE	4.6
32	CE	154	ASP	4.6
36	CJ	64	ASP	4.6
7	BG	35	LYS	4.6
31	CA	345	A	4.6
36	CJ	118	THR	4.6
2	BB	164	ILE	4.6
7	AG	58	GLU	4.6
29	CC	245	VAL	4.5
33	CF	4	LEU	4.5
33	CF	133	ARG	4.5
34	CG	59	ALA	4.5
7	AG	62	PHE	4.5
31	CA	281	C	4.5
46	CT	6	LYS	4.5
10	BJ	36	VAL	4.5
13	BM	57	ARG	4.5
34	CG	69	ARG	4.5
14	AN	25	ALA	4.5
19	BS	40	ILE	4.5
36	DJ	51	LYS	4.5
16	BP	39	PHE	4.5
1	AA	1020	G	4.5
19	AS	56	GLN	4.5
20	BT	82	GLN	4.5
13	BM	38	GLY	4.5
24	C3	17	GLY	4.5
31	CA	1216	G	4.5
31	CA	2801	G	4.5
10	AJ	42	LEU	4.5
26	C5	2	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
43	CQ	95	ALA	4.5
9	AI	32	GLN	4.5
31	CA	1868	C	4.5
54	DA	1063	G	4.5
48	CV	62	GLU	4.5
50	CX	85	GLU	4.5
39	CM	74	THR	4.5
1	BA	1306	A	4.5
41	CO	84	GLY	4.5
1	BA	1023	U	4.5
31	CA	138	U	4.5
43	CQ	86	VAL	4.5
54	DA	885	C	4.5
33	CF	79	ILE	4.5
7	AG	109	ARG	4.5
9	BI	15	SER	4.5
1	BA	196	A	4.5
35	CH	58	LEU	4.5
36	CJ	93	PRO	4.5
43	CQ	31	TRP	4.5
45	CS	60	LYS	4.5
10	BJ	28	THR	4.5
31	CA	2106	U	4.5
31	CA	2180	U	4.5
1	BA	949	A	4.5
2	BB	84	ALA	4.5
14	BN	23	LYS	4.5
46	CT	5	ALA	4.5
34	CG	127	THR	4.5
34	CG	76	VAL	4.5
42	CP	78	VAL	4.5
32	CE	132	LYS	4.5
54	DA	1064	C	4.5
30	CD	126	ASN	4.5
35	CH	47	PHE	4.5
35	CH	133	GLN	4.5
31	CA	880	G	4.5
31	CA	1171	G	4.5
31	CA	1548	A	4.4
31	CA	1052	C	4.4
36	CJ	137	GLY	4.4
42	CP	92	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
49	CW	43	ASP	4.4
40	CN	84	LYS	4.4
45	CS	78	ARG	4.4
48	DV	52	LEU	4.4
49	CW	42	LEU	4.4
54	DA	2131	U	4.4
1	BA	953	G	4.4
31	CA	291	G	4.4
31	CA	1210	G	4.4
31	CA	1530	G	4.4
53	DI	118	ILE	4.4
19	BS	42	PRO	4.4
2	BB	6	MET	4.4
9	BI	57	MET	4.4
30	CD	19	GLY	4.4
1	BA	330	C	4.4
26	C5	8	LYS	4.4
31	CA	1043	C	4.4
9	BI	94	LEU	4.4
3	BC	76	VAL	4.4
17	BQ	72	SER	4.4
36	CJ	66	SER	4.4
50	CX	35	SER	4.4
33	CF	84	PRO	4.4
36	DJ	50	GLU	4.4
1	BA	1005	A	4.4
1	BA	1317	C	4.4
7	BG	89	VAL	4.4
49	CW	65	VAL	4.4
3	BC	53	SER	4.4
1	BA	1209	C	4.4
1	BA	1035	A	4.4
1	BA	1340	A	4.4
17	BQ	83	VAL	4.4
47	CU	28	ASN	4.4
54	DA	2119	A	4.4
7	AG	8	GLY	4.4
45	CS	18	GLN	4.4
36	DJ	26	PRO	4.4
18	AR	55	LEU	4.4
32	CE	126	VAL	4.4
33	CF	94	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
34	CG	48	ASN	4.4
1	BA	842	U	4.4
1	BA	981	U	4.4
31	CA	259	G	4.4
11	BK	21	ALA	4.4
41	CO	25	ALA	4.4
7	BG	77	SER	4.4
14	BN	6	MET	4.4
37	CK	1	MET	4.4
13	BM	101	ARG	4.4
40	CN	80	VAL	4.4
1	BA	83	C	4.4
30	CD	166	GLY	4.4
31	CA	2833	U	4.4
39	CM	130	GLY	4.4
34	CG	99	LYS	4.4
1	BA	212	G	4.4
1	BA	988	G	4.4
1	BA	1236	A	4.4
7	BG	72	THR	4.4
31	CA	2892	G	4.4
39	CM	30	THR	4.4
53	DI	94	ARG	4.4
36	DJ	28	LEU	4.4
42	CP	27	VAL	4.4
13	BM	26	GLY	4.4
48	CV	38	GLY	4.4
25	C4	14	PHE	4.3
7	BG	57	SER	4.3
42	CP	93	ASP	4.3
50	CX	64	ASP	4.3
7	BG	50	LEU	4.3
31	CA	1073	A	4.3
31	CA	1205	A	4.3
32	CE	178	VAL	4.3
34	CG	41	VAL	4.3
41	CO	56	LYS	4.3
3	BC	102	ASN	4.3
23	C2	16	GLY	4.3
41	CO	52	ILE	4.3
48	CV	27	ASN	4.3
19	AS	55	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
39	CM	21	ARG	4.3
2	BB	20	THR	4.3
7	AG	59	LEU	4.3
45	CS	48	LYS	4.3
47	CU	33	LYS	4.3
49	CW	58	SER	4.3
31	CA	2309	A	4.3
54	DA	654	A	4.3
54	DA	1175	A	4.3
7	BG	55	GLY	4.3
54	DA	2128	G	4.3
32	CE	175	ILE	4.3
33	CF	81	GLN	4.3
36	DJ	49	ILE	4.3
41	CO	66	ALA	4.3
52	CZ	5	GLU	4.3
2	AB	210	VAL	4.3
41	CO	76	VAL	4.3
45	CS	94	THR	4.3
31	CA	1057	A	4.3
35	DH	94	ILE	4.3
43	CQ	34	GLU	4.3
14	BN	7	LYS	4.3
53	DI	101	LYS	4.3
2	AB	15	HIS	4.3
13	BM	12	HIS	4.3
13	BM	42	ASP	4.3
3	BC	111	LEU	4.3
31	CA	343	C	4.3
31	CA	1874	C	4.3
43	CQ	8	LEU	4.3
2	AB	5	SER	4.3
10	BJ	32	THR	4.3
36	DJ	139	VAL	4.3
47	CU	67	VAL	4.3
33	CF	27	GLN	4.3
45	CS	24	LYS	4.3
45	CS	45	GLU	4.3
54	DA	2171	A	4.3
7	BG	107	ALA	4.3
1	BA	1312	G	4.3
54	DA	883	G	4.3

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Mol	Chain	Res	Type	RSRZ
2	AB	213	TYR	4.3
24	C3	31	LEU	4.3
32	CE	129	PRO	4.3
44	CR	25	TYR	4.3
33	CF	11	GLU	4.3
35	CH	142	VAL	4.3
46	CT	49	LYS	4.3
1	BA	121	U	4.3
1	BA	216	U	4.3
31	CA	1015	U	4.3
1	BA	1333	A	4.3
26	C5	12	ARG	4.3
36	CJ	10	LYS	4.3
1	BA	1273	C	4.3
48	CV	86	ARG	4.3
26	C5	20	ASP	4.3
31	CA	126	A	4.3
31	CA	505	A	4.3
35	CH	13	GLY	4.3
1	BA	1331	G	4.3
13	AM	4	ILE	4.3
13	BM	49	SER	4.3
16	BP	81	ALA	4.3
40	CN	116	ALA	4.3
46	CT	44	ALA	4.3
32	CE	134	LEU	4.3
43	CQ	13	MET	4.3
13	BM	97	VAL	4.3
52	CZ	11	VAL	4.3
28	CB	19	C	4.3
1	BA	955	U	4.3
9	BI	33	ARG	4.3
20	BT	49	LYS	4.3
14	AN	22	ALA	4.2
30	CD	188	LEU	4.2
36	DJ	34	ASN	4.2
31	CA	1111	A	4.2
31	CA	545	U	4.2
34	CG	110	SER	4.2
14	BN	8	ALA	4.2
35	DH	11	ASN	4.2
47	DU	92	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
48	CV	40	ASN	4.2
15	BO	75	VAL	4.2
33	CF	138	PHE	4.2
1	BA	1363	A	4.2
7	BG	90	GLU	4.2
12	BL	70	GLU	4.2
31	CA	2175	C	4.2
39	CM	19	LEU	4.2
3	BC	62	LYS	4.2
25	C4	36	LYS	4.2
1	BA	174	A	4.2
31	CA	1233	C	4.2
32	CE	190	ALA	4.2
23	C2	40	ASP	4.2
44	CR	102	ASP	4.2
32	CE	32	VAL	4.2
34	CG	79	VAL	4.2
3	BC	60	PRO	4.2
39	CM	75	ALA	4.2
1	BA	153	C	4.2
7	BG	99	LEU	4.2
19	BS	35	SER	4.2
33	CF	142	ASP	4.2
9	BI	103	PHE	4.2
50	CX	51	VAL	4.2
7	BG	60	GLU	4.2
31	CA	1168	G	4.2
36	CJ	110	ALA	4.2
37	CK	94	ALA	4.2
2	BB	10	LEU	4.2
45	CS	7	SER	4.2
1	BA	1281	C	4.2
19	BS	23	VAL	4.2
23	C2	35	GLU	4.2
27	C0	39	GLU	4.2
38	CL	89	ASN	4.2
2	AB	201	PRO	4.2
46	CT	85	ILE	4.2
14	BN	44	ALA	4.2
28	CB	22	U	4.2
27	C0	24	LEU	4.2
31	CA	327	G	4.2

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Mol	Chain	Res	Type	RSRZ
13	AM	11	ASP	4.2
14	AN	100	SER	4.2
1	AA	1027	C	4.2
35	CH	9	VAL	4.2
2	BB	186	ILE	4.2
3	BC	42	TYR	4.2
41	CO	26	GLY	4.2
19	BS	47	LEU	4.2
36	CJ	115	ALA	4.2
33	CF	14	LYS	4.2
31	CA	930	G	4.2
36	CJ	128	SER	4.2
11	AK	81	ASN	4.2
3	BC	177	THR	4.2
52	CZ	56	LEU	4.1
34	CG	35	ARG	4.1
31	CA	638	G	4.1
36	CJ	39	CYS	4.1
19	BS	70	LYS	4.1
31	CA	241	A	4.1
53	DI	40	GLU	4.1
36	DJ	107	GLN	4.1
47	CU	76	ARG	4.1
48	CV	18	ASP	4.1
21	AU	3	VAL	4.1
23	C2	13	SER	4.1
42	CP	39	VAL	4.1
30	CD	58	ASN	4.1
1	BA	108	G	4.1
31	CA	1875	G	4.1
31	CA	2165	C	4.1
31	CA	884	U	4.1
7	BG	102	ARG	4.1
7	BG	120	LEU	4.1
31	CA	603	A	4.1
32	CE	200	LEU	4.1
33	CF	30	ARG	4.1
39	CM	131	ALA	4.1
42	CP	110	ALA	4.1
50	CX	37	ILE	4.1
7	BG	152	ALA	4.1
48	CV	22	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
52	CZ	48	ARG	4.1
31	CA	2412	A	4.1
32	CE	148	ILE	4.1
53	DI	123	ILE	4.1
42	CP	6	ALA	4.1
46	CT	83	LYS	4.1
53	DI	88	HIS	4.1
1	BA	134	G	4.1
1	BA	976	G	4.1
31	CA	1271	G	4.1
31	CA	2799	A	4.1
13	BM	113	ARG	4.1
15	BO	17	ARG	4.1
19	BS	36	ARG	4.1
52	CZ	8	GLU	4.1
33	CF	96	MET	4.1
1	BA	1214	C	4.1
2	AB	16	PHE	4.1
2	AB	30	PHE	4.1
42	CP	36	TYR	4.1
33	DF	74	VAL	4.1
35	CH	127	GLU	4.1
39	CM	135	ILE	4.1
43	CQ	5	ILE	4.1
7	BG	68	ASN	4.1
31	CA	2181	U	4.1
32	CE	161	ALA	4.1
46	CT	19	LEU	4.1
31	CA	1518	C	4.1
25	C4	47	LYS	4.1
46	CT	92	ARG	4.1
48	CV	11	VAL	4.1
31	CA	1538	G	4.1
36	DJ	48	SER	4.1
44	CR	38	ALA	4.1
54	DA	2106	U	4.1
23	C2	46	HIS	4.1
34	CG	113	VAL	4.1
46	CT	36	LEU	4.1
3	BC	51	SER	4.1
11	BK	55	SER	4.1
13	BM	15	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
45	CS	52	PRO	4.0
53	DI	127	ALA	4.1
49	CW	33	GLY	4.0
11	AK	111	THR	4.0
36	CJ	49	ILE	4.0
34	CG	133	LEU	4.0
36	CJ	127	ARG	4.0
52	CZ	21	LEU	4.0
13	AM	36	ALA	4.0
31	CA	2800	A	4.0
31	CA	1235	G	4.0
54	DA	1093	G	4.0
2	BB	199	VAL	4.0
1	BA	1210	C	4.0
31	CA	2628	C	4.0
32	CE	101	TYR	4.0
34	CG	129	THR	4.0
34	CG	131	ILE	4.0
39	CM	5	THR	4.0
42	CP	35	ILE	4.0
3	BC	80	LYS	4.0
2	BB	129	LEU	4.0
13	BM	52	GLN	4.0
16	BP	54	LEU	4.0
32	CE	21	ARG	4.0
7	BG	88	PRO	4.0
13	AM	46	SER	4.0
22	C1	46	ASP	4.0
31	CA	2410	G	4.0
42	CP	88	LYS	4.0
49	CW	70	ILE	4.0
54	DA	277	G	4.0
54	DA	2144	G	4.0
31	CA	1533	C	4.0
31	CA	2000	C	4.0
54	DA	2161	C	4.0
42	CP	60	GLU	4.0
30	CD	31	ALA	4.0
14	BN	72	GLY	4.0
33	CF	29	PRO	4.0
36	DJ	90	SER	4.0
39	CM	119	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
33	CF	10	ASP	4.0
37	CK	35	ARG	4.0
45	CS	79	ARG	4.0
31	CA	1245	G	4.0
50	CX	58	THR	4.0
2	AB	32	PHE	4.0
3	BC	50	ALA	4.0
11	AK	47	ALA	4.0
46	CT	32	ALA	4.0
1	BA	1224	U	4.0
7	BG	110	LYS	4.0
13	AM	13	LYS	4.0
29	CC	249	GLY	4.0
7	BG	80	VAL	4.0
32	CE	67	ARG	4.0
34	CG	109	PHE	4.0
42	CP	97	PHE	4.0
1	BA	102	G	4.0
1	BA	165	G	4.0
36	CJ	104	ALA	4.0
1	BA	843	U	4.0
34	CG	77	ILE	4.0
7	BG	131	LYS	4.0
32	CE	41	GLN	4.0
35	DH	12	LEU	4.0
48	CV	47	LYS	4.0
31	CA	256	A	4.0
14	BN	25	ALA	4.0
31	CA	61	C	4.0
28	CB	56	G	4.0
31	CA	2877	G	4.0
2	AB	4	VAL	4.0
37	CK	139	VAL	4.0
39	CM	106	GLU	4.0
22	C1	34	SER	4.0
50	CX	24	LYS	4.0
33	CF	22	TYR	4.0
1	BA	222	C	4.0
31	CA	357	C	4.0
31	CA	1322	A	4.0
30	CD	180	VAL	4.0
31	CA	1179	G	4.0

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Mol	Chain	Res	Type	RSRZ
7	AG	54	SER	4.0
32	CE	75	SER	4.0
10	BJ	15	HIS	4.0
16	BP	56	ARG	4.0
17	BQ	44	LEU	4.0
24	C3	12	ARG	4.0
34	CG	94	TYR	4.0
44	CR	96	ALA	4.0
44	CR	113	ALA	4.0
31	CA	623	C	3.9
36	DJ	60	THR	3.9
15	BO	12	VAL	3.9
35	CH	134	VAL	3.9
35	DH	138	VAL	3.9
48	DV	53	ASN	3.9
31	CA	315	G	3.9
49	CW	91	PHE	3.9
39	CM	139	GLY	3.9
11	AK	21	ALA	3.9
23	C2	30	LYS	3.9
32	CE	98	LYS	3.9
1	BA	89	U	3.9
31	CA	31	C	3.9
31	CA	89	A	3.9
54	DA	1089	A	3.9
52	CZ	28	LEU	3.9
16	BP	58	ALA	3.9
54	DA	2164	C	3.9
1	BA	1248	A	3.9
1	BA	1534	A	3.9
7	AG	18	PHE	3.9
35	CH	70	GLU	3.9
20	BT	75	HIS	3.9
32	CE	201	ALA	3.9
36	DJ	124	ALA	3.9
1	BA	957	U	3.9
2	AB	225	ARG	3.9
10	BJ	16	ARG	3.9
31	CA	150	U	3.9
31	CA	1217	U	3.9
5	AE	164	ILE	3.9
35	CH	144	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
44	CR	34	VAL	3.9
2	BB	89	GLN	3.9
10	BJ	20	GLN	3.9
29	CC	244	PRO	3.9
35	DH	96	THR	3.9
54	DA	2145	C	3.9
2	AB	214	LEU	3.9
5	BE	109	GLY	3.9
25	C4	29	LEU	3.9
48	CV	90	GLY	3.9
1	BA	1368	A	3.9
31	CA	1551	A	3.9
31	CA	474	G	3.9
31	CA	1863	G	3.9
33	CF	139	PRO	3.9
1	BA	1320	C	3.9
31	CA	550	C	3.9
31	CA	2691	C	3.9
13	AM	8	ASN	3.9
32	CE	179	SER	3.9
36	DJ	104	ALA	3.9
8	BH	110	VAL	3.9
46	CT	87	PRO	3.9
52	CZ	25	GLN	3.9
29	CC	12	GLY	3.9
31	CA	307	G	3.9
7	AG	79	ARG	3.9
51	CY	45	ARG	3.9
52	CZ	4	LYS	3.9
3	BC	61	ALA	3.9
36	DJ	128	SER	3.9
39	CM	137	ALA	3.9
12	BL	117	TYR	3.9
16	AP	17	TYR	3.9
31	CA	1098	A	3.9
31	CA	2287	A	3.9
31	CA	139	U	3.9
17	BQ	46	VAL	3.9
2	BB	90	PHE	3.9
3	BC	172	ARG	3.9
30	CD	46	ARG	3.9
9	BI	9	THR	3.9

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Mol	Chain	Res	Type	RSRZ
20	BT	80	THR	3.9
1	BA	941	G	3.9
31	CA	1056	G	3.9
7	BG	108	ALA	3.9
48	DV	51	ALA	3.9
31	CA	1328	A	3.9
45	CS	87	GLN	3.9
42	CP	76	LYS	3.9
49	CW	46	LYS	3.9
9	AI	89	GLU	3.9
31	CA	32	C	3.9
31	CA	2045	C	3.9
39	CM	71	ALA	3.9
44	CR	81	ASN	3.9
1	AA	82	G	3.9
31	CA	2525	G	3.9
7	AG	56	LYS	3.8
54	DA	2122	U	3.8
14	BN	63	ARG	3.8
42	CP	102	ARG	3.8
16	BP	38	PHE	3.8
20	BT	51	PHE	3.8
54	DA	892	A	3.8
27	C0	41	THR	3.8
30	CD	86	GLU	3.8
46	CT	54	ALA	3.8
53	DI	114	GLU	3.8
29	CC	37	ASN	3.8
32	CE	165	HIS	3.8
46	CT	86	MET	3.8
10	AJ	75	ASP	3.8
21	AU	16	LEU	3.8
31	CA	513	A	3.8
12	BL	108	LYS	3.8
13	BM	44	LYS	3.8
32	CE	87	ALA	3.8
35	CH	67	ALA	3.8
36	DJ	115	ALA	3.8
38	CL	33	ALA	3.8
44	CR	35	ALA	3.8
16	BP	40	ASN	3.8
1	BA	215	C	3.8

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Mol	Chain	Res	Type	RSRZ
31	CA	1018	U	3.8
31	CA	1108	U	3.8
31	CA	1203	U	3.8
33	DF	83	TYR	3.8
34	CG	74	SER	3.8
34	CG	141	ILE	3.8
40	CN	73	ILE	3.8
2	AB	10	LEU	3.8
17	BQ	8	LEU	3.8
33	CF	169	LEU	3.8
33	CF	164	GLU	3.8
54	DA	2140	G	3.8
1	BA	974	A	3.8
47	CU	80	TRP	3.8
17	BQ	5	ILE	3.8
39	CM	103	ILE	3.8
48	CV	93	VAL	3.8
18	BR	51	TYR	3.8
33	CF	150	ARG	3.8
28	CB	23	G	3.8
31	CA	551	G	3.8
31	CA	805	G	3.8
31	CA	477	A	3.8
31	CA	1321	A	3.8
3	BC	2	GLY	3.8
38	CL	15	GLY	3.8
53	DI	122	GLN	3.8
11	AK	18	ASP	3.8
26	C5	3	VAL	3.8
31	CA	1201	U	3.8
31	CA	2111	U	3.8
54	DA	546	U	3.8
31	CA	264	C	3.8
45	CS	34	GLU	3.8
47	CU	84	TYR	3.8
13	AM	32	ALA	3.8
33	CF	54	ALA	3.8
34	CG	5	ALA	3.8
39	CM	83	ALA	3.8
1	BA	107	G	3.8
17	BQ	54	GLY	3.8
28	CB	20	G	3.8

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Mol	Chain	Res	Type	RSRZ
31	CA	1212	G	3.8
31	CA	2502	G	3.8
33	CF	64	LYS	3.8
35	DH	89	LYS	3.8
1	BA	977	A	3.8
31	CA	431	U	3.8
31	CA	1460	U	3.8
31	CA	2167	U	3.8
32	CE	121	VAL	3.8
34	CG	67	THR	3.8
35	CH	61	VAL	3.8
37	CK	128	ASN	3.8
7	BG	59	LEU	3.8
1	BA	1322	C	3.8
1	BA	1336	C	3.8
43	CQ	35	GLY	3.8
44	CR	71	GLN	3.8
47	CU	91	GLN	3.8
21	AU	4	ILE	3.8
30	CD	24	VAL	3.8
33	DF	77	PHE	3.8
1	BA	1000	A	3.8
39	CM	27	LEU	3.8
54	DA	882	G	3.8
8	BH	55	THR	3.8
7	BG	44	TYR	3.8
27	C0	52	SER	3.8
41	CO	94	TYR	3.8
31	CA	1172	C	3.8
2	BB	182	PRO	3.8
34	DG	177	LYS	3.8
36	CJ	72	LYS	3.8
23	C2	6	ARG	3.8
46	CT	105	VAL	3.8
7	BG	130	ASN	3.8
27	C0	17	LEU	3.8
1	BA	205	A	3.8
1	BA	250	A	3.8
30	CD	151	THR	3.8
1	BA	979	C	3.8
31	CA	76	C	3.8
32	CE	177	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
33	DF	176	PRO	3.8
49	CW	37	PRO	3.8
7	BG	119	ARG	3.8
16	AP	82	ALA	3.8
16	BP	11	ALA	3.8
33	CF	119	ALA	3.8
3	BC	77	ILE	3.8
11	AK	110	ILE	3.8
14	BN	11	VAL	3.8
2	BB	57	LEU	3.7
31	CA	1082	U	3.7
39	CM	95	LEU	3.7
49	CW	71	LYS	3.7
54	DA	1094	U	3.7
46	CT	40	ASN	3.7
1	BA	460	A	3.7
31	CA	412	A	3.7
1	BA	1208	C	3.7
1	BA	1323	G	3.7
16	BP	77	GLU	3.7
31	CA	1531	C	3.7
31	CA	2115	G	3.7
41	CO	114	GLU	3.7
49	CW	32	GLY	3.7
22	C1	4	GLN	3.7
48	CV	66	GLN	3.7
36	DJ	58	VAL	3.7
13	AM	42	ASP	3.7
34	CG	38	ASN	3.7
16	BP	10	GLY	3.7
42	CP	101	GLY	3.7
13	AM	35	ALA	3.7
31	CA	311	A	3.7
31	CA	597	G	3.7
31	CA	1207	C	3.7
31	CA	1320	C	3.7
33	CF	6	ASP	3.7
44	CR	91	ASP	3.7
45	CS	39	LEU	3.7
20	BT	5	LYS	3.7
41	CO	93	GLY	3.7
48	CV	15	THR	3.7

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Mol	Chain	Res	Type	RSRZ
7	BG	115	SER	3.7
31	CA	646	U	3.7
31	CA	1862	G	3.7
31	CA	2383	G	3.7
38	CL	56	ASP	3.7
19	BS	65	GLU	3.7
24	C3	26	ASN	3.7
33	CF	7	TYR	3.7
30	CD	73	VAL	3.7
43	CQ	33	VAL	3.7
7	AG	48	GLU	3.7
31	CA	1017	G	3.7
42	CP	34	HIS	3.7
34	CG	152	ARG	3.7
2	BB	212	LEU	3.7
47	CU	31	VAL	3.7
1	BA	218	U	3.7
2	BB	88	ASP	3.7
39	CM	144	GLU	3.7
1	AA	78	A	3.7
27	C0	20	HIS	3.7
31	CA	1228	G	3.7
35	CH	102	ALA	3.7
14	BN	58	SER	3.7
43	CQ	4	ILE	3.7
28	CB	118	C	3.7
31	CA	257	C	3.7
54	DA	1066	U	3.7
7	AG	112	GLY	3.7
54	DA	2114	A	3.7
50	CX	78	LYS	3.7
1	BA	378	G	3.7
25	C4	48	ALA	3.7
13	BM	112	PRO	3.7
28	CB	51	G	3.7
53	DI	120	ALA	3.7
5	BE	120	VAL	3.7
19	BS	25	SER	3.7
40	CN	29	GLY	3.7
13	AM	31	LYS	3.7
31	CA	1385	A	3.7
3	AC	189	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
16	BP	45	GLU	3.7
51	CY	20	HIS	3.7
19	BS	62	VAL	3.7
25	C4	57	LEU	3.7
3	BC	26	THR	3.7
31	CA	2862	G	3.7
1	BA	956	U	3.6
1	BA	1126	U	3.6
1	BA	1375	A	3.6
46	CT	10	ALA	3.6
2	AB	40	ILE	3.6
48	CV	72	ILE	3.6
1	BA	1235	U	3.6
48	CV	84	GLY	3.6
31	CA	1483	G	3.6
45	CS	6	GLN	3.6
1	BA	135	C	3.6
28	CB	63	C	3.6
33	CF	45	ALA	3.6
39	CM	133	ALA	3.6
29	CC	242	LYS	3.6
31	CA	53	A	3.6
31	CA	502	A	3.6
35	DH	99	ILE	3.6
39	CM	127	VAL	3.6
3	BC	179	ARG	3.6
8	AH	54	ASP	3.6
41	CO	46	ARG	3.6
53	DI	90	GLY	3.6
30	CD	35	THR	3.6
31	CA	1173	U	3.6
1	BA	1015	G	3.6
1	BA	1220	G	3.6
1	BA	1356	G	3.6
31	CA	2405	G	3.6
8	BH	130	ALA	3.6
14	BN	17	ALA	3.6
36	DJ	10	LYS	3.6
3	BC	39	VAL	3.6
5	BE	91	GLY	3.6
1	BA	1252	A	3.6
31	CA	2117	A	3.6

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Mol	Chain	Res	Type	RSRZ
9	AI	59	GLU	3.6
31	CA	328	U	3.6
31	CA	405	U	3.6
31	CA	767	U	3.6
31	CA	1325	U	3.6
49	CW	45	ASP	3.6
26	C5	35	GLN	3.6
23	C2	20	PHE	3.6
39	CM	64	PHE	3.6
43	CQ	59	PHE	3.6
48	CV	73	PHE	3.6
1	BA	1442	G	3.6
31	CA	353	C	3.6
53	DI	100	ALA	3.6
54	DA	2162	G	3.6
35	CH	44	ILE	3.6
36	DJ	61	VAL	3.6
44	CR	117	LEU	3.6
35	CH	60	GLU	3.6
54	DA	2180	U	3.6
36	CJ	117	MET	3.6
7	BG	145	ALA	3.6
11	AK	66	ALA	3.6
20	BT	87	ALA	3.6
52	CZ	63	ALA	3.6
13	AM	16	VAL	3.6
13	AM	34	LEU	3.6
35	DH	107	GLY	3.6
49	CW	64	VAL	3.6
48	CV	101	GLU	3.6
37	CK	141	ASP	3.6
31	CA	1234	U	3.6
1	BA	1280	A	3.6
13	BM	76	SER	3.6
24	C3	5	PHE	3.6
32	CE	125	SER	3.6
37	CK	95	ARG	3.6
9	AI	54	LEU	3.6
34	CG	18	LYS	3.6
1	BA	175	C	3.6
3	BC	109	PRO	3.6
34	CG	73	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	BA	1341	U	3.6
31	CA	367	G	3.6
32	CE	9	GLN	3.6
19	BS	44	MET	3.6
1	BA	935	A	3.6
36	CJ	63	ALA	3.6
48	CV	91	LYS	3.6
13	AM	25	VAL	3.6
20	BT	67	ILE	3.6
23	C2	7	GLU	3.6
27	C0	33	GLY	3.6
35	DH	127	GLU	3.6
28	CB	27	C	3.6
31	CA	1289	C	3.6
1	BA	986	U	3.6
13	BM	71	ARG	3.6
33	CF	51	ASP	3.6
2	BB	9	MET	3.6
7	AG	116	MET	3.6
30	CD	101	PHE	3.6
31	CA	266	G	3.6
31	CA	1869	G	3.6
33	CF	47	LYS	3.6
54	DA	2168	G	3.6
10	BJ	50	THR	3.6
11	BK	67	ALA	3.6
25	C4	27	ALA	3.6
33	CF	171	ALA	3.6
49	CW	28	ALA	3.6
31	CA	332	A	3.6
31	CA	478	A	3.6
32	CE	73	ILE	3.6
38	CL	35	VAL	3.6
48	DV	49	VAL	3.6
17	BQ	45	HIS	3.6
46	CT	7	HIS	3.6
31	CA	413	C	3.5
35	DH	139	PHE	3.5
49	CW	48	MET	3.5
1	BA	201	G	3.5
31	CA	1112	G	3.5
31	CA	1239	G	3.5

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Mol	Chain	Res	Type	RSRZ
3	BC	127	ARG	3.5
13	BM	53	ILE	3.5
16	AP	71	VAL	3.5
45	CS	80	ARG	3.5
48	CV	94	ARG	3.5
1	BA	389	A	3.5
31	CA	1285	A	3.5
40	CN	88	ASN	3.5
51	CY	77	LYS	3.5
1	AA	1037	C	3.5
1	BA	206	C	3.5
1	BA	219	U	3.5
31	CA	1251	C	3.5
2	AB	44	GLU	3.5
2	BB	206	ALA	3.5
9	BI	63	LEU	3.5
14	AN	36	ALA	3.5
44	CR	82	GLY	3.5
18	BR	48	ARG	3.5
36	CJ	134	ARG	3.5
42	CP	58	ILE	3.5
16	AP	39	PHE	3.5
43	CQ	11	GLU	3.5
32	CE	199	MET	3.5
51	CY	18	ARG	3.5
3	BC	104	ALA	3.5
20	BT	50	ALA	3.5
33	CF	103	LEU	3.5
43	CQ	97	LEU	3.5
27	C0	44	ILE	3.5
30	CD	48	ILE	3.5
1	BA	1048	G	3.5
2	AB	82	ASP	3.5
22	C1	8	PRO	3.5
34	CG	126	PRO	3.5
45	CS	82	HIS	3.5
45	CS	93	PHE	3.5
49	CW	35	GLU	3.5
2	BB	11	LYS	3.5
39	CM	88	GLY	3.5
33	CF	49	LEU	3.5
44	CR	99	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
3	BC	120	ILE	3.5
35	CH	14	SER	3.5
5	BE	140	THR	3.5
9	BI	59	GLU	3.5
36	DJ	46	THR	3.5
45	CS	29	THR	3.5
35	CH	68	ARG	3.5
47	CU	69	ARG	3.5
11	AK	43	GLY	3.5
31	CA	514	A	3.5
31	CA	2306	C	3.5
35	CH	75	LEU	3.5
7	AG	42	ILE	3.5
17	BQ	61	ILE	3.5
44	CR	65	ILE	3.5
42	CP	98	GLN	3.5
14	BN	19	LYS	3.5
22	C1	16	ARG	3.5
30	CD	39	ASP	3.5
8	BH	120	GLY	3.5
13	AM	24	GLY	3.5
1	BA	1013	G	3.5
1	BA	1369	C	3.5
28	CB	49	C	3.5
28	CB	117	G	3.5
31	CA	93	G	3.5
31	CA	409	G	3.5
7	AG	69	VAL	3.5
13	AM	7	ILE	3.5
47	CU	2	ILE	3.5
54	DA	1098	A	3.5
30	CD	189	VAL	3.5
50	CX	41	ARG	3.5
5	BE	108	GLY	3.5
31	CA	2796	U	3.5
34	CG	49	THR	3.5
44	CR	45	TYR	3.5
53	DI	126	LEU	3.5
7	BG	63	GLU	3.5
9	BI	75	GLN	3.5
28	CB	97	C	3.5
42	CP	85	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
49	CW	68	LYS	3.5
28	CB	98	G	3.5
54	DA	2108	A	3.5
30	CD	3	GLY	3.5
54	DA	1060	U	3.5
35	DH	125	THR	3.5
30	CD	84	LEU	3.5
7	AG	43	VAL	3.5
31	CA	1143	A	3.5
26	C5	6	SER	3.4
33	CF	87	CYS	3.4
36	DJ	82	LYS	3.4
48	DV	55	PRO	3.4
2	AB	27	MET	3.4
41	CO	96	ARG	3.4
30	CD	206	ALA	3.4
44	CR	39	VAL	3.4
43	CQ	74	PHE	3.4
28	CB	52	A	3.4
30	CD	44	GLY	3.4
1	AA	1015	G	3.4
1	BA	933	G	3.4
16	BP	47	GLU	3.4
31	CA	361	G	3.4
18	BR	74	HIS	3.4
41	CO	1	MET	3.4
36	DJ	8	TYR	3.4
46	CT	15	GLN	3.4
2	BB	16	PHE	3.4
25	C4	22	PHE	3.4
31	CA	544	C	3.4
31	CA	2078	C	3.4
1	BA	632	U	3.4
47	CU	6	ARG	3.4
22	C1	26	THR	3.4
29	CC	46	ASN	3.4
31	CA	2112	G	3.4
33	CF	13	VAL	3.4
46	CT	100	THR	3.4
53	DI	67	THR	3.4
16	AP	16	PHE	3.4
36	DJ	25	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
33	CF	101	GLU	3.4
31	CA	288	U	3.4
2	BB	31	ILE	3.4
20	BT	48	GLN	3.4
25	C4	4	ILE	3.4
44	CR	21	ALA	3.4
44	CR	116	ALA	3.4
46	CT	9	HIS	3.4
52	CZ	54	LYS	3.4
1	BA	1272	G	3.4
2	BB	130	THR	3.4
3	BC	56	VAL	3.4
9	BI	47	VAL	3.4
31	CA	1309	G	3.4
31	CA	1332	G	3.4
32	CE	173	THR	3.4
45	CS	19	THR	3.4
47	CU	62	VAL	3.4
54	DA	879	G	3.4
30	CD	90	PHE	3.4
42	CP	86	GLY	3.4
14	AN	54	ASP	3.4
1	BA	1212	U	3.4
1	BA	1286	U	3.4
22	C1	37	LYS	3.4
31	CA	314	C	3.4
35	CH	141	LYS	3.4
54	DA	2105	U	3.4
36	CJ	48	SER	3.4
36	CJ	105	GLN	3.4
1	BA	151	A	3.4
1	BA	195	A	3.4
42	CP	28	VAL	3.4
13	AM	57	ARG	3.4
29	CC	43	ARG	3.4
31	CA	1042	G	3.4
31	CA	1984	G	3.4
31	CA	2904	U	3.4
25	C4	46	PRO	3.4
32	CE	30	GLN	3.4
46	CT	69	LEU	3.4
14	AN	99	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
29	CC	2	ALA	3.4
39	CM	42	SER	3.4
45	CS	15	SER	3.4
2	BB	36	ASN	3.4
2	BB	93	ASN	3.4
1	BA	1319	A	3.4
13	AM	26	GLY	3.4
3	BC	108	LYS	3.4
20	BT	8	LYS	3.4
23	C2	22	THR	3.4
1	BA	100	G	3.4
1	BA	198	G	3.4
34	CG	116	GLN	3.4
35	DH	6	LEU	3.4
43	CQ	22	PRO	3.4
19	BS	50	ALA	3.4
39	CM	24	GLY	3.4
1	BA	1014	A	3.4
31	CA	598	U	3.4
44	CR	95	LEU	3.4
47	DU	91	GLN	3.4
3	AC	195	VAL	3.4
7	AG	57	SER	3.4
10	BJ	88	MET	3.4
13	AM	60	VAL	3.4
35	CH	56	ALA	3.4
16	BP	30	GLY	3.4
35	CH	16	GLY	3.4
35	DH	95	GLY	3.4
51	CY	46	PHE	3.4
9	AI	7	TYR	3.4
7	BG	140	ASP	3.4
41	CO	36	THR	3.4
24	C3	41	ARG	3.3
2	AB	131	LYS	3.3
31	CA	2861	U	3.3
48	DV	54	GLN	3.3
52	CZ	18	LEU	3.3
35	DH	100	ALA	3.3
36	CJ	140	VAL	3.3
49	CW	54	ALA	3.3
52	DZ	63	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
53	DI	2	ALA	3.3
3	BC	78	GLY	3.3
12	BL	71	GLY	3.3
1	BA	1355	G	3.3
31	CA	30	G	3.3
31	CA	1653	G	3.3
10	AJ	91	ASP	3.3
13	BM	20	THR	3.3
3	BC	144	LEU	3.3
29	CC	213	TRP	3.3
53	DI	5	LEU	3.3
1	AA	1016	A	3.3
31	CA	270	A	3.3
31	CA	1253	A	3.3
31	CA	2872	A	3.3
3	BC	194	GLY	3.3
7	AG	134	ALA	3.3
19	BS	59	PRO	3.3
27	C0	42	PRO	3.3
42	CP	96	GLY	3.3
50	CX	36	ILE	3.3
35	CH	78	VAL	3.3
35	DH	103	VAL	3.3
31	CA	611	C	3.3
31	CA	1041	G	3.3
32	CE	168	ASP	3.3
35	DH	5	LEU	3.3
53	DI	3	LEU	3.3
20	BT	81	ALA	3.3
31	CA	1244	A	3.3
31	CA	2660	A	3.3
44	CR	17	ILE	3.3
50	CX	65	GLY	3.3
6	AF	62	MET	3.3
25	C4	58	VAL	3.3
29	CC	5	LYS	3.3
24	C3	16	HIS	3.3
36	DJ	37	GLU	3.3
1	BA	963	G	3.3
31	CA	446	G	3.3
31	CA	1599	U	3.3
16	AP	43	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
16	BP	51	ARG	3.3
20	BT	56	PRO	3.3
32	CE	196	VAL	3.3
1	BA	306	A	3.3
45	CS	1	MET	3.3
31	CA	2313	C	3.3
48	CV	69	ASN	3.3
1	BA	354	G	3.3
31	CA	2677	G	3.3
2	AB	134	ALA	3.3
6	BF	8	PHE	3.3
21	AU	19	PHE	3.3
32	CE	135	ALA	3.3
37	CK	42	ALA	3.3
45	CS	75	VAL	3.3
49	CW	7	GLU	3.3
1	BA	1262	C	3.3
14	BN	3	LYS	3.3
52	CZ	58	ASN	3.3
1	BA	1125	U	3.3
14	BN	13	ARG	3.3
31	CA	290	U	3.3
33	CF	148	ARG	3.3
19	BS	79	THR	3.3
29	CC	228	VAL	3.3
40	CN	7	THR	3.3
1	BA	1006	G	3.3
9	AI	51	PRO	3.3
28	CB	54	G	3.3
14	AN	101	TRP	3.3
1	BA	101	A	3.3
1	BA	845	A	3.3
1	BA	946	A	3.3
31	CA	1089	A	3.3
41	CO	59	SER	3.3
47	CU	81	LYS	3.3
53	DI	105	LYS	3.3
2	AB	117	LEU	3.3
2	AB	139	ARG	3.3
6	BF	79	ARG	3.3
17	BQ	6	ARG	3.3
30	CD	187	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
47	CU	73	ARG	3.3
1	BA	980	C	3.3
31	CA	1729	U	3.3
31	CA	2786	U	3.3
13	BM	73	ILE	3.3
42	CP	50	ALA	3.3
45	CS	46	GLU	3.3
52	CZ	13	GLU	3.3
1	BA	1297	G	3.3
24	C3	11	LYS	3.3
31	CA	1341	G	3.3
42	CP	56	LYS	3.3
20	BT	59	ASP	3.3
27	C0	27	LEU	3.3
1	BA	1362	A	3.3
20	BT	78	ASN	3.3
31	CA	262	A	3.3
1	BA	1237	C	3.3
31	CA	1330	C	3.3
35	CH	76	GLU	3.3
35	DH	64	ALA	3.3
24	D3	46	LYS	3.3
33	CF	33	LYS	3.3
41	CO	85	PRO	3.3
45	CS	92	TRP	3.3
9	AI	24	GLY	3.3
39	CM	140	GLY	3.3
9	AI	92	GLU	3.2
13	BM	59	GLU	3.2
15	AO	69	TYR	3.2
18	AR	51	TYR	3.2
1	BA	110	C	3.2
11	AK	97	ILE	3.2
34	CG	20	ASN	3.2
6	BF	10	VAL	3.2
14	BN	12	LYS	3.2
31	CA	1596	A	3.2
31	CA	1958	C	3.2
54	DA	2143	C	3.2
16	BP	50	THR	3.2
36	DJ	71	THR	3.2
37	CK	21	THR	3.2

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Mol	Chain	Res	Type	RSRZ
7	AG	52	GLN	3.2
34	CG	21	GLY	3.2
3	BC	154	SER	3.2
31	CA	224	U	3.2
31	CA	1539	U	3.2
54	DA	141	G	3.2
1	BA	54	C	3.2
17	AQ	83	VAL	3.2
21	AU	26	ALA	3.2
31	CA	47	C	3.2
31	CA	279	A	3.2
31	CA	2158	A	3.2
31	CA	2632	A	3.2
31	CA	2651	C	3.2
3	BC	204	LYS	3.2
36	CJ	37	GLU	3.2
47	CU	40	LYS	3.2
1	BA	1364	U	3.2
31	CA	894	U	3.2
33	CF	24	SER	3.2
45	CS	5	PHE	3.2
33	CF	127	ASN	3.2
51	CY	47	VAL	3.2
53	DI	35	VAL	3.2
1	BA	260	G	3.2
31	CA	128	C	3.2
31	CA	619	G	3.2
31	CA	1138	G	3.2
31	CA	1546	G	3.2
1	BA	109	A	3.2
33	CF	98	GLU	3.2
5	BE	103	THR	3.2
9	BI	61	LEU	3.2
11	AK	100	LEU	3.2
13	BM	102	THR	3.2
39	CM	118	THR	3.2
5	BE	112	ARG	3.2
21	AU	17	ARG	3.2
41	CO	103	ARG	3.2
30	CD	96	ILE	3.2
31	CA	2122	U	3.2
20	BT	77	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
34	CG	165	ALA	3.2
39	CM	13	LYS	3.2
1	BA	1037	C	3.2
1	BA	1041	G	3.2
23	C2	41	PRO	3.2
29	CC	251	GLN	3.2
31	CA	624	C	3.2
31	CA	1319	C	3.2
31	CA	2844	G	3.2
32	CE	188	MET	3.2
31	CA	1614	A	3.2
44	CR	23	GLY	3.2
7	AG	23	LEU	3.2
30	CD	103	ASP	3.2
1	BA	950	U	3.2
30	CD	14	ILE	3.2
32	CE	77	ILE	3.2
54	DA	1078	U	3.2
7	BG	85	TYR	3.2
32	CE	35	TYR	3.2
43	CQ	2	SER	3.2
45	CS	47	VAL	3.2
46	CT	48	LYS	3.2
47	CU	49	LYS	3.2
48	CV	64	ALA	3.2
39	DM	104	GLN	3.2
1	BA	106	C	3.2
1	BA	186	C	3.2
22	C1	51	GLY	3.2
31	CA	33	C	3.2
31	CA	184	C	3.2
31	CA	1600	C	3.2
33	CF	62	GLY	3.2
1	BA	1357	A	3.2
31	CA	43	G	3.2
31	CA	124	G	3.2
31	CA	1237	A	3.2
31	CA	1279	G	3.2
31	CA	1643	G	3.2
14	BN	73	PHE	3.2
42	CP	53	THR	3.2
44	CR	101	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	BA	96	U	3.2
23	D2	5	ILE	3.2
39	CM	141	LYS	3.2
48	CV	92	LYS	3.2
32	CE	187	VAL	3.2
39	CM	15	ALA	3.2
42	CP	70	ALA	3.2
9	BI	45	ARG	3.2
16	BP	18	GLN	3.2
1	BA	470	C	3.2
7	AG	47	LEU	3.2
12	BL	81	LEU	3.2
31	CA	236	C	3.2
32	CE	184	ASP	3.2
36	DJ	47	ASP	3.2
30	CD	121	THR	3.2
1	BA	1121	U	3.2
31	CA	389	G	3.2
31	CA	1395	A	3.2
2	AB	53	ALA	3.2
9	BI	42	GLU	3.2
31	CA	1060	U	3.2
32	CE	197	GLU	3.2
33	CF	19	GLU	3.2
47	CU	35	ALA	3.2
47	CU	45	ALA	3.2
30	CD	191	GLY	3.2
52	CZ	30	MET	3.2
31	CA	2245	U	3.2
34	CG	42	GLU	3.2
1	BA	223	A	3.2
40	CN	56	ALA	3.2
31	CA	2819	G	3.2
45	CS	66	HIS	3.2
46	CT	11	ARG	3.2
7	BG	13	LEU	3.2
15	AO	21	ASP	3.2
35	CH	139	PHE	3.2
3	BC	85	GLU	3.2
1	AA	1025	U	3.1
14	BN	69	ARG	3.1
31	CA	1176	U	3.1

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Mol	Chain	Res	Type	RSRZ
37	CK	6	ALA	3.1
46	CT	3	THR	3.1
30	CD	198	GLY	3.1
53	DI	32	GLY	3.1
31	CA	406	G	3.1
31	CA	881	G	3.1
31	CA	1334	G	3.1
31	CA	1734	G	3.1
31	CA	2808	G	3.1
7	BG	101	MET	3.1
9	BI	52	LEU	3.1
25	C4	49	MET	3.1
43	CQ	93	ARG	3.1
19	BS	18	LYS	3.1
31	CA	11	C	3.1
31	CA	151	C	3.1
31	CA	1615	C	3.1
15	AO	16	GLY	3.1
8	AH	121	LEU	3.1
9	BI	6	TYR	3.1
2	BB	62	SER	3.1
1	BA	86	G	3.1
1	BA	1002	G	3.1
3	BC	105	GLU	3.1
7	BG	2	PRO	3.1
7	BG	70	ARG	3.1
31	CA	70	G	3.1
31	CA	1185	G	3.1
31	CA	1252	G	3.1
31	CA	2895	G	3.1
32	CE	22	ASP	3.1
36	DJ	75	PRO	3.1
48	CV	9	ASP	3.1
7	BG	149	LYS	3.1
3	AC	103	ILE	3.1
41	CO	113	ILE	3.1
25	C4	65	ALA	3.1
54	DA	2130	U	3.1
32	CE	103	GLY	3.1
45	CS	100	GLY	3.1
24	C3	14	ARG	3.1
30	CD	89	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
35	CH	6	LEU	3.1
14	BN	57	PRO	3.1
31	CA	1059	G	3.1
1	BA	1211	U	3.1
2	AB	47	VAL	3.1
13	AM	15	ALA	3.1
1	BA	1038	C	3.1
1	BA	1263	C	3.1
19	BS	56	GLN	3.1
31	CA	1224	U	3.1
31	CA	2334	U	3.1
32	CE	34	ALA	3.1
37	CK	40	HIS	3.1
13	BM	87	ARG	3.1
13	BM	92	ARG	3.1
26	C5	19	ARG	3.1
36	CJ	65	ARG	3.1
44	CR	89	GLU	3.1
9	AI	62	ASP	3.1
21	BU	2	PRO	3.1
29	DC	272	SER	3.1
36	DJ	136	MET	3.1
1	BA	172	A	3.1
31	CA	104	A	3.1
31	CA	368	A	3.1
31	CA	443	A	3.1
35	CH	21	VAL	3.1
45	CS	30	GLY	3.1
45	CS	56	GLY	3.1
1	BA	326	G	3.1
1	BA	1064	G	3.1
31	CA	2627	G	3.1
54	DA	2113	U	3.1
54	DA	2133	G	3.1
10	BJ	17	LEU	3.1
15	BO	87	LEU	3.1
27	C0	23	THR	3.1
29	CC	50	THR	3.1
33	DF	117	LEU	3.1
6	AF	63	ASN	3.1
30	CD	176	ASP	3.1
12	BL	37	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
16	AP	78	VAL	3.1
3	AC	82	GLU	3.1
19	AS	50	ALA	3.1
22	C1	30	VAL	3.1
25	C4	39	LYS	3.1
31	CA	1387	A	3.1
40	CN	89	VAL	3.1
41	CO	7	GLY	3.1
26	C5	29	ALA	3.1
49	CW	23	ALA	3.1
1	BA	187	G	3.1
1	BA	379	C	3.1
31	CA	1471	G	3.1
31	CA	2159	G	3.1
14	AN	18	ASP	3.1
14	BN	38	ASP	3.1
32	CE	156	ASN	3.1
2	BB	45	LYS	3.1
29	CC	49	ILE	3.1
35	DH	16	GLY	3.1
2	BB	145	GLU	3.1
13	AM	64	VAL	3.1
35	DH	65	ALA	3.1
31	CA	423	A	3.1
31	CA	849	A	3.1
2	AB	157	LEU	3.1
33	CF	57	LEU	3.1
34	CG	50	LEU	3.1
1	BA	214	C	3.1
1	BA	1366	C	3.1
49	CW	2	PHE	3.1
31	CA	625	G	3.1
54	DA	2148	G	3.1
12	BL	50	ARG	3.1
19	AS	32	ARG	3.1
37	CK	137	PRO	3.1
53	DI	119	PRO	3.1
7	BG	105	VAL	3.1
48	CV	37	GLU	3.1
53	DI	47	GLU	3.1
7	AG	151	PHE	3.1
22	C1	53	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
31	CA	233	A	3.1
31	CA	508	A	3.1
31	CA	1133	A	3.1
31	CA	2725	A	3.1
31	CA	2749	A	3.1
54	DA	2309	A	3.1
9	AI	85	ARG	3.1
10	BJ	45	ARG	3.1
30	CD	179	ARG	3.1
1	BA	191	G	3.1
19	AS	46	GLY	3.1
31	CA	215	G	3.1
31	CA	313	G	3.1
32	CE	56	GLY	3.1
17	BQ	82	ALA	3.0
19	BS	51	VAL	3.0
36	DJ	57	VAL	3.0
31	CA	100	U	3.0
31	CA	1864	U	3.0
51	CY	30	LEU	3.0
2	AB	35	ARG	3.0
45	CS	12	HIS	3.0
46	CT	95	ARG	3.0
1	BA	1001	C	3.0
29	CC	225	MET	3.0
34	CG	16	ASP	3.0
35	DH	126	GLY	3.0
36	CJ	36	MET	3.0
11	BK	110	ILE	3.0
27	C0	18	PRO	3.0
30	CD	91	THR	3.0
49	CW	24	ASN	3.0
3	BC	200	VAL	3.0
27	C0	55	VAL	3.0
12	BL	48	ALA	3.0
31	CA	494	G	3.0
31	CA	518	G	3.0
43	CQ	6	LYS	3.0
31	CA	1468	U	3.0
47	CU	23	ALA	3.0
52	CZ	34	SER	3.0
22	C1	52	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
29	CC	235	GLY	3.0
43	CQ	16	ASP	3.0
51	CY	55	GLY	3.0
1	BA	1327	C	3.0
33	CF	8	TYR	3.0
37	CK	138	GLN	3.0
41	CO	18	GLN	3.0
44	CR	59	GLN	3.0
2	AB	36	ASN	3.0
45	CS	64	VAL	3.0
2	AB	69	PHE	3.0
31	CA	1099	G	3.0
32	CE	5	LEU	3.0
3	BC	31	ASP	3.0
19	BS	26	GLY	3.0
20	BT	9	LYS	3.0
26	C5	33	HIS	3.0
29	CC	98	ASP	3.0
34	CG	158	LYS	3.0
7	BG	64	VAL	3.0
30	CD	29	VAL	3.0
31	CA	1275	A	3.0
1	BA	473	U	3.0
8	AH	55	THR	3.0
35	DH	124	THR	3.0
39	CM	134	ALA	3.0
2	BB	162	PHE	3.0
7	BG	118	LEU	3.0
19	BS	15	LEU	3.0
33	CF	162	SER	3.0
35	CH	5	LEU	3.0
36	CJ	108	GLU	3.0
39	CM	86	GLU	3.0
51	CY	61	LYS	3.0
1	BA	847	G	3.0
28	CB	102	G	3.0
31	CA	86	G	3.0
31	CA	1324	G	3.0
32	CE	141	MET	3.0
41	CO	97	ILE	3.0
2	BB	29	PRO	3.0
30	CD	60	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
32	CE	69	ARG	3.0
35	DH	25	TYR	3.0
1	AA	1441	A	3.0
1	BA	975	A	3.0
1	BA	1239	A	3.0
7	BG	122	ASN	3.0
31	CA	504	A	3.0
31	CA	1204	A	3.0
35	CH	36	ALA	3.0
39	CM	94	THR	3.0
32	CE	15	SER	3.0
47	CU	93	LEU	3.0
1	BA	105	G	3.0
1	BA	1310	G	3.0
9	BI	119	ARG	3.0
13	AM	17	ILE	3.0
31	CA	1016	G	3.0
50	CX	67	VAL	3.0
31	CA	1396	U	3.0
35	CH	22	LYS	3.0
10	BJ	83	THR	3.0
31	CA	2406	A	3.0
31	CA	2820	A	3.0
52	CZ	10	SER	3.0
2	AB	156	GLY	3.0
44	CR	7	GLY	3.0
30	CD	77	ARG	3.0
30	CD	83	ARG	3.0
11	BK	86	VAL	3.0
25	C4	15	LYS	3.0
30	CD	30	GLU	3.0
31	CA	2668	G	3.0
33	CF	109	PRO	3.0
34	CG	125	CYS	3.0
38	CL	69	VAL	3.0
39	CM	98	ALA	3.0
48	CV	2	ALA	3.0
31	CA	1542	U	3.0
31	CA	16	C	3.0
31	CA	1229	C	3.0
54	DA	2153	C	3.0
54	DA	2177	C	3.0

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Mol	Chain	Res	Type	RSRZ
2	BB	13	GLY	3.0
9	BI	10	GLY	3.0
32	CE	65	THR	3.0
33	CF	159	THR	3.0
7	BG	76	LYS	3.0
30	CD	18	ASP	3.0
29	CC	236	GLU	3.0
30	CD	98	VAL	3.0
34	DG	173	GLU	3.0
21	AU	11	PRO	3.0
1	BA	324	G	3.0
7	AG	68	ASN	3.0
31	CA	2166	U	3.0
54	DA	1729	U	3.0
38	CL	49	ARG	3.0
54	DA	1731	G	3.0
1	AA	1019	A	3.0
31	CA	1383	A	3.0
12	BL	82	ILE	3.0
42	CP	90	VAL	3.0
10	AJ	39	PRO	2.9
35	DH	132	PHE	2.9
43	CQ	42	ALA	2.9
1	AA	4	U	2.9
30	CD	42	ASN	2.9
39	CM	60	ARG	2.9
1	BA	380	G	2.9
14	AN	32	SER	2.9
31	CA	1277	G	2.9
35	DH	136	SER	2.9
13	AM	45	ILE	2.9
42	CP	80	GLU	2.9
15	AO	27	VAL	2.9
24	C3	23	ALA	2.9
42	CP	100	HIS	2.9
1	BA	1065	U	2.9
12	BL	24	LEU	2.9
31	CA	2783	U	2.9
43	CQ	38	LYS	2.9
11	BK	68	GLU	2.9
28	CB	110	C	2.9
31	CA	115	C	2.9

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Mol	Chain	Res	Type	RSRZ
1	BA	1347	G	2.9
17	AQ	53	CYS	2.9
54	DA	1087	G	2.9
2	AB	74	ARG	2.9
11	BK	65	VAL	2.9
14	BN	97	LYS	2.9
19	BS	58	VAL	2.9
40	CN	36	VAL	2.9
43	CQ	17	VAL	2.9
51	CY	56	MET	2.9
5	AE	115	LEU	2.9
16	BP	6	LEU	2.9
20	AT	20	HIS	2.9
35	CH	106	ALA	2.9
36	DJ	119	GLY	2.9
40	CN	78	LEU	2.9
1	BA	1313	U	2.9
1	BA	1330	U	2.9
2	BB	42	ASN	2.9
15	BO	26	GLU	2.9
30	CD	185	ASN	2.9
34	CG	173	GLU	2.9
31	CA	1092	C	2.9
31	CA	2129	C	2.9
32	CE	191	ASP	2.9
39	CM	73	ILE	2.9
19	AS	39	THR	2.9
44	CR	13	ARG	2.9
2	BB	217	VAL	2.9
10	AJ	36	VAL	2.9
1	BA	104	G	2.9
31	CA	1236	G	2.9
31	CA	1622	G	2.9
36	DJ	44	ALA	2.9
20	BT	65	GLY	2.9
31	CA	272	A	2.9
34	CG	28	GLY	2.9
6	BF	59	TYR	2.9
16	AP	45	GLU	2.9
3	AC	80	LYS	2.9
9	BI	22	LYS	2.9
29	CC	26	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
16	BP	35	ARG	2.9
46	CT	55	ILE	2.9
1	BA	95	C	2.9
2	BB	189	THR	2.9
14	AN	55	SER	2.9
30	CD	5	VAL	2.9
9	BI	69	GLY	2.9
17	BQ	60	GLU	2.9
30	CD	134	HIS	2.9
31	CA	34	U	2.9
31	CA	850	U	2.9
50	CX	70	GLU	2.9
1	BA	167	A	2.9
28	CB	119	A	2.9
31	CA	1088	A	2.9
46	CT	16	LYS	2.9
46	CT	90	LYS	2.9
54	DA	1090	A	2.9
2	BB	208	ARG	2.9
11	BK	98	ARG	2.9
44	CR	92	ARG	2.9
9	AI	28	ILE	2.9
20	BT	32	ILE	2.9
46	CT	103	ILE	2.9
29	CC	240	PHE	2.9
31	CA	2364	C	2.9
2	AB	12	ALA	2.9
4	AD	117	LEU	2.9
34	CG	61	GLY	2.9
1	BA	133	U	2.9
1	BA	1315	U	2.9
3	BC	73	PRO	2.9
31	CA	102	U	2.9
33	CF	72	LYS	2.9
18	AR	48	ARG	2.9
1	BA	1046	A	2.9
1	BA	1246	A	2.9
31	CA	271	G	2.9
31	CA	2742	G	2.9
38	CL	21	CYS	2.9
42	CP	89	ASP	2.9
47	CU	30	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
23	C2	32	GLU	2.9
1	BA	1230	C	2.9
3	AC	43	LEU	2.9
7	AG	110	LYS	2.9
33	CF	61	SER	2.9
31	CA	1454	C	2.9
35	DH	15	LEU	2.9
37	CK	15	TRP	2.9
29	CC	238	ARG	2.9
31	CA	1326	U	2.9
33	CF	5	HIS	2.9
31	CA	1590	A	2.9
38	CL	38	ILE	2.9
31	CA	2414	G	2.9
19	BS	67	VAL	2.9
29	CC	100	GLU	2.9
33	CF	89	VAL	2.9
37	CK	98	GLU	2.9
47	CU	68	LYS	2.9
2	AB	85	LEU	2.9
17	BQ	75	LEU	2.9
20	BT	41	ALA	2.9
24	C3	22	MET	2.9
39	CM	52	GLY	2.9
27	C0	12	SER	2.9
6	AF	97	THR	2.9
7	BG	143	ARG	2.9
34	CG	107	LEU	2.9
1	BA	67	C	2.9
19	BS	33	THR	2.9
31	CA	2863	C	2.9
36	CJ	112	THR	2.9
46	CT	8	ARG	2.9
31	CA	335	C	2.9
54	DA	897	C	2.9
1	BA	943	U	2.9
31	CA	114	U	2.9
39	CM	38	GLN	2.9
44	CR	14	HIS	2.9
51	CY	31	PRO	2.9
29	CC	44	ASN	2.9
32	CE	16	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
33	CF	140	GLU	2.9
30	CD	153	GLY	2.9
33	CF	146	VAL	2.9
37	CK	56	VAL	2.9
38	CL	112	PHE	2.9
43	CQ	30	VAL	2.9
1	BA	377	G	2.9
2	AB	34	ALA	2.9
2	BB	134	ALA	2.9
7	BG	127	ALA	2.9
29	CC	33	LEU	2.9
31	CA	411	G	2.9
31	CA	776	G	2.9
31	CA	1026	G	2.9
31	CA	1166	G	2.9
31	CA	2838	G	2.9
31	CA	198	C	2.8
31	CA	816	C	2.8
31	CA	838	C	2.8
40	CN	60	GLN	2.8
13	BM	78	LYS	2.8
17	AQ	4	LYS	2.8
22	C1	32	LYS	2.8
3	BC	125	GLU	2.8
29	CC	64	ILE	2.8
32	CE	171	ASP	2.8
33	CF	104	ILE	2.8
46	CT	4	ILE	2.8
29	CC	101	ARG	2.8
43	CQ	32	VAL	2.8
46	CT	20	VAL	2.8
53	DI	42	ARG	2.8
53	DI	125	ARG	2.8
1	AA	412	A	2.8
9	AI	16	ALA	2.8
13	AM	40	ALA	2.8
31	CA	866	A	2.8
54	DA	613	A	2.8
1	BA	993	G	2.8
18	AR	24	LYS	2.8
31	CA	583	G	2.8
31	CA	906	U	2.8

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Mol	Chain	Res	Type	RSRZ
31	CA	1037	G	2.8
31	CA	2890	G	2.8
42	CP	68	LYS	2.8
1	AA	1277	C	2.8
1	BA	972	C	2.8
1	BA	999	C	2.8
1	BA	1136	C	2.8
31	CA	1764	C	2.8
34	CG	156	PRO	2.8
36	DJ	118	THR	2.8
37	CK	3	THR	2.8
29	CC	248	TRP	2.8
35	CH	137	GLU	2.8
9	AI	18	ARG	2.8
34	CG	55	ARG	2.8
35	CH	27	ARG	2.8
47	CU	12	ARG	2.8
9	BI	8	GLY	2.8
33	CF	100	PHE	2.8
39	CM	122	VAL	2.8
7	BG	98	ALA	2.8
51	CY	54	LYS	2.8
52	CZ	2	LYS	2.8
1	AA	1492	A	2.8
1	BA	969	A	2.8
31	CA	1871	A	2.8
1	BA	951	G	2.8
1	BA	1370	G	2.8
28	CB	4	C	2.8
28	CB	21	G	2.8
31	CA	242	G	2.8
31	CA	2876	G	2.8
47	CU	29	THR	2.8
37	CK	125	TYR	2.8
29	CC	19	VAL	2.8
35	DH	142	VAL	2.8
36	DJ	140	VAL	2.8
7	AG	66	LEU	2.8
32	DE	11	ALA	2.8
36	DJ	120	ALA	2.8
14	BN	26	GLU	2.8
30	CD	28	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	BA	1227	A	2.8
30	CD	184	ARG	2.8
31	CA	810	U	2.8
31	CA	1443	U	2.8
31	CA	1880	U	2.8
31	CA	1439	A	2.8
31	CA	2147	A	2.8
1	BA	194	C	2.8
1	BA	1277	C	2.8
2	AB	151	ILE	2.8
5	BE	80	THR	2.8
32	CE	48	THR	2.8
46	CT	39	THR	2.8
47	CU	70	HIS	2.8
2	AB	90	PHE	2.8
15	BO	15	PHE	2.8
28	CB	26	C	2.8
29	CC	59	LYS	2.8
31	CA	435	C	2.8
32	CE	158	PHE	2.8
32	CE	176	ASP	2.8
35	CH	17	ASP	2.8
39	CM	11	GLY	2.8
23	C2	42	VAL	2.8
14	AN	27	LEU	2.8
29	CC	202	LEU	2.8
39	CM	61	LEU	2.8
40	CN	124	LEU	2.8
20	BT	55	GLN	2.8
49	CW	75	GLN	2.8
1	BA	1264	U	2.8
14	BN	70	PRO	2.8
29	CC	28	LYS	2.8
1	AA	205	A	2.8
1	AA	1022	A	2.8
1	AA	1534	A	2.8
19	BS	57	HIS	2.8
30	CD	76	GLY	2.8
30	CD	87	GLY	2.8
31	CA	182	A	2.8
31	CA	1525	A	2.8
31	CA	2835	A	2.8

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Mol	Chain	Res	Type	RSRZ
48	CV	58	ILE	2.8
21	AU	12	PHE	2.8
31	CA	2896	C	2.8
9	BI	19	VAL	2.8
37	CK	17	VAL	2.8
6	AF	98	GLU	2.8
31	CA	261	G	2.8
31	CA	1206	G	2.8
1	BA	103	U	2.8
1	BA	1295	U	2.8
31	CA	615	U	2.8
2	AB	17	GLY	2.8
7	BG	14	PRO	2.8
35	DH	88	GLY	2.8
1	AA	1036	A	2.8
19	AS	27	ASP	2.8
31	CA	310	A	2.8
31	CA	666	A	2.8
32	CE	13	THR	2.8
49	CW	60	VAL	2.8
54	DA	2173	A	2.8
31	CA	1708	C	2.8
37	CK	129	GLU	2.8
45	CS	13	ARG	2.8
7	AG	65	ALA	2.8
9	AI	4	ASN	2.8
50	CX	84	ALA	2.8
1	BA	1231	G	2.8
31	CA	1651	G	2.8
31	CA	2046	G	2.8
31	CA	29	U	2.8
3	AC	68	ILE	2.8
32	CE	151	GLY	2.8
49	CW	84	PRO	2.8
9	BI	56	ASP	2.8
7	BG	139	GLU	2.8
9	AI	63	LEU	2.8
32	CE	17	THR	2.8
34	CG	87	LEU	2.8
34	CG	122	THR	2.8
48	CV	82	ARG	2.8
52	CZ	46	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	BA	352	C	2.8
1	BA	1254	A	2.8
20	BT	71	LYS	2.8
28	CB	50	A	2.8
30	CD	75	ALA	2.8
31	CA	179	C	2.8
31	CA	815	C	2.8
52	CZ	60	LYS	2.8
13	BM	8	ASN	2.8
16	BP	29	ASN	2.8
1	AA	1286	U	2.8
1	BA	455	G	2.8
1	BA	1343	G	2.8
28	CB	25	U	2.8
31	CA	408	G	2.8
31	CA	2307	G	2.8
31	CA	2629	U	2.8
31	CA	2859	G	2.8
35	DH	143	ILE	2.8
48	CV	55	PRO	2.8
53	DI	76	PHE	2.8
2	BB	64	LYS	2.8
2	BB	133	GLU	2.8
25	C4	25	LYS	2.8
42	CP	45	SER	2.8
47	CU	27	SER	2.8
34	CG	4	VAL	2.8
48	CV	41	LEU	2.8
53	DI	86	THR	2.8
10	AJ	29	ALA	2.8
31	CA	1327	A	2.7
31	CA	1730	C	2.8
31	CA	2072	C	2.8
9	AI	31	ASN	2.7
16	BP	26	ASN	2.7
54	DA	1088	A	2.7
13	BM	111	GLY	2.7
2	BB	44	GLU	2.7
13	AM	41	GLU	2.7
1	BA	220	G	2.7
1	BA	457	G	2.7
1	BA	1266	G	2.7

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Mol	Chain	Res	Type	RSRZ
1	BA	1334	G	2.7
29	CC	227	PRO	2.7
30	CD	88	GLU	2.7
35	CH	4	ILE	2.7
47	CU	88	LYS	2.7
31	CA	7	G	2.7
31	CA	230	G	2.7
31	CA	535	G	2.7
31	CA	1036	G	2.7
31	CA	1529	G	2.7
2	AB	68	LEU	2.7
8	BH	59	LEU	2.7
49	CW	12	GLN	2.7
32	CE	53	THR	2.7
35	CH	10	ALA	2.7
31	CA	903	C	2.7
54	DA	1076	C	2.7
1	BA	1287	A	2.7
31	CA	71	A	2.7
31	CA	1528	A	2.7
31	CA	1532	A	2.7
31	CA	1609	A	2.7
31	CA	2657	A	2.7
34	CG	66	GLY	2.7
31	CA	87	U	2.7
31	CA	1467	U	2.7
31	CA	1742	U	2.7
35	CH	41	LYS	2.7
40	CN	59	ARG	2.7
3	AC	66	VAL	2.7
18	AR	29	LEU	2.7
1	BA	1003	G	2.7
20	BT	68	HIS	2.7
31	CA	1731	G	2.7
34	DG	111	HIS	2.7
53	DI	55	VAL	2.7
31	CA	273	G	2.7
31	CA	989	G	2.7
34	CG	145	ALA	2.7
10	BJ	31	ARG	2.7
29	CC	127	GLY	2.7
42	CP	75	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
35	DH	76	GLU	2.7
1	BA	1044	A	2.7
3	BC	14	ILE	2.7
3	BC	203	PHE	2.7
31	CA	227	A	2.7
31	CA	432	A	2.7
37	CK	89	PHE	2.7
2	AB	43	LEU	2.7
30	CD	104	VAL	2.7
13	AM	12	HIS	2.7
14	BN	59	ARG	2.7
19	AS	22	ALA	2.7
25	C4	60	ALA	2.7
44	CR	68	ALA	2.7
1	AA	1276	G	2.7
1	BA	1386	G	2.7
1	BA	1454	G	2.7
6	AF	88	MET	2.7
27	C0	10	THR	2.7
31	CA	1311	G	2.7
31	CA	1524	G	2.7
31	CA	1861	G	2.7
45	CS	83	TYR	2.7
1	AA	1028	C	2.7
29	CC	45	ASN	2.7
31	CA	57	C	2.7
12	BL	67	ILE	2.7
16	BP	4	ILE	2.7
31	CA	235	U	2.7
54	DA	1072	C	2.7
2	BB	114	LEU	2.7
3	BC	181	ASP	2.7
31	CA	1608	A	2.7
31	CA	2101	A	2.7
11	AK	80	LYS	2.7
7	BG	51	ALA	2.7
19	AS	57	HIS	2.7
32	CE	72	SER	2.7
42	CP	111	ARG	2.7
48	CV	56	GLY	2.7
1	AA	89	U	2.7
1	BA	1316	G	2.7

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Mol	Chain	Res	Type	RSRZ
31	CA	1250	G	2.7
31	CA	1543	G	2.7
31	CA	2100	G	2.7
31	CA	2130	U	2.7
35	CH	119	ASN	2.7
35	DH	29	PHE	2.7
54	DA	881	G	2.7
1	BA	1342	C	2.7
31	CA	510	C	2.7
31	CA	1079	C	2.7
1	BA	199	A	2.7
10	AJ	77	VAL	2.7
31	CA	216	A	2.7
31	CA	354	A	2.7
40	CN	16	ARG	2.7
16	BP	27	ALA	2.7
32	DE	2	GLU	2.7
42	CP	5	SER	2.7
37	CK	53	TYR	2.7
1	BA	952	U	2.7
3	AC	64	ILE	2.7
7	AG	49	THR	2.7
25	C4	6	THR	2.7
31	CA	1113	U	2.7
34	CG	84	THR	2.7
47	CU	86	THR	2.7
51	CY	29	PHE	2.7
53	DI	11	ILE	2.7
31	CA	1450	G	2.7
47	CU	77	ARG	2.7
11	AK	84	VAL	2.7
43	CQ	41	GLN	2.7
52	DZ	6	LEU	2.7
35	CH	149	GLU	2.7
3	AC	190	HIS	2.7
14	BN	29	ALA	2.7
15	BO	19	ALA	2.7
31	CA	1722	A	2.7
24	C3	15	SER	2.7
34	CG	138	LYS	2.7
47	CU	44	LYS	2.7
2	AB	208	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
3	AC	101	ILE	2.7
28	CB	74	U	2.7
29	CC	212	ARG	2.7
31	CA	1340	U	2.7
31	CA	1963	U	2.7
31	CA	2798	U	2.7
44	CR	94	ILE	2.7
52	CZ	55	THR	2.7
53	DI	82	ILE	2.7
3	BC	84	VAL	2.7
31	CA	1363	C	2.7
35	DH	98	ASP	2.7
35	DH	110	VAL	2.7
36	CJ	106	LEU	2.7
39	CM	143	GLU	2.7
43	CQ	112	GLU	2.7
44	CR	18	LEU	2.7
53	DI	81	LEU	2.7
1	AA	1127	G	2.7
31	CA	258	G	2.7
31	CA	386	G	2.7
31	CA	512	G	2.7
31	CA	799	G	2.7
31	CA	2365	G	2.7
13	BM	106	ALA	2.7
14	BN	101	TRP	2.7
48	CV	71	ALA	2.7
53	DI	91	ALA	2.7
31	CA	1652	A	2.7
31	CA	2766	A	2.7
7	BG	78	ARG	2.7
40	CN	50	ARG	2.7
52	CZ	26	PHE	2.7
1	BA	157	U	2.7
31	CA	112	U	2.7
3	AC	39	VAL	2.7
6	AF	96	VAL	2.7
7	BG	30	LEU	2.7
41	CO	23	ASN	2.7
13	AM	114	LYS	2.7
19	AS	60	VAL	2.7
37	CK	49	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
39	CM	116	VAL	2.7
31	CA	237	C	2.7
31	CA	565	C	2.7
30	CD	182	ALA	2.7
1	BA	177	G	2.7
1	BA	945	G	2.7
25	C4	45	ARG	2.7
31	CA	326	G	2.7
31	CA	855	G	2.7
31	CA	926	G	2.7
31	CA	2148	G	2.7
31	CA	2583	G	2.7
39	CM	50	PHE	2.6
51	CY	50	ARG	2.7
12	BL	105	SER	2.6
1	BA	65	A	2.6
31	CA	1272	A	2.6
31	CA	2358	A	2.6
37	CK	92	MET	2.6
33	CF	44	ILE	2.6
53	DI	98	GLU	2.6
12	AL	73	ASN	2.6
35	DH	18	GLN	2.6
32	CE	120	VAL	2.6
29	CC	237	GLY	2.6
1	BA	87	C	2.6
1	BA	307	C	2.6
10	BJ	79	PRO	2.6
31	CA	433	C	2.6
31	CA	795	C	2.6
39	CM	132	ARG	2.6
1	BA	1475	G	2.6
11	BK	85	MET	2.6
23	C2	9	ILE	2.6
31	CA	1333	G	2.6
31	CA	2692	G	2.6
53	DI	52	MET	2.6
31	CA	1487	U	2.6
31	CA	2109	U	2.6
1	BA	468	A	2.6
1	BA	482	A	2.6
23	C2	34	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
31	CA	94	A	2.6
31	CA	609	A	2.6
31	CA	2814	A	2.6
52	CZ	38	GLN	2.6
7	AG	64	VAL	2.6
7	BG	113	ASP	2.6
42	CP	47	VAL	2.6
49	CW	5	ASN	2.6
51	CY	48	THR	2.6
17	BQ	66	PRO	2.6
34	CG	154	PRO	2.6
11	BK	63	ALA	2.6
31	CA	1135	C	2.6
44	CR	10	ALA	2.6
18	AR	74	HIS	2.6
1	BA	1007	U	2.6
7	BG	83	SER	2.6
29	CC	272	SER	2.6
31	CA	390	U	2.6
1	BA	1215	G	2.6
5	BE	36	LEU	2.6
11	BK	64	GLN	2.6
31	CA	808	G	2.6
31	CA	1867	G	2.6
42	CP	48	LEU	2.6
2	AB	65	GLY	2.6
10	AJ	5	ARG	2.6
20	BT	52	ASN	2.6
31	CA	941	A	2.6
42	CP	74	VAL	2.6
42	CP	81	ARG	2.6
2	BB	46	THR	2.6
37	CK	50	THR	2.6
39	CM	121	THR	2.6
20	BT	16	LYS	2.6
33	CF	70	ALA	2.6
41	CO	68	ALA	2.6
45	CS	81	LYS	2.6
46	CT	58	ALA	2.6
1	BA	1265	C	2.6
21	AU	36	GLU	2.6
2	AB	186	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
14	BN	100	SER	2.6
54	DA	1061	U	2.6
52	CZ	43	LEU	2.6
34	CG	90	VAL	2.6
39	CM	91	ASP	2.6
1	BA	139	A	2.6
1	BA	1039	G	2.6
1	BA	1361	G	2.6
31	CA	48	G	2.6
19	AS	30	PRO	2.6
31	CA	278	A	2.6
31	CA	1024	G	2.6
31	CA	1070	A	2.6
31	CA	2318	G	2.6
31	CA	2363	G	2.6
31	CA	2526	G	2.6
35	DH	104	THR	2.6
40	CN	69	PRO	2.6
44	CR	57	PHE	2.6
1	BA	1149	C	2.6
1	BA	1228	C	2.6
1	BA	1383	C	2.6
31	CA	581	C	2.6
20	BT	39	ILE	2.6
9	BI	85	ARG	2.6
9	BI	87	LEU	2.6
31	CA	653	U	2.6
36	DJ	39	CYS	2.6
47	CU	32	LEU	2.6
53	DI	59	LEU	2.6
23	C2	25	LYS	2.6
36	DJ	16	GLY	2.6
11	BK	94	GLU	2.6
22	C1	45	ALA	2.6
1	BA	1339	A	2.6
3	AC	191	THR	2.6
8	BH	49	PHE	2.6
31	CA	575	A	2.6
2	BB	151	ILE	2.6
20	BT	29	ARG	2.6
14	BN	66	GLN	2.6
31	CA	2177	C	2.6

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Mol	Chain	Res	Type	RSRZ
31	CA	2260	C	2.6
32	CE	136	GLN	2.6
1	BA	1301	U	2.6
31	CA	2244	U	2.6
39	CM	1	MET	2.6
48	CV	44	LYS	2.6
49	CW	50	MET	2.6
2	AB	114	LEU	2.6
42	CP	44	GLY	2.6
42	CP	83	LEU	2.6
12	BL	16	VAL	2.6
30	CD	45	TYR	2.6
44	CR	27	ALA	2.6
44	CR	42	ALA	2.6
12	BL	14	ARG	2.6
1	BA	1067	A	2.6
24	C3	24	THR	2.6
31	CA	377	G	2.6
31	CA	488	G	2.6
31	CA	526	A	2.6
31	CA	633	A	2.6
31	CA	1091	G	2.6
31	CA	1225	G	2.6
38	CL	3	GLN	2.6
3	BC	74	GLY	2.6
7	AG	55	GLY	2.6
9	AI	82	GLY	2.6
24	D3	1	MET	2.6
29	CC	243	HIS	2.6
31	CA	2423	U	2.6
34	CG	91	GLY	2.6
38	CL	68	GLY	2.6
54	DA	143	C	2.6
46	CT	45	VAL	2.6
42	CP	82	ALA	2.6
2	AB	45	LYS	2.6
47	CU	92	ASN	2.6
49	CW	10	LYS	2.6
2	AB	60	ILE	2.6
22	C1	33	THR	2.6
3	AC	81	GLY	2.6
1	BA	1290	G	2.6

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Mol	Chain	Res	Type	RSRZ
10	BJ	56	HIS	2.6
31	CA	2149	U	2.6
31	CA	2157	G	2.6
31	CA	2449	U	2.6
39	CM	112	LEU	2.6
29	CC	180	GLU	2.6
34	CG	130	GLU	2.6
54	DA	893	C	2.6
38	CL	37	ASP	2.6
45	CS	102	SER	2.6
39	CM	29	LYS	2.6
41	CO	8	ARG	2.6
12	BL	23	ALA	2.6
20	AT	87	ALA	2.6
33	CF	2	ALA	2.6
35	CH	111	ALA	2.6
48	CV	99	ASN	2.6
40	CN	45	GLN	2.5
40	CN	54	THR	2.5
41	CO	33	ILE	2.5
48	CV	103	ILE	2.5
52	CZ	39	GLN	2.5
11	AK	96	THR	2.5
40	CN	90	GLU	2.5
52	DZ	5	GLU	2.5
1	BA	532	A	2.5
1	BA	221	C	2.5
5	BE	159	LYS	2.5
27	C0	19	LYS	2.5
31	CA	1909	C	2.5
33	CF	145	LYS	2.5
34	CG	15	VAL	2.5
37	CK	34	ARG	2.5
48	CV	70	VAL	2.5
53	DI	8	LYS	2.5
53	DI	26	VAL	2.5
53	DI	50	VAL	2.5
3	AC	168	TYR	2.5
9	AI	64	TYR	2.5
28	CB	116	G	2.5
29	CC	62	TYR	2.5
31	CA	46	G	2.5

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Mol	Chain	Res	Type	RSRZ
31	CA	178	G	2.5
31	CA	536	G	2.5
7	BG	26	PHE	2.5
2	BB	65	GLY	2.5
2	BB	202	GLY	2.5
13	AM	47	GLU	2.5
33	CF	16	LEU	2.5
47	CU	4	GLU	2.5
29	CC	265	LYS	2.5
31	CA	2132	U	2.5
53	DI	80	THR	2.5
16	BP	19	VAL	2.5
35	DH	108	VAL	2.5
1	AA	183	C	2.5
1	BA	848	C	2.5
1	BA	1145	A	2.5
31	CA	1302	A	2.5
45	CS	95	ASP	2.5
1	BA	1223	C	2.5
45	CS	53	PHE	2.5
48	CV	85	PHE	2.5
54	DA	2179	C	2.5
28	CB	41	G	2.5
31	CA	2186	G	2.5
9	AI	23	PRO	2.5
29	CC	60	GLN	2.5
32	DE	9	GLN	2.5
32	CE	108	ILE	2.5
37	CK	83	GLY	2.5
18	AR	68	LEU	2.5
24	C3	21	ARG	2.5
46	CT	46	LEU	2.5
31	CA	2871	U	2.5
32	CE	100	MET	2.5
19	AS	67	VAL	2.5
20	BT	58	VAL	2.5
23	C2	19	HIS	2.5
51	CY	4	VAL	2.5
42	CP	2	ASP	2.5
53	DI	29	ASP	2.5
1	BA	1226	C	2.5
31	CA	222	A	2.5

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Mol	Chain	Res	Type	RSRZ
31	CA	2047	C	2.5
31	CA	2411	A	2.5
43	CQ	19	SER	2.5
10	AJ	43	PRO	2.5
10	BJ	78	GLU	2.5
5	BE	157	ARG	2.5
9	AI	33	ARG	2.5
9	BI	65	ILE	2.5
19	AS	3	ARG	2.5
19	BS	46	GLY	2.5
20	BT	84	ASN	2.5
31	CA	1355	G	2.5
31	CA	1430	G	2.5
31	CA	1910	G	2.5
31	CA	2238	G	2.5
44	CR	66	ASN	2.5
54	DA	2152	G	2.5
29	CC	93	LEU	2.5
43	CQ	114	LEU	2.5
1	BA	88	U	2.5
16	AP	21	VAL	2.5
30	CD	20	VAL	2.5
31	CA	1438	U	2.5
10	BJ	70	HIS	2.5
30	CD	133	THR	2.5
33	CF	18	THR	2.5
10	BJ	66	GLU	2.5
14	AN	47	LYS	2.5
32	DE	6	LYS	2.5
31	CA	394	C	2.5
31	CA	1278	C	2.5
35	CH	69	ALA	2.5
53	DI	107	GLU	2.5
3	BC	54	ARG	2.5
7	AG	82	GLY	2.5
11	AK	98	ARG	2.5
17	BQ	64	CYS	2.5
31	CA	52	A	2.5
31	CA	244	A	2.5
31	CA	1254	A	2.5
33	CF	82	GLY	2.5
39	CM	65	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	BB	41	ILE	2.5
2	BB	214	LEU	2.5
1	AA	1034	G	2.5
1	BA	61	G	2.5
28	CB	64	G	2.5
31	CA	1455	G	2.5
31	CA	1647	U	2.5
31	CA	2242	G	2.5
35	CH	103	VAL	2.5
13	BM	27	LYS	2.5
18	AR	47	THR	2.5
20	BT	19	LYS	2.5
22	C1	12	LYS	2.5
22	C1	44	THR	2.5
35	CH	135	HIS	2.5
43	CQ	25	THR	2.5
37	CK	9	GLU	2.5
38	CL	83	ALA	2.5
44	CR	67	ALA	2.5
39	CM	34	GLY	2.5
1	BA	461	A	2.5
19	BS	16	LEU	2.5
31	CA	118	A	2.5
31	CA	631	A	2.5
35	CH	80	ILE	2.5
37	CK	140	LEU	2.5
1	AA	121	U	2.5
5	BE	46	VAL	2.5
33	CF	78	LYS	2.5
48	CV	17	LYS	2.5
2	BB	30	PHE	2.5
8	BH	90	ASP	2.5
31	CA	15	G	2.5
31	CA	260	G	2.5
31	CA	277	G	2.5
31	CA	1719	G	2.5
31	CA	2732	G	2.5
35	CH	123	ARG	2.5
35	CH	128	HIS	2.5
39	CM	76	GLU	2.5
23	C2	17	THR	2.5
34	CG	13	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
41	CO	111	ALA	2.5
2	AB	124	GLY	2.5
41	CO	105	GLY	2.5
22	C1	29	SER	2.5
31	CA	240	C	2.5
31	CA	1986	C	2.5
31	CA	2178	C	2.5
31	CA	2787	C	2.5
50	CX	74	PRO	2.5
1	BA	197	A	2.5
1	BA	1324	A	2.5
31	CA	1847	A	2.5
54	DA	1084	A	2.5
2	AB	187	VAL	2.5
17	BQ	13	VAL	2.5
17	BQ	23	VAL	2.5
35	CH	45	GLU	2.5
54	DA	1176	U	2.5
46	CT	110	ARG	2.5
13	AM	38	GLY	2.5
15	BO	7	ALA	2.5
31	CA	333	G	2.5
31	CA	604	G	2.5
31	CA	883	G	2.5
31	CA	1248	G	2.5
31	CA	1361	G	2.5
31	CA	1521	G	2.5
32	CE	50	ALA	2.5
33	CF	168	ALA	2.5
35	DH	148	ALA	2.5
2	AB	31	ILE	2.5
29	CC	74	ILE	2.5
30	CD	204	LYS	2.5
1	BA	469	C	2.5
2	BB	191	SER	2.5
5	BE	115	LEU	2.5
29	CC	259	SER	2.5
31	CA	385	C	2.5
31	CA	1726	C	2.5
26	C5	13	ASN	2.5
28	CB	32	U	2.5
1	BA	1269	A	2.5

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Mol	Chain	Res	Type	RSRZ
2	AB	50	PHE	2.5
3	BC	112	ASP	2.5
31	CA	1598	A	2.5
31	CA	1635	A	2.5
54	DA	1073	A	2.5
2	AB	64	LYS	2.5
3	BC	123	GLN	2.5
29	CC	15	HIS	2.5
39	CM	72	ALA	2.5
25	C4	38	THR	2.5
1	BA	1365	G	2.5
11	AK	42	LEU	2.5
15	BO	67	LEU	2.5
28	CB	96	G	2.5
31	CA	54	G	2.5
31	CA	2816	G	2.5
43	DQ	114	LEU	2.5
14	AN	26	GLU	2.4
48	DV	48	PRO	2.4
1	BA	1148	U	2.4
1	BA	1205	U	2.4
12	BL	119	VAL	2.4
21	BU	9	ASN	2.4
28	CB	28	C	2.4
31	CA	2066	C	2.4
31	CA	2146	C	2.4
41	CO	107	ASN	2.4
44	CR	110	VAL	2.4
54	DA	1058	U	2.4
2	BB	153	ASP	2.4
1	BA	1213	A	2.4
13	BM	91	HIS	2.4
13	BM	100	GLN	2.4
6	BF	92	THR	2.4
49	CW	20	LEU	2.4
3	BC	122	SER	2.4
14	BN	5	SER	2.4
31	CA	1633	G	2.4
54	DA	1059	G	2.4
1	AA	1148	U	2.4
21	AU	37	PHE	2.4
31	CA	306	U	2.4

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Mol	Chain	Res	Type	RSRZ
31	CA	817	C	2.4
31	CA	1507	C	2.4
31	CA	2522	U	2.4
43	CQ	14	LYS	2.4
2	BB	156	GLY	2.4
39	CM	53	GLY	2.4
41	CO	101	GLY	2.4
29	CC	210	ALA	2.4
30	CD	102	ALA	2.4
1	BA	152	A	2.4
14	BN	71	HIS	2.4
31	CA	255	A	2.4
11	BK	97	ILE	2.4
12	BL	86	ARG	2.4
2	BB	193	PRO	2.4
33	CF	120	LYS	2.4
50	CX	66	LYS	2.4
14	BN	14	VAL	2.4
16	AP	38	PHE	2.4
31	CA	67	U	2.4
1	BA	351	G	2.4
31	CA	27	G	2.4
31	CA	690	G	2.4
31	CA	897	C	2.4
31	CA	1466	U	2.4
31	CA	1732	C	2.4
31	CA	2275	C	2.4
34	CG	101	ASN	2.4
54	DA	1083	U	2.4
5	AE	82	GLN	2.4
11	BK	43	GLY	2.4
2	AB	83	ALA	2.4
11	AK	56	ARG	2.4
14	BN	15	ALA	2.4
26	C5	24	ARG	2.4
35	CH	59	ALA	2.4
35	CH	65	ALA	2.4
26	C5	30	GLU	2.4
31	CA	547	A	2.4
31	CA	2059	A	2.4
31	CA	2322	A	2.4
31	CA	2346	A	2.4

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Mol	Chain	Res	Type	RSRZ
33	CF	9	LYS	2.4
40	CN	74	THR	2.4
29	CC	231	PRO	2.4
29	CC	204	VAL	2.4
45	CS	77	PHE	2.4
53	DI	33	VAL	2.4
31	CA	366	C	2.4
31	CA	420	C	2.4
31	CA	509	C	2.4
31	CA	540	C	2.4
31	CA	2310	C	2.4
39	CM	33	ARG	2.4
1	AA	1033	G	2.4
10	BJ	29	ALA	2.4
31	CA	2152	G	2.4
33	CF	134	GLU	2.4
34	CG	123	ALA	2.4
2	BB	15	HIS	2.4
7	BG	124	LEU	2.4
30	CD	2	ILE	2.4
36	DJ	122	ILE	2.4
11	AK	16	VAL	2.4
16	BP	15	PRO	2.4
31	CA	6	A	2.4
31	CA	1260	A	2.4
50	CX	43	THR	2.4
43	CQ	92	VAL	2.4
9	BI	34	SER	2.4
33	CF	166	GLY	2.4
3	AC	105	GLU	2.4
51	CY	16	ASN	2.4
11	BK	25	ALA	2.4
35	CH	39	ALA	2.4
37	CK	20	ALA	2.4
42	CP	71	ALA	2.4
53	DI	83	ALA	2.4
54	DA	1727	C	2.4
2	AB	41	ILE	2.4
7	AG	120	LEU	2.4
8	BH	121	LEU	2.4
12	BL	49	LEU	2.4
54	DA	2107	G	2.4

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Mol	Chain	Res	Type	RSRZ
2	BB	107	VAL	2.4
29	CC	29	PRO	2.4
8	BH	122	GLY	2.4
31	CA	149	A	2.4
31	CA	1096	A	2.4
31	CA	1142	A	2.4
35	DH	123	ARG	2.4
43	CQ	101	ARG	2.4
2	BB	226	SER	2.4
20	BT	13	GLN	2.4
24	C3	2	LYS	2.4
31	CA	1486	U	2.4
31	CA	2079	U	2.4
36	DJ	64	ASP	2.4
41	CO	99	LYS	2.4
45	CS	71	LYS	2.4
40	CN	17	ASN	2.4
5	BE	75	ALA	2.4
12	BL	113	ALA	2.4
16	BP	7	ALA	2.4
34	CG	68	ALA	2.4
35	CH	105	ALA	2.4
31	CA	854	C	2.4
15	BO	3	LEU	2.4
30	CD	138	LEU	2.4
36	CJ	109	ILE	2.4
50	CX	80	ILE	2.4
53	DI	95	LEU	2.4
1	AA	1024	G	2.4
1	BA	944	G	2.4
11	BK	13	ARG	2.4
21	BU	17	ARG	2.4
31	CA	205	G	2.4
31	CA	489	G	2.4
31	CA	539	G	2.4
3	BC	15	VAL	2.4
13	AM	62	LYS	2.4
31	CA	1186	G	2.4
33	CF	108	VAL	2.4
39	CM	36	LYS	2.4
40	CN	9	PHE	2.4
1	BA	992	U	2.4

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Mol	Chain	Res	Type	RSRZ
7	BG	123	GLU	2.4
15	BO	79	THR	2.4
35	DH	92	GLY	2.4
31	CA	392	U	2.4
1	BA	66	A	2.4
1	BA	1036	A	2.4
11	AK	38	GLN	2.4
31	CA	677	A	2.4
31	CA	1354	A	2.4
31	CA	1508	A	2.4
31	CA	1522	A	2.4
51	CY	39	TRP	2.4
35	CH	20	ASN	2.4
53	DI	22	ALA	2.4
9	BI	72	ILE	2.4
31	CA	672	C	2.4
35	CH	12	LEU	2.4
22	C1	42	HIS	2.4
24	C3	39	ARG	2.4
32	CE	44	ARG	2.4
34	CG	29	LYS	2.4
39	CM	69	ARG	2.4
41	CO	45	ARG	2.4
9	AI	47	VAL	2.4
19	BS	20	GLU	2.4
34	CG	135	GLY	2.4
40	CN	77	PRO	2.4
50	CX	27	GLY	2.4
51	CY	15	GLY	2.4
18	AR	32	TYR	2.4
3	BC	70	THR	2.4
31	CA	543	G	2.4
31	CA	1983	G	2.4
31	CA	2061	G	2.4
31	CA	2409	G	2.4
42	CP	19	GLN	2.4
46	CT	68	ASP	2.4
28	CB	29	A	2.4
30	CD	95	SER	2.4
31	CA	1496	A	2.4
31	CA	2060	A	2.4
31	CA	2154	A	2.4

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Mol	Chain	Res	Type	RSRZ
31	CA	2758	A	2.4
31	CA	2778	A	2.4
42	CP	77	ALA	2.4
54	DA	1080	A	2.4
16	AP	74	LEU	2.4
17	BQ	67	LEU	2.4
21	AU	34	ARG	2.4
23	C2	48	ILE	2.4
36	CJ	103	ARG	2.4
1	BA	990	C	2.4
31	CA	351	C	2.4
31	CA	680	C	2.4
2	AB	39	HIS	2.3
7	BG	27	VAL	2.3
10	BJ	51	VAL	2.3
45	CS	4	VAL	2.3
43	CQ	18	PRO	2.3
1	AA	1029	U	2.3
31	CA	1865	U	2.3
2	AB	211	THR	2.3
32	CE	84	THR	2.3
7	AG	39	ALA	2.3
8	BH	116	ALA	2.3
31	CA	185	G	2.3
31	CA	620	G	2.3
31	CA	875	G	2.3
31	CA	1116	G	2.3
45	CS	42	ALA	2.3
24	C3	13	ASN	2.3
46	CT	96	ILE	2.3
48	CV	74	ASN	2.3
49	CW	79	ARG	2.3
1	AA	80	A	2.3
1	BA	55	A	2.3
28	CB	15	A	2.3
31	CA	2071	A	2.3
31	CA	2639	A	2.3
31	CA	517	C	2.3
31	CA	1306	C	2.3
31	CA	2888	C	2.3
2	BB	159	ASP	2.3
23	C2	38	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
31	CA	1097	U	2.3
34	CG	164	TYR	2.3
45	CS	76	LYS	2.3
24	C3	28	ARG	2.3
6	AF	66	ALA	2.3
29	CC	257	THR	2.3
42	CP	72	ALA	2.3
49	CW	74	ALA	2.3
37	CK	36	LEU	2.3
1	BA	69	G	2.3
1	BA	846	G	2.3
6	AF	42	TRP	2.3
31	CA	26	G	2.3
31	CA	248	G	2.3
31	CA	2633	G	2.3
1	AA	1	A	2.3
1	BA	1042	A	2.3
2	AB	162	PHE	2.3
31	CA	2753	A	2.3
54	DA	2311	A	2.3
1	BA	381	C	2.3
1	BA	1066	C	2.3
11	AK	32	VAL	2.3
20	AT	61	GLN	2.3
21	BU	6	VAL	2.3
29	CC	65	VAL	2.3
30	CD	203	VAL	2.3
31	CA	2248	C	2.3
34	CG	22	GLN	2.3
35	DH	141	LYS	2.3
13	BM	82	ASP	2.3
21	AU	13	ASP	2.3
31	CA	2296	U	2.3
13	AM	37	ALA	2.3
34	CG	65	ALA	2.3
41	CO	91	ALA	2.3
21	BU	8	GLU	2.3
34	CG	34	THR	2.3
40	CN	126	ILE	2.3
47	CU	78	SER	2.3
2	AB	115	LYS	2.3
14	AN	98	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	BA	1150	A	2.3
17	BQ	29	VAL	2.3
1	BA	1132	C	2.3
2	AB	21	ARG	2.3
5	BE	123	VAL	2.3
10	AJ	37	ARG	2.3
29	CC	232	HIS	2.3
31	CA	515	A	2.3
31	CA	1137	G	2.3
31	CA	1616	A	2.3
31	CA	1866	A	2.3
31	CA	2311	A	2.3
31	CA	2367	G	2.3
31	CA	2435	A	2.3
31	CA	2654	A	2.3
41	CO	64	ARG	2.3
54	DA	278	A	2.3
31	CA	898	C	2.3
31	CA	1117	C	2.3
31	CA	1208	C	2.3
31	CA	2830	C	2.3
8	BH	54	ASP	2.3
13	AM	10	PRO	2.3
31	CA	2312	U	2.3
31	CA	2818	U	2.3
39	CM	56	PRO	2.3
37	CK	118	MET	2.3
40	CN	103	TYR	2.3
9	BI	78	ALA	2.3
8	BH	89	LYS	2.3
14	AN	3	LYS	2.3
32	CE	63	LYS	2.3
19	BS	4	SER	2.3
35	CH	34	GLY	2.3
6	BF	91	ARG	2.3
13	AM	113	ARG	2.3
26	C5	36	ARG	2.3
25	C4	26	HIS	2.3
1	AA	1001	C	2.3
1	BA	1367	C	2.3
31	CA	381	G	2.3
19	BS	64	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
31	CA	393	C	2.3
31	CA	584	C	2.3
31	CA	622	G	2.3
31	CA	640	C	2.3
31	CA	1621	U	2.3
31	CA	2527	C	2.3
31	CA	2815	C	2.3
31	CA	2903	U	2.3
9	BI	13	LYS	2.3
11	AK	75	LYS	2.3
11	BK	66	ALA	2.3
44	CR	15	LYS	2.3
7	BG	7	ILE	2.3
29	CC	41	GLY	2.3
14	BN	62	ASN	2.3
18	AR	73	ARG	2.3
21	BU	19	PHE	2.3
30	CD	82	PHE	2.3
34	CG	53	GLY	2.3
50	DX	10	THR	2.3
13	AM	50	GLU	2.3
37	CK	47	HIS	2.3
31	CA	2321	U	2.3
31	CA	1353	A	2.3
31	CA	1358	G	2.3
31	CA	1456	G	2.3
31	CA	1922	G	2.3
31	CA	2325	G	2.3
31	CA	2630	G	2.3
31	CA	2795	C	2.3
33	CF	46	ASP	2.3
49	CW	14	LYS	2.3
1	BA	973	G	2.3
2	AB	111	ILE	2.3
14	BN	96	LEU	2.3
19	AS	47	LEU	2.3
29	CC	112	ALA	2.3
31	CA	132	G	2.3
31	CA	971	G	2.3
54	DA	1870	C	2.3
41	CO	88	ALA	2.3
33	CF	115	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
32	CE	70	SER	2.3
36	CJ	102	SER	2.3
37	CK	131	ASN	2.3
31	CA	2845	U	2.3
7	BG	10	ARG	2.3
30	CD	71	ALA	2.3
31	CA	105	C	2.3
31	CA	1323	C	2.3
31	CA	1728	C	2.3
31	CA	2104	C	2.3
7	BG	29	ILE	2.3
11	AK	107	ILE	2.3
26	C5	23	ILE	2.3
31	CA	320	A	2.3
31	CA	1021	A	2.3
31	CA	1134	A	2.3
31	CA	1469	A	2.3
42	CP	15	ARG	2.3
6	AF	8	PHE	2.3
12	BL	34	CYS	2.3
29	CC	266	PHE	2.3
31	CA	175	G	2.3
31	CA	254	G	2.3
31	CA	1555	G	2.3
31	CA	1642	G	2.3
30	CD	49	GLN	2.3
7	AG	105	VAL	2.3
11	AK	129	VAL	2.3
11	BK	84	VAL	2.3
30	CD	17	GLU	2.3
35	DH	20	ASN	2.3
36	CJ	40	LYS	2.3
32	DE	14	VAL	2.3
42	CP	84	GLU	2.3
1	AA	84	U	2.3
1	BA	1358	U	2.3
2	BB	74	ARG	2.3
2	BB	104	TRP	2.3
17	BQ	11	ARG	2.3
31	CA	25	U	2.3
32	CE	29	HIS	2.3
35	DH	128	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
2	AB	202	GLY	2.3
31	CA	1472	C	2.3
31	CA	2793	C	2.3
54	DA	1075	C	2.3
1	BA	74	A	2.3
1	BA	994	A	2.3
31	CA	804	A	2.3
35	DH	8	LYS	2.3
54	DA	1057	A	2.3
2	AB	89	GLN	2.3
31	CA	491	G	2.3
31	CA	1445	G	2.3
31	CA	2688	G	2.3
32	CE	51	GLU	2.3
36	DJ	141	GLU	2.3
22	C1	54	VAL	2.2
30	CD	34	VAL	2.2
53	DI	4	ASN	2.2
39	CM	40	SER	2.2
4	AD	154	ARG	2.2
25	C4	8	ARG	2.2
34	CG	3	ARG	2.2
1	BA	960	U	2.2
3	BC	190	HIS	2.2
15	BO	18	ASP	2.2
31	CA	2491	U	2.2
35	DH	7	ASP	2.2
7	AG	61	ALA	2.2
15	BO	11	ILE	2.2
17	AQ	10	GLY	2.2
34	CG	37	LEU	2.2
36	DJ	74	PRO	2.2
21	AU	5	LYS	2.2
37	CK	126	ALA	2.2
1	BA	1384	C	2.2
2	BB	69	PHE	2.2
11	AK	94	GLU	2.2
31	CA	2153	C	2.2
32	CE	2	GLU	2.2
27	C0	38	ARG	2.2
39	CM	110	VAL	2.2
16	BP	3	THR	2.2

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Mol	Chain	Res	Type	RSRZ
28	CB	18	G	2.2
31	CA	396	G	2.2
31	CA	1401	G	2.2
31	CA	2852	G	2.2
35	CH	79	THR	2.2
1	AA	1125	U	2.2
1	BA	84	U	2.2
2	AB	84	ALA	2.2
22	C1	19	HIS	2.2
40	CN	71	LYS	2.2
45	CS	57	GLY	2.2
26	C5	37	GLN	2.2
31	CA	995	C	2.2
9	AI	58	VAL	2.2
46	CT	18	ARG	2.2
49	CW	9	ARG	2.2
1	BA	71	A	2.2
1	BA	609	A	2.2
28	CB	53	A	2.2
29	CC	97	LYS	2.2
54	DA	2154	A	2.2
54	DA	2169	A	2.2
54	DA	2886[A]	A	2.2
3	BC	44	THR	2.2
1	AA	1187	G	2.2
1	BA	991	U	2.2
9	AI	91	ASP	2.2
5	BE	124	LEU	2.2
10	AJ	10	LEU	2.2
26	C5	21	GLY	2.2
31	CA	1296	G	2.2
31	CA	1429	G	2.2
35	DH	13	GLY	2.2
41	CO	72	ASP	2.2
31	CA	1	G	2.2
31	CA	58	G	2.2
31	CA	801	G	2.2
3	AC	77	ILE	2.2
10	BJ	18	ILE	2.2
16	AP	75	ILE	2.2
35	DH	44	ILE	2.2
35	DH	69	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
42	CP	57	ALA	2.2
49	CW	16	ALA	2.2
29	CC	6	CYS	2.2
46	CT	1	MET	2.2
2	AB	7	ARG	2.2
3	AC	127	ARG	2.2
34	CG	149	ARG	2.2
9	BI	120	LYS	2.2
20	AT	58	VAL	2.2
23	C2	50	LYS	2.2
29	CC	268	VAL	2.2
31	CA	1488	C	2.2
48	CV	97	LYS	2.2
20	BT	70	ASN	2.2
43	DQ	115	ASN	2.2
1	BA	263	A	2.2
3	BC	87	LEU	2.2
31	CA	1779	U	2.2
31	CA	2690	U	2.2
35	DH	54	LEU	2.2
39	CM	37	GLY	2.2
36	DJ	123	GLU	2.2
37	CK	78	THR	2.2
51	CY	2	SER	2.2
15	BO	14	GLU	2.2
39	CM	51	GLU	2.2
27	C0	14	ILE	2.2
35	DH	4	ILE	2.2
51	CY	73	ALA	2.2
10	AJ	62	ARG	2.2
23	D2	28	ARG	2.2
29	CC	270	ARG	2.2
31	CA	1300	G	2.2
31	CA	1382	G	2.2
31	CA	1540	G	2.2
40	CN	6	ARG	2.2
40	CN	40	ARG	2.2
2	BB	87	CYS	2.2
16	AP	46	LYS	2.2
24	C3	25	LYS	2.2
1	BA	1200	C	2.2
27	C0	36	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
28	CB	47	C	2.2
30	CD	92	VAL	2.2
31	CA	334	C	2.2
31	CA	1053	C	2.2
31	CA	1398	C	2.2
31	CA	2200	C	2.2
31	CA	2681	C	2.2
53	DI	108	VAL	2.2
3	AC	83	ASP	2.2
4	AD	113	GLU	2.2
9	BI	89	GLU	2.2
36	DJ	29	GLY	2.2
37	CK	38	GLY	2.2
39	CM	22	GLY	2.2
39	CM	49	GLY	2.2
1	BA	478	A	2.2
1	BA	978	A	2.2
1	BA	1151	A	2.2
16	AP	50	THR	2.2
31	CA	243	U	2.2
45	CS	23	GLU	2.2
31	CA	1916	A	2.2
31	CA	2433	A	2.2
12	BL	51	LYS	2.2
13	AM	96	PRO	2.2
32	CE	68	ALA	2.2
32	CE	102	ARG	2.2
35	CH	63	ALA	2.2
39	CM	41	ARG	2.2
41	CO	77	ALA	2.2
49	CW	63	ILE	2.2
53	DI	113	PHE	2.2
25	C4	3	LYS	2.2
29	CC	83	TYR	2.2
31	CA	768	G	2.2
31	CA	841	G	2.2
31	CA	1449	G	2.2
31	CA	1860	G	2.2
31	CA	2029	G	2.2
54	DA	1074	G	2.2
3	BC	116	VAL	2.2
11	AK	74	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
36	DJ	9	VAL	2.2
1	BA	995	C	2.2
1	BA	1112	C	2.2
31	CA	238	C	2.2
31	CA	1607	C	2.2
1	BA	1123	U	2.2
2	BB	68	LEU	2.2
12	BL	114	ARG	2.2
22	C1	28	LEU	2.2
30	CD	200	ASP	2.2
26	C5	15	LYS	2.2
31	CA	2743	U	2.2
34	DG	99	LYS	2.2
42	CP	7	ARG	2.2
43	CQ	40	LEU	2.2
44	CR	22	LYS	2.2
54	DA	2797	U	2.2
2	AB	67	ILE	2.2
9	AI	9	THR	2.2
11	BK	102	ALA	2.2
20	AT	80	THR	2.2
24	C3	8	SER	2.2
38	CL	14	SER	2.2
38	CL	109	SER	2.2
1	AA	306	A	2.2
1	BA	459	A	2.2
1	BA	1318	A	2.2
31	CA	1287	A	2.2
31	CA	2837	A	2.2
36	DJ	31	GLN	2.2
36	DJ	105	GLN	2.2
12	BL	52	VAL	2.2
51	CY	7	VAL	2.2
9	BI	53	GLU	2.2
31	CA	1421	G	2.2
34	CG	170	ARG	2.2
40	CN	92	TRP	2.2
1	BA	322	C	2.2
1	BA	1325	C	2.2
1	BA	1460	C	2.2
52	DZ	2	LYS	2.2
9	AI	94	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
31	CA	2807	U	2.2
3	BC	69	HIS	2.2
9	BI	51	PRO	2.2
19	AS	77	THR	2.2
42	CP	91	SER	2.2
47	DU	24	MET	2.2
28	CB	73	A	2.2
31	CA	196	A	2.2
31	CA	699	A	2.2
31	CA	1156	A	2.2
31	CA	1876	A	2.2
7	AG	60	GLU	2.2
8	BH	71	VAL	2.2
21	AU	8	GLU	2.2
29	CC	18	LYS	2.2
39	CM	136	GLU	2.2
47	CU	18	GLU	2.2
9	AI	8	GLY	2.2
30	CD	135	GLY	2.2
32	CE	40	ARG	2.2
44	CR	28	ARG	2.2
45	CS	90	ARG	2.2
1	AA	1320	C	2.2
1	BA	64	G	2.2
1	BA	93	U	2.2
31	CA	246	C	2.2
31	CA	537	G	2.2
31	CA	585	G	2.2
31	CA	1071	G	2.2
31	CA	1148	U	2.2
31	CA	1408	G	2.2
31	CA	1409	U	2.2
31	CA	2712	C	2.2
43	CQ	24	ASP	2.2
37	CK	67	ASN	2.2
39	CM	66	PHE	2.2
41	CO	11	ASN	2.2
49	CW	26	PHE	2.2
54	DA	2156	G	2.2
8	BH	36	ILE	2.2
11	AK	45	ALA	2.2
17	AQ	21	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
32	CE	39	ALA	2.2
32	CE	182	ALA	2.2
49	CW	40	ILE	2.2
2	AB	154	MET	2.2
4	AD	178	MET	2.2
30	CD	23	PRO	2.2
41	CO	39	PRO	2.2
9	AI	66	THR	2.2
3	BC	72	ARG	2.2
3	BC	88	ARG	2.2
19	AS	51	VAL	2.2
31	CA	1877	A	2.2
43	CQ	26	VAL	2.2
2	AB	57	LEU	2.1
19	AS	15	LEU	2.1
1	BA	1051	C	2.1
17	AQ	9	GLN	2.1
31	CA	106	C	2.1
31	CA	667	U	2.1
42	CP	23	ALA	2.1
1	BA	112	G	2.1
9	AI	27	LYS	2.1
31	CA	914	G	2.1
31	CA	1645	G	2.1
31	CA	1992	G	2.1
31	CA	2286	G	2.1
31	CA	2659	G	2.1
52	CZ	9	LYS	2.1
2	BB	108	ARG	2.1
9	BI	49	ARG	2.1
16	BP	28	ARG	2.1
29	CC	223	THR	2.1
29	CC	230	HIS	2.1
11	BK	20	VAL	2.1
29	CC	172	VAL	2.1
34	CG	14	GLY	2.1
31	CA	2850	A	2.1
11	BK	100	LEU	2.1
13	AM	63	PHE	2.1
19	AS	74	PHE	2.1
20	BT	31	PHE	2.1
37	CK	60	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
46	CT	109	ASP	2.1
52	DZ	49	ASP	2.1
1	BA	467	U	2.1
2	AB	132	LYS	2.1
2	BB	111	ILE	2.1
6	AF	6	ILE	2.1
10	AJ	20	GLN	2.1
30	CD	146	ILE	2.1
31	CA	2473	U	2.1
34	CG	97	ALA	2.1
35	DH	39	ALA	2.1
1	BA	267	C	2.1
31	CA	445	C	2.1
31	CA	1102	C	2.1
32	CE	25	GLU	2.1
40	CN	47	GLU	2.1
45	CS	43	ASN	2.1
2	BB	154	MET	2.1
53	DI	89	PRO	2.1
1	AA	201	G	2.1
1	BA	1309	G	2.1
30	CD	199	SER	2.1
31	CA	17	G	2.1
54	DA	1171	G	2.1
12	BL	93	VAL	2.1
32	CE	14	VAL	2.1
45	CS	67	GLY	2.1
16	BP	32	PHE	2.1
32	CE	99	LYS	2.1
35	CH	89	LYS	2.1
42	CP	3	LYS	2.1
48	CV	4	LYS	2.1
31	CA	429	A	2.1
31	CA	637	A	2.1
31	CA	1373	A	2.1
39	CM	18	ARG	2.1
9	AI	125	PRO	2.1
31	CA	436	C	2.1
31	CA	2362	C	2.1
2	AB	217	VAL	2.1
12	BL	87	VAL	2.1
29	CC	209	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
40	CN	135	VAL	2.1
48	CV	100	SER	2.1
1	BA	148	G	2.1
1	BA	1144	G	2.1
11	BK	30	THR	2.1
23	C2	8	LYS	2.1
31	CA	24	G	2.1
31	CA	1038	G	2.1
31	CA	1452	G	2.1
31	CA	2067	G	2.1
31	CA	2444	G	2.1
33	DF	78	LYS	2.1
9	BI	35	LEU	2.1
3	BC	110	GLU	2.1
4	BD	35	GLU	2.1
13	AM	3	ARG	2.1
18	AR	25	ASP	2.1
30	CD	156	PHE	2.1
34	CG	64	GLN	2.1
51	CY	28	ARG	2.1
1	BA	1122	U	2.1
3	BC	55	ILE	2.1
8	BH	35	ALA	2.1
9	BI	121	ALA	2.1
31	CA	10	A	2.1
31	CA	528	A	2.1
31	CA	2873	A	2.1
46	CT	93	ALA	2.1
10	AJ	58	ASN	2.1
2	AB	224	GLY	2.1
8	BH	123	GLY	2.1
10	BJ	54	SER	2.1
30	CD	50	VAL	2.1
35	CH	126	GLY	2.1
39	CM	87	GLY	2.1
39	DM	102	GLY	2.1
44	CR	84	LYS	2.1
52	CZ	50	VAL	2.1
4	BD	47	ARG	2.1
24	C3	3	ARG	2.1
47	CU	51	PHE	2.1
47	DU	87	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
31	CA	618	G	2.1
31	CA	649	G	2.1
31	CA	831	G	2.1
31	CA	1063	G	2.1
31	CA	1266	G	2.1
31	CA	1475	G	2.1
1	BA	224	U	2.1
10	AJ	8	ILE	2.1
13	AM	53	ILE	2.1
37	CK	81	ILE	2.1
14	BN	76	LYS	2.1
29	CC	253	LYS	2.1
19	BS	8	GLY	2.1
20	BT	21	ASN	2.1
25	C4	21	GLY	2.1
30	CD	11	MET	2.1
31	CA	1008	A	2.1
42	CP	22	GLY	2.1
1	BA	1140	C	2.1
1	BA	1267	C	2.1
5	BE	114	VAL	2.1
17	BQ	22	VAL	2.1
6	BF	58	HIS	2.1
28	CB	30	C	2.1
31	CA	678	C	2.1
31	CA	1295	C	2.1
36	DJ	70	VAL	2.1
35	DH	135	HIS	2.1
37	CK	120	ARG	2.1
49	CW	44	HIS	2.1
2	BB	220	THR	2.1
3	BC	170	GLU	2.1
5	AE	76	LEU	2.1
7	BG	84	THR	2.1
10	AJ	102	LEU	2.1
41	CO	43	GLU	2.1
45	CS	99	THR	2.1
51	CY	38	PHE	2.1
2	AB	8	ASP	2.1
10	BJ	60	ASP	2.1
18	BR	23	TYR	2.1
24	C3	6	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
41	CO	106	ASP	2.1
1	BA	1308	U	2.1
11	BK	45	ALA	2.1
38	CL	2	ILE	2.1
1	BA	1187	G	2.1
13	BM	114	LYS	2.1
42	CP	113	ALA	2.1
28	CB	67	G	2.1
31	CA	370	G	2.1
31	CA	407	G	2.1
31	CA	859	G	2.1
31	CA	1124	G	2.1
31	CA	2087	G	2.1
53	DI	103	ASN	2.1
1	BA	1216	A	2.1
14	AN	13	ARG	2.1
31	CA	422	A	2.1
31	CA	2336	A	2.1
31	CA	2868	A	2.1
37	CK	124	VAL	2.1
44	CR	53	ARG	2.1
54	DA	2142	A	2.1
1	BA	316	C	2.1
1	BA	1443	C	2.1
31	CA	692	C	2.1
31	CA	853	C	2.1
31	CA	994	C	2.1
31	CA	1462	C	2.1
4	AD	21	LEU	2.1
30	CD	100	LEU	2.1
32	CE	107	SER	2.1
8	BH	48	ASP	2.1
35	CH	18	GLN	2.1
46	CT	42	LYS	2.1
1	BA	1232	U	2.1
3	BC	180	ALA	2.1
11	AK	79	ILE	2.1
20	BT	12	ILE	2.1
30	CD	85	ALA	2.1
31	CA	2401	U	2.1
9	AI	117	GLY	2.1
2	BB	63	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
6	AF	90	MET	2.1
6	BF	84	VAL	2.1
31	CA	68	G	2.1
31	CA	245	G	2.1
31	CA	561	G	2.1
31	CA	612	G	2.1
31	CA	1055	G	2.1
31	CA	2857	G	2.1
39	CM	123	ARG	2.1
7	AG	123	GLU	2.1
8	AH	110	VAL	2.1
1	BA	1045	C	2.1
2	BB	50	PHE	2.1
16	BP	12	LYS	2.1
30	CD	140	HIS	2.1
31	CA	125	A	2.1
31	CA	734	A	2.1
31	CA	972	A	2.1
16	BP	68	SER	2.1
16	BP	74	LEU	2.1
21	BU	16	LEU	2.1
31	CA	1039	A	2.1
31	CA	1646	C	2.1
31	CA	2160	C	2.1
31	CA	2882	A	2.1
37	CK	23	LYS	2.1
46	CT	33	LEU	2.1
50	CX	45	PHE	2.1
17	BQ	9	GLN	2.1
41	CO	100	CYS	2.1
12	BL	97	THR	2.1
14	AN	20	TYR	2.1
16	BP	67	ILE	2.1
31	CA	2585	U	2.1
32	CE	26	ALA	2.1
42	CP	37	ALA	2.1
45	CS	41	ILE	2.1
15	BO	29	VAL	2.1
34	CG	124	GLU	2.1
46	CT	2	GLU	2.1
30	CD	152	PRO	2.1
1	BA	111	G	2.1

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Mol	Chain	Res	Type	RSRZ
1	BA	275	G	2.1
31	CA	1517	G	2.1
31	CA	2669	G	2.1
31	CA	2822	G	2.1
31	CA	2846	G	2.1
33	CF	20	PHE	2.1
54	DA	1091	G	2.1
54	DA	2885[A]	G	2.1
7	BG	23	LEU	2.0
1	BA	176	C	2.0
1	BA	1285	A	2.0
30	CD	94	GLN	2.0
31	CA	275	C	2.0
31	CA	1286	A	2.0
31	CA	2176	A	2.0
35	DH	72	ILE	2.0
12	BL	104	CYS	2.0
24	C3	38	GLY	2.0
31	CA	2299	U	2.0
47	CU	39	THR	2.0
19	BS	17	LYS	2.0
29	CC	36	LYS	2.0
38	CL	53	LYS	2.0
40	CN	8	LYS	2.0
47	CU	54	GLU	2.0
34	CG	11	VAL	2.0
5	AE	81	LEU	2.0
41	CO	87	PHE	2.0
1	AA	95	C	2.0
1	BA	136	C	2.0
1	BA	217	C	2.0
1	BA	1186	G	2.0
1	BA	1385	G	2.0
3	BC	65	ARG	2.0
1	BA	1251	A	2.0
15	AO	11	ILE	2.0
30	CD	145	SER	2.0
31	CA	107	G	2.0
31	CA	239	C	2.0
31	CA	953	G	2.0
31	CA	1170	C	2.0
31	CA	1807	G	2.0

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Mol	Chain	Res	Type	RSRZ
31	CA	1811	G	2.0
31	CA	2156	G	2.0
41	CO	2	ARG	2.0
52	CZ	7	ARG	2.0
53	DI	31	ARG	2.0
1	BA	323	U	2.0
22	C1	49	TYR	2.0
22	C1	56	ALA	2.0
30	CD	209	ALA	2.0
31	CA	665	U	2.0
35	DH	52	ALA	2.0
12	BL	39	THR	2.0
15	AO	22	THR	2.0
18	AR	45	THR	2.0
48	DV	47	LYS	2.0
20	BT	35	VAL	2.0
27	C0	57	VAL	2.0
30	CD	122	VAL	2.0
37	CK	48	VAL	2.0
44	CR	104	VAL	2.0
48	CV	34	VAL	2.0
5	BE	150	PRO	2.0
29	CC	86	ASN	2.0
35	CH	73	ASN	2.0
35	DH	47	PHE	2.0
51	CY	32	ASN	2.0
15	BO	54	ARG	2.0
20	BT	61	GLN	2.0
44	CR	64	ARG	2.0
2	BB	127	ASP	2.0
3	BC	75	ILE	2.0
14	AN	28	LYS	2.0
32	CE	91	ASP	2.0
47	CU	17	SER	2.0
51	DY	77	LYS	2.0
1	BA	92	U	2.0
16	AP	72	ALA	2.0
31	CA	440	C	2.0
1	AA	1188	A	2.0
1	AA	1285	A	2.0
1	BA	331	G	2.0
9	AI	53	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
31	CA	1497	U	2.0
31	CA	1644	C	2.0
31	CA	2259	U	2.0
31	CA	2455	G	2.0
31	CA	2716	C	2.0
31	CA	1735	A	2.0
31	CA	2722	G	2.0
42	CP	112	GLU	2.0
54	DA	1733	G	2.0
2	BB	210	VAL	2.0
3	BC	173	VAL	2.0
5	AE	74	VAL	2.0
7	AG	141	VAL	2.0
16	BP	36	VAL	2.0
2	AB	158	PRO	2.0
3	BC	164	ARG	2.0
41	CO	4	ARG	2.0
43	CQ	20	PHE	2.0
19	AS	31	LEU	2.0
34	DG	101	ASN	2.0
53	DI	46	ARG	2.0
4	AD	31	LYS	2.0
38	CL	84	CYS	2.0
51	CY	44	LYS	2.0
32	CE	198	GLU	2.0
37	CK	71	ASP	2.0
48	CV	65	ILE	2.0
8	AH	116	ALA	2.0
20	AT	26	SER	2.0
20	BT	6	SER	2.0
21	BU	15	ALA	2.0
48	DV	57	GLY	2.0
1	BA	132	C	2.0
1	BA	1354	U	2.0
31	CA	564	C	2.0
31	CA	1447	C	2.0
31	CA	1493	C	2.0
31	CA	2179	C	2.0
31	CA	2616	C	2.0
1	BA	1329	A	2.0
31	CA	127	A	2.0
31	CA	324	A	2.0

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Mol	Chain	Res	Type	RSRZ
31	CA	911	A	2.0
31	CA	1193	G	2.0
31	CA	1478	G	2.0
31	CA	2135	A	2.0
31	CA	2813	A	2.0
54	DA	2159	G	2.0
29	CC	13	ARG	2.0
2	BB	128	LYS	2.0
3	BC	89	LYS	2.0
6	AF	104	LYS	2.0
23	D2	53	LYS	2.0
34	CG	134	LYS	2.0
34	CG	176	LYS	2.0
47	CU	9	LYS	2.0
5	BE	135	ASN	2.0
35	CH	43	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
1	5MC	BA	967	21/22	0.72	0.33	149,158,161,161	0
31	2MA	CA	2503	23/24	0.78	0.30	107,109,110,110	0
1	2MG	BA	966	24/25	0.78	0.29	149,156,167,168	0
31	3TD	CA	1915	21/22	0.80	0.30	149,155,157,158	0
31	PSU	CA	1917	20/21	0.81	0.26	120,125,134,134	0
31	5MU	CA	747	21/22	0.83	0.23	116,120,122,123	0
31	PSU	CA	955	20/21	0.83	0.23	100,105,108,108	0
31	G7M	CA	2069	24/25	0.83	0.27	102,104,108,109	0
31	PSU	CA	2504	20/21	0.84	0.23	93,103,106,106	0
31	6MZ	CA	2030	23/24	0.84	0.26	101,104,106,107	0
31	PSU	CA	746	20/21	0.84	0.22	116,118,119,120	0
31	2MG	CA	2445	24/25	0.86	0.34	97,100,102,102	0
31	PSU	CA	1911	20/21	0.86	0.26	127,137,139,140	0
31	PSU	CA	2580	20/21	0.86	0.20	93,99,101,101	0
31	OMU	CA	2552	21/22	0.86	0.43	88,92,94,95	0
1	2MG	BA	1207	24/25	0.87	0.27	150,152,156,160	0
1	5MC	BA	1407	21/22	0.87	0.21	98,109,111,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	D2T	BL	89	10/11	0.88	0.28	83,85,93,94	0
30	MEQ	CD	150	9/11	0.88	0.28	92,98,133,136	0
1	2MG	BA	1516	24/25	0.88	0.20	79,86,93,95	0
31	OMG	CA	2251	24/25	0.88	0.23	85,90,93,93	0
40	4D4	CN	81	12/13	0.89	0.30	108,112,131,132	0
31	6MZ	CA	1618	23/24	0.89	0.25	134,138,143,145	0
1	PSU	BA	516	20/21	0.90	0.16	80,89,91,94	0
31	PSU	CA	2457	20/21	0.91	0.17	96,97,99,99	0
31	1MG	CA	745	24/25	0.91	0.25	103,107,111,114	0
54	3TD	DA	1915	21/22	0.91	0.20	105,110,116,117	0
31	OMC	CA	2498	21/22	0.91	0.26	91,94,95,95	0
1	2MG	AA	1207	24/25	0.92	0.15	99,103,105,108	0
31	5MU	CA	1939	21/22	0.92	0.17	70,77,78,80	0
31	PSU	CA	2605	20/21	0.92	0.20	79,81,83,84	0
1	MA6	BA	1519	24/25	0.92	0.23	80,82,87,88	0
12	D2T	AL	89	10/11	0.92	0.23	60,63,71,72	0
1	MA6	BA	1518	24/25	0.92	0.23	84,86,92,93	0
1	2MG	AA	966	24/25	0.93	0.15	79,84,91,91	0
31	2MG	CA	1835	24/25	0.93	0.17	71,73,76,77	0
31	5MC	CA	1962	21/22	0.93	0.18	70,77,80,82	0
1	UR3	BA	1498	21/22	0.93	0.14	84,87,94,94	0
1	5MC	AA	967	21/22	0.93	0.16	74,88,90,91	0
1	4OC	BA	1402	22/23	0.94	0.16	74,77,79,80	0
54	PSU	DA	1917	20/21	0.94	0.15	80,84,91,91	0
1	G7M	BA	527	24/25	0.94	0.14	70,73,78,79	0
54	PSU	DA	1911	20/21	0.94	0.17	83,90,91,92	0
30	MEQ	DD	150[B]	10/11	0.96	0.24	25,29,41,41	10
40	4D4	DN	81[B]	12/13	0.96	0.23	26,28,31,32	9
30	MEQ	DD	150[A]	10/11	0.96	0.24	17,22,27,29	10
54	PSU	DA	2604	20/21	0.96	0.20	36,42,53,53	0
1	2MG	AA	1516	24/25	0.96	0.15	52,54,56,57	0
1	PSU	AA	516	20/21	0.96	0.14	76,78,82,82	0
40	4D4	DN	81[A]	12/13	0.96	0.23	30,36,49,50	9
1	UR3	AA	1498	21/22	0.97	0.16	54,56,61,63	0
54	5MC	DA	1962	21/22	0.97	0.20	44,46,49,50	0
1	4OC	AA	1402	22/23	0.97	0.16	52,59,61,62	0
54	PSU	DA	2605	20/21	0.97	0.18	33,42,46,46	0
1	5MC	AA	1407	21/22	0.97	0.13	51,52,54,55	0
54	2MG	DA	1835	24/25	0.97	0.20	53,55,56,58	0
1	G7M	AA	527	24/25	0.97	0.15	55,58,62,63	0
1	MA6	AA	1519	24/25	0.97	0.16	53,56,61,65	0
54	2MG	DA	2445	24/25	0.98	0.20	14,25,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	OMG	DA	2251	24/25	0.98	0.17	23,27,30,30	0
54	H2U	DA	2449	20/21	0.98	0.20	24,27,28,32	0
54	PSU	DA	2580	20/21	0.98	0.21	24,30,36,37	0
54	PSU	DA	746	20/21	0.98	0.18	28,30,33,36	0
54	5MU	DA	1939	21/22	0.98	0.19	31,36,38,39	0
54	2MA	DA	2503	23/24	0.98	0.19	26,42,46,47	0
54	5MU	DA	747	21/22	0.98	0.17	26,28,32,37	0
54	OMU	DA	2552	21/22	0.98	0.22	35,37,44,47	0
1	MA6	AA	1518	24/25	0.98	0.16	50,54,56,57	0
54	PSU	DA	2504	20/21	0.98	0.18	45,53,56,57	0
54	1MG	DA	745	24/25	0.99	0.20	19,26,31,33	0
54	6MZ	DA	2030	23/24	0.99	0.21	13,23,28,28	0
54	OMC	DA	2498	21/22	0.99	0.20	21,22,27,29	0
54	PSU	DA	2457	20/21	0.99	0.18	20,28,30,31	0
54	G7M	DA	2069	24/25	0.99	0.19	24,30,37,38	0
54	6MZ	DA	1618	23/24	0.99	0.19	25,28,31,33	0
54	PSU	DA	955	20/21	0.99	0.20	25,26,29,30	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. 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	B-factors(\AA^2)	Q<0.9
55	MG	AA	1622	1/1	-0.27	1.24	119,119,119,119	0
55	MG	CA	3122	1/1	-0.23	1.55	182,182,182,182	0
55	MG	CA	3133	1/1	-0.20	0.62	194,194,194,194	0
55	MG	CA	3139	1/1	-0.18	0.64	128,128,128,128	0
55	MG	CA	3037	1/1	-0.11	0.45	256,256,256,256	0
55	MG	CA	3128	1/1	-0.10	0.47	135,135,135,135	0
55	MG	CA	3129	1/1	-0.02	0.76	118,118,118,118	0
55	MG	CA	3155	1/1	-0.02	0.24	240,240,240,240	0
55	MG	CA	3059	1/1	0.02	0.73	240,240,240,240	0
55	MG	CA	3109	1/1	0.04	0.99	175,175,175,175	0
55	MG	CA	3004	1/1	0.12	1.51	243,243,243,243	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CB	203	1/1	0.13	0.11	146,146,146,146	0
55	MG	CA	3121	1/1	0.16	1.41	125,125,125,125	0
55	MG	AA	1628	1/1	0.18	0.58	142,142,142,142	0
55	MG	DA	3168	1/1	0.19	0.75	109,109,109,109	0
55	MG	CA	3145	1/1	0.21	0.49	234,234,234,234	0
55	MG	CA	3138	1/1	0.21	0.97	125,125,125,125	0
55	MG	AA	1654	1/1	0.22	0.37	241,241,241,241	0
55	MG	CA	3025	1/1	0.24	0.48	180,180,180,180	0
55	MG	CA	3053	1/1	0.26	0.18	134,134,134,134	0
55	MG	CA	3141	1/1	0.26	0.41	115,115,115,115	0
55	MG	CA	3055	1/1	0.27	0.58	94,94,94,94	0
55	MG	AA	1616	1/1	0.28	0.72	94,94,94,94	0
55	MG	CA	3032	1/1	0.29	0.33	194,194,194,194	0
55	MG	CA	3110	1/1	0.30	1.04	141,141,141,141	0
55	MG	CA	3002	1/1	0.30	2.03	278,278,278,278	0
55	MG	AA	1606	1/1	0.32	0.45	108,108,108,108	0
55	MG	DA	3179	1/1	0.34	0.71	100,100,100,100	0
55	MG	DA	3130	1/1	0.35	0.34	81,81,81,81	0
55	MG	BA	1626	1/1	0.36	0.20	264,264,264,264	0
55	MG	BA	1632	1/1	0.37	0.07	219,219,219,219	0
55	MG	DA	3171	1/1	0.37	0.55	83,83,83,83	0
55	MG	BA	1619	1/1	0.40	0.13	122,122,122,122	0
55	MG	CA	3054	1/1	0.41	0.16	201,201,201,201	0
55	MG	DA	3145	1/1	0.41	0.80	111,111,111,111	0
55	MG	CA	3074	1/1	0.42	1.08	243,243,243,243	0
55	MG	CA	3070	1/1	0.42	0.20	188,188,188,188	0
55	MG	DA	3159	1/1	0.43	0.63	74,74,74,74	0
55	MG	DB	206	1/1	0.43	0.48	106,106,106,106	0
55	MG	CA	3031	1/1	0.43	0.41	257,257,257,257	0
55	MG	CA	3001	1/1	0.43	0.28	258,258,258,258	0
55	MG	DA	3182	1/1	0.45	0.43	65,65,65,65	0
55	MG	CA	3009	1/1	0.46	0.23	217,217,217,217	0
55	MG	CA	3027	1/1	0.46	0.26	277,277,277,277	0
55	MG	CA	3007	1/1	0.46	0.11	175,175,175,175	0
61	PEG	DQ	201	7/7	0.47	0.95	104,105,105,106	0
55	MG	CA	3075	1/1	0.47	0.11	215,215,215,215	0
55	MG	BA	1608	1/1	0.47	0.18	243,243,243,243	0
55	MG	AA	1626	1/1	0.47	1.84	104,104,104,104	0
55	MG	BA	1640	1/1	0.48	0.77	101,101,101,101	0
55	MG	CA	3153	1/1	0.48	0.48	138,138,138,138	0
55	MG	CA	3033	1/1	0.48	0.42	246,246,246,246	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	C3	101	1/1	0.48	0.47	299,299,299,299	0
55	MG	DA	3180	1/1	0.49	1.30	99,99,99,99	0
55	MG	DA	3178	1/1	0.49	0.55	100,100,100,100	0
55	MG	CA	3105	1/1	0.50	0.36	92,92,92,92	0
55	MG	CA	3119	1/1	0.50	0.61	188,188,188,188	0
55	MG	AA	1661	1/1	0.51	1.16	182,182,182,182	0
55	MG	BA	1606	1/1	0.54	0.26	190,190,190,190	0
55	MG	AA	1605	1/1	0.54	0.64	97,97,97,97	0
55	MG	DA	3172	1/1	0.54	0.59	86,86,86,86	0
55	MG	CA	3098	1/1	0.54	0.27	231,231,231,231	0
55	MG	AA	1603	1/1	0.55	0.60	110,110,110,110	0
55	MG	CA	3092	1/1	0.56	0.13	113,113,113,113	0
55	MG	DA	3163	1/1	0.56	0.19	76,76,76,76	0
55	MG	DA	3173	1/1	0.56	0.89	77,77,77,77	0
62	EDO	DA	3208	4/4	0.57	0.57	88,90,91,91	0
55	MG	CA	3146	1/1	0.58	0.49	76,76,76,76	1
55	MG	DA	3175	1/1	0.58	0.60	85,85,85,85	0
55	MG	CA	3060	1/1	0.58	0.15	256,256,256,256	0
55	MG	AA	1615	1/1	0.59	0.55	81,81,81,81	0
57	MPD	AA	1676	8/8	0.59	0.64	97,99,100,103	0
55	MG	CA	3038	1/1	0.60	0.58	154,154,154,154	0
55	MG	CA	3011	1/1	0.60	0.27	120,120,120,120	0
55	MG	AA	1624	1/1	0.61	1.12	92,92,92,92	0
55	MG	BA	1620	1/1	0.61	0.14	97,97,97,97	0
55	MG	BA	1625	1/1	0.61	1.01	231,231,231,231	0
55	MG	CA	3013	1/1	0.62	0.22	251,251,251,251	0
55	MG	BA	1629	1/1	0.63	1.63	124,124,124,124	0
55	MG	DA	3112	1/1	0.63	0.49	291,291,291,291	0
55	MG	DA	3167	1/1	0.63	0.50	80,80,80,80	0
55	MG	CA	3147	1/1	0.64	0.82	80,80,80,80	1
61	PEG	DA	3217	7/7	0.64	0.64	92,95,99,99	0
55	MG	AA	1617	1/1	0.64	0.42	93,93,93,93	0
55	MG	CA	3076	1/1	0.65	0.59	246,246,246,246	0
55	MG	DA	3124	1/1	0.65	0.32	102,102,102,102	0
55	MG	AA	1636	1/1	0.65	0.24	103,103,103,103	0
55	MG	CA	3039	1/1	0.65	0.12	124,124,124,124	0
55	MG	BA	1635	1/1	0.65	0.13	226,226,226,226	0
55	MG	AA	1614	1/1	0.65	0.51	126,126,126,126	0
55	MG	CA	3067	1/1	0.66	0.18	239,239,239,239	0
55	MG	BA	1610	1/1	0.66	0.15	119,119,119,119	0
55	MG	AA	1642	1/1	0.66	0.40	153,153,153,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
63	PGE	D1	102	10/10	0.66	0.67	89,92,93,93	0
63	PGE	D3	101	10/10	0.67	0.61	82,83,87,87	0
55	MG	DA	3138	1/1	0.67	0.25	80,80,80,80	0
55	MG	BA	1605	1/1	0.67	0.31	250,250,250,250	0
55	MG	CA	3134	1/1	0.67	0.59	99,99,99,99	0
58	PUT	AA	1672	6/6	0.67	0.72	98,98,100,101	0
55	MG	CA	3132	1/1	0.68	0.98	129,129,129,129	0
55	MG	CA	3106	1/1	0.68	0.52	83,83,83,83	0
55	MG	CA	3066	1/1	0.68	0.77	284,284,284,284	0
55	MG	BA	1627	1/1	0.68	0.21	264,264,264,264	0
55	MG	CA	3101	1/1	0.68	0.24	115,115,115,115	0
55	MG	CA	3085	1/1	0.69	0.18	82,82,82,82	0
55	MG	DA	3176	1/1	0.69	0.46	91,91,91,91	0
55	MG	CA	3148	1/1	0.69	0.70	80,80,80,80	0
55	MG	AA	1632	1/1	0.69	0.15	110,110,110,110	0
55	MG	CA	3140	1/1	0.70	0.47	91,91,91,91	0
55	MG	CA	3046	1/1	0.70	0.44	228,228,228,228	0
55	MG	AA	1601	1/1	0.70	1.54	100,100,100,100	0
55	MG	CA	3057	1/1	0.70	0.34	128,128,128,128	0
68	TRS	DA	3219	8/8	0.71	0.47	95,98,100,101	0
55	MG	DA	3170	1/1	0.71	0.45	80,80,80,80	0
55	MG	CA	3104	1/1	0.71	0.40	252,252,252,252	0
55	MG	DA	3181	1/1	0.71	0.49	58,58,58,58	0
60	ZN	AB	301	1/1	0.71	0.18	198,198,198,198	0
55	MG	CA	3127	1/1	0.72	0.27	85,85,85,85	0
55	MG	DA	3129	1/1	0.72	1.15	69,69,69,69	0
55	MG	BA	1636	1/1	0.72	0.08	112,112,112,112	0
55	MG	CA	3012	1/1	0.72	0.21	134,134,134,134	0
57	MPD	DA	3206	8/8	0.72	0.53	93,94,95,95	0
55	MG	DA	3157	1/1	0.72	0.46	69,69,69,69	0
55	MG	DA	3147	1/1	0.72	0.37	98,98,98,98	0
55	MG	CA	3116	1/1	0.72	0.78	101,101,101,101	0
55	MG	CA	3056	1/1	0.72	0.19	119,119,119,119	0
55	MG	AA	1627	1/1	0.73	0.36	88,88,88,88	0
55	MG	CA	3006	1/1	0.73	0.61	242,242,242,242	0
55	MG	CA	3026	1/1	0.73	0.30	123,123,123,123	0
55	MG	AA	1657	1/1	0.73	0.20	144,144,144,144	0
58	PUT	AA	1675	6/6	0.73	0.55	82,83,84,84	0
55	MG	CA	3081	1/1	0.73	0.35	153,153,153,153	0
61	PEG	D3	102	7/7	0.73	1.16	73,79,82,82	0
55	MG	DA	3125	1/1	0.74	0.46	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MPD	DT	202	8/8	0.74	0.41	88,89,90,92	0
57	MPD	DA	3203	8/8	0.74	0.60	89,92,98,99	0
55	MG	BA	1644	1/1	0.74	0.12	87,87,87,87	0
55	MG	AA	1621	1/1	0.74	0.43	88,88,88,88	0
55	MG	CA	3082	1/1	0.74	0.20	229,229,229,229	0
55	MG	CA	3136	1/1	0.74	0.58	156,156,156,156	0
55	MG	DB	209	1/1	0.74	0.81	87,87,87,87	0
55	MG	CA	3118	1/1	0.74	0.74	123,123,123,123	0
55	MG	BA	1643	1/1	0.75	0.32	134,134,134,134	0
55	MG	CA	3048	1/1	0.75	0.12	92,92,92,92	0
57	MPD	DT	201	8/8	0.76	0.36	85,87,92,92	0
55	MG	CA	3015	1/1	0.76	0.29	143,143,143,143	0
55	MG	DA	3155	1/1	0.76	0.58	71,71,71,71	0
62	EDO	DA	3004	4/4	0.76	0.42	112,113,114,114	0
55	MG	CA	3125	1/1	0.76	0.39	120,120,120,120	0
55	MG	AA	1623	1/1	0.76	0.69	74,74,74,74	0
55	MG	CA	3093	1/1	0.76	0.26	151,151,151,151	0
55	MG	CA	3111	1/1	0.76	0.60	91,91,91,91	0
55	MG	CA	3044	1/1	0.76	0.09	93,93,93,93	0
55	MG	AA	1609	1/1	0.76	0.28	96,96,96,96	0
55	MG	AA	1610	1/1	0.76	0.52	97,97,97,97	0
55	MG	AA	1644	1/1	0.76	0.14	83,83,83,83	0
55	MG	CA	3016	1/1	0.77	0.07	106,106,106,106	0
67	GUN	DA	3210	11/11	0.77	0.32	66,68,71,71	0
58	PUT	AA	1674	6/6	0.77	0.57	88,90,91,91	0
61	PEG	DP	201	7/7	0.77	0.60	90,92,94,94	0
55	MG	CA	3091	1/1	0.77	0.35	202,202,202,202	0
55	MG	CA	3063	1/1	0.77	0.61	257,257,257,257	0
55	MG	DA	3136	1/1	0.77	0.14	100,100,100,100	0
55	MG	CA	3079	1/1	0.77	0.51	177,177,177,177	0
57	MPD	DE	302	8/8	0.77	0.61	92,94,95,96	0
55	MG	CA	3131	1/1	0.78	0.47	145,145,145,145	0
55	MG	AA	1665	1/1	0.78	0.31	158,158,158,158	0
55	MG	CA	3123	1/1	0.78	0.24	199,199,199,199	0
55	MG	CB	202	1/1	0.78	0.08	128,128,128,128	0
55	MG	DA	3126	1/1	0.78	0.26	70,70,70,70	0
58	PUT	DA	3221	6/6	0.78	0.40	45,46,49,51	0
55	MG	CA	3144	1/1	0.78	0.29	62,62,62,62	0
55	MG	AA	1611	1/1	0.78	0.18	88,88,88,88	0
61	PEG	DA	3200	7/7	0.78	0.55	56,57,59,61	0
55	MG	CA	3030	1/1	0.79	0.33	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DR	201	1/1	0.79	0.63	55,55,55,55	0
58	PUT	DA	3218	6/6	0.79	0.41	73,74,75,75	0
61	PEG	AL	201	7/7	0.79	0.33	78,79,82,82	0
55	MG	DA	3131	1/1	0.79	0.31	85,85,85,85	0
56	PG4	DR	202	13/13	0.79	0.48	55,64,74,75	0
55	MG	DA	3166	1/1	0.79	0.97	92,92,92,92	0
55	MG	BA	1641	1/1	0.79	0.35	98,98,98,98	0
57	MPD	DE	301	8/8	0.80	0.64	98,102,104,105	0
64	SPD	DA	3205	10/10	0.80	0.34	76,83,85,85	0
55	MG	CA	3103	1/1	0.80	0.47	260,260,260,260	0
55	MG	BA	1623	1/1	0.80	0.28	37,37,37,37	0
55	MG	DA	3153	1/1	0.80	0.26	100,100,100,100	0
55	MG	CA	3114	1/1	0.80	0.37	102,102,102,102	0
55	MG	CA	3151	1/1	0.80	0.33	209,209,209,209	0
66	ACY	DA	3196	4/4	0.80	0.29	79,80,80,80	0
61	PEG	DA	3225	7/7	0.80	0.34	60,63,70,71	0
55	MG	DA	3151	1/1	0.80	0.10	54,54,54,54	0
58	PUT	DA	3195	6/6	0.81	0.40	49,55,59,60	0
55	MG	BA	1639	1/1	0.81	0.67	88,88,88,88	0
55	MG	CA	3112	1/1	0.81	0.48	77,77,77,77	0
55	MG	CA	3069	1/1	0.81	0.06	95,95,95,95	0
55	MG	CA	3064	1/1	0.81	0.14	107,107,107,107	0
55	MG	CA	3068	1/1	0.81	0.19	107,107,107,107	0
58	PUT	AA	1673	6/6	0.81	0.35	122,122,123,123	0
55	MG	CA	3102	1/1	0.81	0.18	115,115,115,115	0
55	MG	AA	1635	1/1	0.81	0.09	96,96,96,96	0
55	MG	BA	1616	1/1	0.81	0.17	136,136,136,136	0
55	MG	DA	3134	1/1	0.81	0.25	65,65,65,65	0
55	MG	CA	3143	1/1	0.81	0.08	85,85,85,85	0
55	MG	AA	1625	1/1	0.81	0.35	63,63,63,63	0
61	PEG	D1	103	7/7	0.81	0.36	57,60,61,63	0
55	MG	CA	3071	1/1	0.82	0.83	257,257,257,257	0
55	MG	CA	3137	1/1	0.82	0.13	95,95,95,95	0
56	PG4	BA	1601	13/13	0.82	0.33	90,95,98,99	0
58	PUT	DA	3220	6/6	0.82	0.42	93,96,99,100	0
55	MG	DA	3133	1/1	0.82	0.22	70,70,70,70	0
63	PGE	DA	3213	10/10	0.82	0.48	83,85,89,89	0
55	MG	CA	3065	1/1	0.82	0.17	119,119,119,119	0
55	MG	AA	1633	1/1	0.83	0.12	110,110,110,110	0
56	PG4	DA	3215	13/13	0.83	0.28	91,98,100,100	0
55	MG	AA	1604	1/1	0.83	0.35	64,64,64,64	0
57	MPD	DK	201	8/8	0.83	0.25	91,92,94,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3107	1/1	0.83	0.35	90,90,90,90	0
55	MG	DA	3161	1/1	0.83	0.39	69,69,69,69	0
55	MG	DA	3148	1/1	0.83	0.20	123,123,123,123	0
55	MG	AA	1619	1/1	0.83	0.35	94,94,94,94	0
55	MG	CA	3100	1/1	0.83	0.10	135,135,135,135	0
55	MG	CA	3062	1/1	0.83	0.24	196,196,196,196	0
63	PGE	DA	3224	10/10	0.83	0.34	79,85,88,88	0
61	PEG	DA	3199	7/7	0.84	0.41	62,66,69,69	0
55	MG	DA	3154	1/1	0.84	0.40	58,58,58,58	0
55	MG	AA	1655	1/1	0.84	0.07	100,100,100,100	0
58	PUT	DA	3211	6/6	0.84	0.29	57,65,66,66	0
63	PGE	DA	3216	10/10	0.84	0.44	57,60,68,70	0
55	MG	BA	1631	1/1	0.84	0.68	151,151,151,151	0
62	EDO	D1	101	4/4	0.84	0.29	63,64,67,70	0
63	PGE	DS	201	10/10	0.84	0.32	61,66,67,68	0
62	EDO	DB	210	4/4	0.84	0.34	76,77,77,78	0
63	PGE	DD	301	10/10	0.84	0.34	63,66,69,69	0
55	MG	CA	3152	1/1	0.84	0.23	87,87,87,87	0
55	MG	DA	3164	1/1	0.85	0.40	75,75,75,75	0
57	MPD	DA	3192	8/8	0.85	0.45	68,72,74,74	0
55	MG	DA	3174	1/1	0.85	0.39	79,79,79,79	0
63	PGE	DU	101	10/10	0.85	0.44	62,68,78,78	0
55	MG	CA	3005	1/1	0.85	0.18	224,224,224,224	0
56	PG4	AA	1670	13/13	0.85	0.22	80,86,94,94	0
55	MG	CA	3130	1/1	0.85	0.35	101,101,101,101	0
55	MG	BA	1611	1/1	0.85	0.13	191,191,191,191	0
65	1PE	DA	3202	16/16	0.85	0.42	52,59,65,67	0
55	MG	DA	3045	1/1	0.85	0.14	90,90,90,90	0
55	MG	CA	3154	1/1	0.85	0.37	200,200,200,200	0
55	MG	CA	3124	1/1	0.85	0.49	127,127,127,127	0
59	TAC	BA	1602	32/32	0.85	0.15	170,172,172,172	0
57	MPD	DN	201	8/8	0.85	0.40	83,88,90,91	0
55	MG	CA	3040	1/1	0.85	0.11	71,71,71,71	0
55	MG	CA	3041	1/1	0.86	0.10	90,90,90,90	0
55	MG	AA	1660	1/1	0.86	0.28	275,275,275,275	0
55	MG	DA	3165	1/1	0.86	0.29	74,74,74,74	0
55	MG	AA	1679	1/1	0.86	0.19	163,163,163,163	0
55	MG	AA	1608	1/1	0.86	0.52	97,97,97,97	0
55	MG	CA	3017	1/1	0.86	0.17	124,124,124,124	0
55	MG	CA	3150	1/1	0.86	0.30	80,80,80,80	0
55	MG	AA	1618	1/1	0.86	0.71	81,81,81,81	0
55	MG	CA	3080	1/1	0.86	0.08	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3049	1/1	0.86	0.13	81,81,81,81	0
55	MG	AA	1634	1/1	0.86	0.11	106,106,106,106	0
56	PG4	DA	3193	13/13	0.86	0.69	59,61,70,71	0
62	EDO	DA	3003	4/4	0.86	0.44	47,49,50,50	0
55	MG	CA	3028	1/1	0.86	0.31	172,172,172,172	0
62	EDO	DA	3001	4/4	0.86	0.37	74,76,76,77	0
56	PG4	DQ	202	13/13	0.86	0.26	62,65,71,71	0
55	MG	CA	3095	1/1	0.86	0.10	112,112,112,112	0
55	MG	CA	3021	1/1	0.86	0.79	182,182,182,182	0
55	MG	AA	1637	1/1	0.86	0.08	49,49,49,49	0
55	MG	AA	1630	1/1	0.86	0.17	124,124,124,124	0
55	MG	AA	1612	1/1	0.86	0.30	65,65,65,65	0
57	MPD	DA	3209	8/8	0.86	0.35	65,68,71,72	0
55	MG	BA	1612	1/1	0.87	0.07	101,101,101,101	0
58	PUT	DA	3184	6/6	0.87	0.36	45,45,47,48	0
55	MG	CA	3019	1/1	0.87	0.09	102,102,102,102	0
55	MG	DA	3144	1/1	0.87	0.46	65,65,65,65	0
55	MG	BA	1618	1/1	0.87	0.12	144,144,144,144	0
55	MG	DA	3097	1/1	0.87	0.12	45,45,45,45	0
55	MG	DA	3122	1/1	0.87	0.26	86,86,86,86	0
55	MG	BA	1624	1/1	0.87	0.12	97,97,97,97	0
55	MG	CA	3090	1/1	0.88	0.12	106,106,106,106	0
55	MG	AA	1663	1/1	0.88	0.17	76,76,76,76	0
55	MG	CA	3035	1/1	0.88	0.32	201,201,201,201	0
55	MG	CA	3034	1/1	0.88	0.31	144,144,144,144	0
55	MG	CA	3120	1/1	0.88	0.38	75,75,75,75	0
55	MG	CA	3089	1/1	0.88	0.94	209,209,209,209	0
62	EDO	DA	3194	4/4	0.88	0.29	60,61,62,63	0
55	MG	DA	3118	1/1	0.88	0.24	65,65,65,65	0
55	MG	CA	3096	1/1	0.88	0.14	117,117,117,117	0
55	MG	DA	3005	1/1	0.88	0.12	69,69,69,69	0
55	MG	CA	3003	1/1	0.88	0.34	218,218,218,218	0
55	MG	AA	1639	1/1	0.88	0.07	120,120,120,120	0
55	MG	DA	3099	1/1	0.88	0.15	81,81,81,81	0
62	EDO	DA	3214	4/4	0.88	0.28	74,74,74,75	0
61	PEG	DL	201	7/7	0.88	0.21	69,70,71,71	0
55	MG	CA	3051	1/1	0.88	0.10	82,82,82,82	0
55	MG	DA	3160	1/1	0.88	0.16	56,56,56,56	0
55	MG	DA	3053	1/1	0.88	0.12	78,78,78,78	0
55	MG	CA	3078	1/1	0.88	0.21	134,134,134,134	0
55	MG	DA	3132	1/1	0.88	0.29	66,66,66,66	0
57	MPD	DA	3190	8/8	0.89	0.26	87,88,89,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	PUT	DA	3212	6/6	0.89	0.65	47,53,59,60	0
55	MG	BA	1642	1/1	0.89	0.70	164,164,164,164	0
55	MG	BA	1609	1/1	0.89	0.35	172,172,172,172	0
55	MG	BA	1633	1/1	0.89	0.08	57,57,57,57	0
55	MG	CA	3022	1/1	0.89	0.16	142,142,142,142	0
55	MG	CA	3020	1/1	0.89	0.54	269,269,269,269	0
55	MG	AA	1620	1/1	0.89	0.35	67,67,67,67	0
55	MG	BA	1607	1/1	0.89	0.09	118,118,118,118	0
55	MG	DA	3022	1/1	0.89	0.14	50,50,50,50	0
55	MG	CA	3088	1/1	0.89	0.23	90,90,90,90	0
62	EDO	DA	3207	4/4	0.89	0.33	57,58,59,59	0
55	MG	CA	3142	1/1	0.89	0.41	85,85,85,85	0
55	MG	DA	3143	1/1	0.89	0.39	93,93,93,93	0
55	MG	AA	1641	1/1	0.89	0.08	81,81,81,81	0
61	PEG	DA	3226	7/7	0.89	0.32	55,59,63,64	0
55	MG	DA	3065	1/1	0.89	0.37	59,59,59,59	0
55	MG	DD	303	1/1	0.89	0.26	53,53,53,53	0
55	MG	BA	1628	1/1	0.90	0.22	97,97,97,97	0
55	MG	DA	3114	1/1	0.90	0.10	59,59,59,59	0
65	1PE	DA	3185	16/16	0.90	0.22	42,50,62,64	0
58	PUT	DA	3204	6/6	0.90	0.33	63,65,68,69	0
59	TAC	AA	1678	32/32	0.90	0.19	64,73,81,82	0
55	MG	CA	3087	1/1	0.90	0.10	91,91,91,91	0
55	MG	DA	3108	1/1	0.90	0.18	39,39,39,39	0
55	MG	DA	3079	1/1	0.90	0.08	76,76,76,76	0
55	MG	CA	3099	1/1	0.90	0.21	101,101,101,101	0
57	MPD	AA	1671	8/8	0.90	0.71	96,98,99,101	0
55	MG	DB	207	1/1	0.90	0.90	99,99,99,99	0
56	PG4	DS	202	13/13	0.90	0.30	49,51,61,62	0
55	MG	BA	1613	1/1	0.90	0.14	54,54,54,54	0
55	MG	CA	3008	1/1	0.90	0.23	244,244,244,244	0
66	ACY	DA	3201	4/4	0.91	0.28	53,56,57,57	0
55	MG	AA	1613	1/1	0.91	0.97	68,68,68,68	0
55	MG	CA	3058	1/1	0.91	0.22	137,137,137,137	0
55	MG	CA	3047	1/1	0.91	0.15	94,94,94,94	0
58	PUT	DA	3189	6/6	0.91	0.32	38,44,47,47	0
55	MG	AA	1640	1/1	0.91	0.09	61,61,61,61	0
55	MG	DA	3128	1/1	0.91	0.20	73,73,73,73	0
55	MG	DA	3135	1/1	0.91	0.40	73,73,73,73	0
55	MG	DB	208	1/1	0.91	0.26	66,66,66,66	0
55	MG	BA	1604	1/1	0.91	0.07	99,99,99,99	0
55	MG	AA	1656	1/1	0.91	0.14	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	1645	1/1	0.91	0.07	48,48,48,48	0
55	MG	DA	3081	1/1	0.91	0.13	94,94,94,94	0
55	MG	DA	3139	1/1	0.91	0.64	58,58,58,58	1
55	MG	AA	1651	1/1	0.92	0.14	68,68,68,68	0
55	MG	DA	3156	1/1	0.92	0.27	74,74,74,74	0
55	MG	DR	203	1/1	0.92	0.44	108,108,108,108	0
64	SPD	DA	3183	10/10	0.92	0.41	48,57,60,60	0
55	MG	CA	3115	1/1	0.92	0.60	76,76,76,76	0
55	MG	CA	3097	1/1	0.92	0.10	110,110,110,110	0
55	MG	DA	3142	1/1	0.92	0.36	73,73,73,73	0
55	MG	DA	3013	1/1	0.92	0.15	67,67,67,67	0
55	MG	CA	3149	1/1	0.92	0.63	73,73,73,73	0
62	EDO	DA	3197	4/4	0.92	0.27	66,66,67,67	0
55	MG	DA	3091	1/1	0.92	0.23	28,28,28,28	0
55	MG	CA	3023	1/1	0.92	0.13	134,134,134,134	0
55	MG	DA	3090	1/1	0.92	0.20	21,21,21,21	0
55	MG	CA	3024	1/1	0.92	0.25	104,104,104,104	0
64	SPD	DA	3223	10/10	0.92	0.27	39,42,46,46	0
55	MG	CA	3077	1/1	0.92	0.23	189,189,189,189	0
55	MG	DA	3073	1/1	0.92	0.18	45,45,45,45	0
55	MG	AA	1669	1/1	0.92	0.11	109,109,109,109	0
55	MG	DA	3063	1/1	0.92	0.24	219,219,219,219	0
55	MG	DB	204	1/1	0.92	0.15	65,65,65,65	0
55	MG	AA	1649	1/1	0.92	0.10	58,58,58,58	0
55	MG	BA	1603	1/1	0.92	0.28	95,95,95,95	0
55	MG	DA	3227	1/1	0.92	0.14	52,52,52,52	0
55	MG	DA	3080	1/1	0.93	0.08	105,105,105,105	0
55	MG	AA	1667	1/1	0.93	0.12	51,51,51,51	0
55	MG	DA	3040	1/1	0.93	0.16	30,30,30,30	0
55	MG	DA	3177	1/1	0.93	0.33	84,84,84,84	0
55	MG	DA	3121	1/1	0.93	0.40	90,90,90,90	0
55	MG	BA	1614	1/1	0.93	0.14	123,123,123,123	0
55	MG	CA	3083	1/1	0.93	0.30	209,209,209,209	0
62	EDO	DB	211	4/4	0.93	0.26	74,74,75,75	0
55	MG	DA	3103	1/1	0.93	0.10	46,46,46,46	0
55	MG	AA	1659	1/1	0.93	0.04	73,73,73,73	0
55	MG	DA	3049	1/1	0.93	0.13	31,31,31,31	0
55	MG	DA	3027	1/1	0.93	0.25	76,76,76,76	0
55	MG	DA	3087	1/1	0.93	0.18	45,45,45,45	0
55	MG	CA	3073	1/1	0.93	0.28	197,197,197,197	0
55	MG	DA	3050	1/1	0.93	0.14	35,35,35,35	0
55	MG	DA	3096	1/1	0.93	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3061	1/1	0.93	0.21	227,227,227,227	0
55	MG	DA	3082	1/1	0.93	0.08	57,57,57,57	0
64	SPD	DA	3187	10/10	0.93	0.25	32,35,43,46	0
55	MG	DA	3042	1/1	0.93	0.21	28,28,28,28	0
55	MG	CA	3108	1/1	0.93	0.41	72,72,72,72	0
55	MG	DA	3068	1/1	0.93	0.08	67,67,67,67	0
55	MG	BA	1634	1/1	0.93	0.09	66,66,66,66	0
58	PUT	DA	3188	6/6	0.93	0.25	30,31,33,39	0
55	MG	DA	3043	1/1	0.94	0.13	34,34,34,34	0
55	MG	BA	1615	1/1	0.94	0.18	70,70,70,70	0
55	MG	DA	3146	1/1	0.94	0.13	73,73,73,73	0
55	MG	CA	3029	1/1	0.94	0.16	113,113,113,113	0
55	MG	CA	3050	1/1	0.94	0.16	102,102,102,102	0
55	MG	CA	3117	1/1	0.94	0.54	85,85,85,85	0
55	MG	DM	201	1/1	0.94	0.04	55,55,55,55	0
55	MG	DA	3036	1/1	0.94	0.18	41,41,41,41	0
55	MG	BA	1621	1/1	0.94	0.15	103,103,103,103	0
55	MG	CA	3052	1/1	0.94	0.19	96,96,96,96	0
55	MG	DA	3149	1/1	0.94	0.20	66,66,66,66	0
55	MG	DA	3162	1/1	0.94	0.20	70,70,70,70	0
62	EDO	DA	3198	4/4	0.94	0.25	53,55,55,55	0
55	MG	CA	3113	1/1	0.94	0.38	57,57,57,57	0
58	PUT	DA	3222	6/6	0.94	0.25	46,49,51,52	0
55	MG	DA	3158	1/1	0.94	0.09	55,55,55,55	0
55	MG	DB	205	1/1	0.94	0.20	64,64,64,64	0
55	MG	CA	3018	1/1	0.94	0.18	78,78,78,78	0
55	MG	AA	1664	1/1	0.94	0.13	161,161,161,161	0
55	MG	DA	3029	1/1	0.94	0.14	49,49,49,49	0
55	MG	DA	3041	1/1	0.94	0.08	50,50,50,50	0
55	MG	DA	3152	1/1	0.94	0.29	43,43,43,43	0
55	MG	CA	3094	1/1	0.94	0.08	73,73,73,73	0
55	MG	CA	3126	1/1	0.94	0.15	78,78,78,78	0
55	MG	BA	1638	1/1	0.94	0.86	175,175,175,175	0
55	MG	CA	3086	1/1	0.94	0.07	93,93,93,93	0
55	MG	DA	3123	1/1	0.95	0.15	83,83,83,83	0
55	MG	DA	3032	1/1	0.95	0.19	34,34,34,34	0
55	MG	DA	3141	1/1	0.95	0.20	82,82,82,82	0
55	MG	CA	3045	1/1	0.95	0.08	142,142,142,142	0
55	MG	AA	1607	1/1	0.95	0.56	91,91,91,91	0
55	MG	DA	3083	1/1	0.95	0.07	60,60,60,60	0
55	MG	BA	1637	1/1	0.95	0.20	99,99,99,99	0
55	MG	DA	3093	1/1	0.95	0.16	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3036	1/1	0.95	0.30	235,235,235,235	0
55	MG	CA	3014	1/1	0.95	0.26	71,71,71,71	0
66	ACY	DA	3191	4/4	0.95	0.18	55,55,56,57	0
55	MG	BA	1622	1/1	0.95	0.11	82,82,82,82	0
55	MG	DA	3077	1/1	0.95	0.14	22,22,22,22	0
55	MG	DA	3071	1/1	0.95	0.08	90,90,90,90	0
55	MG	DA	3105	1/1	0.95	0.17	31,31,31,31	0
55	MG	DA	3009	1/1	0.95	0.08	89,89,89,89	0
55	MG	AA	1653	1/1	0.95	0.06	81,81,81,81	0
55	MG	DA	3057	1/1	0.96	0.12	49,49,49,49	0
55	MG	DA	3111	1/1	0.96	0.21	38,38,38,38	0
55	MG	CA	3084	1/1	0.96	0.06	75,75,75,75	0
55	MG	CB	201	1/1	0.96	0.06	157,157,157,157	0
55	MG	CA	3135	1/1	0.96	0.23	90,90,90,90	0
55	MG	DA	3115	1/1	0.96	0.16	35,35,35,35	0
55	MG	DA	3088	1/1	0.96	0.14	56,56,56,56	0
55	MG	CA	3043	1/1	0.96	0.10	73,73,73,73	0
55	MG	DA	3038	1/1	0.96	0.23	27,27,27,27	0
63	PGE	DA	3186	10/10	0.96	0.15	29,33,36,37	0
55	MG	AA	1629	1/1	0.96	0.08	82,82,82,82	0
55	MG	DA	3100	1/1	0.96	0.16	34,34,34,34	0
55	MG	CA	3042	1/1	0.96	0.09	92,92,92,92	0
55	MG	AA	1658	1/1	0.96	0.13	83,83,83,83	0
55	MG	AA	1602	1/1	0.96	0.29	82,82,82,82	0
55	MG	DA	3150	1/1	0.96	0.10	51,51,51,51	0
55	MG	DA	3117	1/1	0.96	0.06	32,32,32,32	0
55	MG	DA	3020	1/1	0.96	0.31	11,11,11,11	0
55	MG	DA	3078	1/1	0.96	0.10	32,32,32,32	0
55	MG	AA	1646	1/1	0.96	0.07	53,53,53,53	0
55	MG	DA	3102	1/1	0.96	0.11	52,52,52,52	0
58	PUT	DA	3002	6/6	0.96	0.21	39,41,44,47	0
55	MG	DB	201	1/1	0.96	0.14	63,63,63,63	0
55	MG	DA	3006	1/1	0.96	0.10	60,60,60,60	0
55	MG	DA	3007	1/1	0.96	0.10	111,111,111,111	0
55	MG	CA	3072	1/1	0.97	0.51	255,255,255,255	0
55	MG	AA	1647	1/1	0.97	0.20	201,201,201,201	0
55	MG	DA	3140	1/1	0.97	0.12	43,43,43,43	0
55	MG	AA	1650	1/1	0.97	0.08	75,75,75,75	0
55	MG	BA	1630	1/1	0.97	0.12	101,101,101,101	0
55	MG	DA	3066	1/1	0.97	0.14	22,22,22,22	0
55	MG	DA	3054	1/1	0.97	0.09	47,47,47,47	0
55	MG	DA	3012	1/1	0.97	0.14	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3052	1/1	0.97	0.12	33,33,33,33	0
55	MG	DA	3098	1/1	0.97	0.08	39,39,39,39	0
55	MG	DA	3016	1/1	0.97	0.18	62,62,62,62	0
55	MG	AA	1638	1/1	0.97	0.22	94,94,94,94	0
60	ZN	C5	101	1/1	0.97	0.08	139,139,139,139	0
55	MG	DA	3116	1/1	0.97	0.12	45,45,45,45	0
55	MG	DA	3008	1/1	0.97	0.07	73,73,73,73	0
55	MG	DA	3064	1/1	0.97	0.12	63,63,63,63	0
55	MG	DA	3030	1/1	0.97	0.13	14,14,14,14	0
57	MPD	DS	203	8/8	0.97	0.23	36,40,42,44	0
55	MG	DA	3120	1/1	0.97	0.33	48,48,48,48	0
55	MG	DA	3011	1/1	0.97	0.16	24,24,24,24	0
55	MG	AA	1668	1/1	0.97	0.14	40,40,40,40	0
55	MG	AA	1643	1/1	0.97	0.14	64,64,64,64	0
55	MG	AA	1662	1/1	0.97	0.19	84,84,84,84	0
55	MG	DA	3033	1/1	0.97	0.19	19,19,19,19	0
55	MG	DA	3086	1/1	0.97	0.16	41,41,41,41	0
55	MG	DA	3056	1/1	0.97	0.21	39,39,39,39	0
55	MG	DA	3230	1/1	0.97	0.34	37,37,37,37	0
55	MG	DD	302	1/1	0.97	0.09	53,53,53,53	0
55	MG	DA	3084	1/1	0.97	0.10	44,44,44,44	0
55	MG	DA	3169	1/1	0.97	0.20	72,72,72,72	0
55	MG	DA	3119	1/1	0.97	0.07	53,53,53,53	0
55	MG	BA	1617	1/1	0.97	0.07	65,65,65,65	0
55	MG	CA	3010	1/1	0.97	0.27	99,99,99,99	0
55	MG	AA	1677	1/1	0.97	0.12	78,78,78,78	0
55	MG	DA	3028	1/1	0.98	0.17	41,41,41,41	0
55	MG	DA	3018	1/1	0.98	0.19	29,29,29,29	0
55	MG	DA	3072	1/1	0.98	0.12	49,49,49,49	0
55	MG	DA	3044	1/1	0.98	0.13	36,36,36,36	0
55	MG	DA	3039	1/1	0.98	0.15	27,27,27,27	0
55	MG	AA	1652	1/1	0.98	0.24	40,40,40,40	0
55	MG	DA	3060	1/1	0.98	0.13	29,29,29,29	0
55	MG	DA	3113	1/1	0.98	0.21	25,25,25,25	0
55	MG	DA	3017	1/1	0.98	0.12	56,56,56,56	0
55	MG	DA	3101	1/1	0.98	0.19	30,30,30,30	0
55	MG	AA	1631	1/1	0.98	0.07	60,60,60,60	0
55	MG	DA	3062	1/1	0.98	0.15	33,33,33,33	0
55	MG	DA	3070	1/1	0.98	0.18	54,54,54,54	0
55	MG	DA	3229	1/1	0.98	0.08	38,38,38,38	0
55	MG	DA	3074	1/1	0.98	0.16	32,32,32,32	0
55	MG	DA	3023	1/1	0.98	0.20	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3127	1/1	0.98	0.34	71,71,71,71	0
55	MG	DA	3021	1/1	0.98	0.09	55,55,55,55	0
55	MG	DA	3015	1/1	0.98	0.18	17,17,17,17	0
55	MG	DA	3109	1/1	0.98	0.10	29,29,29,29	0
55	MG	DA	3075	1/1	0.98	0.06	39,39,39,39	0
55	MG	AA	1666	1/1	0.98	0.04	54,54,54,54	0
55	MG	DA	3228	1/1	0.98	0.07	44,44,44,44	0
55	MG	DA	3034	1/1	0.98	0.15	29,29,29,29	0
55	MG	DA	3051	1/1	0.98	0.14	24,24,24,24	0
55	MG	DA	3089	1/1	0.98	0.11	46,46,46,46	0
55	MG	DA	3085	1/1	0.98	0.15	45,45,45,45	0
55	MG	DA	3025	1/1	0.98	0.21	26,26,26,26	0
55	MG	DA	3076	1/1	0.98	0.12	25,25,25,25	0
55	MG	DA	3058	1/1	0.98	0.06	37,37,37,37	0
60	ZN	D5	101	1/1	0.98	0.15	55,55,55,55	0
55	MG	DA	3055	1/1	0.98	0.09	55,55,55,55	0
55	MG	DA	3061	1/1	0.98	0.16	19,19,19,19	0
55	MG	DA	3019	1/1	0.98	0.12	47,47,47,47	0
55	MG	DA	3010	1/1	0.98	0.15	24,24,24,24	0
55	MG	DA	3137	1/1	0.98	0.25	55,55,55,55	0
55	MG	DA	3094	1/1	0.98	0.19	25,25,25,25	0
55	MG	BA	1645	1/1	0.98	0.06	87,87,87,87	0
55	MG	DA	3059	1/1	0.98	0.14	32,32,32,32	0
55	MG	DA	3046	1/1	0.98	0.05	47,47,47,47	0
55	MG	DA	3035	1/1	0.98	0.17	20,20,20,20	0
55	MG	AA	1648	1/1	0.98	0.09	63,63,63,63	0
55	MG	DA	3014	1/1	0.98	0.29	24,24,24,24	0
55	MG	DA	3048	1/1	0.99	0.12	47,47,47,47	0
55	MG	DA	3092	1/1	0.99	0.15	18,18,18,18	0
55	MG	DB	203	1/1	0.99	0.09	37,37,37,37	0
55	MG	DA	3106	1/1	0.99	0.17	32,32,32,32	0
55	MG	DA	3110	1/1	0.99	0.20	20,20,20,20	0
55	MG	DA	3069	1/1	0.99	0.19	36,36,36,36	0
55	MG	DA	3067	1/1	0.99	0.09	51,51,51,51	0
55	MG	DA	3037	1/1	0.99	0.21	26,26,26,26	0
55	MG	DB	202	1/1	0.99	0.14	33,33,33,33	0
55	MG	DA	3031	1/1	0.99	0.17	35,35,35,35	0
55	MG	DA	3024	1/1	0.99	0.23	42,42,42,42	0
55	MG	DA	3095	1/1	0.99	0.22	38,38,38,38	0
55	MG	DA	3047	1/1	0.99	0.20	34,34,34,34	0
55	MG	DA	3104	1/1	0.99	0.13	59,59,59,59	0
55	MG	DA	3107	1/1	1.00	0.16	39,39,39,39	0

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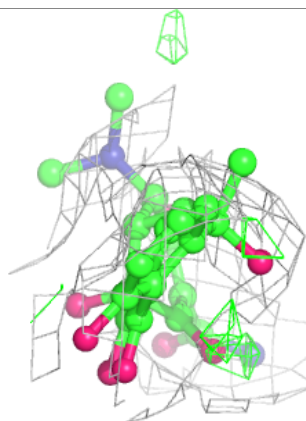
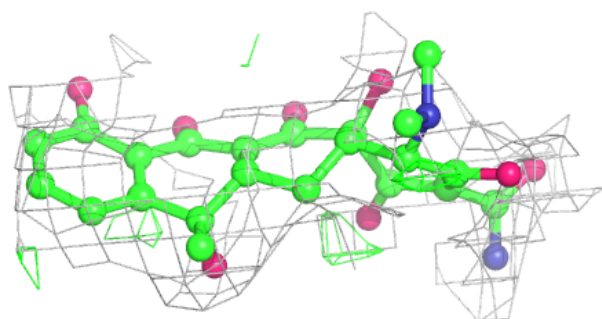
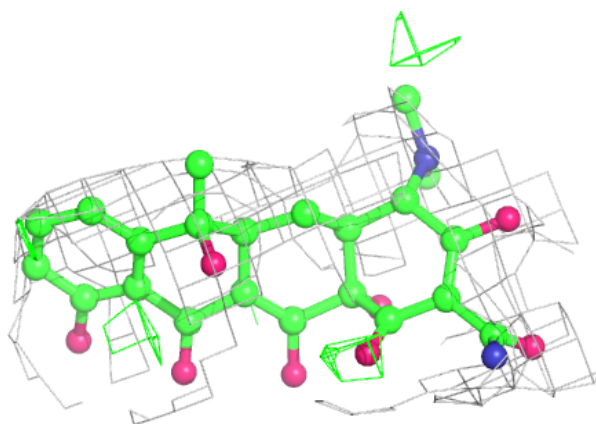
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	3026	1/1	1.00	0.10	29,29,29,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

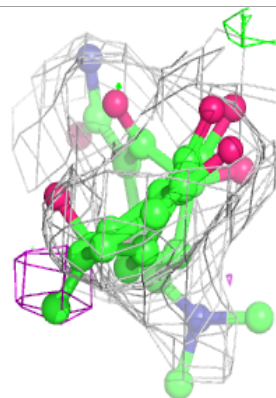
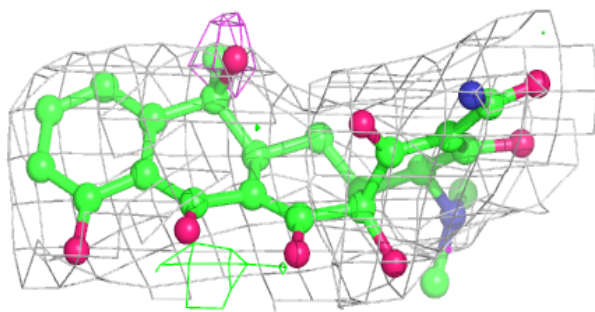
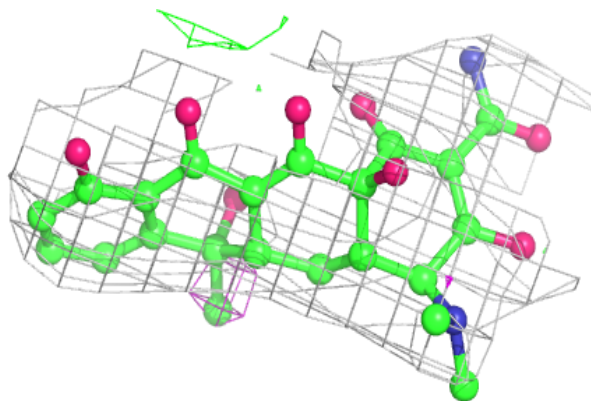
Electron density around TAC BA 1602:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TAC AA 1678:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.