



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2016 – 10:35 AM EDT

PDB ID : 5JC9  
Title : Structure of the Escherichia coli ribosome with the U1052G mutation in the 16S rRNA  
Authors : Cocozaki, A.; Ferguson, A.  
Deposited on : 2016-04-14  
Resolution : 3.03 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

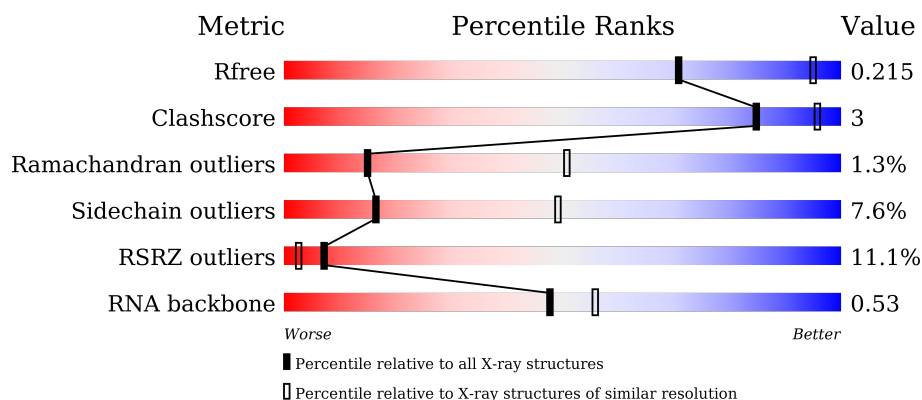
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.03 Å.

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



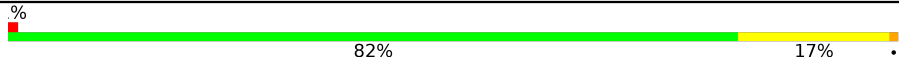

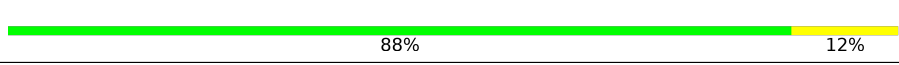

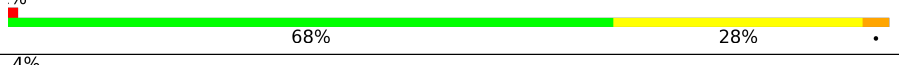
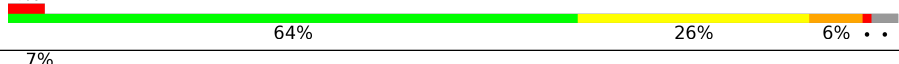
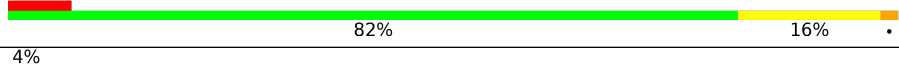

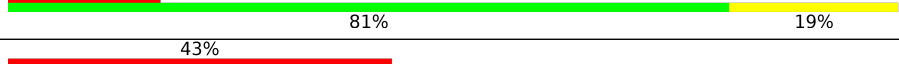


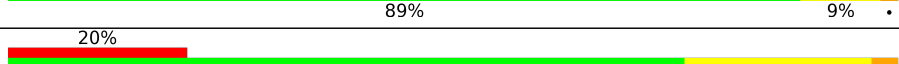
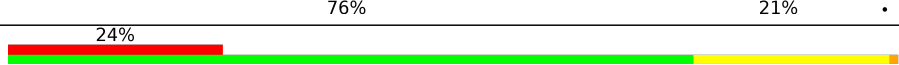
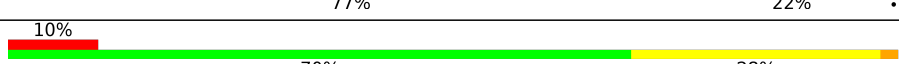

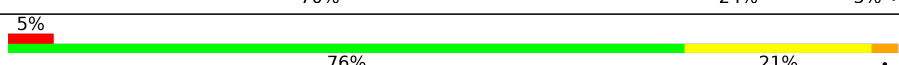
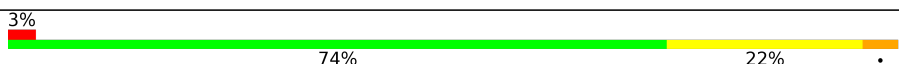
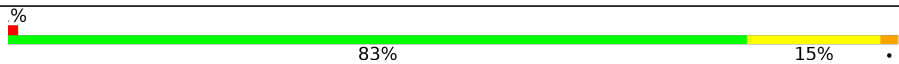
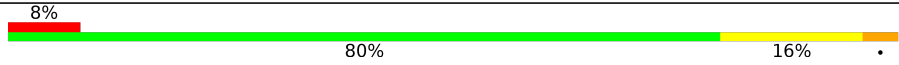


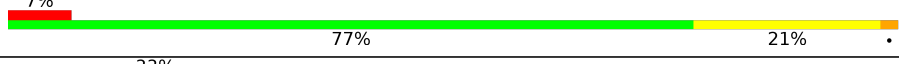
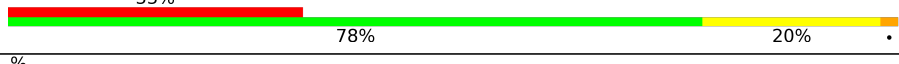
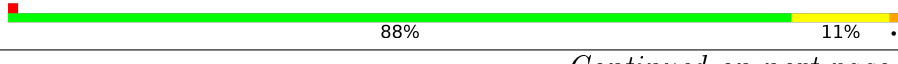

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1995 (3.08-3.00)
Clashscore	102246	2351 (3.08-3.00)
Ramachandran outliers	100387	2272 (3.08-3.00)
Sidechain outliers	100360	2275 (3.08-3.00)
RSRZ outliers	91569	2013 (3.08-3.00)
RNA backbone	2183	1061 (3.48-2.60)

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

Mol	Chain	Length	Quality of chain
1	AA	1534	<div> <div>2%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
1	BA	1534	<div> <div>10%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>
2	AB	224	<div> <div>7%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
2	BB	224	<div> <div>16%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>

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

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

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


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

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Mol	Chain	Length	Quality of chain
55	DA	2904	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	1608	-	-	-	X
56	MG	AA	1612	-	-	-	X
56	MG	AA	1642	-	-	-	X
56	MG	BA	1612	-	-	-	X
56	MG	BA	1627	-	-	-	X
56	MG	CA	3003	-	-	-	X
56	MG	CA	3026	-	-	-	X
56	MG	CA	3039	-	-	-	X
56	MG	CA	3105	-	-	-	X
56	MG	CA	3122	-	-	-	X
56	MG	CA	3133	-	-	-	X
56	MG	CA	3137	-	-	-	X
56	MG	DA	3039	-	-	-	X
56	MG	DA	3126	-	-	-	X
56	MG	DA	3128	-	-	-	X
56	MG	DA	3129	-	-	-	X
56	MG	DA	3142	-	-	-	X
56	MG	DA	3175	-	-	-	X
56	MG	DA	3180	-	-	-	X
57	PG4	AA	1670	-	-	-	X
57	PG4	BA	1642	-	-	-	X
57	PG4	DA	3196	-	-	-	X
57	PG4	DA	3218	-	-	-	X
57	PG4	DS	202	-	-	-	X
58	MPD	AA	1671	-	-	-	X
58	MPD	AA	1676	-	-	-	X
58	MPD	DA	3004	-	-	-	X
58	MPD	DA	3195	-	-	-	X
58	MPD	DA	3206	-	-	-	X
58	MPD	DA	3209	-	-	-	X
58	MPD	DE	301	-	-	-	X
58	MPD	DE	302	-	-	-	X
58	MPD	DT	201	-	-	-	X
59	PUT	AA	1673	-	-	-	X
59	PUT	AA	1674	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	PUT	DA	3187	-	-	-	X
59	PUT	DA	3192	-	-	-	X
59	PUT	DA	3198	-	-	-	X
59	PUT	DA	3207	-	-	-	X
59	PUT	DA	3215	-	-	-	X
59	PUT	DA	3221	-	-	-	X
59	PUT	DA	3223	-	-	-	X
59	PUT	DA	3224	-	-	-	X
59	PUT	DM	201	-	-	-	X
61	PEG	AL	201	-	-	-	X
61	PEG	D1	103	-	-	-	X
61	PEG	D3	102	-	-	-	X
61	PEG	DA	3203	-	-	-	X
61	PEG	DA	3220	-	-	-	X
61	PEG	DA	3228	-	-	-	X
61	PEG	DL	201	-	-	-	X
61	PEG	DQ	201	-	-	-	X
62	EDO	DA	3002	-	-	-	X
62	EDO	DA	3200	-	-	-	X
62	EDO	DA	3201	-	-	-	X
62	EDO	DA	3211	-	-	-	X
63	PGE	D1	102	-	-	-	X
63	PGE	D3	101	-	-	-	X
63	PGE	DA	3216	-	-	-	X
63	PGE	DA	3219	-	-	-	X
63	PGE	DD	301	-	-	-	X
63	PGE	DS	201	-	-	-	X
63	PGE	DU	101	-	-	-	X
64	SPD	DA	3186	-	-	-	X
64	SPD	DA	3190	-	-	-	X
64	SPD	DA	3208	-	-	-	X
64	SPD	DA	3226	-	-	-	X
65	1PE	DA	3205	-	-	-	X
66	ACY	DA	3204	-	-	-	X
67	GUN	DA	3213	-	-	-	X



## 2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295130 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
			32933	14695	6044	10660	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32911	14685	6039	10654	1533			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1052	G	U	engineered mutation	GB 731469900
BA	1052	G	U	engineered mutation	GB 731469900

- 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			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	0
			796	498	152	145	1			
10	BJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0	0
			670	414	138	115	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	C5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
26	D5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

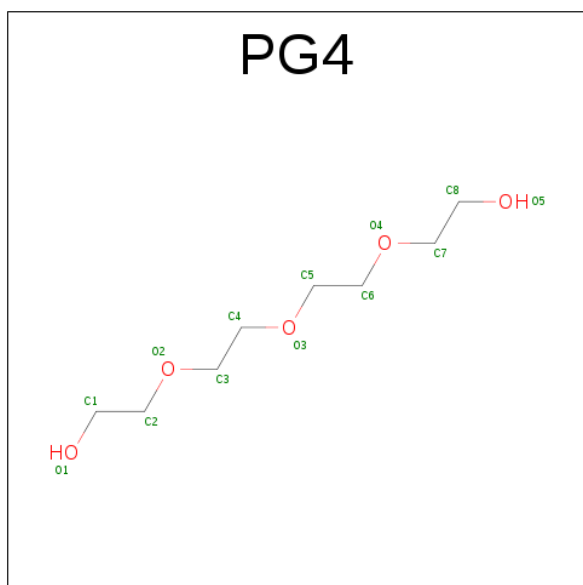
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BA	43	Total	Mg	0	0
			43	43		
56	CA	156	Total	Mg	0	0
			156	156		
56	CB	3	Total	Mg	0	0
			3	3		
56	DM	1	Total	Mg	0	0
			1	1		
56	DR	1	Total	Mg	0	0
			1	1		
56	AA	71	Total	Mg	0	0
			71	71		
56	DA	184	Total	Mg	0	0
			184	184		

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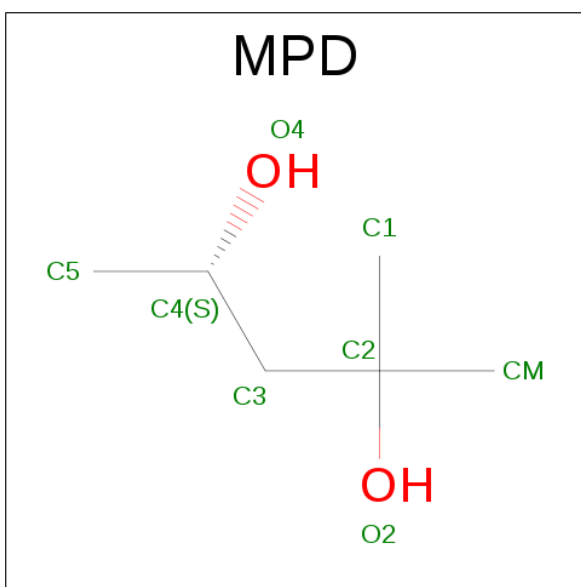
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DB	9	Total	Mg	0	0
			9	9		
56	DD	1	Total	Mg	0	0
			1	1		

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



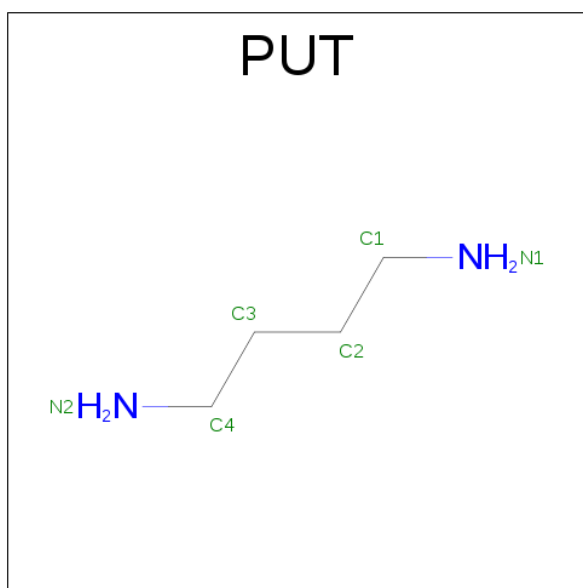
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			13	8	5		
57	BA	1	Total	C	O	0	0
			13	8	5		
57	DQ	1	Total	C	O	0	0
			13	8	5		
57	DR	1	Total	C	O	0	0
			13	8	5		
57	DS	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		

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



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

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



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

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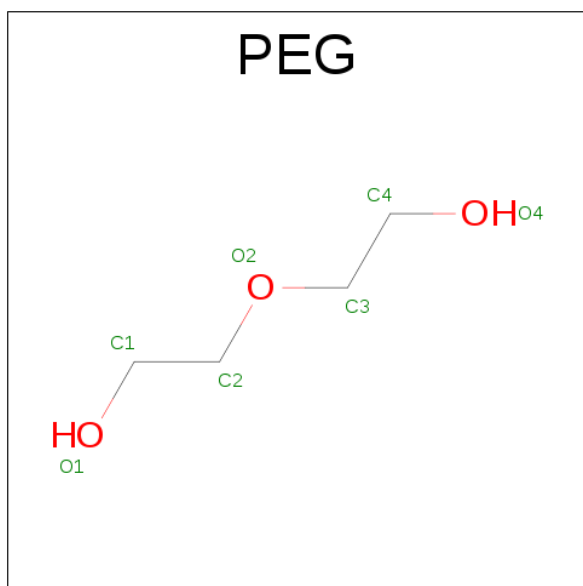
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		

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

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

- Molecule 61 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



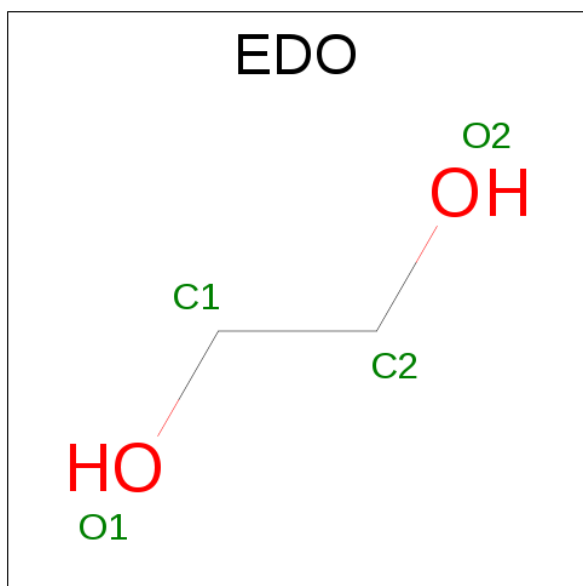
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	AL	1	Total	C	O	0	0
			7	4	3		
61	D1	1	Total	C	O	0	0
			7	4	3		
61	D3	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	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: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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		

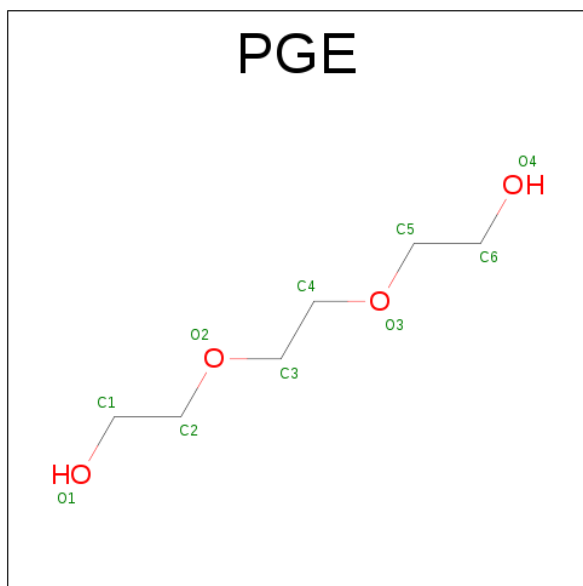
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1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

- Molecule 63 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



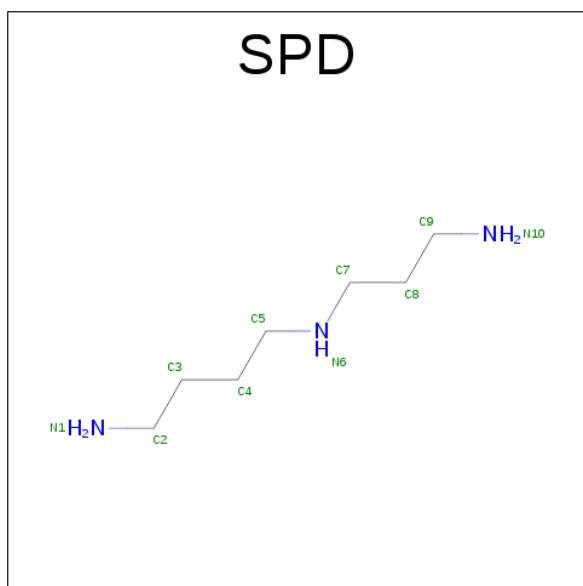
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			10	6	4		
63	D3	1	Total	C	O	0	0
			10	6	4		

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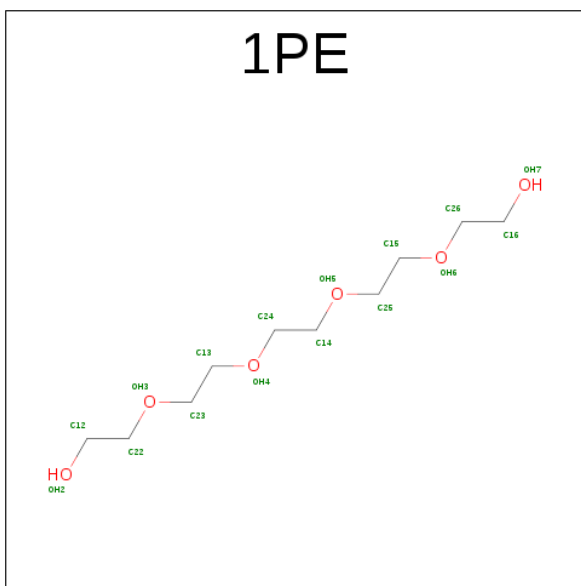
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	DD	1	Total	C	O	0	0
			10	6	4		
63	DS	1	Total	C	O	0	0
			10	6	4		
63	DU	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		

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



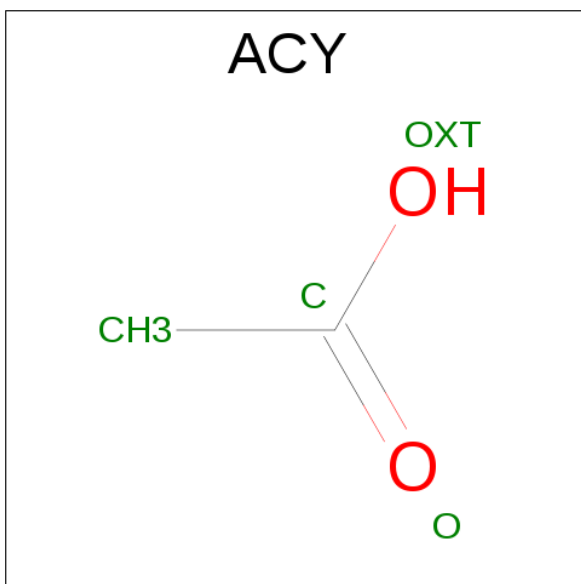
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		

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



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

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



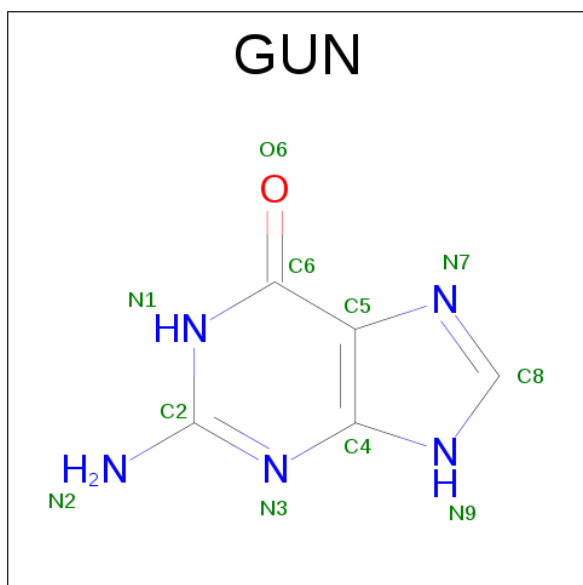
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		

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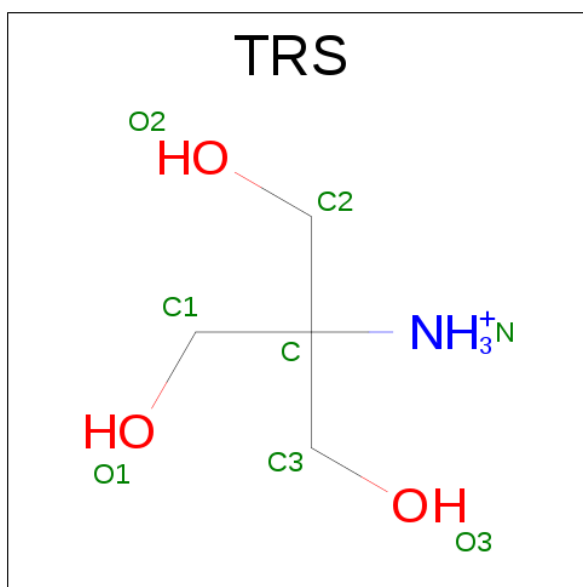
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		

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



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

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



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

- Molecule 69 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AA	508	Total	O	0	0
			508	508		
69	AC	5	Total	O	0	0
			5	5		
69	AD	1	Total	O	0	0
			1	1		
69	AE	5	Total	O	0	0
			5	5		
69	AF	1	Total	O	0	0
			1	1		
69	AG	1	Total	O	0	0
			1	1		
69	AJ	3	Total	O	0	0
			3	3		
69	AK	6	Total	O	0	0
			6	6		
69	AL	10	Total	O	0	0
			10	10		
69	AM	4	Total	O	0	0
			4	4		
69	AN	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AO	2	Total 2	O 2	0	0
69	AP	2	Total 2	O 2	0	0
69	AT	4	Total 4	O 4	0	0
69	AU	2	Total 2	O 2	0	0
69	C3	2	Total 2	O 2	0	0
69	C4	1	Total 1	O 1	0	0
69	C5	1	Total 1	O 1	0	0
69	BA	282	Total 282	O 282	0	0
69	BD	12	Total 12	O 12	0	0
69	BE	1	Total 1	O 1	0	0
69	BF	1	Total 1	O 1	0	0
69	BK	3	Total 3	O 3	0	0
69	BL	6	Total 6	O 6	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	3	Total 3	O 3	0	0
69	BU	3	Total 3	O 3	0	0
69	D1	46	Total 46	O 46	0	0
69	D2	6	Total 6	O 6	0	0

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*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	D3	28	Total 28	O 28	0	0
69	D4	33	Total 33	O 33	0	0
69	D5	11	Total 11	O 11	0	0
69	D0	26	Total 26	O 26	0	0
69	CB	13	Total 13	O 13	0	0
69	CC	8	Total 8	O 8	0	0
69	CD	7	Total 7	O 7	0	0
69	CA	693	Total 693	O 693	0	0
69	DC	102	Total 102	O 102	0	0
69	DD	95	Total 95	O 95	0	0
69	CE	4	Total 4	O 4	0	0
69	CL	1	Total 1	O 1	0	0
69	CM	4	Total 4	O 4	0	0
69	CO	2	Total 2	O 2	0	0
69	CQ	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	16	Total 16	O 16	0	0

*Continued on next page...*

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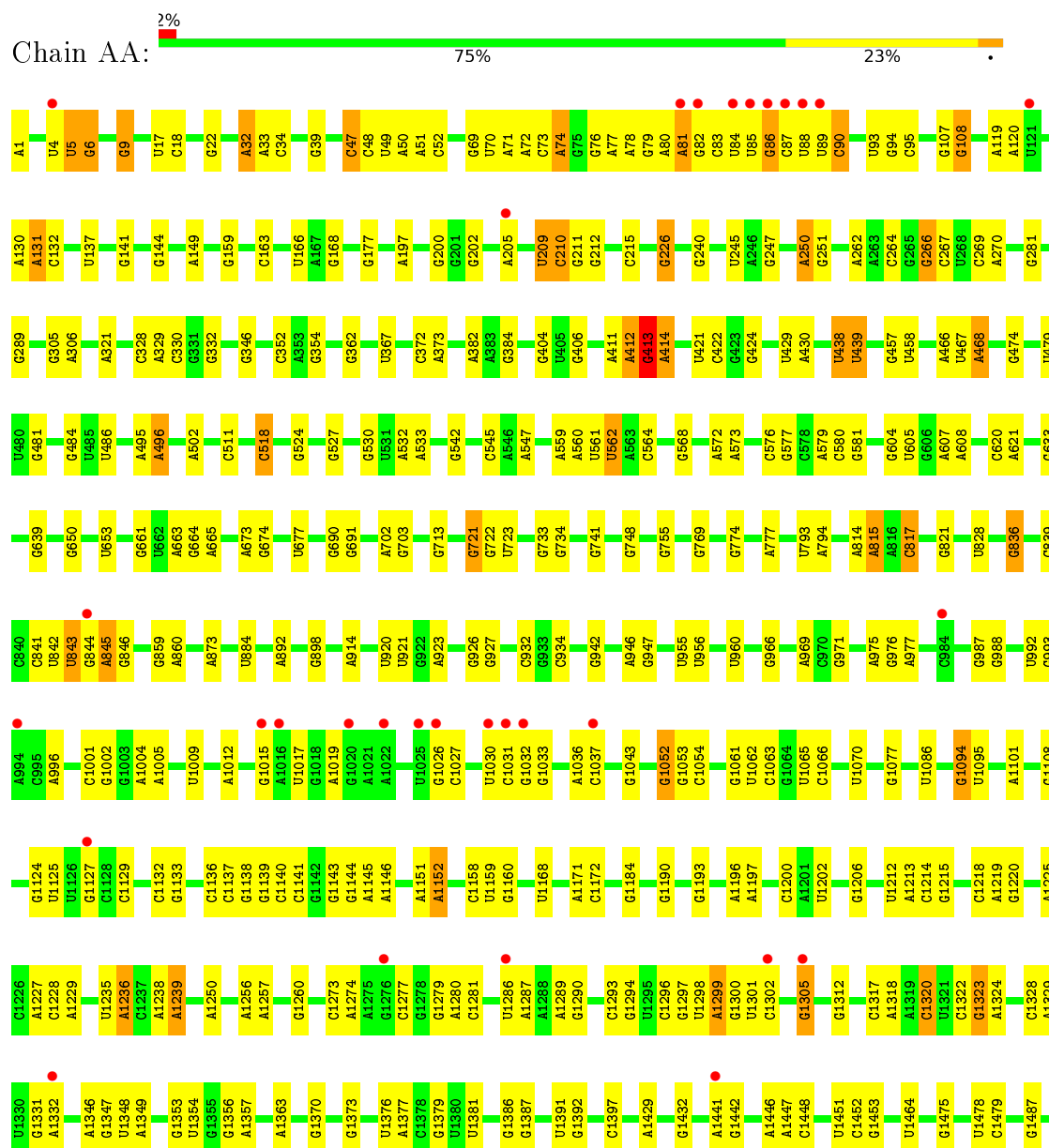
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DG	7	Total 7	O 7	0	0
69	DH	2	Total 2	O 2	0	0
69	DK	60	Total 60	O 60	0	0
69	DL	51	Total 51	O 51	0	0
69	DM	68	Total 68	O 68	0	0
69	DN	73	Total 73	O 73	0	0
69	DO	49	Total 49	O 49	0	0
69	DP	38	Total 38	O 38	0	0
69	DQ	29	Total 29	O 29	0	0
69	DR	61	Total 61	O 61	0	0
69	DS	50	Total 50	O 50	0	0
69	DT	66	Total 66	O 66	0	0
69	DU	19	Total 19	O 19	0	0
69	DV	21	Total 21	O 21	0	0
69	DW	32	Total 32	O 32	0	0
69	DX	25	Total 25	O 25	0	0
69	DY	10	Total 10	O 10	0	0
69	DZ	6	Total 6	O 6	0	0
69	DB	203	Total 203	O 203	0	0
69	DA	4830	Total 4830	O 4830	0	0

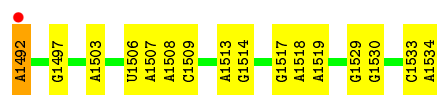


### 3 Residue-property plots

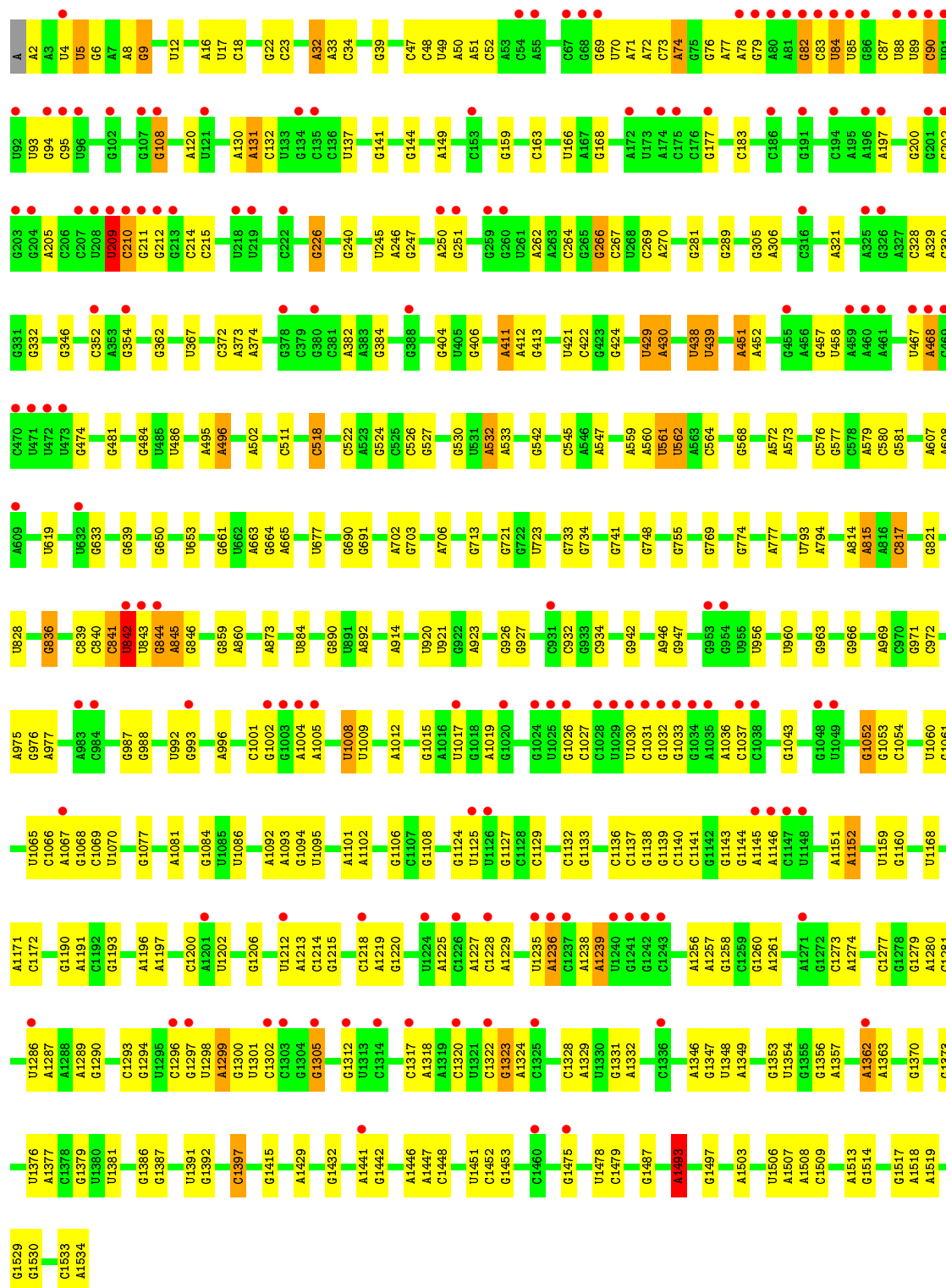
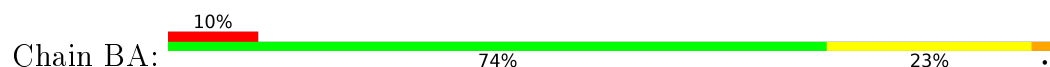
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: 16S rRNA

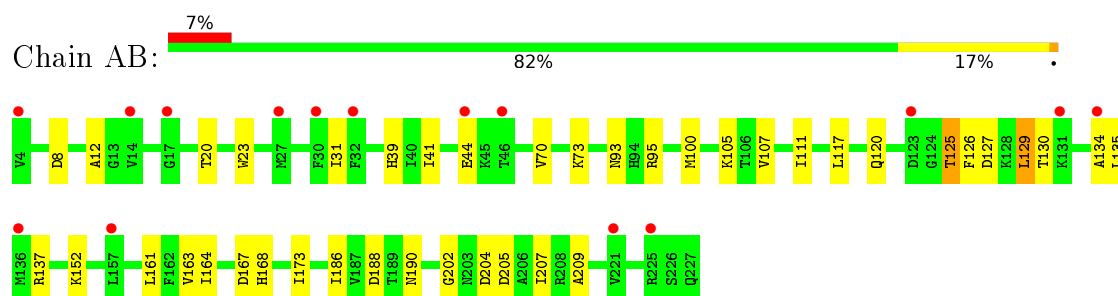




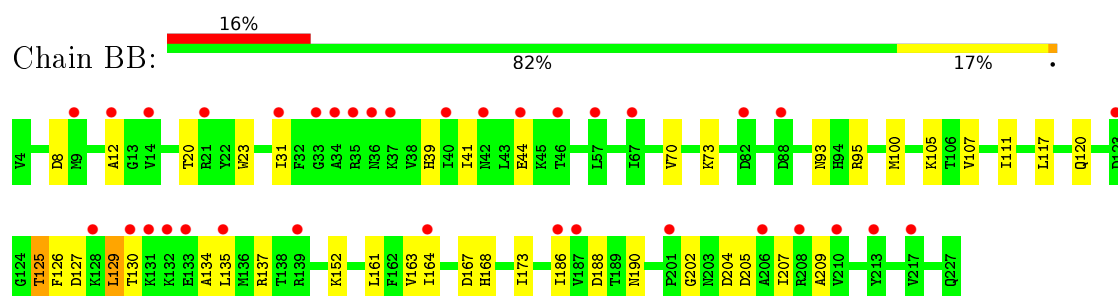
• Molecule 1: 16S rRNA



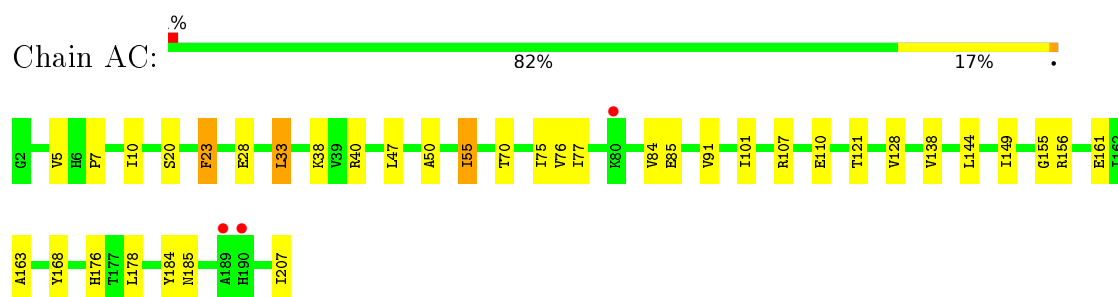
- Molecule 2: 30S ribosomal protein S2



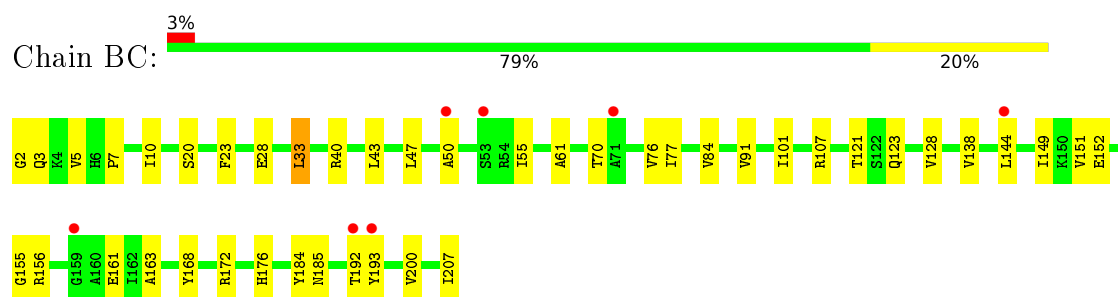
- Molecule 2: 30S ribosomal protein S2



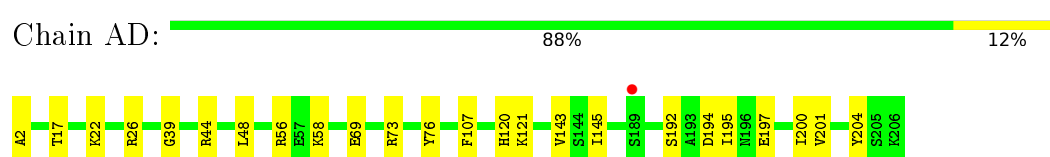
- Molecule 3: 30S ribosomal protein S3



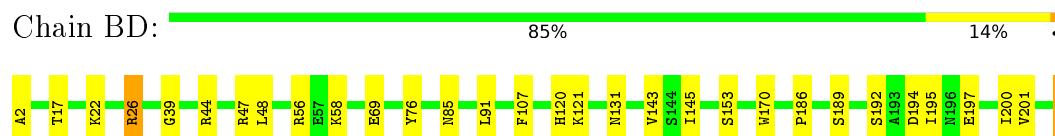
- Molecule 3: 30S ribosomal protein S3



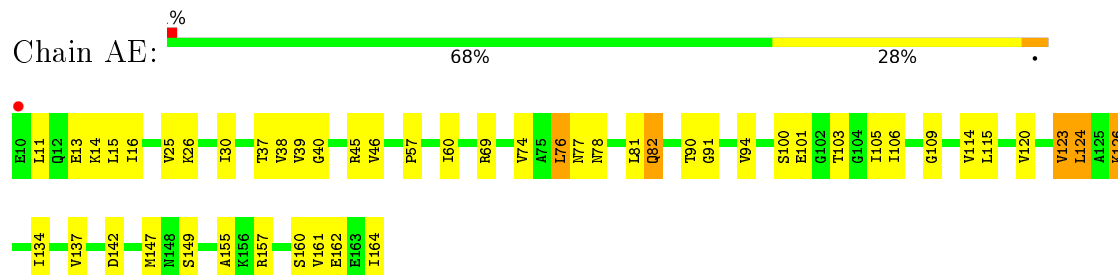
- Molecule 4: 30S ribosomal protein S4



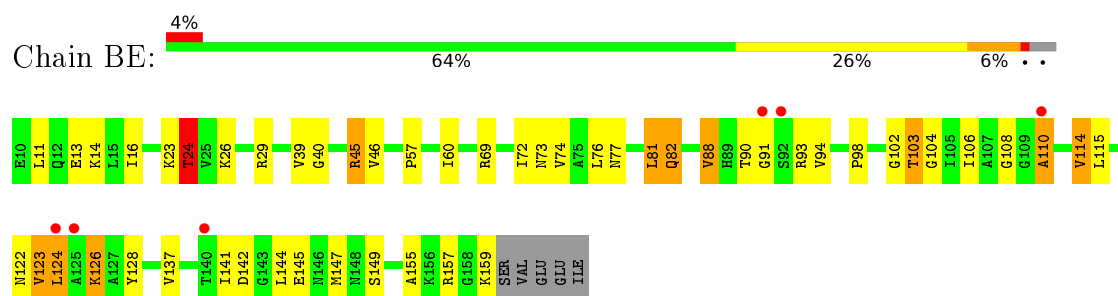
- Molecule 4: 30S ribosomal protein S4



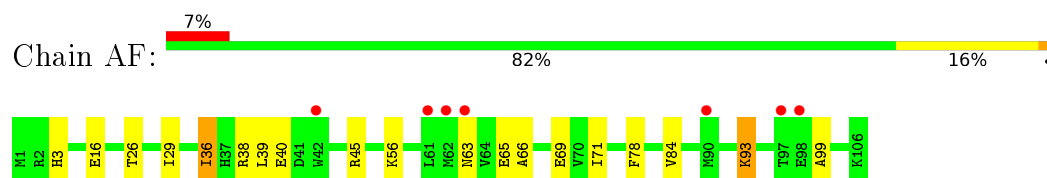
- Molecule 5: 30S ribosomal protein S5



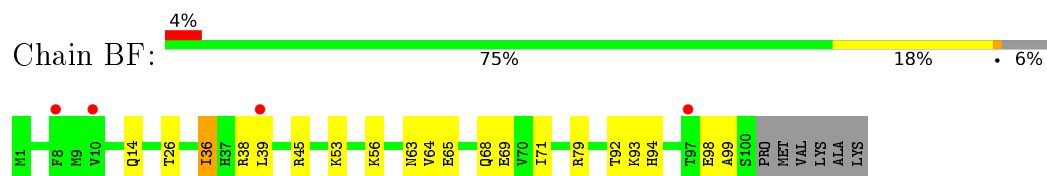
- Molecule 5: 30S ribosomal protein S5



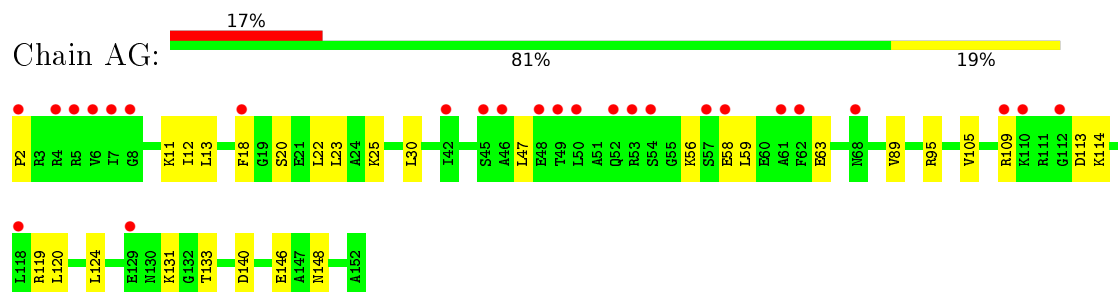
- Molecule 6: 30S ribosomal protein S6



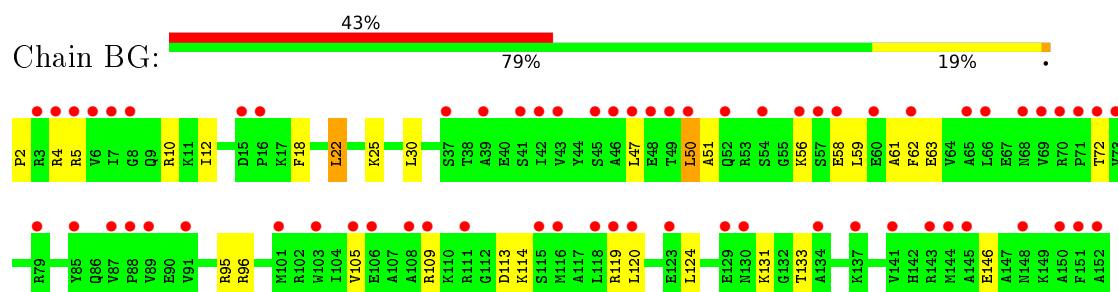
- Molecule 6: 30S ribosomal protein S6



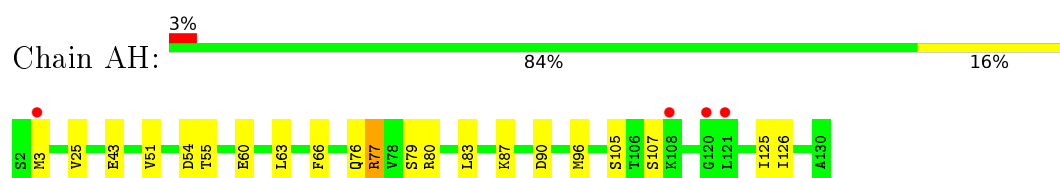
- Molecule 7: 30S ribosomal protein S7



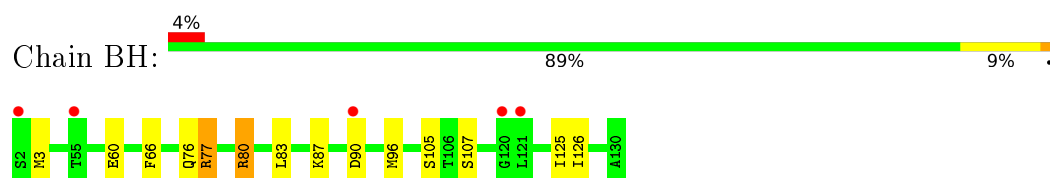
- Molecule 7: 30S ribosomal protein S7



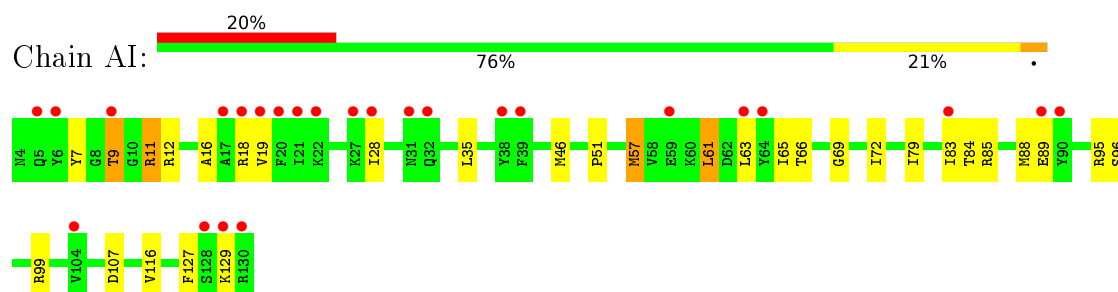
- Molecule 8: 30S ribosomal protein S8



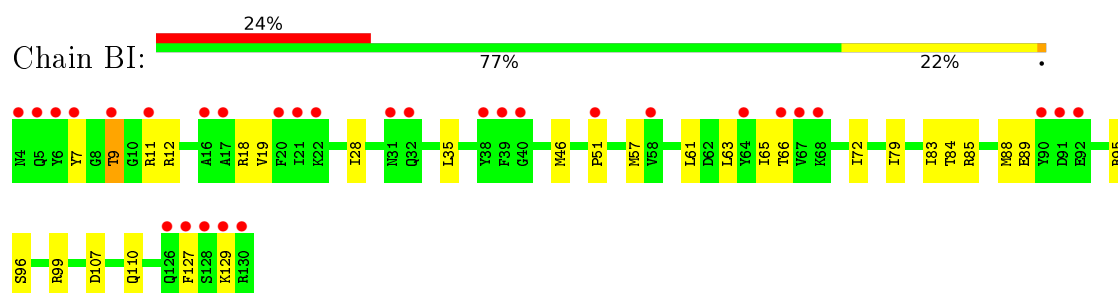
- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9



- Molecule 9: 30S ribosomal protein S9

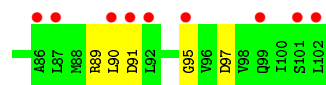
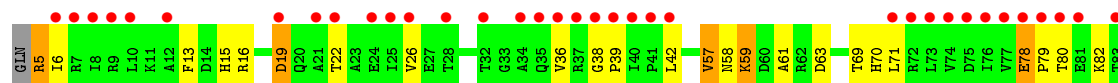
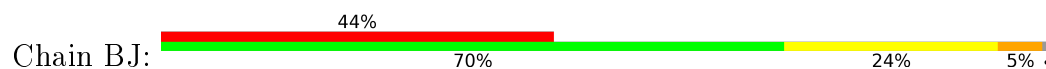


- Molecule 10: 30S ribosomal protein S10

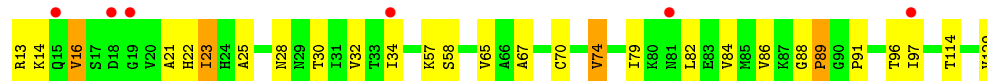
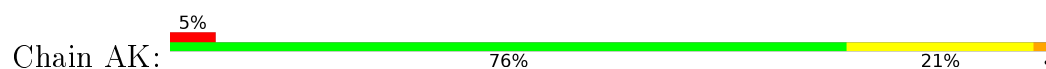




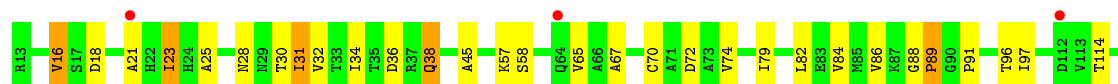
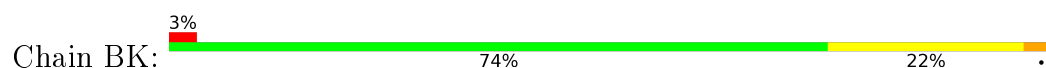
- Molecule 10: 30S ribosomal protein S10



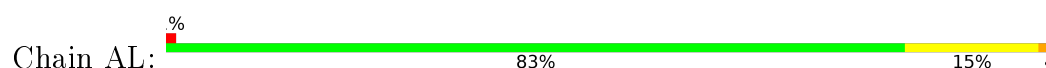
- Molecule 11: 30S ribosomal protein S11



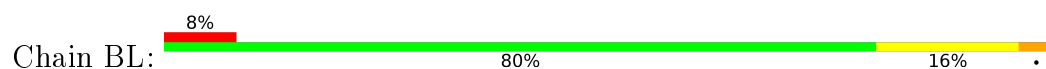
- Molecule 11: 30S ribosomal protein S11



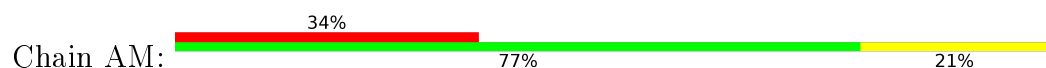
- Molecule 12: 30S ribosomal protein S12

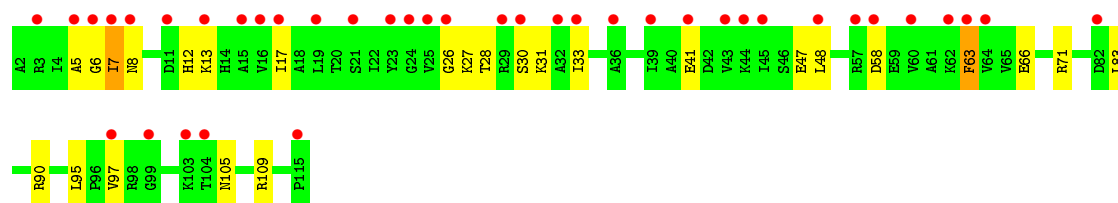


- Molecule 12: 30S ribosomal protein S12

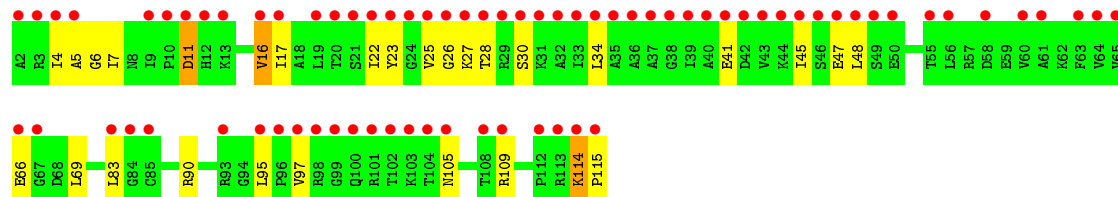
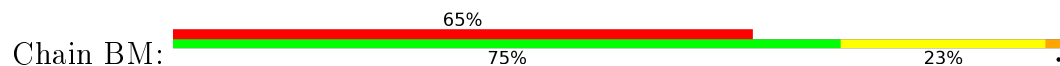


- Molecule 13: 30S ribosomal protein S13





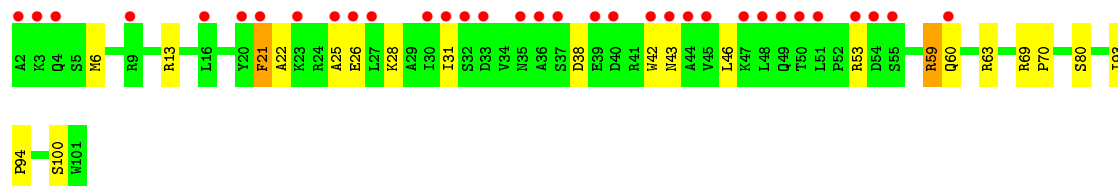
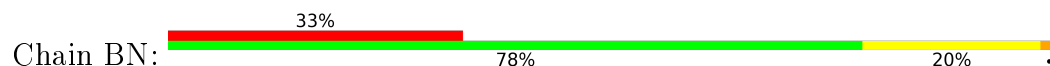
• Molecule 13: 30S ribosomal protein S13



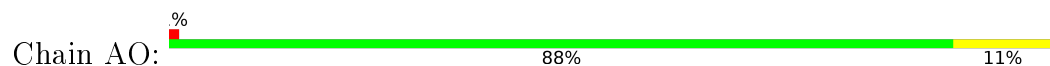
• Molecule 14: 30S ribosomal protein S14



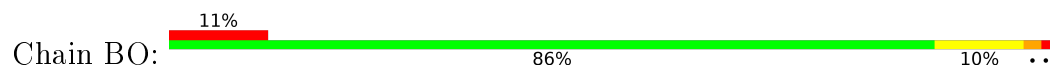
• Molecule 14: 30S ribosomal protein S14



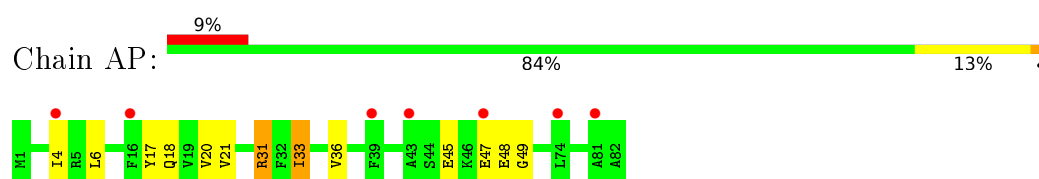
• Molecule 15: 30S ribosomal protein S15



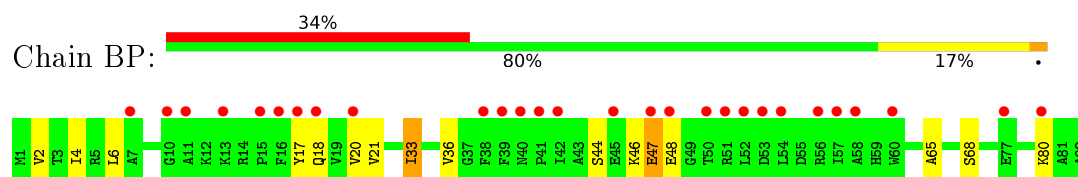
• Molecule 15: 30S ribosomal protein S15



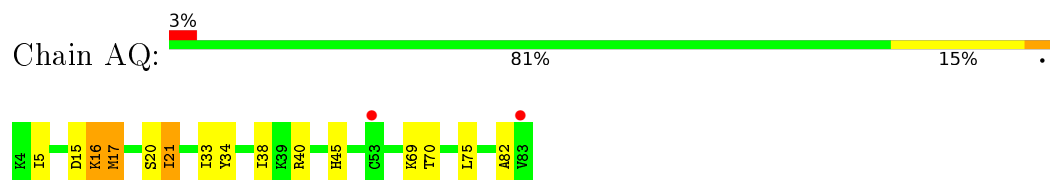
• Molecule 16: 30S ribosomal protein S16



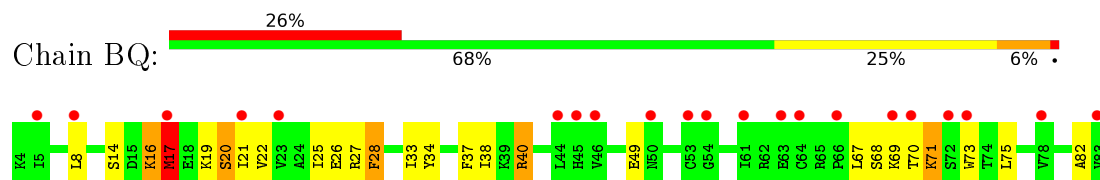
- Molecule 16: 30S ribosomal protein S16



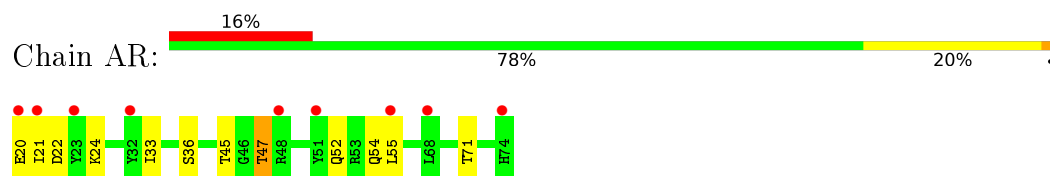
- Molecule 17: 30S ribosomal protein S17



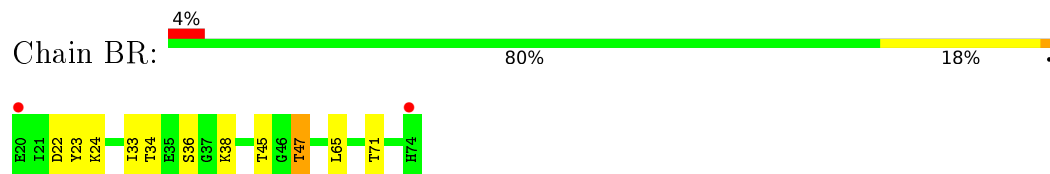
- Molecule 17: 30S ribosomal protein S17



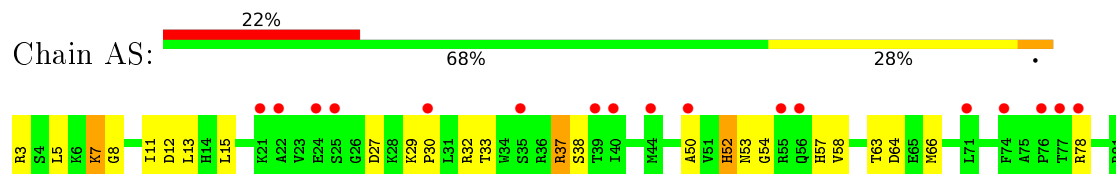
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18

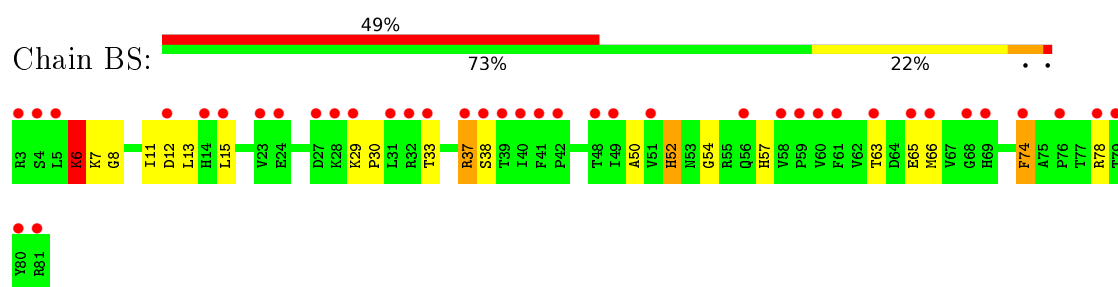


- Molecule 19: 30S ribosomal protein S19

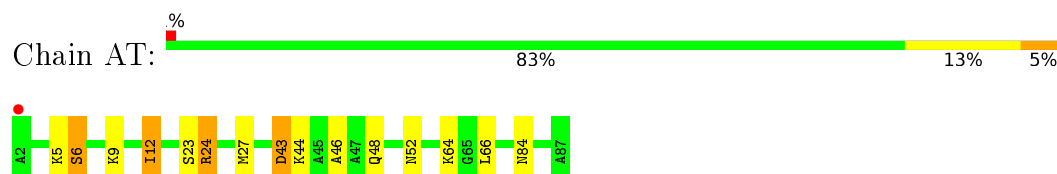


- Molecule 19: 30S ribosomal protein S19

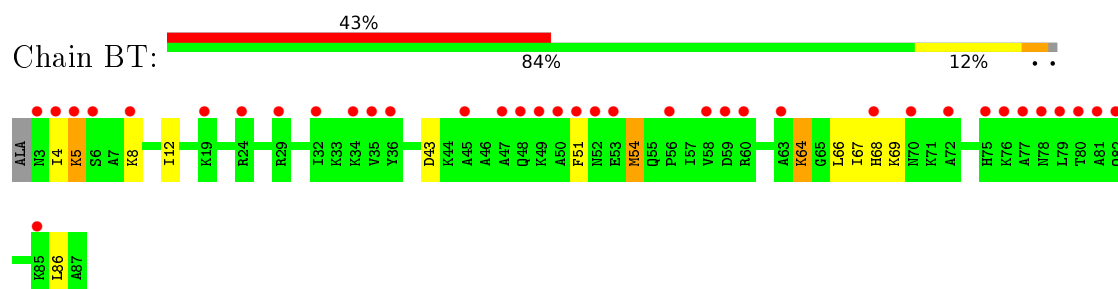




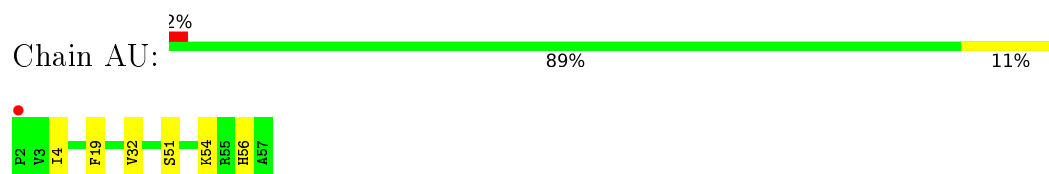
- Molecule 20: 30S ribosomal protein S20



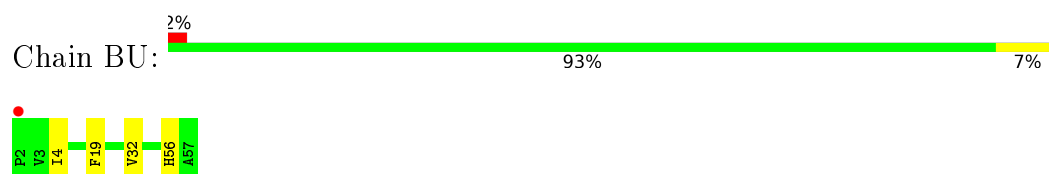
- Molecule 20: 30S ribosomal protein S20



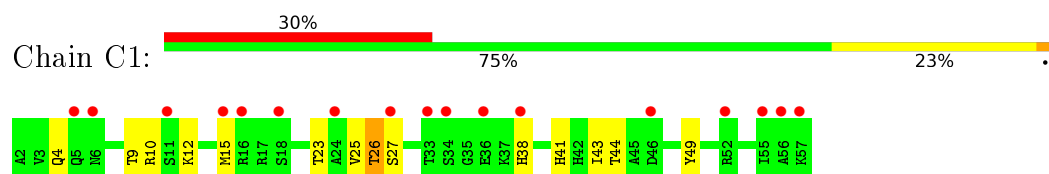
- Molecule 21: 30S ribosomal protein S21



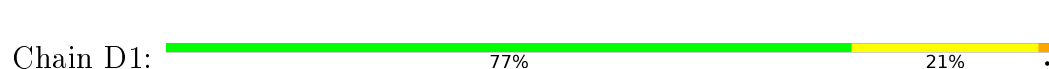
- Molecule 21: 30S ribosomal protein S21

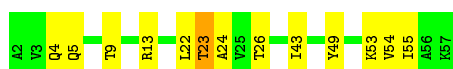


- Molecule 22: 50S ribosomal protein L32

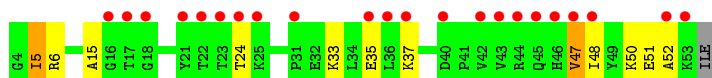
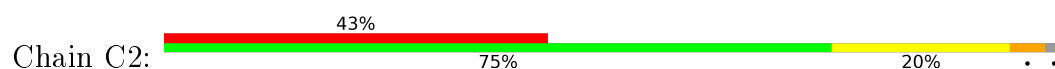


- Molecule 22: 50S ribosomal protein L32

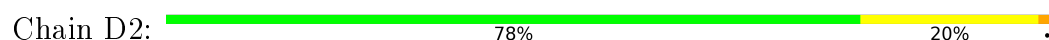




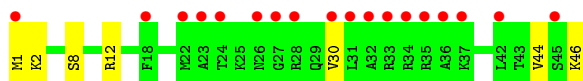
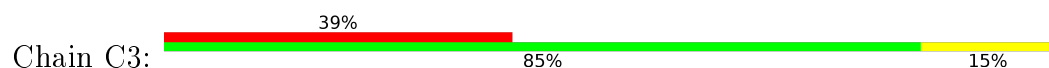
- Molecule 23: 50S ribosomal protein L33



- Molecule 23: 50S ribosomal protein L33



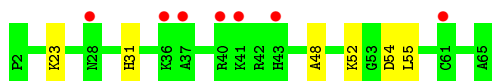
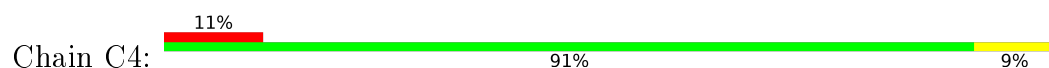
- Molecule 24: 50S ribosomal protein L34



- Molecule 24: 50S ribosomal protein L34



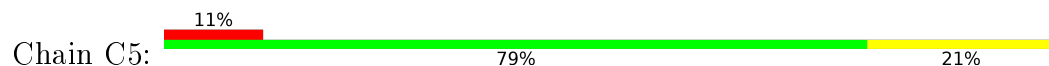
- Molecule 25: 50S ribosomal protein L35



- Molecule 25: 50S ribosomal protein L35



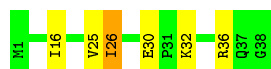
- Molecule 26: 50S ribosomal protein L36





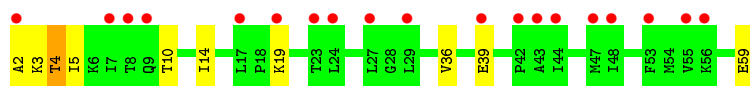
- Molecule 26: 50S ribosomal protein L36

Chain D5: 84% 13%



- Molecule 27: 50S ribosomal protein L30

Chain C0: 33% 83% 16%



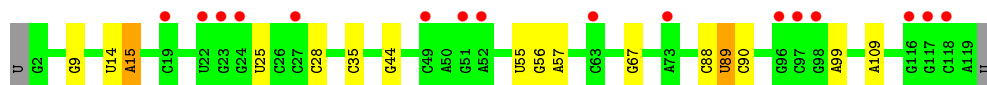
- Molecule 27: 50S ribosomal protein L30

Chain D0: 81% 16%



- Molecule 28: 5S rRNA

Chain CB: 13% 85% 12%



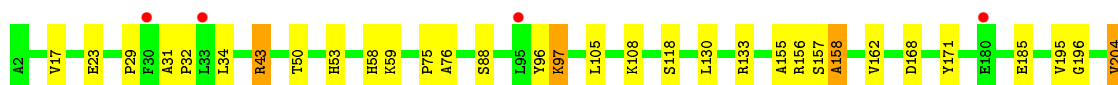
- Molecule 28: 5S rRNA

Chain DB: 87% 13%




- Molecule 29: 50S ribosomal protein L2

Chain CC: 3% 82% 15%




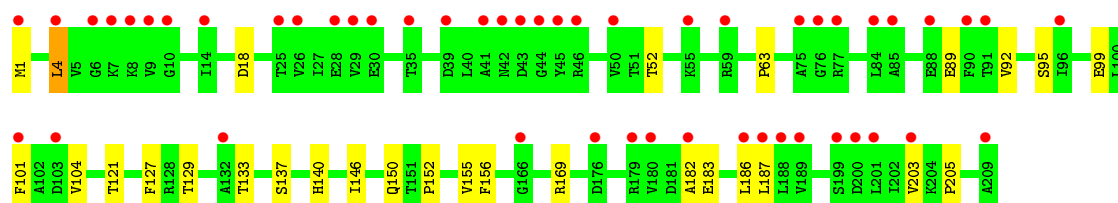
- Molecule 29: 50S ribosomal protein L2

Chain DC:  89% 10%




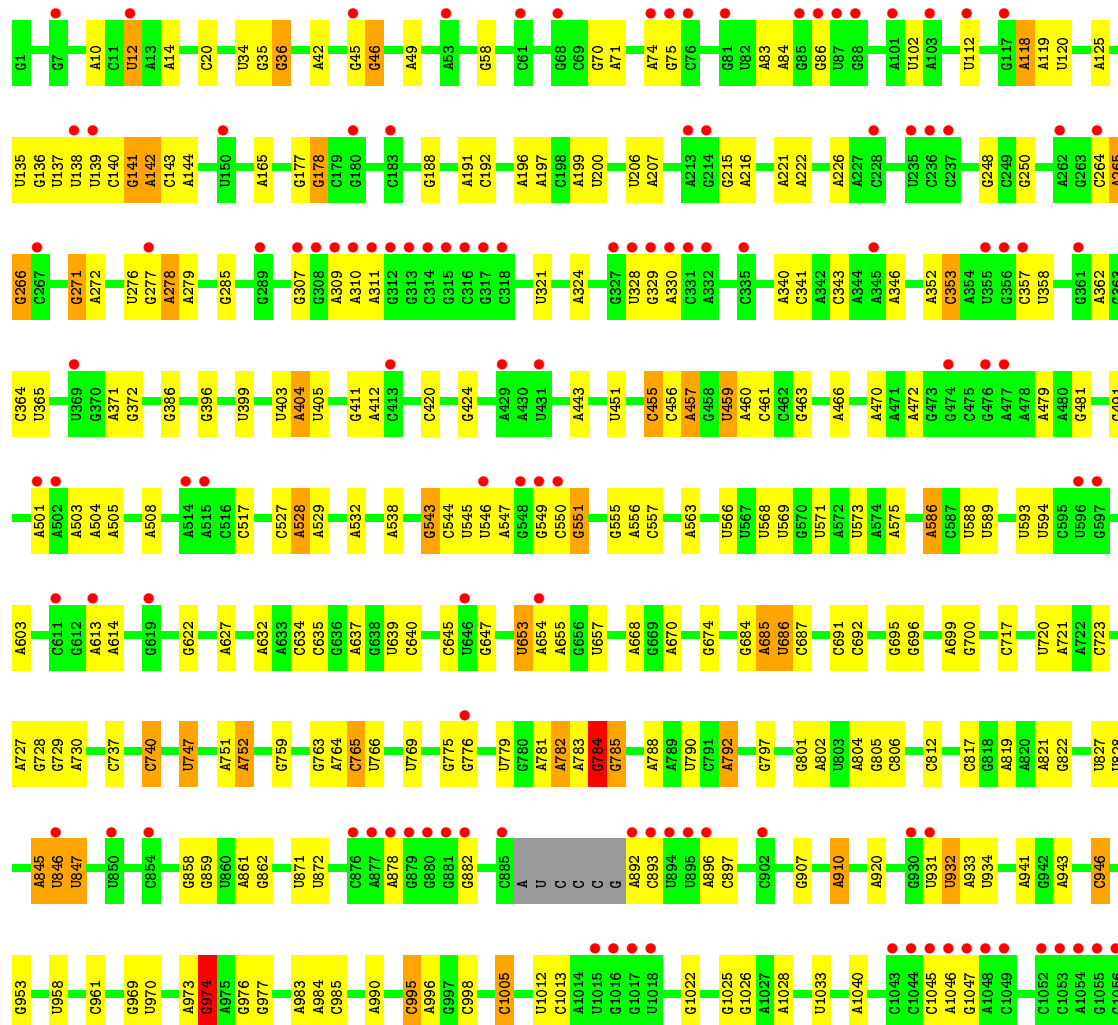
• Molecule 30: 50S ribosomal protein L3

Chain CD:  24% 86% 13%

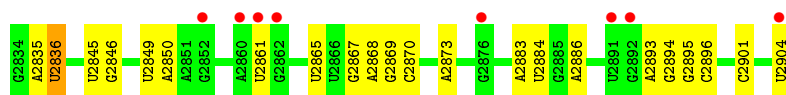


• Molecule 31: 23S rRNA

Chain CA:  10% 73% 23%



A1057	U1058	G1059	U1060	U1061	G1062	G1063	C1064	U1065	U1066	A1067	G1068	A1069	A1070	G1071	G1072	A1073	G1074	C1075	C1076	A1077	U1078	U1082	U1083	A1084	A1085	G1086	G1087	A1088	A1089	A1090	U1093	U1094	A1095	A1096	U1097	A1098	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	A1111	G1112	U1119	G1122	G1123	G1124	A1255	G1128	A1129
U1130	G1131	U1132	A1133	C1134	G1135	G1136	U1141	A1142	A1143	A1156	G1166	G1167	G1168	G1169	G1170	G1171	G1172	U1173	U1174	U1175	U1176	U1177	G1178	G1179	U1180	G1186	G1196	G1206	G1210	G1211	G1212	A1213	A1214	G1215	G1218	U1224	G1227	G1236	G1237	G1238	A1247	G1248	A1253	G1256									
A1262	G1266	U1267	A1268	A1269	G1270	G1271	A1272	U1273	A1286	A1287	G1288	G1300	A1301	C1306	G1311	G1319	C1320	A1321	G1324	U1325	A1328	U1329	C1330	U1340	U1344	U1352	G1360	A1365	C1376	U1379	G1380	G1386	A1387	A1383	C1386	A1387	U1394	U1405	U1406	G1407	G1416												
C1417	A1420	G1428	A1429	G1430	A1431	A1434	G1435	C1447	G1448	G1452	A1453	G1454	G1455	U1460	G1478	G1482	A1490	G1491	G1492	A1493	A1494	A1495	U1496	U1497	A1504	A1509	G1510	G1511	A1515	U1523	G1524	G1529	G1530	G1531	A1532	C1533	U1534	C1536	U1537	C1538	U1539	U1554	G1555										
C1556	C1557	C1565	A1566	G1567	G1568	A1569	U1578	A1583	U1584	C1585	A1586	G1587	G1588	A1603	G1606	A1607	A1608	A1616	G1633	U1636	A1637	C1638	U1647	U1648	G1649	A1650	A1651	A1652	G1653	A1654	C1658	U1682	A1685	G1686	G1687	A1688	G1674	C1675	G1681	C1708	U1709	G1710	G1715										
U1716	A1717	U1729	G1731	G1732	G1733	G1734	G1738	A1744	G1750	A1754	A1757	C1764	A1773	C1774	G1775	G1776	U1777	U1778	U1779	U1782	A1783	A1784	A1787	C1788	A1789	C1790	A1791	G1800	A1801	A1805	A1808	A1809	A1810	G1811	U1812	C1816	G1817	U1818	A1819	U1820	A1821	C1822											
U1825	G1826	U1827	G1828	A1829	A1847	A1848	G1862	G1863	U1864	G1867	A1868	G1869	C1870	A1871	A1872	G1873	G1874	U1882	A1885	U1886	A1889	A1900	A1901	G1902	G1903	C1906	G1907	A1913	C1914	G1929	G1930	U1931	A1932	G1933	G1934	G1935	A1936	A1937	A1938	U1943	G1945	A1955	U1963	G1964									
C1967	A1970	G1971	G1972	G1973	C1974	U1991	G1992	U1993	C1997	A1998	C1999	A2014	A2015	U2016	U2017	G2018	A2019	C2021	U2022	C2023	U2026	G2027	U2030	A2031	G2032	A2033	G2034	G2035	C2036	A2037	G2038	U2039	C2043	C2044	C2045	G2046	G2049	C2050	A2051	C2055	G2056	A2060	G2061	A2062	C2063	C2065							
G2069	C2072	G2078	U2092	A2093	A2094	A2095	U2106	G2107	U2108	U2109	U2110	U2111	G2112	U2113	A2114	G2115	G2116	A2117	U2118	A2119	G2120	G2121	U2122	G2123	G2124	G2125	A2126	G2127	G2128	U2129	U2130	U2131	U2132	G2133	G2136	G2146	A2147	C2150	G2157	A2158	G2159	C2160	C2161	A2163	G2164	C2165	U2166	U2167	C2168				
A2169	A2170	U2172	C2174	G2175	C2178	A2183	A2184	G2190	A2191	A2198	A2199	U2203	G2204	A2211	A2225	C2226	A2227	C2232	U2233	C2234	G2235	A2237	A2238	A2239	U2245	G2251	U2259	C2260	C2261	U2262	A2266	C2267	A2268	G2271	U2272	A2273	A2274	C2275	A2278	G2279	G2280	A2281	G2282	C2283	G2286								
A2287	U2291	U2292	A2298	U2299	C2300	G2304	U2305	A2311	U2312	U2321	A2322	G2323	U2324	G2325	A2327	A2328	A2333	U2334	A2335	C2339	A2340	G2345	A2346	C2347	C2350	C2354	A2358	G2361	C2367	C2368	G2383	U2384	C2385	U2402	C2403	A2406	G2409	G2410	U2423	C2424													
A2425	A2426	G2429	A2430	A2435	U2441	A2448	U2449	A2450	C2465	C2466	U2474	C2475	A2476	A2482	U2491	C2498	C2499	G2502	A2503	U2504	G2505	A2518	U2519	C2520	G2529	G2535	C2539	G2543	G2544	A2547	C2551	U2554	U2555	C2556	A2566	G2567	C2573	G2578															
G2581	G2582	U2585	A2590	A2602	G2603	U2609	U2613	A2614	U2615	G2618	U2629	G2630	C2636	U2637	G2638	C2642	G2646	U2647	A2660	G2661	G2662	G2663	G2664	A2665	C2666	C2667	G2668	U2680	C2681	A2682	U2687	G2688	U2689	U2690	G2693	C2710	G2714	A2718	U2719	G2720	A2721												
A2726	U2727	G2728	G2729	G2744	G2747	A2748	C2755	A2765	U2766	C2773	G2777	A2778	U2779	G2780	A2781	G2782	C2787	C2788	C2789	U2790	G2791	A2792	G2793	C2794	U2795	U2796	U2797	U2798	A2799	A2800	G2801	G2802	G2803	G2811	A2813	G2815	G2816	U2817	U2818	G2819	A2820	A2821	G2822	A2823	G2824	G2825	U2833						



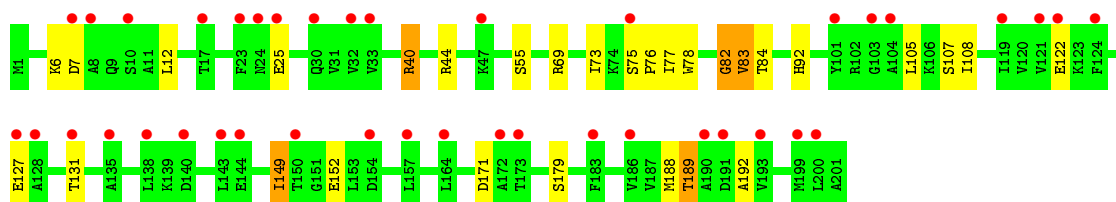
- Molecule 32: 50S ribosomal protein L3

Chain DD: 86% 14%



- Molecule 33: 50S ribosomal protein L4

Chain CE: 20% 85% 12%



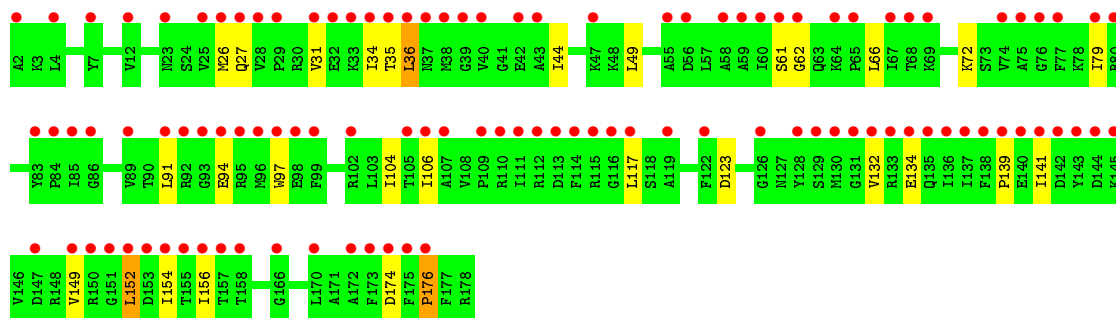
- Molecule 33: 50S ribosomal protein L4

Chain DE: 95% 5%



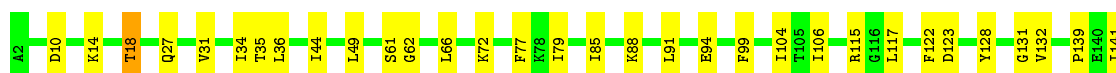
- Molecule 34: 50S ribosomal protein L5

Chain CF: 60% 83% 15%



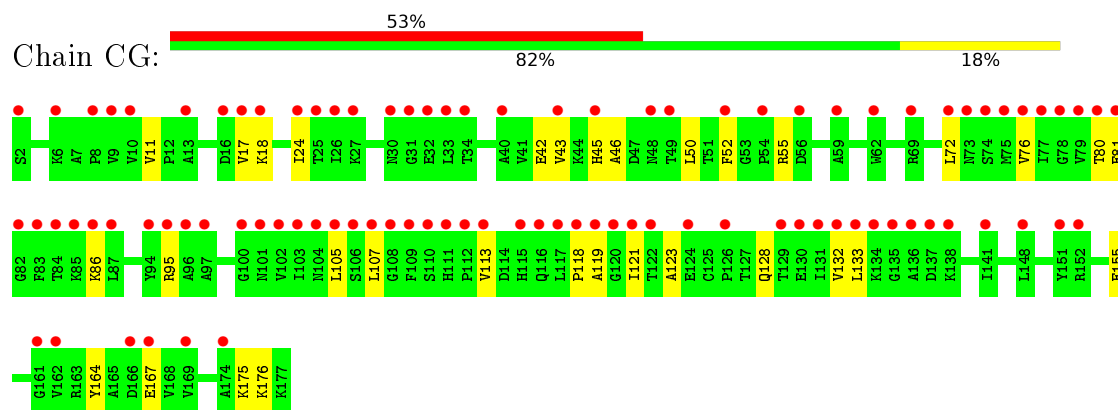
- Molecule 34: 50S ribosomal protein L5

Chain DF: 76% 22%

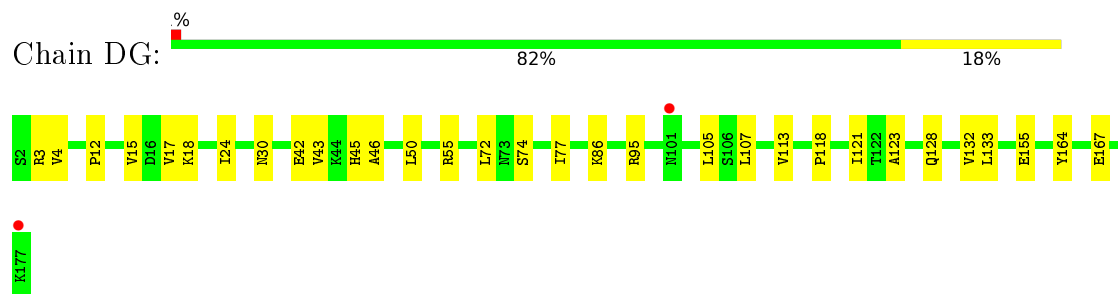




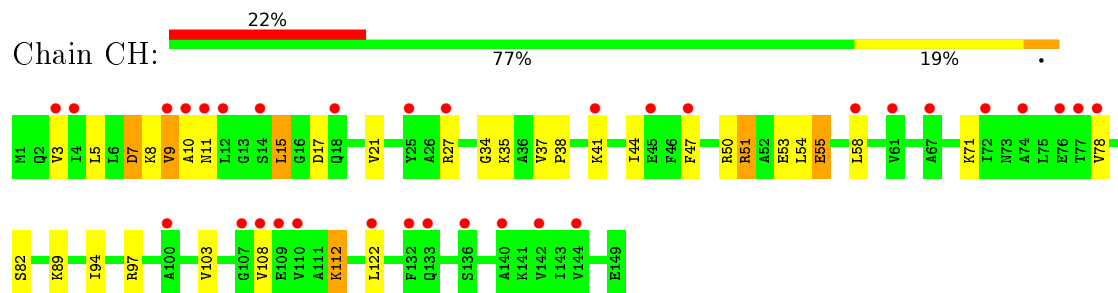
- Molecule 35: 50S ribosomal protein L6



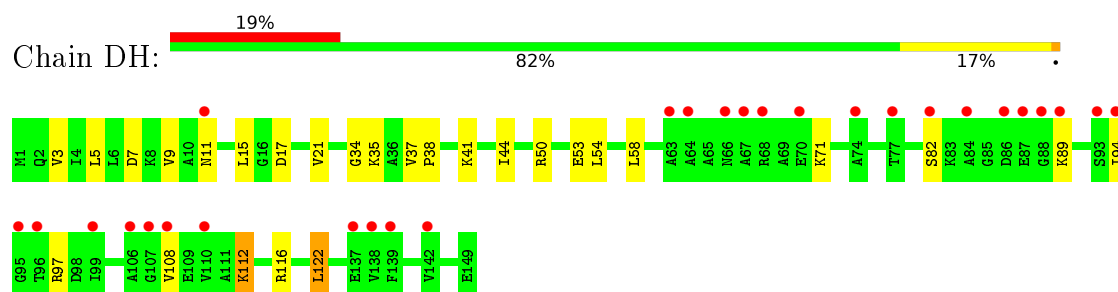
- Molecule 35: 50S ribosomal protein L6



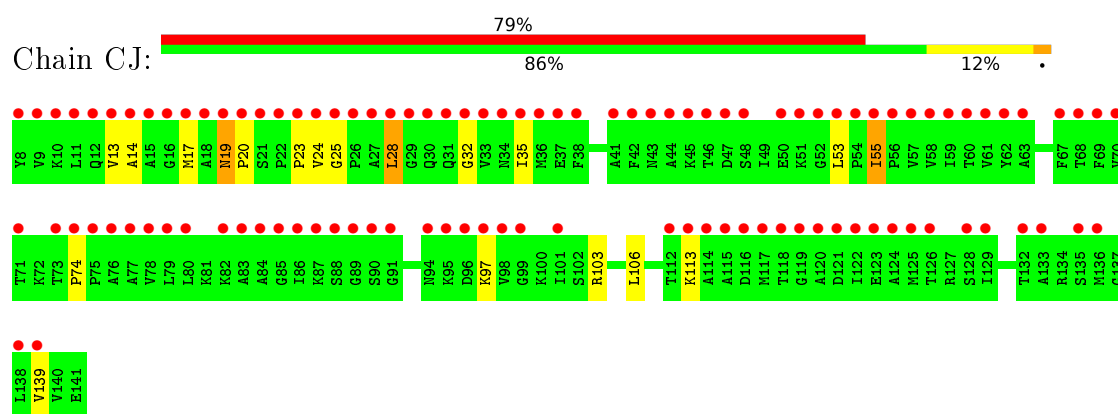
- Molecule 36: 50S ribosomal protein L9



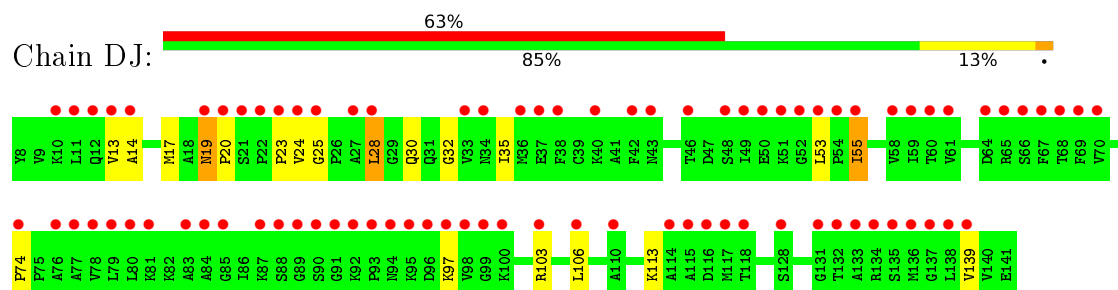
- Molecule 36: 50S ribosomal protein L9



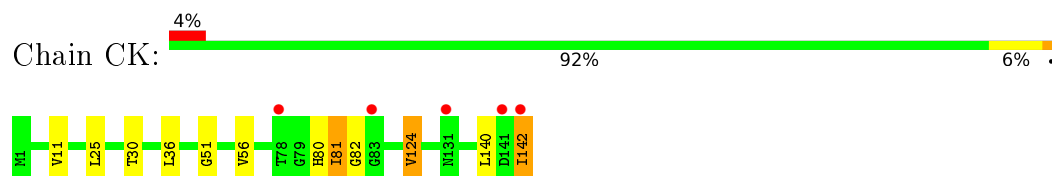
- Molecule 37: 50S ribosomal protein L11



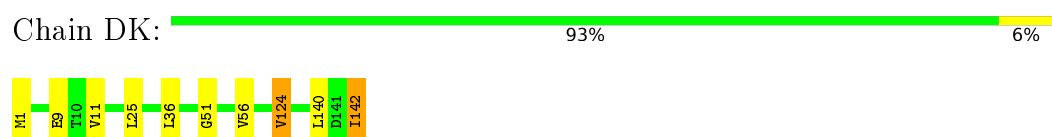
- Molecule 37: 50S ribosomal protein L11



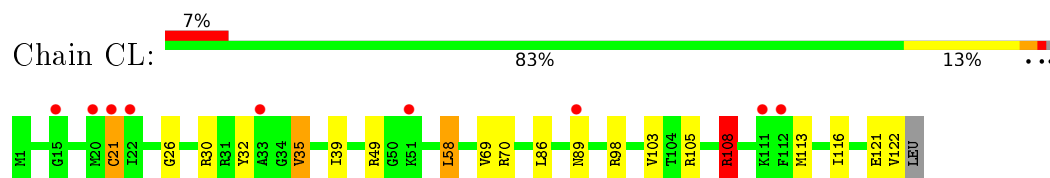
- Molecule 38: 50S ribosomal protein L13



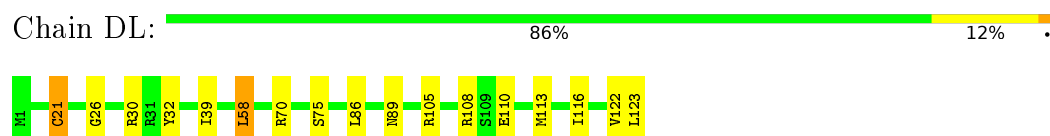
- Molecule 38: 50S ribosomal protein L13



- Molecule 39: 50S ribosomal protein L14

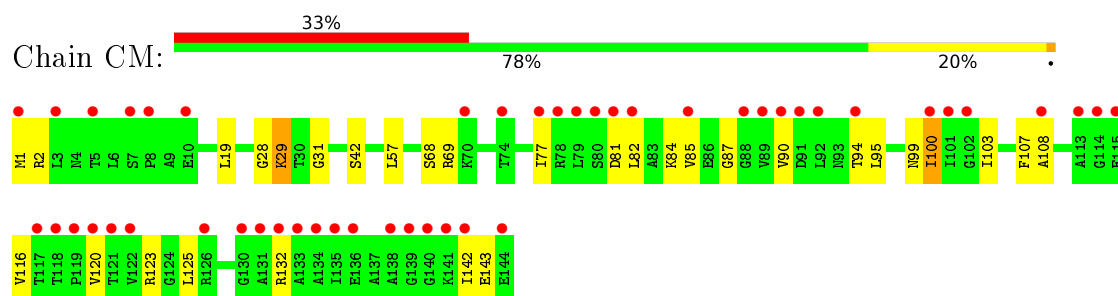


- Molecule 39: 50S ribosomal protein L14

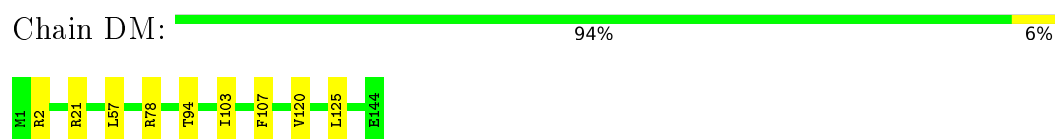




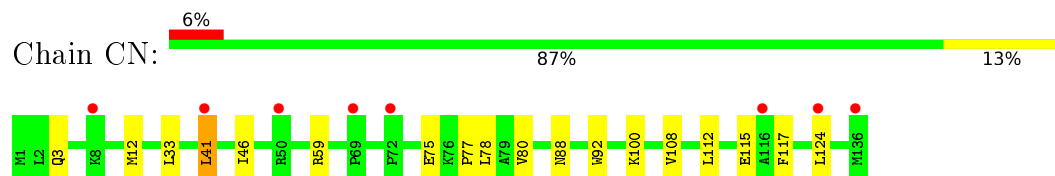
- Molecule 40: 50S ribosomal protein L15



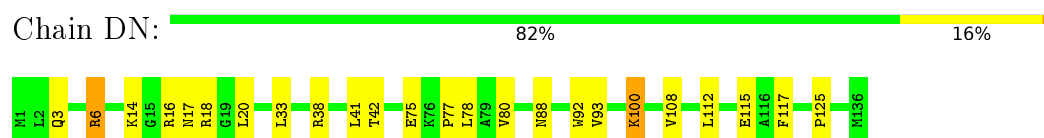
- Molecule 40: 50S ribosomal protein L15



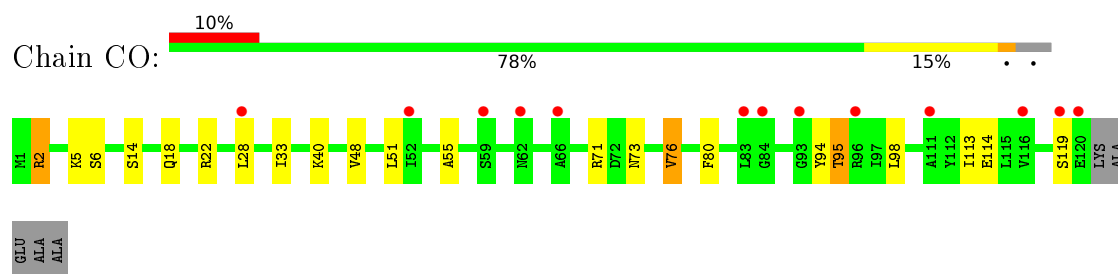
- Molecule 41: 50S ribosomal protein L16



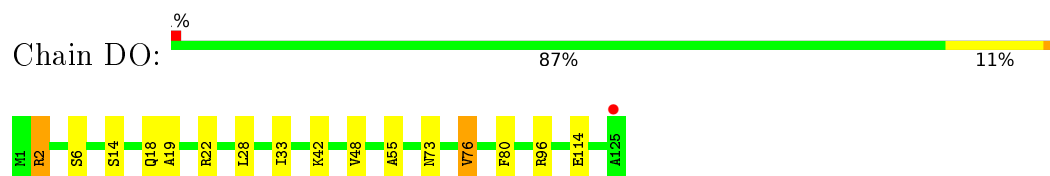
- Molecule 41: 50S ribosomal protein L16



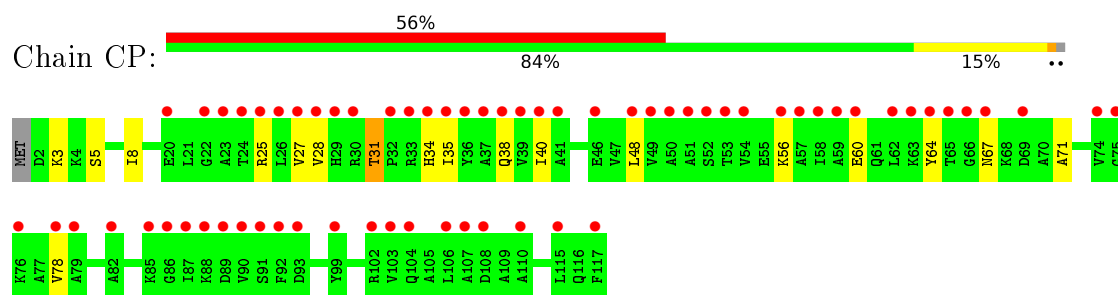
- Molecule 42: 50S ribosomal protein L17



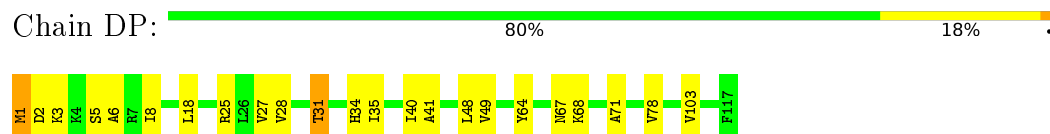
- Molecule 42: 50S ribosomal protein L17



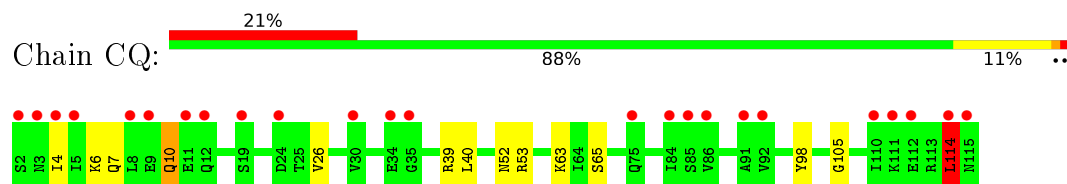
- Molecule 43: 50S ribosomal protein L18



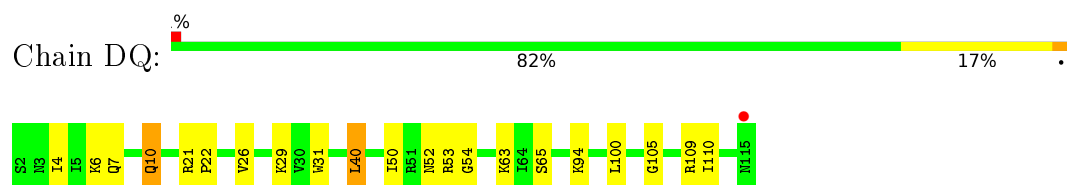
- Molecule 43: 50S ribosomal protein L18



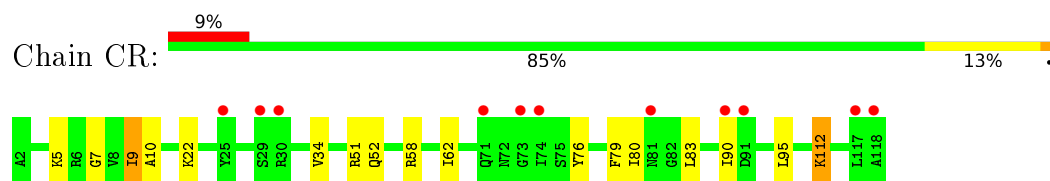
- Molecule 44: 50S ribosomal protein L19



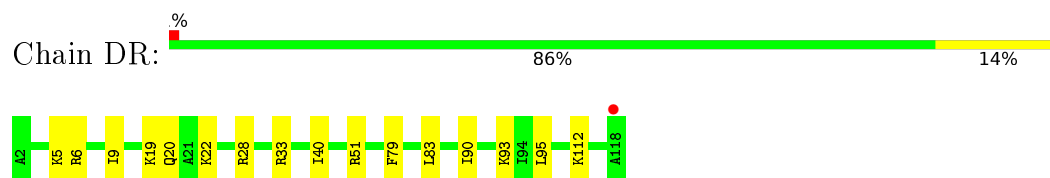
- Molecule 44: 50S ribosomal protein L19



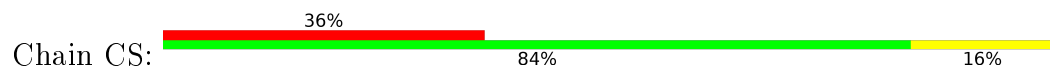
- Molecule 45: 50S ribosomal protein L20

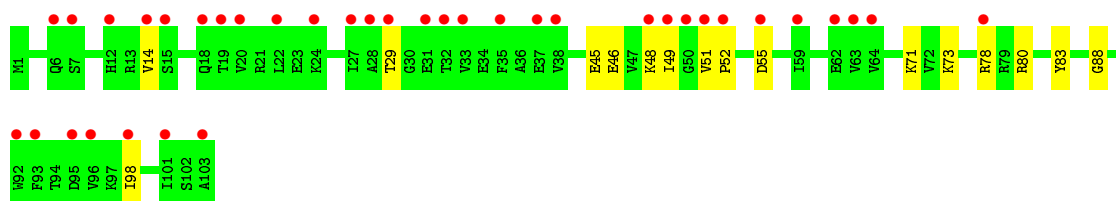


- Molecule 45: 50S ribosomal protein L20



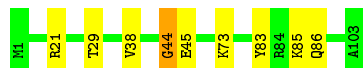
- Molecule 46: 50S ribosomal protein L21





- Molecule 46: 50S ribosomal protein L21

Chain DS: 91% 8% .



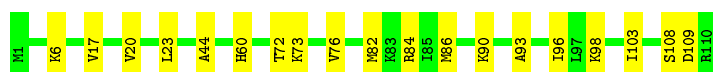
- Molecule 47: 50S ribosomal protein L22

Chain CT: 15% 80% 19% .



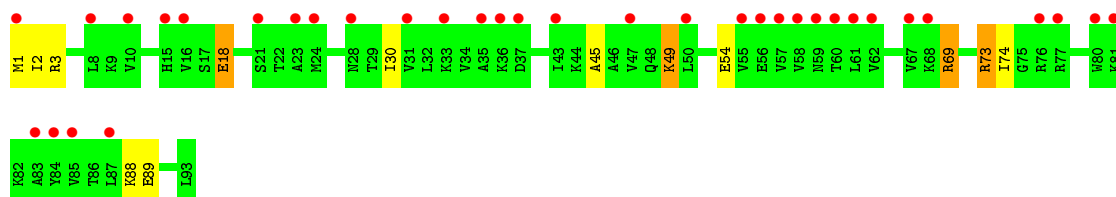
- Molecule 47: 50S ribosomal protein L22

Chain DT: 83% 17% .



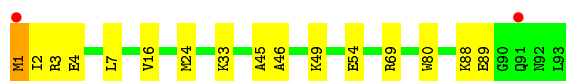
- Molecule 48: 50S ribosomal protein L23

Chain CU: 38% 86% 10% .



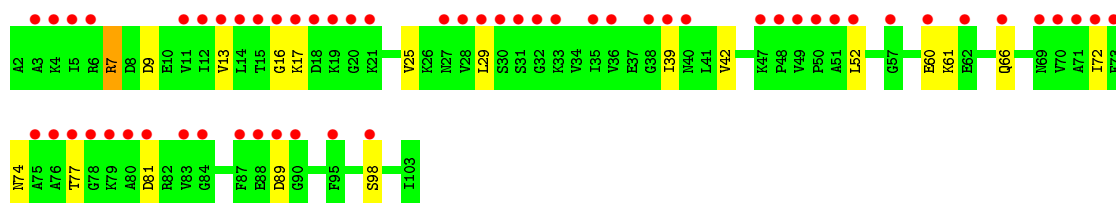
- Molecule 48: 50S ribosomal protein L23

Chain DU: 2% 83% 16% .

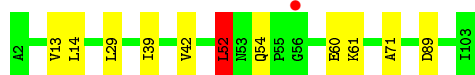
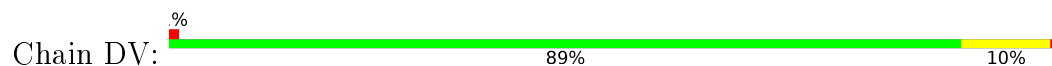


- Molecule 49: 50S ribosomal protein L24

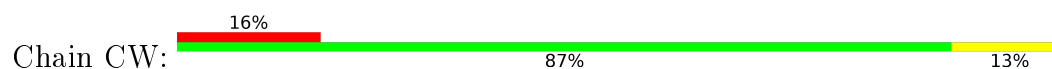
Chain CV: 56% 81% 18% .



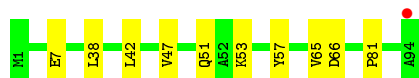
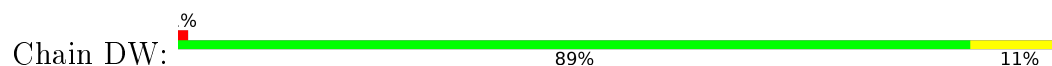
- Molecule 49: 50S ribosomal protein L24



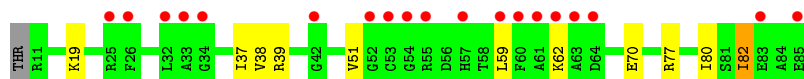
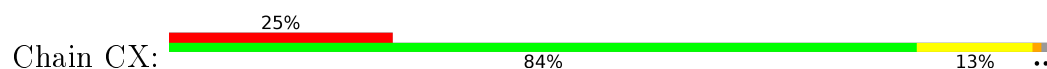
- Molecule 50: 50S ribosomal protein L25



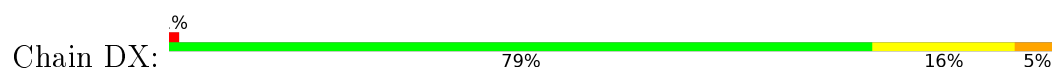
- Molecule 50: 50S ribosomal protein L25



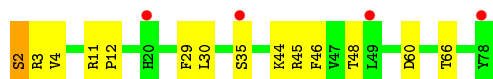
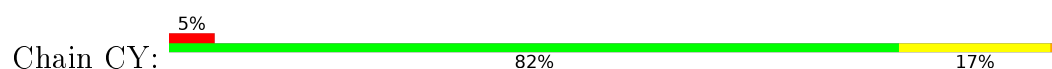
- Molecule 51: 50S ribosomal protein L27




- Molecule 51: 50S ribosomal protein L27



- Molecule 52: 50S ribosomal protein L28



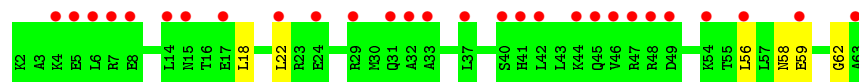
- Molecule 52: 50S ribosomal protein L28

Chain DY:  79% 19% .



- Molecule 53: 50S ribosomal protein L29

Chain CZ:  45% 90% 10%




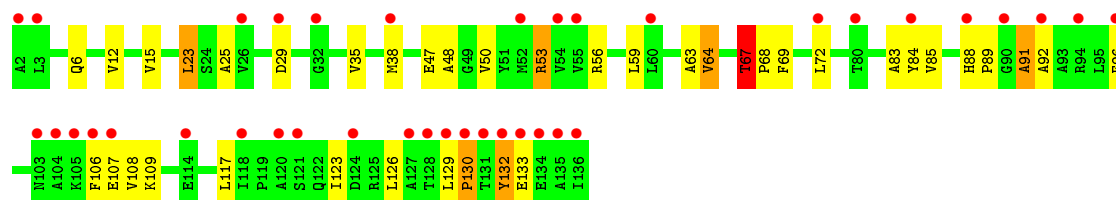
- Molecule 53: 50S ribosomal protein L29

Chain DZ:  2% 95% 5%




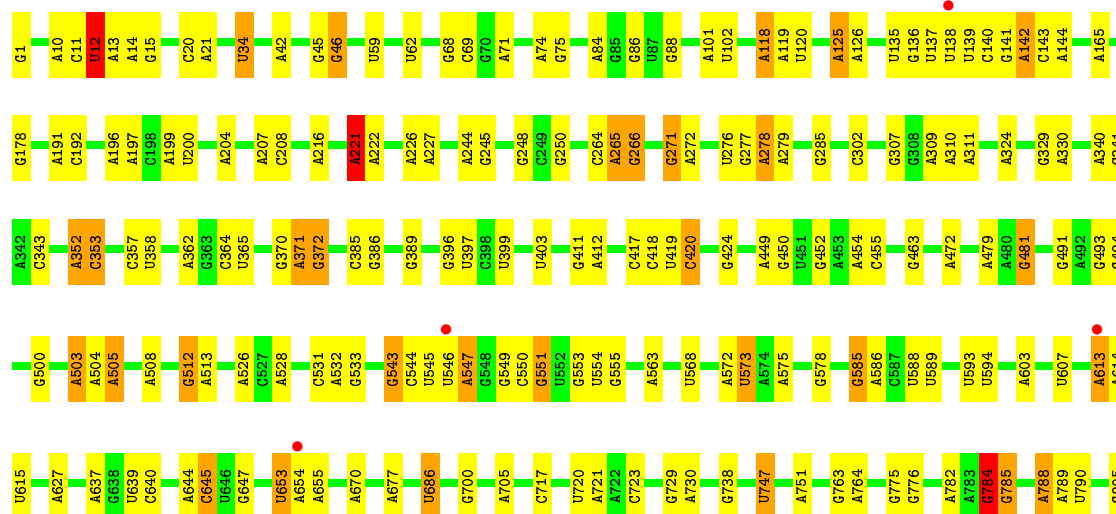
- Molecule 54: 50S ribosomal protein L10

Chain DI:  28% 71% 24% . .



- Molecule 55: 23S rRNA

Chain DA:  3% 76% 21% .





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	213.04Å 436.85Å 628.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 3.03 48.02 – 3.03	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.39-3.03) 96.8 (48.02-3.03)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 3.01Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, $R_{free}$	0.172 , 0.200 0.186 , 0.215	Depositor DCC
$R_{free}$ test set	4333 reflections (0.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.4	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 93.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	295130	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AA	0.98	10/36597 (0.0%)	0.86	2/57088 (0.0%)
1	BA	0.98	10/36572 (0.0%)	0.86	3/57049 (0.0%)
2	AB	0.47	0/1784	0.66	0/2403
2	BB	0.47	0/1784	0.66	0/2403
3	AC	0.44	0/1652	0.67	0/2225
3	BC	0.44	0/1652	0.67	0/2225
4	AD	0.46	0/1665	0.68	0/2227
4	BD	0.44	0/1665	0.69	0/2227
5	AE	0.47	0/1157	0.76	0/1557
5	BE	0.48	0/1118	0.78	0/1504
6	AF	0.46	0/881	0.70	0/1189
6	BF	0.47	0/835	0.80	0/1128
7	AG	0.46	0/1196	0.63	0/1602
7	BG	0.45	0/1196	0.62	0/1602
8	AH	0.44	0/989	0.71	0/1326
8	BH	0.43	0/989	0.69	0/1326
9	AI	0.45	0/1034	0.69	0/1375
9	BI	0.45	0/1034	0.67	0/1375
10	AJ	0.43	0/806	0.67	0/1089
10	BJ	0.47	0/797	0.70	0/1077
11	AK	0.44	0/893	0.65	0/1205
11	BK	0.45	0/893	0.69	0/1205
12	AL	0.45	0/960	0.71	0/1286
12	BL	0.42	0/960	0.72	0/1286
13	AM	0.52	0/893	0.77	0/1193
13	BM	0.51	0/893	0.74	0/1193
14	AN	0.45	0/817	0.65	0/1088
14	BN	0.44	0/817	0.63	0/1088
15	AO	0.46	0/722	0.63	0/964
15	BO	0.44	0/722	0.62	0/964
16	AP	0.46	0/659	0.70	0/884



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	BP	0.48	0/659	0.74	0/884
17	AQ	0.48	0/658	0.75	0/881
17	BQ	0.50	0/658	0.76	0/881
18	AR	0.51	0/463	0.66	0/621
18	BR	0.49	0/463	0.65	0/621
19	AS	0.47	0/653	0.61	0/877
19	BS	0.47	0/653	0.63	0/877
20	AT	0.49	0/676	0.70	0/895
20	BT	0.52	0/671	0.67	0/888
21	AU	0.40	0/472	0.60	0/627
21	BU	0.39	0/472	0.61	0/627
22	C1	0.48	0/450	0.70	0/599
22	D1	0.59	0/450	0.73	0/599
23	C2	0.48	0/416	0.73	0/554
23	D2	0.49	0/421	0.74	0/561
24	C3	0.45	0/380	0.71	0/498
24	D3	0.58	0/380	0.73	0/498
25	C4	0.44	0/513	0.64	0/676
25	D4	0.51	0/513	0.68	0/676
26	C5	0.44	0/303	0.69	0/397
26	D5	0.59	0/303	0.73	0/397
27	C0	0.51	0/453	0.76	0/605
27	D0	0.66	0/467	0.77	0/623
28	CB	0.94	0/2828	0.89	2/4410 (0.0%)
28	DB	1.08	1/2872 (0.0%)	0.90	0/4478
29	CC	0.46	0/2122	0.75	0/2852
29	DC	0.52	0/2122	0.76	0/2852
30	CD	0.44	0/1586	0.70	0/2134
31	CA	1.02	45/69165 (0.1%)	0.88	19/107896 (0.0%)
32	DD	0.51	0/1576	0.70	0/2119
33	CE	0.43	0/1571	0.72	0/2113
33	DE	0.51	0/1571	0.70	0/2113
34	CF	0.43	0/1435	0.69	0/1926
34	DF	0.52	0/1435	0.73	0/1926
35	CG	0.41	0/1343	0.67	0/1816
35	DG	0.45	0/1343	0.66	0/1816
36	CH	0.47	0/1121	0.68	0/1515
36	DH	0.47	0/1121	0.68	0/1515
37	CJ	0.51	0/993	0.64	0/1341
37	DJ	0.51	0/993	0.64	0/1341
38	CK	0.42	0/1152	0.68	0/1551
38	DK	0.56	0/1152	0.71	0/1551
39	CL	0.44	0/947	0.69	0/1268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	DL	0.53	0/955	0.70	0/1279
40	CM	0.45	0/1062	0.74	1/1413 (0.1%)
40	DM	0.49	0/1062	0.72	0/1413
41	CN	0.45	0/1081	0.70	0/1443
41	DN	0.57	0/1092	0.76	1/1457 (0.1%)
42	CO	0.45	0/973	0.72	1/1301 (0.1%)
42	DO	0.58	0/1006	0.78	0/1345
43	CP	0.44	0/902	0.72	0/1209
43	DP	0.53	0/910	0.73	0/1219
44	CQ	0.44	0/929	0.73	1/1242 (0.1%)
44	DQ	0.51	0/929	0.72	0/1242
45	CR	0.48	0/960	0.68	0/1278
45	DR	0.58	0/960	0.70	0/1278
46	CS	0.43	0/829	0.74	0/1107
46	DS	0.52	0/829	0.75	0/1107
47	CT	0.41	0/864	0.73	0/1156
47	DT	0.60	0/864	0.72	0/1156
48	CU	0.47	0/745	0.73	0/994
48	DU	0.54	0/745	0.75	0/994
49	CV	0.45	0/788	0.76	0/1051
49	DV	0.51	0/788	0.76	0/1051
50	CW	0.41	0/766	0.66	0/1025
50	DW	0.52	0/766	0.71	0/1025
51	CX	0.40	0/576	0.64	0/762
51	DX	0.54	0/598	0.70	0/790
52	CY	0.45	0/635	0.70	0/848
52	DY	0.51	0/635	0.73	1/848 (0.1%)
53	CZ	0.41	0/502	0.63	0/667
53	DZ	0.48	0/502	0.62	0/667
54	DI	0.54	0/1037	0.78	1/1402 (0.1%)
55	DA	1.19	63/69364 (0.1%)	0.93	15/108207 (0.0%)
All	All	0.93	129/309281 (0.0%)	0.84	47/462224 (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	1
20	AT	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	CA	0	3
55	DA	0	37
All	All	0	45

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2095	A	O5'-C5'	-9.10	1.28	1.42
31	CA	12	U	C1'-N1	8.94	1.62	1.48
55	DA	1237	A	C3'-O3'	-8.70	1.29	1.42
31	CA	1936	A	N9-C4	-8.66	1.32	1.37
31	CA	2225	A	C3'-O3'	8.52	1.54	1.42
55	DA	2097	A	O5'-C5'	-8.26	1.29	1.42
31	CA	769	U	C1'-N1	7.67	1.60	1.48
55	DA	2585	U	C3'-O3'	7.30	1.52	1.42
31	CA	1379	U	C3'-O3'	7.25	1.52	1.42
55	DA	829	A	N7-C5	-7.24	1.34	1.39
1	BA	1397	C	N1-C2	7.10	1.47	1.40
55	DA	2820	A	N3-C4	6.99	1.39	1.34
31	CA	790	U	C1'-N1	6.90	1.59	1.48
31	CA	946	C	C1'-N1	6.83	1.58	1.48
1	AA	956	U	C1'-N1	6.77	1.58	1.48
31	CA	2425	A	C3'-O3'	6.77	1.51	1.42
55	DA	2016	U	C3'-O3'	-6.46	1.33	1.42
55	DA	788	A	N7-C5	-6.42	1.35	1.39
1	BA	5	U	C1'-N1	6.39	1.58	1.48
1	BA	956	U	C1'-N1	6.28	1.58	1.48
31	CA	995	C	O5'-C5'	-6.27	1.32	1.42
31	CA	1658	C	C1'-N1	6.25	1.58	1.48
31	CA	2017	U	C1'-N1	6.25	1.58	1.48
55	DA	2585	U	C1'-N1	6.24	1.58	1.48
31	CA	2233	U	C1'-N1	6.24	1.58	1.48
55	DA	578	G	N7-C5	-6.21	1.35	1.39
31	CA	2232	C	C1'-N1	6.18	1.58	1.48
1	AA	1354	U	C1'-N1	6.12	1.57	1.48
31	CA	692	C	C1'-N1	6.10	1.57	1.48
55	DA	1607	C	N1-C6	6.08	1.40	1.37
31	CA	1777	U	C1'-N1	6.07	1.57	1.48
1	AA	5	U	C1'-N1	6.05	1.57	1.48
55	DA	705	A	C6-N6	6.04	1.38	1.33
55	DA	820	A	N9-C4	6.00	1.41	1.37
31	CA	1774	C	C1'-N1	5.98	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2326	C	C3'-O3'	5.94	1.50	1.42
31	CA	12	U	N1-C2	5.93	1.43	1.38
55	DA	613	A	N9-C4	5.91	1.41	1.37
55	DA	547	A	C3'-O3'	5.89	1.50	1.42
55	DA	2127	G	C3'-O3'	5.88	1.50	1.42
1	BA	842	U	C3'-O3'	5.87	1.50	1.42
55	DA	2547	A	P-O5'	-5.87	1.53	1.59
55	DA	12	U	C1'-N1	5.79	1.57	1.48
31	CA	817	C	C1'-N1	5.76	1.57	1.48
55	DA	2820	A	C6-N1	5.74	1.39	1.35
31	CA	2146	C	C3'-O3'	5.73	1.50	1.42
55	DA	204	A	N3-C4	-5.71	1.31	1.34
31	CA	685	A	C3'-O3'	5.70	1.50	1.42
55	DA	653	U	C1'-N1	5.67	1.57	1.48
1	AA	119	A	C3'-O3'	5.65	1.50	1.42
1	BA	1354	U	C1'-N1	5.65	1.57	1.48
55	DA	34	U	O3'-P	-5.62	1.54	1.61
1	AA	1397	C	N1-C6	5.62	1.40	1.37
55	DA	59	U	C3'-O3'	-5.62	1.34	1.42
55	DA	1534	U	C1'-N1	5.58	1.57	1.48
31	CA	2647	U	C1'-N1	5.57	1.57	1.48
55	DA	2867	G	C3'-O3'	5.57	1.50	1.42
55	DA	2585	U	N1-C2	5.56	1.43	1.38
31	CA	801	G	C3'-O3'	5.55	1.50	1.42
55	DA	353	C	C1'-N1	5.54	1.57	1.48
1	BA	1008	U	O5'-C5'	-5.53	1.33	1.42
55	DA	2769	U	O5'-C5'	-5.52	1.34	1.42
31	CA	1376	C	C1'-N1	5.52	1.57	1.48
1	BA	1493	A	C3'-O3'	5.50	1.49	1.42
1	AA	932	C	C1'-N1	5.50	1.57	1.48
31	CA	404	A	C3'-O3'	5.50	1.49	1.42
31	CA	2261	C	C1'-N1	5.49	1.56	1.48
31	CA	459	U	C1'-N1	5.47	1.56	1.48
55	DA	1136	G	C5-C4	-5.47	1.34	1.38
1	BA	209	U	C1'-N1	5.46	1.56	1.48
55	DA	2227	A	N7-C5	-5.44	1.35	1.39
31	CA	691	C	C1'-N1	5.43	1.56	1.48
31	CA	653	U	C1'-N1	5.41	1.56	1.48
31	CA	1708	C	C1'-N1	5.40	1.56	1.48
1	BA	16	A	C3'-O3'	-5.40	1.34	1.42
55	DA	1872	A	N7-C5	-5.39	1.36	1.39
55	DA	513	A	N7-C5	-5.35	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	1902	C	C1'-N1	5.35	1.56	1.48
55	DA	1971	U	C2-N3	5.35	1.41	1.37
31	CA	657	U	C1'-N1	5.32	1.56	1.48
55	DA	1610	A	O5'-C5'	-5.32	1.34	1.42
55	DA	1759	A	N7-C5	-5.31	1.36	1.39
55	DA	2224	G	C3'-O3'	-5.29	1.34	1.42
55	DA	88	G	N7-C5	-5.29	1.36	1.39
31	CA	1584	U	C1'-N1	5.29	1.56	1.48
55	DA	670	A	N7-C5	-5.29	1.36	1.39
55	DA	1022	G	O5'-C5'	-5.28	1.34	1.42
55	DA	2158	A	C3'-O3'	5.26	1.49	1.42
55	DA	1584	U	C1'-N1	5.26	1.56	1.48
55	DA	2715	C	C3'-O3'	-5.26	1.34	1.42
31	CA	1825	U	C1'-N1	5.24	1.56	1.48
55	DA	2547	A	O5'-C5'	-5.24	1.34	1.42
55	DA	2781	A	N7-C5	-5.23	1.36	1.39
31	CA	2016	U	C1'-N1	5.23	1.56	1.48
1	AA	1397	C	C1'-N1	5.23	1.56	1.48
1	AA	955	U	C1'-N1	5.22	1.56	1.48
31	CA	353	C	C1'-N1	5.22	1.56	1.48
55	DA	1234	U	C3'-O3'	-5.21	1.34	1.42
31	CA	20	C	C1'-N1	5.19	1.56	1.48
31	CA	1788	C	C1'-N1	5.18	1.56	1.48
55	DA	21	A	N3-C4	5.18	1.38	1.34
55	DA	1001	A	C3'-O3'	-5.18	1.34	1.42
55	DA	481	G	N3-C4	5.17	1.39	1.35
55	DA	911	A	N3-C4	5.17	1.38	1.34
55	DA	271	G	C3'-O3'	5.17	1.49	1.42
1	AA	892	A	N7-C5	-5.16	1.36	1.39
55	DA	1453	A	N3-C4	5.16	1.38	1.34
55	DA	2578	G	N7-C5	-5.13	1.36	1.39
55	DA	2051	A	N7-C5	-5.12	1.36	1.39
28	DB	90	C	O5'-C5'	-5.11	1.34	1.42
1	AA	250	A	C3'-O3'	5.11	1.49	1.42
55	DA	784	G	C3'-O3'	5.10	1.49	1.42
55	DA	1971	U	C2-O2	5.10	1.26	1.22
31	CA	1889	A	N9-C4	5.09	1.41	1.37
55	DA	1965	C	C3'-O3'	-5.09	1.35	1.42
1	BA	932	C	C1'-N1	5.08	1.56	1.48
55	DA	1174	U	C1'-N1	5.07	1.56	1.48
31	CA	2794	C	C1'-N1	5.07	1.56	1.48
55	DA	1350	C	C3'-O3'	-5.07	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	461	C	C1'-N1	5.06	1.56	1.48
31	CA	1196	C	C1'-N1	5.05	1.56	1.48
55	DA	585	G	C8-N7	-5.05	1.27	1.30
55	DA	859	G	C3'-O3'	5.03	1.49	1.42
55	DA	2473	U	N1-C2	5.03	1.43	1.38
31	CA	2491	U	C1'-N1	5.02	1.56	1.48
55	DA	1254	A	N7-C5	-5.02	1.36	1.39
31	CA	271	G	C3'-O3'	5.01	1.49	1.42
31	CA	1306	C	C1'-N1	5.01	1.56	1.48
55	DA	2847	U	C4-O4	-5.01	1.19	1.23

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	CB	15	A	O4'-C1'-N9	10.42	116.54	108.20
31	CA	752	A	O4'-C1'-N9	10.40	116.52	108.20
55	DA	1936	A	O4'-C1'-N9	9.02	115.41	108.20
55	DA	2406	A	C5'-C4'-O4'	-7.61	99.97	109.10
54	DI	132	TYR	C-N-CA	7.10	139.44	121.70
55	DA	892	A	OP1-P-OP2	-7.07	108.99	119.60
1	AA	1	A	OP1-P-OP2	-7.05	109.02	119.60
31	CA	892	A	OP1-P-OP2	-7.00	109.10	119.60
55	DA	1	G	OP1-P-OP2	-6.99	109.12	119.60
55	DA	784	G	P-O3'-C3'	6.96	128.06	119.70
1	BA	2	A	OP1-P-OP2	-6.95	109.18	119.60
1	BA	1362	A	C1'-O4'-C4'	-6.85	104.42	109.90
55	DA	512	G	O4'-C1'-N9	6.71	113.57	108.20
31	CA	271	G	P-O3'-C3'	6.47	127.46	119.70
31	CA	2406	A	C5'-C4'-O4'	6.44	116.82	109.10
55	DA	271	G	P-O3'-C3'	6.29	127.25	119.70
31	CA	2825	G	O4'-C1'-N9	6.23	113.18	108.20
31	CA	2225	A	P-O3'-C3'	6.13	127.06	119.70
31	CA	2326	C	P-O3'-C3'	6.00	126.90	119.70
31	CA	752	A	C1'-O4'-C4'	-5.95	105.14	109.90
31	CA	752	A	C3'-C2'-C1'	-5.89	96.79	101.50
1	AA	413	G	C1'-O4'-C4'	-5.77	105.28	109.90
55	DA	2848	G	O4'-C1'-N9	5.75	112.80	108.20
31	CA	974	G	N9-C1'-C2'	5.74	121.46	114.00
55	DA	807	U	C4'-C3'-C2'	-5.68	96.92	102.60
31	CA	2425	A	P-O3'-C3'	5.60	126.42	119.70
41	DN	6	ARG	CA-CB-CG	5.48	125.46	113.40
40	CM	68	SER	C-N-CA	5.48	135.40	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	784	G	P-O3'-C3'	5.44	126.23	119.70
31	CA	479	A	C3'-C2'-C1'	-5.38	97.19	101.50
55	DA	1936	A	C1'-O4'-C4'	-5.38	105.60	109.90
55	DA	479	A	C3'-C2'-C1'	-5.35	97.22	101.50
1	BA	890	G	O4'-C1'-N9	5.31	112.45	108.20
55	DA	2645	G	O4'-C1'-N9	5.29	112.43	108.20
55	DA	2825	G	O4'-C1'-N9	5.28	112.42	108.20
55	DA	2715	C	O4'-C1'-N1	5.27	112.42	108.20
28	CB	15	A	C1'-O4'-C4'	-5.25	105.70	109.90
31	CA	974	G	C1'-O4'-C4'	-5.21	105.73	109.90
31	CA	2680	U	P-O3'-C3'	5.20	125.94	119.70
31	CA	752	A	N9-C1'-C2'	5.20	120.75	114.00
55	DA	2817	U	O4'-C1'-N1	5.14	112.31	108.20
31	CA	2095	A	C5'-C4'-C3'	-5.10	107.84	116.00
52	DY	11	ARG	CA-CB-CG	5.09	124.59	113.40
31	CA	1379	U	P-O3'-C3'	5.08	125.80	119.70
42	CO	71	ARG	CA-CB-CG	5.07	124.55	113.40
44	CQ	114	LEU	CA-CB-CG	5.06	126.94	115.30
31	CA	2035	G	C1'-O4'-C4'	-5.03	105.87	109.90

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1077	G	Sidechain
1	AA	1094	G	Sidechain
1	AA	898	G	Sidechain
20	AT	24	ARG	Sidechain
1	BA	1077	G	Sidechain
31	CA	2267	A	Sidechain
31	CA	250	G	Sidechain
31	CA	463	G	Sidechain
55	DA	1142	A	Sidechain
55	DA	1188	U	Sidechain
55	DA	1288	G	Sidechain
55	DA	1324	G	Sidechain
55	DA	1425	G	Sidechain
55	DA	1631	G	Sidechain
55	DA	1753	G	Sidechain
55	DA	1872	A	Sidechain
55	DA	1938	A	Sidechain
55	DA	2048	G	Sidechain

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Mol	Chain	Res	Type	Group
55	DA	221	A	Sidechain
55	DA	2267	A	Sidechain
55	DA	2375	G	Sidechain
55	DA	2481	G	Sidechain
55	DA	250	G	Sidechain
55	DA	2516	A	Sidechain
55	DA	2529	G	Sidechain
55	DA	2578	G	Sidechain
55	DA	2595	G	Sidechain
55	DA	2597	G	Sidechain
55	DA	2641	G	Sidechain
55	DA	2645	G	Sidechain
55	DA	2779	U	Sidechain
55	DA	2835	A	Sidechain
55	DA	452	G	Sidechain
55	DA	463	G	Sidechain
55	DA	500	G	Sidechain
55	DA	512	G	Sidechain
55	DA	555	G	Sidechain
55	DA	607	U	Sidechain
55	DA	700	G	Sidechain
55	DA	858	G	Sidechain
55	DA	864	G	Sidechain
55	DA	956	G	Sidechain
55	DA	980	A	Sidechain
55	DA	983	A	Sidechain
55	DA	984	A	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32933	0	16592	102	0
1	BA	32911	0	16581	118	0
2	AB	1753	0	1780	14	0
2	BB	1753	0	1780	13	0
3	AC	1625	0	1696	17	0
3	BC	1625	0	1696	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AD	1643	0	1707	12	0
4	BD	1643	0	1707	18	0
5	AE	1144	0	1185	24	0
5	BE	1105	0	1148	29	0
6	AF	862	0	864	10	0
6	BF	817	0	808	4	0
7	AG	1182	0	1238	7	0
7	BG	1182	0	1238	11	0
8	AH	979	0	1031	6	0
8	BH	979	0	1031	4	0
9	AI	1022	0	1070	14	0
9	BI	1022	0	1070	10	0
10	AJ	796	0	836	13	0
10	BJ	787	0	828	13	0
11	AK	877	0	887	15	0
11	BK	877	0	887	19	0
12	AL	957	0	1017	9	0
12	BL	957	0	1017	14	0
13	AM	884	0	941	11	0
13	BM	884	0	941	13	0
14	AN	805	0	844	14	0
14	BN	805	0	844	12	0
15	AO	714	0	734	2	0
15	BO	714	0	734	3	0
16	AP	649	0	666	4	0
16	BP	649	0	666	5	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	14	0
18	AR	456	0	478	5	0
18	BR	456	0	478	4	0
19	AS	638	0	665	13	0
19	BS	638	0	665	11	0
20	AT	670	0	719	6	0
20	BT	665	0	714	3	0
21	AU	465	0	491	3	0
21	BU	465	0	491	2	0
22	C1	444	0	458	9	0
22	D1	444	0	458	13	0
23	C2	409	0	440	5	0
23	D2	414	0	442	5	0
24	C3	377	0	418	3	0
24	D3	377	0	418	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	C4	504	0	572	2	0
25	D4	504	0	572	3	0
26	C5	302	0	340	4	0
26	D5	302	0	340	4	0
27	C0	449	0	488	2	0
27	D0	463	0	504	5	0
28	CB	2529	0	1281	5	0
28	DB	2569	0	1301	7	0
29	CC	2083	0	2154	27	0
29	DC	2083	0	2154	19	0
30	CD	1565	0	1616	18	0
31	CA	62229	0	31318	216	0
32	DD	1576	0	1627	17	0
33	CE	1552	0	1619	13	0
33	DE	1552	0	1619	4	0
34	CF	1411	0	1444	12	0
34	DF	1411	0	1444	18	0
35	CG	1323	0	1371	13	0
35	DG	1323	0	1371	13	0
36	CH	1110	0	1148	17	0
36	DH	1110	0	1148	9	0
37	CJ	979	0	1028	7	0
37	DJ	979	0	1028	8	0
38	CK	1129	0	1162	10	0
38	DK	1129	0	1162	4	0
39	CL	938	0	1012	10	0
39	DL	946	0	1023	6	0
40	CM	1053	0	1129	13	0
40	DM	1053	0	1129	3	0
41	CN	1075	0	1154	7	0
41	DN	1092	0	1177	14	0
42	CO	960	0	1000	9	0
42	DO	993	0	1034	7	0
43	CP	892	0	923	9	0
43	DP	900	0	935	13	0
44	CQ	917	0	962	9	0
44	DQ	917	0	962	17	0
45	CR	947	0	1019	10	0
45	DR	947	0	1019	12	0
46	CS	816	0	839	11	0
46	DS	816	0	839	7	0
47	CT	857	0	922	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	DT	857	0	922	11	0
48	CU	739	0	807	5	0
48	DU	739	0	807	7	0
49	CV	780	0	831	6	0
49	DV	780	0	831	4	0
50	CW	753	0	780	4	0
50	DW	753	0	780	4	0
51	CX	569	0	581	4	0
51	DX	591	0	606	10	0
52	CY	625	0	652	8	0
52	DY	625	0	652	8	0
53	CZ	501	0	531	1	0
53	DZ	501	0	531	1	0
54	DI	1023	0	1052	19	0
55	DA	62423	0	31411	199	0
56	AA	71	0	0	0	0
56	BA	43	0	0	0	0
56	CA	156	0	0	0	0
56	CB	3	0	0	0	0
56	DA	184	0	0	0	0
56	DB	9	0	0	0	0
56	DD	1	0	0	0	0
56	DM	1	0	0	0	0
56	DR	1	0	0	0	0
57	AA	13	0	18	1	0
57	BA	13	0	18	1	0
57	DA	26	0	36	2	0
57	DQ	13	0	18	1	0
57	DR	13	0	18	3	0
57	DS	13	0	18	1	0
58	AA	16	0	28	2	0
58	DA	48	0	84	4	0
58	DE	16	0	28	0	0
58	DK	8	0	14	0	0
58	DN	8	0	14	0	0
58	DS	8	0	14	3	0
58	DT	8	0	14	0	0
59	AA	24	0	48	0	0
59	DA	66	0	132	4	0
59	DM	6	0	12	0	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	0	0
61	DL	7	0	10	0	0
61	DP	7	0	10	1	0
61	DQ	7	0	10	1	0
62	D1	4	0	6	0	0
62	DA	36	0	54	3	0
62	DB	8	0	12	1	0
63	D1	10	0	14	3	0
63	D3	10	0	14	0	0
63	DA	40	0	56	4	0
63	DD	10	0	14	0	0
63	DS	10	0	14	0	0
63	DU	10	0	14	1	0
64	DA	40	0	76	2	0
65	DA	32	0	44	1	0
66	DA	12	0	9	0	0
67	DA	11	0	5	0	0
68	DA	8	0	12	2	0
69	AA	508	0	0	1	0
69	AC	5	0	0	0	0
69	AD	1	0	0	0	0
69	AE	5	0	0	0	0
69	AF	1	0	0	0	0
69	AG	1	0	0	0	0
69	AJ	3	0	0	0	0
69	AK	6	0	0	0	0
69	AL	10	0	0	0	0
69	AM	4	0	0	1	0
69	AN	5	0	0	2	0
69	AO	2	0	0	0	0
69	AP	2	0	0	1	0
69	AT	4	0	0	0	0
69	AU	2	0	0	0	0
69	BA	282	0	0	1	0
69	BD	12	0	0	0	0
69	BE	1	0	0	0	0
69	BF	1	0	0	0	0
69	BK	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	BL	6	0	0	0	0
69	BN	2	0	0	0	0
69	BO	1	0	0	0	0
69	BP	3	0	0	1	0
69	BR	1	0	0	0	0
69	BT	3	0	0	0	0
69	BU	3	0	0	0	0
69	C3	2	0	0	0	0
69	C4	1	0	0	0	0
69	C5	1	0	0	0	0
69	CA	693	0	0	4	0
69	CB	13	0	0	0	0
69	CC	8	0	0	0	0
69	CD	7	0	0	0	0
69	CE	4	0	0	0	0
69	CL	1	0	0	0	0
69	CM	4	0	0	0	0
69	CO	2	0	0	0	0
69	CQ	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	26	0	0	0	0
69	D1	46	0	0	1	0
69	D2	6	0	0	0	0
69	D3	28	0	0	1	0
69	D4	33	0	0	0	0
69	D5	11	0	0	0	0
69	DA	4830	0	0	20	0
69	DB	203	0	0	1	0
69	DC	102	0	0	1	0
69	DD	95	0	0	1	0
69	DE	63	0	0	2	0
69	DF	16	0	0	0	0
69	DG	7	0	0	0	0
69	DH	2	0	0	0	0
69	DK	60	0	0	1	0
69	DL	51	0	0	0	0
69	DM	68	0	0	1	0
69	DN	73	0	0	1	0
69	DO	49	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	DP	38	0	0	0	0
69	DQ	29	0	0	0	0
69	DR	61	0	0	1	0
69	DS	50	0	0	0	0
69	DT	66	0	0	1	0
69	DU	19	0	0	0	0
69	DV	21	0	0	0	0
69	DW	32	0	0	0	0
69	DX	25	0	0	1	0
69	DY	10	0	0	0	0
69	DZ	6	0	0	0	0
All	All	295130	0	194412	1415	0

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

All (1415) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D5:26:ILE:CD1	26:D5:26:ILE:CG1	1.82	1.56
46:CS:14:VAL:HG21	46:CS:98:ILE:HG13	1.28	1.11
31:CA:1005:C:O2'	38:CK:30:THR:HG21	1.60	1.01
18:AR:21:ILE:HG21	18:AR:54:GLN:HB3	1.39	1.00
40:CM:77:ILE:HD11	40:CM:108:ALA:HB1	1.46	0.96
12:BL:65:SER:HB2	12:BL:82:ILE:HD11	1.48	0.95
31:CA:1847:A:HO2'	31:CA:1848:A:H8	0.99	0.95
46:CS:14:VAL:CG2	46:CS:98:ILE:HG13	1.97	0.94
11:BK:88:GLY:H	11:BK:114:THR:HG22	1.31	0.93
55:DA:1847:A:HO2'	55:DA:1848:A:H8	0.99	0.93
11:AK:88:GLY:H	11:AK:114:THR:HG22	1.30	0.93
55:DA:2796:U:H3	55:DA:2799:A:H61	1.18	0.91
31:CA:1779:U:H5	31:CA:1784:A:N7	1.69	0.90
31:CA:1936:A:H2	31:CA:1943:U:N3	1.70	0.88
31:CA:2728:U:HO2'	31:CA:2729:G:H8	0.92	0.88
31:CA:528:A:C2	31:CA:2043:C:H4'	2.09	0.87
31:CA:2796:U:H3	31:CA:2799:A:H61	1.19	0.86
31:CA:1936:A:H2	31:CA:1943:U:H3	0.91	0.86
54:DI:67:THR:HG22	54:DI:68:PRO:HA	1.56	0.85
55:DA:1913:A:H4'	55:DA:1913:A:OP1	1.78	0.83
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.59	0.83
47:CT:59:GLU:HA	47:CT:64:ALA:HA	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:CT:86:MET:HB2	47:CT:96:ILE:HD11	1.59	0.83
30:CD:129:THR:HG23	30:CD:140:HIS:O	1.79	0.83
55:DA:135:U:H3	55:DA:144:A:H61	1.27	0.82
1:AA:664:G:H22	1:AA:741:G:H1	1.27	0.82
43:DP:31:THR:HG22	43:DP:34:HIS:H	1.45	0.82
1:AA:1518:MA6:H103	1:AA:1519:MA6:H102	1.61	0.81
43:CP:31:THR:HG22	43:CP:34:HIS:H	1.46	0.81
46:CS:14:VAL:HG21	46:CS:98:ILE:CG1	2.09	0.81
8:BH:87:LYS:HB2	8:BH:125:ILE:HD11	1.62	0.80
24:C3:12:ARG:HD2	24:C3:44:VAL:HG11	1.62	0.80
31:CA:1779:U:C5	31:CA:1784:A:N7	2.49	0.80
40:CM:82:LEU:HD11	40:CM:116:VAL:HG23	1.62	0.80
31:CA:135:U:H3	31:CA:144:A:H61	1.27	0.80
31:CA:740:C:H5'	31:CA:1784:A:H3'	1.65	0.79
1:BA:1518:MA6:H103	1:BA:1519:MA6:H102	1.62	0.79
1:BA:664:G:H22	1:BA:741:G:H1	1.26	0.79
11:AK:88:GLY:N	11:AK:114:THR:HG22	1.97	0.79
13:BM:114:LYS:HB3	13:BM:115:PRO:HD3	1.64	0.79
11:BK:88:GLY:N	11:BK:114:THR:HG22	1.98	0.78
51:DX:23:VAL:HA	51:DX:38:VAL:HG23	1.66	0.78
13:BM:83:LEU:HD21	19:BS:65:GLU:HB2	1.68	0.76
5:BE:104:GLY:HA3	5:BE:122:ASN:HA	1.66	0.76
29:CC:75:PRO:HG2	29:CC:97:LYS:HD3	1.68	0.76
24:D3:29:GLN:HG2	61:D3:102:PEG:H21	1.68	0.76
8:AH:87:LYS:HB2	8:AH:125:ILE:HD11	1.66	0.76
29:DC:233:GLY:HA3	69:DC:306:HOH:O	1.85	0.75
31:CA:2728:U:O2'	31:CA:2729:G:H8	1.68	0.75
46:DS:21:ARG:HH21	57:DS:202:PG4:H71	1.50	0.75
46:DS:73:LYS:HE2	58:DS:203:MPD:H53	1.66	0.75
31:CA:846:U:H1'	31:CA:847:U:H5	1.50	0.74
40:CM:77:ILE:CD1	40:CM:108:ALA:HB1	2.16	0.74
10:AJ:7:ARG:HB3	10:AJ:101:SER:HB2	1.68	0.74
1:BA:451:A:H2'	69:BA:1701:HOH:O	1.88	0.74
5:BE:106:ILE:HD11	5:BE:124:LEU:HD23	1.71	0.73
13:AM:33:ILE:HD11	13:AM:63:PHE:HE1	1.53	0.73
1:BA:522:C:H41	12:BL:50:ARG:HH12	1.35	0.72
31:CA:752:A:H62	31:CA:2609:U:H3	1.36	0.72
35:CG:24:ILE:HD11	35:CG:43:VAL:HG11	1.71	0.72
58:AA:1671:MPD:H31	20:AT:24:ARG:NH1	2.05	0.72
22:D1:24:ALA:HB3	63:D1:102:PGE:H5	1.71	0.72
30:CD:133:THR:HG22	31:CA:1993:U:H4'	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BK:89:PRO:HG3	21:BU:32:VAL:HG11	1.72	0.71
38:CK:81:ILE:HG23	38:CK:82:GLY:H	1.55	0.71
19:AS:15:LEU:HD13	19:AS:33:THR:HG21	1.72	0.71
31:CA:460:A:H5'	48:CU:73:ARG:HH22	1.56	0.71
35:DG:24:ILE:HD11	35:DG:43:VAL:HG11	1.73	0.71
1:AA:1323:G:H2'	1:AA:1324:A:C8	2.26	0.71
40:CM:85:VAL:HG11	40:CM:90:VAL:HG22	1.71	0.71
55:DA:1853:A:N1	55:DA:2087:G:H1'	2.05	0.71
45:DR:28:ARG:HD3	69:DR:305:HOH:O	1.91	0.70
1:BA:1323:G:H2'	1:BA:1324:A:C8	2.27	0.69
19:BS:15:LEU:HD13	19:BS:33:THR:HG21	1.73	0.69
3:BC:40:ARG:HD3	3:BC:55:ILE:HG23	1.73	0.69
17:BQ:14:SER:HB3	17:BQ:22:VAL:HG12	1.74	0.69
5:AE:38:VAL:HG11	5:AE:114:VAL:HG22	1.74	0.69
25:C4:54:ASP:HB3	40:CM:57:LEU:HD22	1.74	0.69
43:DP:31:THR:HG21	28:DB:28:C:OP1	1.91	0.69
41:DN:18[B]:ARG:HG3	28:DB:90:C:H5''	1.72	0.69
11:AK:89:PRO:HG3	21:AU:32:VAL:HG11	1.75	0.69
11:AK:34:ILE:HG12	11:AK:70:CYS:SG	2.33	0.68
29:CC:88:SER:HB2	29:CC:158:ALA:HB2	1.75	0.68
1:BA:73:C:HO2'	1:BA:74:A:H8	1.42	0.68
31:CA:699:A:H2'	31:CA:700:G:O4'	1.94	0.67
5:BE:72:ILE:HG12	5:BE:145:GLU:HG3	1.75	0.67
1:AA:81:A:H61	1:AA:86:G:H1	1.42	0.67
45:CR:58:ARG:HH11	45:CR:62:ILE:HD11	1.60	0.67
13:AM:33:ILE:HD11	13:AM:63:PHE:CE1	2.29	0.67
1:AA:86:G:H21	1:AA:87:C:H41	1.43	0.67
31:CA:634:C:H2'	31:CA:635:C:C6	2.30	0.66
24:D3:44:VAL:HG23	69:D3:222:HOH:O	1.96	0.66
19:BS:52:HIS:HD2	19:BS:54:GLY:H	1.41	0.66
30:CD:99:GLU:HG2	30:CD:182:ALA:HB2	1.78	0.66
40:CM:95:LEU:HD22	40:CM:100:ILE:HG12	1.77	0.66
1:BA:1218:C:H2'	1:BA:1219:A:C8	2.31	0.66
55:DA:568:U:H1'	55:DA:2030:6MZ:H9C1	1.77	0.65
32:DD:99:GLU:HG2	32:DD:182:ALA:HB2	1.78	0.65
38:CK:81:ILE:CG2	38:CK:82:GLY:H	2.10	0.65
32:DD:186:LEU:HD21	44:DQ:4:ILE:HG21	1.79	0.65
55:DA:789:A:OP1	59:DA:3224:PUT:H11	1.95	0.65
17:BQ:68:SER:OG	17:BQ:71:LYS:HB3	1.97	0.65
31:CA:1311:G:H21	31:CA:1603:A:H62	1.44	0.65
49:CV:7:ARG:O	49:CV:25:VAL:HB	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:DN:20:LEU:HD22	50:DW:81:PRO:HG2	1.79	0.65
1:AA:1218:C:H2'	1:AA:1219:A:C8	2.31	0.65
33:DE:33:VAL:HG22	58:DA:3195:MPD:H12	1.79	0.65
1:AA:1492:A:H5'	1:AA:1492:A:H8	1.61	0.64
17:BQ:8:LEU:HD23	17:BQ:25:ILE:HG21	1.79	0.64
11:BK:23:ILE:HG22	11:BK:32:VAL:HG13	1.80	0.64
13:BM:11:ASP:HA	13:BM:45:ILE:HD13	1.79	0.64
55:DA:1746:A:H2'	55:DA:1747:U:C6	2.33	0.64
45:DR:20:GLN:HG3	57:DR:202:PG4:H42	1.78	0.64
31:CA:1653:G:H3'	42:CO:2:ARG:HG2	1.78	0.64
41:DN:77:PRO:HG2	41:DN:80:VAL:HG21	1.78	0.64
6:AF:45:ARG:O	6:AF:56:LYS:HA	1.98	0.64
13:AM:83:LEU:HD11	19:AS:66:MET:HG3	1.78	0.64
18:AR:21:ILE:CG2	18:AR:54:GLN:HB3	2.22	0.64
46:CS:49:ILE:HB	46:CS:51:VAL:O	1.98	0.64
47:CT:82:MET:HB2	47:CT:98:LYS:HB2	1.79	0.64
29:DC:29:PRO:HG2	29:DC:34:LEU:HD11	1.79	0.64
48:CU:18:GLU:H	48:CU:18:GLU:CD	1.99	0.63
47:DT:82:MET:HB2	47:DT:98:LYS:HB2	1.79	0.63
35:CG:76:VAL:O	35:CG:80:THR:HG22	1.97	0.63
29:CC:105:LEU:H	29:CC:105:LEU:HD12	1.63	0.63
11:AK:23:ILE:HG22	11:AK:32:VAL:HG13	1.80	0.63
57:DA:3218:PG4:H31	69:DA:6906:HOH:O	1.98	0.63
13:AM:6:GLY:HA3	13:AM:66:GLU:HG3	1.81	0.63
31:CA:1105:U:H2'	31:CA:1106:G:H8	1.63	0.63
6:BF:45:ARG:O	6:BF:56:LYS:HA	1.98	0.62
13:BM:6:GLY:HA3	13:BM:66:GLU:HG3	1.80	0.62
19:AS:52:HIS:HD2	19:AS:54:GLY:H	1.47	0.62
33:DE:21:ARG:HD2	69:DE:430:HOH:O	1.97	0.62
5:AE:105:ILE:HG23	5:AE:123:VAL:HG23	1.80	0.62
55:DA:2127:G:H4'	55:DA:2128:G:OP1	1.98	0.62
22:D1:9:THR:CG2	55:DA:2020:A:H5'	2.29	0.62
2:AB:129:LEU:HD13	2:AB:134:ALA:HB2	1.82	0.62
31:CA:568:U:H1'	31:CA:2030:6MZ:H9C1	1.80	0.62
31:CA:846:U:H1'	31:CA:847:U:C5	2.33	0.62
36:CH:15:LEU:HD22	36:CH:15:LEU:H	1.65	0.62
55:DA:1105:U:H2'	55:DA:1106:G:H8	1.64	0.62
14:AN:66:GLN:HB2	69:AN:205:HOH:O	1.99	0.61
1:AA:1151:A:HO2'	1:AA:1152:A:H8	1.48	0.61
1:BA:841:C:H3'	1:BA:842:U:C5'	2.30	0.61
29:CC:29:PRO:HG2	29:CC:34:LEU:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:DG:42:GLU:HG3	35:DG:55:ARG:HH21	1.66	0.61
19:BS:50:ALA:HB1	19:BS:57:HIS:HB3	1.81	0.61
12:AL:3:THR:HB	12:AL:6:GLN:HB2	1.82	0.61
22:C1:43:ILE:HG22	22:C1:49:TYR:HB2	1.82	0.61
54:DI:15:VAL:HG23	54:DI:53:ARG:HH21	1.66	0.61
31:CA:2226:C:H2'	31:CA:2227:A:O4'	2.01	0.61
38:DK:9:GLU:HG2	69:DA:4873:HOH:O	2.01	0.61
38:CK:81:ILE:HG23	38:CK:82:GLY:N	2.16	0.61
55:DA:1105:U:H2'	55:DA:1106:G:C8	2.36	0.61
1:BA:841:C:H3'	1:BA:842:U:H5''	1.82	0.60
1:BA:619:U:H3	4:BD:131:ASN:HB3	1.66	0.60
8:BH:77:ARG:NH1	8:BH:80:ARG:HA	2.16	0.60
31:CA:784:G:H5'	31:CA:785:G:OP1	2.01	0.60
31:CA:1105:U:H2'	31:CA:1106:G:C8	2.36	0.60
31:CA:910:A:H62	41:CN:12:MET:HA	1.65	0.60
28:CB:28:C:OP1	43:CP:31:THR:HG21	2.01	0.60
17:BQ:8:LEU:HD13	17:BQ:73:TRP:CH2	2.37	0.60
31:CA:1936:A:C2	31:CA:1943:U:N3	2.51	0.60
35:CG:42:GLU:HG3	35:CG:55:ARG:HH21	1.67	0.60
49:CV:74:ASN:HD22	49:CV:77:THR:H	1.49	0.60
55:DA:2751:G:H2'	69:DA:4610:HOH:O	2.01	0.60
31:CA:528:A:H2	31:CA:2043:C:H4'	1.66	0.60
28:CB:89:U:C6	31:CA:958:U:H2'	2.37	0.60
36:CH:41:LYS:HA	36:CH:44:ILE:HG12	1.84	0.60
1:AA:1518:MA6:H103	1:AA:1519:MA6:C10	2.32	0.60
14:BN:31:ILE:HG23	14:BN:42:TRP:HZ2	1.66	0.60
31:CA:2573:C:H5	69:CA:3275:HOH:O	1.84	0.60
42:CO:33:ILE:HD12	42:CO:114:GLU:HB3	1.83	0.60
42:DO:33:ILE:HD12	42:DO:114:GLU:HB3	1.83	0.59
19:AS:50:ALA:HB1	19:AS:57:HIS:HB3	1.82	0.59
44:DQ:6:LYS:O	44:DQ:10:GLN:HG2	2.02	0.59
5:AE:90:THR:HG22	5:AE:91:GLY:H	1.67	0.59
31:CA:2065:C:H4'	31:CA:2251:OMG:HM22	1.85	0.59
29:CC:219:THR:O	31:CA:1789:A:H5''	2.02	0.59
41:DN:42:THR:HG22	41:DN:93:VAL:HG12	1.85	0.59
49:DV:52:LEU:HB3	49:DV:54:GLN:HB2	1.84	0.59
2:BB:129:LEU:HD13	2:BB:134:ALA:HB2	1.84	0.59
34:CF:31:VAL:HG11	34:CF:97:TRP:CH2	2.38	0.59
38:DK:56:VAL:HB	38:DK:124:VAL:HB	1.85	0.59
42:DO:73:ASN:HA	42:DO:76:VAL:HG13	1.84	0.59
36:CH:27:ARG:HH11	52:CY:60:ASP:HA	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D1:43:ILE:HG22	22:D1:49:TYR:HB2	1.84	0.59
39:CL:103:VAL:O	39:CL:122:VAL:HB	2.02	0.59
36:DH:41:LYS:HA	36:DH:44:ILE:HG12	1.84	0.59
45:DR:6:ARG:NH1	55:DA:585:G:N7	2.50	0.59
5:AE:16:ILE:HD13	5:AE:137:VAL:HG11	1.84	0.59
5:BE:90:THR:HG22	5:BE:91:GLY:H	1.67	0.59
1:BA:1493:A:H1'	31:CA:1913:A:H61	1.68	0.59
31:CA:822:G:O6	31:CA:943:A:H2	1.86	0.59
5:BE:16:ILE:HD13	5:BE:137:VAL:HG11	1.85	0.58
30:CD:1:MET:HB3	30:CD:205:PRO:HG2	1.84	0.58
34:CF:31:VAL:CG1	34:CF:97:TRP:CH2	2.86	0.58
41:CN:41:LEU:HD22	41:CN:46:ILE:HG13	1.84	0.58
22:D1:54:VAL:HG23	22:D1:55:ILE:HG12	1.85	0.58
5:AE:76:LEU:HD11	5:AE:120:VAL:HG22	1.85	0.58
32:DD:1:MET:HB3	32:DD:205:PRO:HG2	1.85	0.58
1:BA:202:G:H1	1:BA:215:C:H42	1.51	0.58
8:AH:105:SER:HB2	8:AH:126:ILE:HD11	1.86	0.58
5:AE:157:ARG:HD2	8:AH:43:GLU:O	2.03	0.58
17:BQ:17:MET:HB3	17:BQ:20:SER:HB3	1.84	0.58
25:D4:54:ASP:HB3	40:DM:57:LEU:HD22	1.83	0.58
1:BA:1060:U:C5	3:BC:2:GLY:HA3	2.39	0.58
9:BI:12:ARG:HG3	9:BI:107:ASP:HB3	1.84	0.58
55:DA:2886[A]:A:C2	55:DA:2887[A]:A:H1'	2.39	0.58
1:BA:502:A:OP1	12:BL:115:SER:HB3	2.04	0.58
42:CO:73:ASN:HA	42:CO:76:VAL:HG13	1.85	0.58
52:DY:61:LYS:HD3	55:DA:372:G:H5''	1.86	0.58
41:CN:77:PRO:HG2	41:CN:80:VAL:HG21	1.84	0.58
47:CT:69:LEU:HG	47:CT:107:VAL:HG22	1.85	0.58
31:CA:1394:U:H4'	31:CA:1603:A:H4'	1.86	0.58
48:CU:54:GLU:HB3	48:CU:88:LYS:HD2	1.86	0.58
55:DA:11:C:H2'	55:DA:12:U:H5'	1.86	0.58
58:AA:1671:MPD:H31	20:AT:24:ARG:HH12	1.68	0.58
1:BA:923:A:OP1	5:BE:26:LYS:HG2	2.04	0.57
31:CA:396:G:H1'	52:CY:29:PHE:HB3	1.86	0.57
44:CQ:114:LEU:H	44:CQ:114:LEU:CD2	2.17	0.57
51:DX:59:LEU:HD12	51:DX:80:ILE:HD12	1.86	0.57
17:AQ:15:ASP:HA	17:AQ:21:ILE:HG22	1.87	0.57
31:CA:118:A:N3	31:CA:178:G:H1'	2.19	0.57
55:DA:551:G:H8	55:DA:551:G:H5''	1.69	0.57
9:AI:12:ARG:HG3	9:AI:107:ASP:HB3	1.86	0.57
1:AA:923:A:OP1	5:AE:26:LYS:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:774:G:H21	57:AA:1670:PG4:H51	1.69	0.57
6:BF:38:ARG:HB3	6:BF:63:ASN:HB2	1.85	0.57
31:CA:783:A:H4'	31:CA:1779:U:O2	2.05	0.57
38:CK:56:VAL:HB	38:CK:124:VAL:HB	1.85	0.57
19:AS:32:ARG:HE	19:AS:57:HIS:CE1	2.23	0.57
4:BD:107:PHE:HB3	4:BD:145:ILE:HD11	1.85	0.57
29:CC:227:PRO:HA	29:CC:233:GLY:HA2	1.86	0.57
36:CH:82:SER:HB2	36:CH:94:ILE:HD11	1.85	0.57
6:AF:38:ARG:HB3	6:AF:63:ASN:HB2	1.86	0.57
1:BA:1397:C:H2'	1:BA:1397:C:O2	2.05	0.57
13:BM:90:ARG:HD3	13:BM:97:VAL:HA	1.87	0.57
4:AD:107:PHE:HB3	4:AD:145:ILE:HD11	1.85	0.57
28:DB:85:G:H1'	62:DB:211:EDO:H11	1.87	0.57
31:CA:2190:G:H2'	31:CA:2191:A:C8	2.40	0.57
31:CA:2796:U:H3	31:CA:2799:A:N6	1.97	0.57
44:CQ:6:LYS:O	44:CQ:10:GLN:HG2	2.04	0.56
36:DH:82:SER:HB2	36:DH:94:ILE:HD11	1.86	0.56
1:AA:1062:U:H2'	1:AA:1063:C:C6	2.40	0.56
1:AA:677:U:H3	1:AA:713:G:H22	1.53	0.56
1:BA:1391:U:H2'	1:BA:1392:G:C8	2.39	0.56
12:BL:65:SER:CB	12:BL:82:ILE:HD11	2.30	0.56
13:AM:90:ARG:HD3	13:AM:97:VAL:HA	1.86	0.56
7:BG:22:LEU:HD23	7:BG:62:PHE:HE1	1.70	0.56
23:C2:37:LYS:HG2	23:C2:48:ILE:HG13	1.86	0.56
1:BA:677:U:H3	1:BA:713:G:H22	1.50	0.56
1:BA:209:U:O2	1:BA:209:U:H2'	2.04	0.56
1:BA:1106:G:H5''	3:BC:172:ARG:HG3	1.87	0.56
29:DC:227:PRO:HA	29:DC:233:GLY:HA2	1.86	0.56
1:AA:413:G:H5''	1:AA:414:A:H5'	1.88	0.56
37:CJ:19:ASN:H	37:CJ:20:PRO:HD2	1.71	0.56
39:CL:58:LEU:HD11	39:CL:86:LEU:HD13	1.87	0.56
7:BG:113:ASP:HB2	7:BG:119:ARG:HG3	1.87	0.56
35:CG:80:THR:HG23	35:CG:81:GLU:H	1.69	0.56
51:CX:37:ILE:HG21	51:CX:80:ILE:HG21	1.87	0.56
54:DI:132:TYR:H	54:DI:133:GLU:HB2	1.70	0.56
54:DI:50:VAL:HG11	54:DI:92:ALA:HB2	1.87	0.56
8:BH:105:SER:HB2	8:BH:126:ILE:HD11	1.87	0.56
1:BA:706:A:O2'	11:BK:31:ILE:HD11	2.06	0.56
3:BC:155:GLY:HA2	3:BC:163:ALA:HB1	1.88	0.56
41:CN:41:LEU:HD21	41:CN:124:LEU:HD22	1.88	0.56
1:AA:1391:U:H2'	1:AA:1392:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:202:G:H1	1:AA:215:C:H42	1.54	0.56
1:AA:502:A:OP1	12:AL:115:SER:HB3	2.06	0.56
1:BA:774:G:H21	57:BA:1642:PG4:H62	1.71	0.56
4:BD:197:GLU:HA	4:BD:200:ILE:HD12	1.88	0.56
1:BA:1219:A:H2'	1:BA:1220:G:C8	2.41	0.55
31:CA:1509:A:HO2'	31:CA:1510:G:H8	1.53	0.55
31:CA:528:A:H2'	31:CA:529:A:H5''	1.87	0.55
55:DA:1831:G:H1'	63:DA:3227:PGE:H1	1.88	0.55
4:AD:197:GLU:HA	4:AD:200:ILE:HD12	1.88	0.55
7:AG:113:ASP:HB2	7:AG:119:ARG:HG3	1.87	0.55
55:DA:1509:A:HO2'	55:DA:1510:G:H8	1.53	0.55
29:CC:17:VAL:HB	29:CC:204:VAL:HG13	1.88	0.55
45:CR:9:ILE:HG13	45:CR:10:ALA:N	2.22	0.55
55:DA:788:A:H5''	59:DA:3224:PUT:H12	1.87	0.55
1:BA:518:C:H2'	1:BA:530:G:C8	2.42	0.55
21:BU:4:ILE:HG13	21:BU:19:PHE:HA	1.89	0.55
37:DJ:19:ASN:H	37:DJ:20:PRO:HD2	1.72	0.55
1:BA:1518:MA6:H103	1:BA:1519:MA6:C10	2.34	0.55
29:CC:155:ALA:HB2	29:CC:162:VAL:HG23	1.89	0.55
44:DQ:54:GLY:HA3	61:DQ:201:PEG:H22	1.88	0.55
3:AC:155:GLY:HA2	3:AC:163:ALA:HB1	1.88	0.55
13:AM:90:ARG:NH2	13:AM:95:LEU:HB3	2.22	0.55
21:AU:4:ILE:HG13	21:AU:19:PHE:HA	1.88	0.55
11:BK:23:ILE:HD11	11:BK:86:VAL:HG13	1.88	0.55
19:BS:29:LYS:HB3	19:BS:30:PRO:HD2	1.89	0.55
20:BT:4:ILE:HA	20:BT:8:LYS:HE2	1.89	0.55
31:CA:751:A:H5'	47:CT:90:LYS:HA	1.89	0.55
32:DD:161:MET:HG2	69:DA:5697:HOH:O	2.07	0.55
51:CX:59:LEU:HD12	51:CX:80:ILE:HD12	1.88	0.54
24:D3:12:ARG:HD3	69:DA:7002:HOH:O	2.07	0.54
31:CA:551:G:H8	31:CA:551:G:H5''	1.71	0.54
39:DL:58:LEU:HD11	39:DL:86:LEU:HD13	1.89	0.54
48:DU:54:GLU:HB3	48:DU:88:LYS:HD2	1.90	0.54
51:DX:37:ILE:HG21	51:DX:80:ILE:HG21	1.88	0.54
1:BA:1356:G:H2'	1:BA:1357:A:C8	2.42	0.54
31:CA:1991:U:H2'	31:CA:1992:G:H5''	1.90	0.54
40:CM:28:GLY:O	40:CM:29:LYS:O	2.25	0.54
45:CR:58:ARG:NH1	45:CR:62:ILE:HD11	2.23	0.54
1:AA:1219:A:H2'	1:AA:1220:G:C8	2.43	0.54
1:AA:1356:G:H2'	1:AA:1357:A:C8	2.43	0.54
55:DA:1417:C:H5'	55:DA:1588:G:H1'	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DA:1424:G:H21	63:DA:3216:PGE:H32	1.72	0.54
1:AA:1239:A:H62	1:AA:1299:A:H62	1.55	0.54
3:AC:23:PHE:C	3:AC:23:PHE:CD1	2.81	0.54
1:BA:12:U:H4'	1:BA:526:C:H4'	1.89	0.54
31:CA:2190:G:H2'	31:CA:2191:A:H8	1.71	0.54
55:DA:2796:U:H3	55:DA:2799:A:N6	1.96	0.54
55:DA:686:U:H2'	55:DA:788:A:N1	2.22	0.54
31:CA:686:U:H2'	31:CA:788:A:N1	2.22	0.54
31:CA:1131:G:OP1	38:CK:82:GLY:HA2	2.08	0.54
46:DS:85:LYS:HE3	69:DA:6504:HOH:O	2.08	0.54
9:AI:79:ILE:HG22	9:AI:83:ILE:HD11	1.90	0.54
31:CA:2502:G:H5''	31:CA:2503:2MA:H5''	1.89	0.54
42:CO:95:THR:HG21	42:CO:113:ILE:HD11	1.89	0.54
3:AC:33:LEU:HD21	14:AN:93:ILE:HG12	1.90	0.54
10:BJ:26:VAL:HG21	10:BJ:39:PRO:HD3	1.90	0.54
23:D2:6:ARG:HG2	23:D2:24:THR:HB	1.90	0.54
55:DA:2030:6MZ:H8	69:DA:6158:HOH:O	2.08	0.54
12:BL:80:ILE:HD13	12:BL:97:THR:HG22	1.91	0.53
3:AC:7:PRO:HD2	3:AC:184:TYR:CD1	2.43	0.53
2:BB:31:ILE:HG21	2:BB:39:HIS:HD2	1.74	0.53
29:CC:208:ALA:HB2	31:CA:1790:C:O2'	2.08	0.53
30:CD:133:THR:CG2	31:CA:1993:U:H4'	2.36	0.53
47:DT:17:VAL:HG11	47:DT:103:ILE:HG12	1.89	0.53
1:AA:542:G:H5'	4:AD:39:GLY:HA3	1.90	0.53
13:BM:90:ARG:NH2	13:BM:95:LEU:HB3	2.23	0.53
19:AS:29:LYS:HB3	19:AS:30:PRO:HD2	1.90	0.53
20:AT:48:GLN:HE21	20:AT:52:ASN:ND2	2.05	0.53
3:BC:43:LEU:HD13	3:BC:55:ILE:HD11	1.91	0.53
47:CT:17:VAL:HG11	47:CT:103:ILE:HG12	1.89	0.53
31:CA:2718:G:OP1	44:CQ:98:TYR:HD2	1.92	0.53
11:AK:25:ALA:HA	11:AK:30:THR:HG22	1.90	0.53
14:BN:13:ARG:HB3	14:BN:60:GLN:HG2	1.91	0.53
34:DF:132:VAL:HG22	34:DF:152:LEU:HG	1.90	0.53
1:AA:518:C:H2'	1:AA:530:G:C8	2.44	0.53
2:AB:188:ASP:HB2	2:AB:204:ASP:OD2	2.07	0.53
42:CO:2:ARG:HA	42:CO:5:LYS:HD2	1.91	0.53
11:BK:16:VAL:HG13	11:BK:79:ILE:HG13	1.89	0.53
54:DI:48:ALA:HB1	54:DI:91:ALA:HB1	1.90	0.53
34:CF:36:LEU:HD21	34:CF:91:LEU:HD11	1.91	0.53
48:CU:69:ARG:HB2	48:CU:74:ILE:HG22	1.91	0.53
55:DA:526:A:H2'	69:DA:3655:HOH:O	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:DQ:53:ARG:HG2	44:DQ:53:ARG:HH11	1.74	0.52
10:AJ:57:VAL:HG22	10:AJ:58:ASN:H	1.73	0.52
2:BB:188:ASP:HB2	2:BB:204:ASP:OD2	2.08	0.52
1:BA:1108:G:H5''	3:BC:176:HIS:ND1	2.25	0.52
10:BJ:57:VAL:HG22	10:BJ:58:ASN:H	1.74	0.52
40:CM:82:LEU:HD11	40:CM:116:VAL:CG2	2.37	0.52
55:DA:118:A:N3	55:DA:178:G:H1'	2.24	0.52
55:DA:62:U:O4'	58:DA:3206:MPD:H31	2.09	0.52
29:DC:155:ALA:HB2	29:DC:162:VAL:HG23	1.92	0.52
1:BA:542:G:H5'	4:BD:39:GLY:HA3	1.91	0.52
5:BE:40:GLY:HA2	5:BE:45:ARG:O	2.09	0.52
31:CA:1268:A:H2'	31:CA:1269:A:O4'	2.10	0.52
1:AA:1052:G:H22	1:AA:1206:G:H1	1.56	0.52
1:AA:209:U:H4'	1:AA:210:C:OP2	2.09	0.52
2:BB:111:ILE:HD12	2:BB:152:LYS:HA	1.92	0.52
10:BJ:5:ARG:HG2	10:BJ:79:PRO:HG3	1.90	0.52
24:D3:29:GLN:HB3	61:D3:102:PEG:H32	1.91	0.52
55:DA:2255:G:H21	68:DA:3222:TRS:H12	1.73	0.52
1:BA:1239:A:H62	1:BA:1299:A:H62	1.56	0.52
31:CA:2788:C:H2'	31:CA:2789:C:C6	2.44	0.52
31:CA:528:A:H3'	31:CA:528:A:H8	1.75	0.52
46:DS:83:TYR:CE1	55:DA:1187:G:H5''	2.45	0.52
47:DT:93:ALA:HB2	55:DA:1614:A:C2	2.44	0.52
1:AA:131:A:H2'	1:AA:132:C:C6	2.45	0.52
14:AN:13:ARG:HB3	14:AN:60:GLN:HG2	1.91	0.52
29:CC:266:PHE:N	29:CC:266:PHE:CD1	2.77	0.52
37:DJ:24:VAL:HG22	37:DJ:28:LEU:HD22	1.92	0.52
1:AA:769:G:H4'	1:AA:1513:A:H4'	1.92	0.52
11:BK:25:ALA:HA	11:BK:30:THR:HG22	1.89	0.52
11:BK:67:ALA:HB2	11:BK:96:THR:HG23	1.92	0.52
23:D2:8:LYS:HE2	55:DA:2420:C:H5''	1.90	0.52
16:BP:21:VAL:HG12	16:BP:33:ILE:HD12	1.92	0.52
31:CA:1936:A:H62	31:CA:1963:U:H3	1.57	0.52
36:CH:9:VAL:HG22	36:CH:35:LYS:HD3	1.91	0.52
34:DF:36:LEU:CD2	34:DF:154:ILE:HG12	2.40	0.52
1:BA:1277:C:O2'	1:BA:1279:G:H8	1.93	0.52
3:BC:33:LEU:HD21	14:BN:93:ILE:HG12	1.91	0.52
31:CA:2291:U:H2'	31:CA:2292:U:C6	2.45	0.52
35:CG:17:VAL:HG11	35:CG:50:LEU:HD21	1.92	0.52
37:CJ:97:LYS:HE2	37:CJ:139:VAL:HG11	1.92	0.52
55:DA:2788:C:H2'	55:DA:2789:C:C6	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:DD:167:ASN:HD21	62:DA:3201:EDO:H11	1.73	0.52
2:AB:111:ILE:HD12	2:AB:152:LYS:HA	1.92	0.52
11:AK:23:ILE:HD11	11:AK:86:VAL:HG13	1.90	0.52
1:BA:209:U:H4'	1:BA:210:C:OP2	2.10	0.52
9:BI:79:ILE:HG22	9:BI:83:ILE:HD11	1.91	0.52
23:C2:6:ARG:HG2	23:C2:24:THR:HB	1.90	0.52
29:CC:50:THR:O	31:CA:1805:A:H1'	2.10	0.52
31:CA:566:U:O4	46:CS:80:ARG:HD3	2.09	0.52
34:DF:122:PHE:CE1	34:DF:128:TYR:HB2	2.45	0.52
34:DF:131:GLY:HA3	55:DA:2305:U:H5''	1.92	0.52
5:AE:106:ILE:HD11	5:AE:124:LEU:HD23	1.91	0.51
1:BA:131:A:H2'	1:BA:132:C:C6	2.46	0.51
22:D1:26:THR:HG23	55:DA:2887[B]:A:H2	1.75	0.51
9:BI:7:TYR:HE1	9:BI:18:ARG:HB2	1.75	0.51
19:BS:6:LYS:HD2	19:BS:7:LYS:H	1.76	0.51
31:CA:781:A:H2'	31:CA:1777:U:O2'	2.10	0.51
53:CZ:56:LEU:HA	53:CZ:59:GLU:HG2	1.92	0.51
35:DG:17:VAL:HG11	35:DG:50:LEU:HD21	1.92	0.51
29:CC:50:THR:HB	31:CA:1805:A:N3	2.25	0.51
35:DG:86:LYS:HG2	35:DG:132:VAL:HG22	1.92	0.51
44:DQ:29:LYS:HB3	44:DQ:40:LEU:HD13	1.92	0.51
5:AE:77:ASN:HB2	5:AE:82:GLN:NE2	2.26	0.51
31:CA:2095:A:H8	31:CA:2095:A:H5''	1.74	0.51
39:DL:113:MET:SD	39:DL:116:ILE:HD11	2.51	0.51
53:DZ:56:LEU:HA	53:DZ:59:GLU:HG2	1.93	0.51
9:AI:9:THR:O	9:AI:85:ARG:HD2	2.11	0.51
16:AP:4:ILE:HG12	16:AP:21:VAL:HG22	1.92	0.51
18:AR:22:ASP:OD2	18:AR:24:LYS:HB2	2.10	0.51
1:BA:532:A:H61	3:BC:193:TYR:HD2	1.58	0.51
13:BM:90:ARG:HH21	13:BM:95:LEU:HB3	1.76	0.51
31:CA:1141:U:H4'	31:CA:1142:A:O4'	2.11	0.51
31:CA:1931:U:H2'	31:CA:1932:A:H8	1.76	0.51
29:CC:210:ALA:HA	29:CC:213:TRP:CE2	2.45	0.51
5:AE:90:THR:HG22	5:AE:91:GLY:N	2.24	0.51
1:BA:845:A:H8	1:BA:845:A:O5'	1.94	0.51
5:BE:90:THR:HG22	5:BE:91:GLY:N	2.26	0.51
39:CL:21:CYS:HB2	39:CL:39:ILE:HD12	1.93	0.51
55:DA:207:A:H2'	55:DA:208:C:O4'	2.11	0.51
6:AF:40:GLU:OE2	6:AF:99:ALA:HA	2.11	0.51
19:AS:11:ILE:HD12	19:AS:38:SER:HB3	1.93	0.51
1:BA:404:G:N7	4:BD:2:ALA:HB3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BE:74:VAL:HG11	5:BE:144:LEU:HB3	1.93	0.51
16:BP:4:ILE:HG12	16:BP:21:VAL:HG22	1.93	0.51
34:CF:106:ILE:HD12	34:CF:139:PRO:HG2	1.93	0.51
13:BM:16:VAL:HG13	13:BM:34:LEU:HD12	1.92	0.51
31:CA:206:U:H2'	31:CA:207:A:H8	1.74	0.51
31:CA:278:A:N3	31:CA:278:A:H2'	2.26	0.51
37:CJ:24:VAL:HG22	37:CJ:28:LEU:HD22	1.93	0.51
36:DH:9:VAL:HG22	36:DH:35:LYS:HD3	1.93	0.51
1:AA:1277:C:O2'	1:AA:1279:G:H8	1.93	0.51
33:CE:149:ILE:HG12	33:CE:188:MET:HG2	1.92	0.51
55:DA:2603:G:H5'	69:DA:7522:HOH:O	2.11	0.51
55:DA:278:A:H2'	55:DA:278:A:N3	2.25	0.51
16:AP:21:VAL:HG12	16:AP:33:ILE:HD12	1.92	0.50
46:CS:49:ILE:HD12	46:CS:52:PRO:HA	1.93	0.50
55:DA:493:G:H2'	55:DA:494:G:O4'	2.11	0.50
37:DJ:97:LYS:HE2	37:DJ:139:VAL:HG11	1.93	0.50
45:DR:79:PHE:CZ	45:DR:83:LEU:HD11	2.46	0.50
51:DX:21:LEU:HD11	51:DX:41[A]:ARG:HE	1.75	0.50
11:AK:67:ALA:HB2	11:AK:96:THR:HG23	1.91	0.50
18:AR:45:THR:OG1	18:AR:47:THR:HG23	2.12	0.50
19:BS:11:ILE:HD12	19:BS:38:SER:HB3	1.93	0.50
26:C5:4:ARG:HB2	31:CA:2466:C:OP1	2.11	0.50
25:D4:9:GLY:O	25:D4:13:ARG:HD2	2.12	0.50
34:DF:36:LEU:HD23	34:DF:154:ILE:HG12	1.92	0.50
54:DI:12:VAL:HG13	54:DI:63:ALA:HB2	1.94	0.50
54:DI:69:PHE:CZ	54:DI:84:TYR:HE1	2.29	0.50
1:AA:33:A:H2'	1:AA:34:C:C6	2.46	0.50
1:BA:1052:G:H22	1:BA:1206:G:H1	1.59	0.50
1:BA:33:A:H2'	1:BA:34:C:C6	2.46	0.50
7:BG:72:THR:HG22	7:BG:96:ARG:HH12	1.76	0.50
18:BR:22:ASP:OD2	18:BR:24:LYS:HB2	2.12	0.50
55:DA:2228:G:H2'	55:DA:2229:U:C6	2.46	0.50
55:DA:307:G:N2	55:DA:309:A:H3'	2.27	0.50
55:DA:677:A:OP1	64:DA:3226:SPD:H41	2.11	0.50
9:BI:9:THR:O	9:BI:85:ARG:HD2	2.12	0.50
46:CS:71:LYS:HG2	46:CS:73:LYS:HE3	1.93	0.50
29:DC:50:THR:HB	55:DA:1805:A:N3	2.27	0.50
45:DR:20:GLN:HG3	57:DR:202:PG4:C4	2.41	0.50
17:BQ:28:PHE:HD2	17:BQ:37:PHE:HB3	1.76	0.50
35:CG:86:LYS:HG2	35:CG:132:VAL:HG22	1.94	0.50
55:DA:2799:A:O2'	55:DA:2800:A:H5''	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:DC:231:PRO:C	29:DC:233:GLY:H	2.15	0.50
1:BA:82:G:H1	1:BA:84:U:H5	1.60	0.50
3:BC:23:PHE:CD2	10:BJ:97:ASP:HB2	2.47	0.50
54:DI:126:LEU:HA	54:DI:129:LEU:HD12	1.94	0.50
1:BA:202:G:O2'	1:BA:468:A:H8	1.95	0.50
5:BE:24:THR:HA	5:BE:29:ARG:HA	1.94	0.50
34:CF:132:VAL:HG22	34:CF:152:LEU:HG	1.93	0.50
51:DX:39:ARG:HD3	69:DX:117:HOH:O	2.11	0.50
6:AF:93:LYS:H	6:AF:93:LYS:HE2	1.76	0.50
31:CA:2036:C:H2'	31:CA:2037:A:C8	2.46	0.50
55:DA:45:G:H5''	55:DA:46:G:H5'	1.94	0.50
55:DA:551:G:C8	55:DA:551:G:H5''	2.47	0.50
1:AA:404:G:N7	4:AD:2:ALA:HB3	2.27	0.50
17:BQ:8:LEU:HD13	17:BQ:73:TRP:HH2	1.74	0.50
31:CA:1405:U:H2'	31:CA:1406:U:C6	2.46	0.50
31:CA:674:G:H2'	31:CA:804:A:H61	1.77	0.50
30:CD:4:LEU:HD22	30:CD:101:PHE:CE2	2.46	0.50
5:AE:106:ILE:HG13	5:AE:124:LEU:HA	1.92	0.49
12:AL:79:VAL:HG12	12:AL:102:LEU:HD23	1.94	0.49
10:BJ:80:THR:HG22	10:BJ:82:LYS:H	1.77	0.49
39:DL:21:CYS:HB2	39:DL:39:ILE:HD12	1.93	0.49
43:DP:64:TYR:HB3	43:DP:67:ASN:HD22	1.77	0.49
9:AI:7:TYR:HE1	9:AI:18:ARG:HB2	1.75	0.49
1:AA:1328:C:H5''	13:AM:28:THR:HG21	1.94	0.49
5:BE:77:ASN:HB2	5:BE:82:GLN:NE2	2.27	0.49
31:CA:1955:U:H5'	31:CA:2551:C:O2'	2.13	0.49
55:DA:639:U:H2'	55:DA:640:C:C6	2.47	0.49
29:CC:76:ALA:HB2	29:CC:96:TYR:CD1	2.48	0.49
44:DQ:52:ASN:O	55:DA:2845:U:H5''	2.12	0.49
1:AA:1305:G:H21	1:AA:1332:A:H2	1.60	0.49
1:AA:6:G:H1	5:AE:103:THR:HG21	1.78	0.49
13:AM:90:ARG:HH21	13:AM:95:LEU:HB3	1.76	0.49
31:CA:639:U:H2'	31:CA:640:C:C6	2.47	0.49
34:CF:61:SER:HB2	34:CF:91:LEU:HD21	1.95	0.49
43:CP:64:TYR:HB3	43:CP:67:ASN:HD22	1.77	0.49
23:D2:10:LYS:HE3	23:D2:53:LYS:O	2.13	0.49
29:DC:50:THR:O	55:DA:1805:A:H1'	2.12	0.49
1:AA:47:C:H2'	69:AA:2148:HOH:O	2.13	0.49
3:AC:40:ARG:HG2	3:AC:55:ILE:HG21	1.94	0.49
30:CD:155:VAL:HG21	31:CA:2618:G:H21	1.78	0.49
22:C1:38:HIS:HE1	31:CA:2884:U:O4	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:357:C:H2'	31:CA:358:U:C6	2.48	0.49
34:DF:14:LYS:O	34:DF:18:THR:HG22	2.12	0.49
14:AN:42:TRP:HD1	14:AN:44:ALA:H	1.59	0.49
31:CA:1324:G:H1'	31:CA:1616:A:N6	2.27	0.49
32:DD:84:LEU:HD22	32:DD:88:GLU:HB3	1.94	0.49
49:DV:42:VAL:O	49:DV:60:GLU:HA	2.13	0.49
3:BC:70:THR:HG21	3:BC:76:VAL:HG21	1.95	0.49
16:BP:6:LEU:HB3	16:BP:17:TYR:HB3	1.94	0.49
17:BQ:14:SER:HB3	17:BQ:22:VAL:CG1	2.42	0.49
18:BR:45:THR:OG1	18:BR:47:THR:HG23	2.11	0.49
33:CE:40:ARG:HH21	33:CE:92:HIS:CE1	2.30	0.49
55:DA:1386:C:H2'	55:DA:1387:A:C8	2.47	0.49
5:AE:115:LEU:HD13	5:AE:123:VAL:HG21	1.94	0.49
31:CA:1556:C:H2'	31:CA:1557:C:C6	2.48	0.49
31:CA:45:G:H5''	31:CA:46:G:H5'	1.94	0.49
28:CB:55:U:H1'	34:CF:26:MET:HG3	1.95	0.49
55:DA:2609:U:C5	62:DA:3197:EDO:H12	2.48	0.49
1:AA:202:G:O2'	1:AA:468:A:H8	1.96	0.49
1:AA:137:U:H3	1:AA:226:G:H1	1.61	0.49
9:AI:19:VAL:HG11	9:AI:83:ILE:HA	1.95	0.49
10:AJ:80:THR:HG22	10:AJ:82:LYS:H	1.76	0.49
1:BA:769:G:H4'	1:BA:1513:A:H4'	1.93	0.49
23:C2:35:GLU:HG2	23:C2:50:LYS:HG2	1.95	0.49
47:CT:84:ARG:HB2	47:CT:96:ILE:HB	1.95	0.49
34:DF:61:SER:HB2	34:DF:91:LEU:HD21	1.95	0.49
43:DP:27:VAL:HG21	43:DP:40:ILE:HD12	1.95	0.49
3:AC:70:THR:HG21	3:AC:76:VAL:HG21	1.95	0.49
8:AH:77:ARG:HD2	8:AH:79:SER:O	2.13	0.49
29:CC:208:ALA:CB	31:CA:1790:C:H4'	2.42	0.49
45:DR:22:LYS:HE3	55:DA:20:C:OP1	2.13	0.49
55:DA:2491:U:HO2'	55:DA:2492:U:H5	1.61	0.49
34:DF:106:ILE:HD12	34:DF:139:PRO:HG2	1.94	0.49
1:BA:607:A:H2'	1:BA:608:A:C8	2.48	0.48
3:BC:7:PRO:HD2	3:BC:184:TYR:CD1	2.48	0.48
31:CA:12:U:O2	31:CA:12:U:H2'	2.13	0.48
31:CA:1638:C:H4'	31:CA:2710:C:O2	2.13	0.48
33:CE:108:ILE:HG22	40:CM:1:MET:SD	2.52	0.48
55:DA:357:C:H2'	55:DA:358:U:C6	2.48	0.48
39:DL:113:MET:CE	39:DL:116:ILE:HD11	2.43	0.48
1:AA:1228:C:H2'	1:AA:1229:A:C8	2.48	0.48
7:BG:47:LEU:HD22	7:BG:58:GLU:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C5:16:ILE:HD13	26:C5:25:VAL:HG22	1.95	0.48
31:CA:729:G:H2'	31:CA:1775:U:H1'	1.94	0.48
29:CC:220:VAL:HG21	31:CA:782:A:N7	2.28	0.48
39:DL:26:GLY:HA3	39:DL:30:ARG:HH11	1.78	0.48
11:AK:16:VAL:HG23	11:AK:79:ILE:HG13	1.95	0.48
1:BA:1273:C:H2'	1:BA:1274:A:O4'	2.14	0.48
31:CA:2262:U:H1'	31:CA:2328:A:H1'	1.96	0.48
31:CA:2799:A:O2'	31:CA:2800:A:H5''	2.13	0.48
55:DA:2063:C:O2	55:DA:2450:A:N1	2.47	0.48
55:DA:933:A:H5'	55:DA:934:U:OP2	2.13	0.48
36:DH:97:ARG:HG3	36:DH:112:LYS:HG3	1.96	0.48
1:BA:1328:C:H5''	13:BM:28:THR:HG21	1.96	0.48
31:CA:1709:U:H2'	31:CA:1710:G:C8	2.49	0.48
45:CR:90:ILE:HG22	45:CR:95:LEU:HG	1.96	0.48
55:DA:1515:A:H2'	55:DA:1516:G:O4'	2.13	0.48
55:DA:543:G:H5''	55:DA:543:G:H8	1.78	0.48
1:AA:1464:U:P	44:DQ:109:ARG:HH12	2.36	0.48
29:CC:158:ALA:O	29:CC:196:GLY:O	2.31	0.48
34:CF:44:ILE:HG21	34:CF:79:ILE:HG22	1.95	0.48
43:CP:27:VAL:HG21	43:CP:40:ILE:HD12	1.96	0.48
45:CR:79:PHE:CZ	45:CR:83:LEU:HD11	2.48	0.48
34:DF:34:ILE:HG12	34:DF:156:ILE:HG12	1.95	0.48
54:DI:69:PHE:HB3	54:DI:72:LEU:HD12	1.94	0.48
1:AA:1376:U:H2'	1:AA:1377:A:C8	2.49	0.48
31:CA:2019:A:H4'	45:CR:34:VAL:HG21	1.96	0.48
31:CA:528:A:H3'	31:CA:528:A:C8	2.48	0.48
23:D2:35:GLU:HG2	23:D2:50:LYS:HG2	1.96	0.48
26:D5:16:ILE:HD13	26:D5:25:VAL:HG22	1.95	0.48
37:DJ:30:GLN:HE22	55:DA:1095:A:H61	1.61	0.48
55:DA:1738:G:O2'	55:DA:1739:A:C8	2.65	0.48
55:DA:2547:A:H2'	55:DA:2548:U:C6	2.49	0.48
16:AP:6:LEU:HB3	16:AP:17:TYR:HB3	1.96	0.48
5:BE:72:ILE:HG13	5:BE:73:ASN:N	2.28	0.48
9:BI:19:VAL:HG11	9:BI:83:ILE:HA	1.94	0.48
14:BN:28:LYS:HA	14:BN:31:ILE:HG22	1.94	0.48
39:CL:26:GLY:HA3	39:CL:30:ARG:HH11	1.77	0.48
49:CV:42:VAL:O	49:CV:60:GLU:HA	2.13	0.48
32:DD:150[A]:MEQ:HE3	55:DA:2032:G:C8	2.49	0.48
45:DR:40:ILE:HG12	58:DS:203:MPD:H31	1.96	0.48
9:AI:19:VAL:HG22	9:AI:65:ILE:HG22	1.96	0.48
1:BA:1228:C:H2'	1:BA:1229:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1376:U:H2'	1:BA:1377:A:C8	2.49	0.48
11:BK:45:ALA:HB3	11:BK:70:CYS:HB2	1.95	0.48
31:CA:1386:C:H2'	31:CA:1387:A:C8	2.49	0.48
31:CA:136:G:H1	31:CA:143:C:H42	1.62	0.48
22:D1:4:GLN:HA	55:DA:2615:U:C2	2.49	0.48
11:BK:36:ASP:OD1	11:BK:38:GLN:HG2	2.14	0.48
29:DC:160:THR:HG21	55:DA:1819:A:H5''	1.96	0.48
55:DA:2117:A:H61	55:DA:2171:A:H61	1.61	0.48
1:AA:1001:C:H2'	1:AA:1002:G:H8	1.79	0.48
1:AA:1329:A:H5''	13:AM:26:GLY:H	1.79	0.48
31:CA:2815:C:H2'	31:CA:2816:G:O4'	2.14	0.48
29:CC:231:PRO:C	29:CC:233:GLY:H	2.16	0.48
36:CH:94:ILE:HB	36:CH:122:LEU:HB2	1.95	0.48
41:DN:3:GLN:HG3	41:DN:92:TRP:CD1	2.49	0.48
1:AA:607:A:H2'	1:AA:608:A:C8	2.48	0.47
1:BA:1305:G:H21	1:BA:1332:A:H2	1.60	0.47
22:C1:15:MET:HB3	31:CA:2045:C:O3'	2.14	0.47
38:CK:81:ILE:CG2	38:CK:82:GLY:N	2.76	0.47
22:D1:9:THR:HG22	55:DA:2020:A:H5'	1.95	0.47
55:DA:136:G:H1	55:DA:143:C:H42	1.62	0.47
55:DA:455:C:N3	55:DA:472:A:H2'	2.29	0.47
40:DM:78:ARG:HD3	69:DM:330:HOH:O	2.14	0.47
46:DS:73:LYS:HE2	58:DS:203:MPD:C5	2.38	0.47
1:AA:1273:C:H2'	1:AA:1274:A:O4'	2.14	0.47
7:AG:12:ILE:HD11	7:AG:25:LYS:HG3	1.95	0.47
1:BA:532:A:N1	3:BC:193:TYR:HB3	2.29	0.47
12:BL:79:VAL:HG12	12:BL:102:LEU:HD23	1.95	0.47
17:BQ:19:LYS:HG2	17:BQ:49:GLU:HA	1.96	0.47
41:CN:3:GLN:HG3	41:CN:92:TRP:CD1	2.49	0.47
54:DI:132:TYR:N	54:DI:133:GLU:HB2	2.28	0.47
1:AA:1108:G:H5''	3:AC:176:HIS:HD1	1.79	0.47
1:BA:1092:A:H2'	1:BA:1093:A:C8	2.49	0.47
1:BA:545:C:H5'	4:BD:69:GLU:HB2	1.96	0.47
31:CA:1156:A:H5''	69:CA:3355:HOH:O	2.13	0.47
31:CA:747:5MU:O2	31:CA:2014:A:H1'	2.14	0.47
52:CY:12:PRO:HB3	52:CY:30:LEU:HD23	1.96	0.47
48:DU:80:TRP:HB3	63:DU:101:PGE:H32	1.95	0.47
10:AJ:26:VAL:HG21	10:AJ:39:PRO:HD3	1.96	0.47
31:CA:569:U:H5''	31:CA:821:A:C2	2.49	0.47
34:DF:77:PHE:HE2	55:DA:2310:C:H2'	1.79	0.47
55:DA:2324:U:H3'	55:DA:2325:G:H5''	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:845:A:H2'	1:AA:846:G:O4'	2.14	0.47
2:AB:31:ILE:HG21	2:AB:39:HIS:HD2	1.79	0.47
9:AI:88:MET:SD	9:AI:95:ARG:HG2	2.55	0.47
12:AL:110:ARG:NH2	12:AL:117:TYR:CE2	2.82	0.47
1:BA:32:A:H2'	1:BA:33:A:C8	2.49	0.47
2:BB:120:GLN:HE22	2:BB:137:ARG:HE	1.62	0.47
9:BI:19:VAL:HG22	9:BI:65:ILE:HG22	1.95	0.47
22:C1:9:THR:CG2	31:CA:2020:A:H5'	2.45	0.47
31:CA:1999:C:H1'	31:CA:2687:U:H1'	1.96	0.47
31:CA:792:A:H1'	31:CA:2072:C:O2'	2.14	0.47
55:DA:1384:A:H1'	55:DA:1405:U:H1'	1.97	0.47
36:DH:94:ILE:HB	36:DH:122:LEU:HB2	1.95	0.47
3:BC:23:PHE:HD1	10:BJ:13:PHE:CZ	2.33	0.47
12:BL:110:ARG:NH2	12:BL:117:TYR:CE2	2.82	0.47
23:C2:33:LYS:HA	23:C2:52:ALA:HB3	1.94	0.47
31:CA:2026:U:H2'	31:CA:2027:G:O4'	2.14	0.47
31:CA:2821:A:H2'	31:CA:2822:G:O4'	2.14	0.47
31:CA:974:G:H8	31:CA:990:A:H62	1.63	0.47
39:CL:35:VAL:HG22	39:CL:69:VAL:HG12	1.97	0.47
27:D0:26:GLY:O	55:DA:929:U:H1'	2.13	0.47
37:DJ:55:ILE:HD12	37:DJ:74:PRO:HD3	1.97	0.47
7:AG:47:LEU:HD22	7:AG:58:GLU:HG2	1.96	0.47
3:BC:47:LEU:HD22	3:BC:76:VAL:HG22	1.96	0.47
31:CA:457:A:N1	31:CA:470:A:H5''	2.30	0.47
44:CQ:53:ARG:HH11	44:CQ:53:ARG:HG2	1.79	0.47
45:CR:112:LYS:HD2	46:CS:48:LYS:HG3	1.95	0.47
55:DA:1297:C:OP1	55:DA:2710:C:H4'	2.14	0.47
55:DA:137:U:H3	55:DA:142:A:H61	1.63	0.47
22:D1:24:ALA:HB2	47:DT:23:LEU:HD22	1.96	0.47
18:BR:23:TYR:HE1	18:BR:65:LEU:CD1	2.28	0.47
29:CC:43:ARG:NH2	31:CA:779:U:H5''	2.29	0.47
31:CA:797:G:H5''	33:CE:55:SER:HB2	1.95	0.47
55:DA:2520:C:C6	55:DA:2567:G:H1'	2.49	0.47
54:DI:64:VAL:HG22	54:DI:69:PHE:HB2	1.96	0.47
12:AL:4:VAL:HG13	17:AQ:34:TYR:HB3	1.97	0.47
5:BE:81:LEU:HB3	5:BE:147:MET:SD	2.55	0.47
7:BG:12:ILE:HD11	7:BG:25:LYS:HG3	1.95	0.47
31:CA:2845:U:H5''	44:CQ:52:ASN:O	2.14	0.47
36:CH:97:ARG:HG3	36:CH:112:LYS:HG3	1.96	0.47
1:AA:79:G:H22	1:AA:90:C:H42	1.62	0.47
5:BE:81:LEU:HB2	5:BE:98:PRO:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:240:PHE:HD2	29:CC:242:LYS:H	1.60	0.47
55:DA:2233:U:H2'	55:DA:2234:G:C8	2.50	0.47
41:DN:16:ARG:HG3	41:DN:18[B]:ARG:HH11	1.79	0.47
43:DP:103:VAL:HG23	69:DB:317:HOH:O	2.14	0.47
1:AA:77:A:H2'	1:AA:78:A:C8	2.49	0.47
12:AL:36:ARG:HH11	12:AL:54:ARG:HH12	1.62	0.47
1:BA:1067:A:H1'	1:BA:1068:G:C8	2.49	0.47
1:BA:9:G:OP2	5:BE:126:LYS:HE2	2.15	0.47
31:CA:2688:G:H1'	31:CA:2721:A:N6	2.30	0.47
31:CA:933:A:H5'	31:CA:934:U:OP2	2.15	0.47
29:CC:53:HIS:HA	29:CC:217:ARG:HB2	1.96	0.47
48:CU:45:ALA:O	48:CU:49:LYS:HG2	2.15	0.47
29:DC:156:ARG:NH2	55:DA:1818:U:C5	2.83	0.47
1:AA:545:C:H5'	4:AD:69:GLU:HB2	1.96	0.46
3:AC:47:LEU:HD22	3:AC:76:VAL:HG22	1.97	0.46
33:CE:76:PRO:HA	33:CE:82:GLY:HA2	1.96	0.46
52:CY:2:SER:HB2	52:CY:4:VAL:HG23	1.97	0.46
1:BA:1001:C:H2'	1:BA:1002:G:H8	1.79	0.46
9:BI:28:ILE:HG21	9:BI:35:LEU:HD13	1.96	0.46
31:CA:2869:G:H2'	31:CA:2870:C:O4'	2.15	0.46
26:D5:36:ARG:HH22	55:DA:2539:C:H4'	1.81	0.46
55:DA:1168:G:H2'	55:DA:1169:A:O4'	2.15	0.46
55:DA:1433:A:O2'	55:DA:1434:A:H5'	2.16	0.46
32:DD:140:HIS:HB3	69:DD:470:HOH:O	2.16	0.46
38:DK:140:LEU:HD11	38:DK:142:ILE:HD13	1.97	0.46
52:DY:12:PRO:HB3	52:DY:30:LEU:HD23	1.97	0.46
1:BA:1348:U:H2'	1:BA:1349:A:H8	1.80	0.46
31:CA:551:G:C8	31:CA:551:G:H5''	2.49	0.46
22:D1:5:GLN:O	55:DA:2017:U:H4'	2.16	0.46
46:DS:86:GLN:HG2	69:DA:6211:HOH:O	2.14	0.46
14:AN:21:PHE:HA	14:AN:25:ALA:HB3	1.97	0.46
5:BE:114:VAL:HG21	5:BE:141:ILE:HG13	1.98	0.46
1:BA:562:U:H1'	12:BL:12:ARG:HD2	1.97	0.46
31:CA:2543:G:H2'	31:CA:2544:G:C8	2.51	0.46
36:CH:51:ARG:O	36:CH:55:GLU:HB2	2.15	0.46
55:DA:1171:G:N2	55:DA:1172:C:N4	2.63	0.46
55:DA:1802:A:N1	55:DA:1822:C:H1'	2.30	0.46
55:DA:2339:C:H2'	55:DA:2340:A:C8	2.51	0.46
29:DC:97:LYS:HD3	29:DC:97:LYS:HA	1.79	0.46
1:AA:1347:G:N2	1:AA:1373:G:H2'	2.31	0.46
20:AT:43:ASP:HB3	20:AT:46:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BM:22:ILE:HB	13:BM:25:VAL:CG1	2.45	0.46
31:CA:2817:U:O2	31:CA:2836:U:H1'	2.15	0.46
31:CA:969:G:H2'	31:CA:970:U:C6	2.51	0.46
55:DA:2728:U:O2'	55:DA:2729:G:H5''	2.16	0.46
43:DP:31:THR:HG21	28:DB:28:C:P	2.55	0.46
45:DR:90:ILE:HG22	45:DR:95:LEU:HG	1.96	0.46
10:AJ:21:ALA:HB1	10:AJ:92:LEU:HD22	1.97	0.46
10:AJ:35:GLN:HB2	10:AJ:77:VAL:HB	1.98	0.46
20:AT:9:LYS:HA	20:AT:12:ILE:HD12	1.97	0.46
1:BA:137:U:H3	1:BA:226:G:H1	1.62	0.46
31:CA:2339:C:H2'	31:CA:2340:A:C8	2.50	0.46
22:C1:4:GLN:HA	31:CA:2615:U:C2	2.50	0.46
31:CA:571:U:H5''	69:CA:3849:HOH:O	2.15	0.46
1:AA:6:G:H22	5:AE:103:THR:CG2	2.29	0.46
1:BA:1329:A:H5''	13:BM:26:GLY:H	1.80	0.46
4:BD:58:LYS:HA	4:BD:200:ILE:HG12	1.98	0.46
14:BN:21:PHE:HA	14:BN:25:ALA:HB3	1.97	0.46
12:BL:4:VAL:HG23	17:BQ:34:TYR:HB3	1.98	0.46
31:CA:1028:A:N6	31:CA:1125:G:H2'	2.31	0.46
31:CA:1494:A:H2'	31:CA:1495:A:C8	2.51	0.46
55:DA:191:A:H2'	55:DA:192:C:C6	2.51	0.46
55:DA:265:A:H4'	55:DA:266:G:OP1	2.16	0.46
32:DD:152:PRO:HG3	32:DD:156:PHE:CZ	2.51	0.46
34:DF:44:ILE:HG21	34:DF:79:ILE:HG22	1.98	0.46
47:DT:84:ARG:HB2	47:DT:96:ILE:HB	1.98	0.46
52:DY:3:ARG:HD2	52:DY:30:LEU:HD22	1.98	0.46
1:BA:1305:G:N2	1:BA:1331:G:H1'	2.31	0.46
31:CA:1974:C:H3'	69:CA:3240:HOH:O	2.16	0.46
31:CA:1662:U:O2'	31:CA:2687:U:H5''	2.15	0.46
31:CA:543:G:H8	31:CA:543:G:H5''	1.80	0.46
36:CH:37:VAL:HG22	36:CH:38:PRO:HD2	1.98	0.46
28:CB:28:C:P	43:CP:31:THR:HG21	2.56	0.46
50:CW:42:LEU:HD13	50:CW:47:VAL:HG21	1.97	0.46
55:DA:1093:G:H1'	55:DA:1099:G:N2	2.30	0.46
36:DH:37:VAL:HG22	36:DH:38:PRO:HD2	1.98	0.46
43:DP:35:ILE:HG21	43:DP:71:ALA:HA	1.98	0.46
50:DW:42:LEU:HD13	50:DW:47:VAL:HG21	1.97	0.46
1:AA:1305:G:N2	1:AA:1331:G:H1'	2.31	0.46
1:BA:9:G:H5'	5:BE:108:GLY:HA3	1.97	0.46
2:BB:31:ILE:HG21	2:BB:39:HIS:CD2	2.50	0.46
30:CD:101:PHE:O	30:CD:104:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:DL:105:ARG:HG3	39:DL:122:VAL:CG1	2.46	0.46
46:DS:44:GLY:O	46:DS:45:GLU:HG2	2.15	0.46
52:DY:2:SER:HB2	52:DY:4:VAL:HG23	1.98	0.46
2:AB:120:GLN:HE22	2:AB:137:ARG:HE	1.61	0.46
1:BA:690:G:H2'	1:BA:691:G:O4'	2.16	0.46
34:CF:34:ILE:HG12	34:CF:156:ILE:HG12	1.98	0.46
34:DF:36:LEU:HD21	34:DF:99:PHE:CZ	2.51	0.46
44:DQ:31:TRP:CD1	57:DQ:202:PG4:H31	2.51	0.46
51:DX:41[B]:ARG:HA	51:DX:41[B]:ARG:HD3	1.63	0.46
1:BA:77:A:H2'	1:BA:78:A:C8	2.51	0.45
2:BB:20:THR:HA	2:BB:39:HIS:CE1	2.51	0.45
9:BI:88:MET:SD	9:BI:95:ARG:HG2	2.56	0.45
31:CA:2425:A:H4'	31:CA:2426:A:O5'	2.16	0.45
31:CA:845:A:H61	31:CA:932:U:H3	1.63	0.45
43:CP:35:ILE:HG21	43:CP:71:ALA:HA	1.98	0.45
55:DA:1168:G:H5''	55:DA:1168:G:H8	1.81	0.45
55:DA:2133:G:H21	55:DA:2158:A:N6	2.14	0.45
48:DU:2:ILE:HG21	48:DU:45:ALA:CB	2.45	0.45
49:DV:14:LEU:HD21	49:DV:71:ALA:HB2	1.98	0.45
3:AC:91:VAL:HG21	3:AC:101:ILE:HD11	1.99	0.45
9:AI:28:ILE:HG21	9:AI:35:LEU:HD13	1.97	0.45
19:AS:52:HIS:CD2	19:AS:54:GLY:H	2.30	0.45
23:C2:15:ALA:HB2	23:C2:47:VAL:HG21	1.98	0.45
26:C5:30:GLU:HG3	26:C5:32:LYS:HB2	1.98	0.45
31:CA:1509:A:O2'	31:CA:1510:G:H8	1.99	0.45
22:D1:23:THR:HG22	63:D1:102:PGE:H62	1.98	0.45
55:DA:1794:A:H2'	55:DA:1795:C:C6	2.51	0.45
55:DA:2033:A:H5'	69:DA:3393:HOH:O	2.15	0.45
55:DA:2609:U:H5	62:DA:3197:EDO:H12	1.82	0.45
55:DA:2887[B]:A:O2'	55:DA:2888[B]:C:H5'	2.16	0.45
54:DI:23:LEU:HD13	54:DI:89:PRO:HD3	1.98	0.45
37:DJ:103:ARG:HA	37:DJ:106:LEU:HD12	1.98	0.45
50:DW:51:GLN:HB2	50:DW:57:TYR:OH	2.16	0.45
1:AA:1239:A:H62	1:AA:1299:A:N6	2.14	0.45
2:AB:31:ILE:HG21	2:AB:39:HIS:CD2	2.51	0.45
3:AC:77:ILE:HA	3:AC:84:VAL:HG22	1.98	0.45
1:BA:1347:G:N2	1:BA:1373:G:H2'	2.31	0.45
31:CA:1430:G:H2'	31:CA:1431:A:O4'	2.16	0.45
31:CA:1510:G:H2'	31:CA:1511:G:O4'	2.16	0.45
29:CC:171:TYR:CD1	29:CC:185:GLU:HA	2.51	0.45
38:CK:140:LEU:HD11	38:CK:142:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:CL:121:GLU:HG2	39:CL:122:VAL:HG23	1.97	0.45
22:D1:22:LEU:HD23	61:D1:103:PEG:H31	1.98	0.45
35:DG:4:VAL:HA	58:DA:3209:MPD:H13	1.99	0.45
54:DI:25:ALA:HA	54:DI:83:ALA:O	2.16	0.45
44:DQ:94:LYS:CE	55:DA:1754:A:C8	3.00	0.45
45:DR:6:ARG:HD3	55:DA:1250:G:C5'	2.46	0.45
11:AK:84:VAL:HG21	11:AK:97:ILE:HG23	1.99	0.45
3:BC:91:VAL:HG21	3:BC:101:ILE:HD11	1.97	0.45
17:BQ:16:LYS:HA	17:BQ:16:LYS:HD2	1.84	0.45
55:DA:2123:G:H2'	55:DA:2124:G:H8	1.81	0.45
55:DA:417:C:H2'	55:DA:418:C:H6	1.81	0.45
32:DD:169:ARG:HG2	55:DA:2773:C:H5''	1.98	0.45
54:DI:50:VAL:HG22	54:DI:85:VAL:HG13	1.99	0.45
1:AA:1348:U:H2'	1:AA:1349:A:H8	1.82	0.45
1:BA:972:C:H4'	10:BJ:59:LYS:HG2	1.98	0.45
11:BK:28:ASN:O	11:BK:57:LYS:HE3	2.16	0.45
11:BK:58:SER:O	11:BK:91:PRO:HG3	2.16	0.45
34:DF:85:ILE:HD11	55:DA:2311:A:C2	2.52	0.45
1:AA:1386:G:H2'	1:AA:1387:G:H8	1.80	0.45
1:AA:562:U:H1'	12:AL:12:ARG:HD2	1.98	0.45
13:AM:31:LYS:HA	13:AM:41:GLU:OE2	2.17	0.45
14:AN:13:ARG:HD3	14:AN:59:ARG:O	2.17	0.45
1:BA:214:C:H2'	1:BA:215:C:H6	1.81	0.45
5:BE:72:ILE:HG13	5:BE:73:ASN:H	1.82	0.45
37:CJ:103:ARG:HA	37:CJ:106:LEU:HD12	1.98	0.45
37:CJ:55:ILE:HD12	37:CJ:74:PRO:HD3	1.98	0.45
31:CA:2642:G:H5'	38:CK:80:HIS:CG	2.51	0.45
44:CQ:114:LEU:H	44:CQ:114:LEU:HD23	1.81	0.45
55:DA:244:A:H2'	55:DA:245:G:O4'	2.17	0.45
55:DA:543:G:H5''	55:DA:543:G:C8	2.52	0.45
1:AA:690:G:H2'	1:AA:691:G:O4'	2.16	0.45
5:AE:160:SER:HB2	5:AE:161:VAL:HG22	1.98	0.45
10:AJ:42:LEU:HB2	10:AJ:71:LEU:HB3	1.97	0.45
11:AK:28:ASN:O	11:AK:57:LYS:HE3	2.17	0.45
9:BI:51:PRO:HB3	9:BI:84:THR:HG23	1.99	0.45
31:CA:2636:C:H2'	31:CA:2637:U:C6	2.52	0.45
31:CA:588:U:H2'	31:CA:589:U:C6	2.52	0.45
34:CF:36:LEU:HD12	34:CF:154:ILE:HG12	1.98	0.45
47:DT:73:LYS:HD3	65:DA:3188:1PE:H232	1.98	0.45
34:DF:158:THR:HG23	34:DF:160:ALA:H	1.82	0.45
45:DR:19:LYS:HD3	57:DR:202:PG4:H22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:673:A:H2'	1:AA:674:G:C8	2.52	0.45
5:AE:82:GLN:HG2	5:AE:149:SER:HA	1.98	0.45
1:BA:1084:G:H5'	1:BA:1102:A:OP2	2.17	0.45
1:BA:49:U:O2	1:BA:362:G:H1'	2.16	0.45
5:BE:82:GLN:HG2	5:BE:149:SER:HA	1.99	0.45
7:BG:72:THR:HG22	7:BG:96:ARG:NH1	2.32	0.45
31:CA:2183:A:H2'	31:CA:2184:A:C8	2.52	0.45
31:CA:737:C:H42	31:CA:759:G:H1	1.64	0.45
31:CA:765:C:H2'	31:CA:766:U:C6	2.52	0.45
31:CA:804:A:H2'	31:CA:806:C:C4	2.51	0.45
29:CC:31:ALA:HB3	29:CC:32:PRO:HD3	1.99	0.45
32:DD:150[B]:MEQ:HG3	55:DA:2032:G:N3	2.32	0.45
55:DA:1975:G:H21	63:DA:3227:PGE:H22	1.81	0.45
55:DA:417:C:H2'	55:DA:418:C:C6	2.52	0.45
19:AS:64:ASP:HB3	34:DF:115:ARG:HH22	1.82	0.45
50:DW:38:LEU:HD21	50:DW:65:VAL:HG11	1.98	0.45
52:DY:7:VAL:HG23	52:DY:51:VAL:HG12	1.99	0.45
1:AA:73:C:O2'	1:AA:74:A:H8	1.99	0.45
2:AB:20:THR:HA	2:AB:39:HIS:CE1	2.52	0.45
5:AE:40:GLY:HA2	5:AE:45:ARG:O	2.17	0.45
6:BF:26:THR:HG23	6:BF:36:ILE:HG21	1.99	0.45
10:BJ:42:LEU:HB2	10:BJ:71:LEU:HB3	1.99	0.45
15:BO:64:ARG:HH22	15:BO:88:ARG:NH2	2.15	0.45
31:CA:976:G:H2'	31:CA:977:G:H8	1.80	0.45
45:CR:112:LYS:HD2	46:CS:48:LYS:HE2	1.99	0.45
27:D0:10:THR:HG22	27:D0:11:ARG:HG3	1.98	0.45
55:DA:2637:U:C2'	55:DA:2638:G:H5'	2.46	0.45
55:DA:2800:A:C2	55:DA:2895:G:H1'	2.52	0.45
29:DC:31:ALA:HB3	29:DC:32:PRO:HD3	1.97	0.45
41:DN:108:VAL:HB	41:DN:112:LEU:HD23	1.99	0.45
1:AA:1322:C:P	19:AS:78:ARG:HH22	2.39	0.44
9:BI:127:PHE:CZ	9:BI:129:LYS:HD2	2.53	0.44
24:C3:2:LYS:HE2	31:CA:687:C:H5''	1.99	0.44
31:CA:2298:A:C2	31:CA:2321:U:N3	2.85	0.44
30:CD:129:THR:CG2	30:CD:140:HIS:O	2.59	0.44
31:CA:443:A:H2'	33:CE:40:ARG:NH1	2.32	0.44
55:DA:1509:A:O2'	55:DA:1510:G:H8	1.99	0.44
55:DA:2402:U:H2'	69:DA:7830:HOH:O	2.18	0.44
29:DC:207:LYS:HB2	55:DA:729:G:C6	2.52	0.44
55:DA:845[B]:A:H61	55:DA:932:U:H3	1.65	0.44
12:AL:5:ASN:O	12:AL:9:ARG:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:48:LEU:HD21	4:BD:56:ARG:HG3	1.99	0.44
31:CA:1434:A:H2'	31:CA:1435:G:C8	2.52	0.44
31:CA:2637:U:C2'	31:CA:2638:G:H5'	2.48	0.44
30:CD:152:PRO:HG3	30:CD:156:PHE:CZ	2.52	0.44
55:DA:1510:G:H2'	55:DA:1511:G:O4'	2.18	0.44
55:DA:1733:G:H2'	55:DA:1734:G:H8	1.81	0.44
55:DA:747:5MU:O2	55:DA:2014:A:H1'	2.17	0.44
33:DE:189:THR:HG22	33:DE:192:ALA:H	1.82	0.44
2:AB:12:ALA:HB1	2:AB:209:ALA:HA	1.99	0.44
17:AQ:17:MET:HG2	17:AQ:20:SER:HB2	1.98	0.44
24:C3:30:VAL:HG13	31:CA:466:A:H5''	1.98	0.44
31:CA:2327:A:H2'	31:CA:2328:A:C8	2.53	0.44
30:CD:169:ARG:HG2	31:CA:2773:C:H5''	1.98	0.44
31:CA:396:G:C1'	52:CY:29:PHE:HB3	2.47	0.44
55:DA:142:A:H2'	55:DA:143:C:C6	2.51	0.44
55:DA:588:U:H2'	55:DA:589:U:C6	2.52	0.44
55:DA:644:A:H2'	55:DA:645:C:O4'	2.17	0.44
11:AK:34:ILE:HB	11:AK:74:VAL:HG11	1.98	0.44
13:BM:22:ILE:HB	13:BM:25:VAL:HG12	2.00	0.44
29:DC:240:PHE:HD2	29:DC:242:LYS:H	1.65	0.44
31:CA:191:A:H2'	31:CA:192:C:C6	2.52	0.44
31:CA:2822:G:H2'	31:CA:2823:A:H5''	1.98	0.44
36:CH:3:VAL:HG12	36:CH:38:PRO:HA	1.99	0.44
23:D2:15:ALA:HB2	23:D2:47:VAL:HG21	1.99	0.44
48:DU:4:GLU:HG3	48:DU:49:LYS:HE2	1.98	0.44
1:AA:843:U:H1'	1:AA:845:A:C6	2.53	0.44
4:AD:73:ARG:HG3	4:AD:204:TYR:CE1	2.53	0.44
11:BK:84:VAL:HG21	11:BK:97:ILE:HG23	1.99	0.44
14:BN:6:MET:HE2	14:BN:63:ARG:HH22	1.82	0.44
3:BC:20:SER:HB3	14:BN:94:PRO:HG3	1.99	0.44
31:CA:586:A:H5'	33:CE:84:THR:HG21	1.98	0.44
35:CG:95:ARG:HG2	35:CG:128:GLN:HB3	1.99	0.44
36:CH:27:ARG:HA	36:CH:27:ARG:HD3	1.78	0.44
52:DY:61:LYS:HE2	55:DA:371:A:O2'	2.18	0.44
4:AD:58:LYS:HA	4:AD:200:ILE:HG12	1.99	0.44
6:AF:78:PHE:HD1	6:AF:84:VAL:HG21	1.82	0.44
9:AI:127:PHE:CZ	9:AI:129:LYS:HD2	2.53	0.44
4:BD:76:TYR:HE1	4:BD:201:VAL:HG13	1.82	0.44
5:BE:110:ALA:O	5:BE:114:VAL:HG12	2.18	0.44
1:BA:1322:C:P	19:BS:78:ARG:HH22	2.40	0.44
31:CA:1733:G:H2'	31:CA:1734:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:20:SER:HB3	14:AN:94:PRO:HG3	2.00	0.44
1:BA:1239:A:H62	1:BA:1299:A:N6	2.15	0.44
1:BA:532:A:N6	3:BC:192:THR:HG23	2.33	0.44
3:BC:77:ILE:HA	3:BC:84:VAL:HG22	2.00	0.44
11:BK:21:ALA:HB2	11:BK:82:LEU:HD13	2.00	0.44
12:BL:48:ALA:HB3	12:BL:50:ARG:HE	1.83	0.44
20:BT:51:PHE:HA	20:BT:54:MET:HG2	1.99	0.44
22:C1:43:ILE:CG2	42:CO:98:LEU:HB3	2.48	0.44
31:CA:861:A:H2'	31:CA:862:G:O4'	2.17	0.44
47:CT:66:ILE:HA	47:CT:69:LEU:HD22	1.98	0.44
55:DA:1172:C:C5	55:DA:1173:U:H1'	2.53	0.44
55:DA:1494:A:H2'	55:DA:1495:A:C8	2.52	0.44
55:DA:1733:G:H2'	55:DA:1734:G:C8	2.53	0.44
44:DQ:53:ARG:NH2	55:DA:2720:U:OP1	2.51	0.44
41:DN:14:LYS:HE2	69:DA:4160:HOH:O	2.17	0.44
1:AA:1108:G:H5''	3:AC:176:HIS:ND1	2.32	0.44
1:AA:1320:C:OP2	19:AS:3:ARG:HD3	2.18	0.44
2:BB:12:ALA:HB1	2:BB:209:ALA:HA	1.99	0.44
5:BE:88:VAL:HG12	5:BE:93:ARG:HG2	1.99	0.44
31:CA:142:A:H2'	31:CA:143:C:C6	2.52	0.44
31:CA:1447:C:H2'	31:CA:1448:G:C8	2.52	0.44
44:CQ:4:ILE:H	44:CQ:4:ILE:HD12	1.82	0.44
31:CA:2261:C:H5''	51:CX:19:LYS:NZ	2.33	0.44
22:D1:13:ARG:HB2	69:D1:209:HOH:O	2.17	0.44
55:DA:136:G:H1	55:DA:143:C:N4	2.16	0.44
43:DP:18:LEU:HD23	43:DP:18:LEU:HA	1.91	0.44
1:AA:845:A:O4'	1:AA:845:A:P	2.76	0.43
3:AC:138:VAL:HG13	3:AC:149:ILE:HG23	2.00	0.43
7:AG:30:LEU:HD12	7:AG:105:VAL:HG13	2.00	0.43
1:BA:23:C:H5	1:BA:561:U:O4	2.01	0.43
1:BA:815:A:H4'	1:BA:817:C:C4	2.53	0.43
1:BA:1190:G:H5'	3:BC:176:HIS:NE2	2.33	0.43
5:BE:57:PRO:O	5:BE:60:ILE:HG13	2.17	0.43
31:CA:137:U:H3	31:CA:142:A:H61	1.65	0.43
39:CL:98:ARG:HH11	39:CL:98:ARG:HG2	1.83	0.43
29:DC:156:ARG:NH2	55:DA:1818:U:H5	2.16	0.43
34:DF:88:LYS:HD3	55:DA:2313:C:H5''	2.00	0.43
55:DA:340:A:H2'	55:DA:341:C:O4'	2.18	0.43
55:DA:503:A:H5'	55:DA:505:A:OP1	2.17	0.43
35:DG:95:ARG:HG2	35:DG:128:GLN:HB3	1.99	0.43
54:DI:35:VAL:HA	54:DI:38:MET:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:DP:64:TYR:HB3	43:DP:67:ASN:ND2	2.33	0.43
1:AA:9:G:OP2	5:AE:126:LYS:HE2	2.18	0.43
9:AI:51:PRO:HB3	9:AI:84:THR:HG23	1.99	0.43
1:BA:1061:G:H5'	10:BJ:61:ALA:HB2	2.01	0.43
1:BA:1493:A:H8	1:BA:1493:A:OP2	2.01	0.43
1:BA:73:C:O2'	1:BA:74:A:H8	1.99	0.43
2:BB:164:ILE:HD13	2:BB:186:ILE:HG13	2.00	0.43
31:CA:1810:A:H2'	31:CA:1811:G:O4'	2.16	0.43
31:CA:1938:A:C6	31:CA:2590:A:H1'	2.52	0.43
33:CE:189:THR:HG22	33:CE:192:ALA:H	1.83	0.43
37:CJ:14:ALA:HB3	37:CJ:17:MET:HB2	1.99	0.43
55:DA:2097:A:H8	55:DA:2097:A:H5''	1.83	0.43
55:DA:2266:A:H4'	55:DA:2267:A:O5'	2.19	0.43
1:AA:920:U:H2'	1:AA:921:U:C6	2.54	0.43
2:AB:129:LEU:H	2:AB:129:LEU:HG	1.58	0.43
2:AB:164:ILE:HD13	2:AB:186:ILE:HG13	2.00	0.43
10:AJ:5:ARG:HE	10:AJ:77:VAL:HG22	1.83	0.43
11:AK:58:SER:O	11:AK:91:PRO:HG3	2.17	0.43
21:AU:51:SER:HA	21:AU:54:LYS:HE3	2.00	0.43
1:BA:920:U:H2'	1:BA:921:U:C6	2.52	0.43
31:CA:2747:G:O6	31:CA:2755:C:H5''	2.18	0.43
39:CL:113:MET:SD	39:CL:116:ILE:HD11	2.58	0.43
22:D1:53:LYS:HE3	22:D1:55:ILE:O	2.18	0.43
24:D3:19:ARG:HG3	55:DA:126:A:O5'	2.19	0.43
42:DO:2:ARG:NH1	42:DO:2:ARG:HB3	2.34	0.43
5:AE:81:LEU:HB3	5:AE:147:MET:SD	2.59	0.43
19:AS:53:ASN:HD22	19:AS:58:VAL:HG23	1.83	0.43
55:DA:2291:U:H2'	55:DA:2292:U:C6	2.53	0.43
1:BA:411:A:P	4:BD:26:ARG:HH12	2.41	0.43
5:BE:155:ALA:HB1	8:BH:66:PHE:CZ	2.54	0.43
10:BJ:15:HIS:HB3	10:BJ:70:HIS:CE1	2.54	0.43
31:CA:727:A:H2'	31:CA:728:G:C8	2.53	0.43
31:CA:1224:U:H4'	46:CS:88:GLY:O	2.19	0.43
50:CW:38:LEU:HD21	50:CW:65:VAL:HG11	2.01	0.43
44:DQ:53:ARG:HG2	44:DQ:53:ARG:NH1	2.34	0.43
1:AA:1293:C:H2'	1:AA:1294:G:C8	2.54	0.43
14:AN:53:ARG:HH21	19:AS:37:ARG:HH22	1.67	0.43
2:BB:163:VAL:HG11	2:BB:173:ILE:HD11	2.00	0.43
1:BA:1108:G:H5''	3:BC:176:HIS:CE1	2.54	0.43
7:BG:30:LEU:HD12	7:BG:105:VAL:HG13	2.01	0.43
17:BQ:27:ARG:NH2	17:BQ:40:ARG:HG2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:1935:G:H1'	31:CA:1964:G:N2	2.33	0.43
30:CD:150:GLN:NE2	31:CA:2032:G:H1'	2.34	0.43
55:DA:2110:G:H5'	55:DA:2145:C:N4	2.33	0.43
47:DT:6:LYS:HB2	55:DA:494:G:H4'	2.01	0.43
44:DQ:21:ARG:HD2	69:DA:6724:HOH:O	2.19	0.43
5:AE:155:ALA:HB1	8:AH:66:PHE:CZ	2.53	0.43
1:BA:1513:A:H2'	1:BA:1514:G:C8	2.54	0.43
31:CA:1168:G:H5''	31:CA:1168:G:H8	1.83	0.43
34:CF:104:ILE:HG23	34:CF:176:PRO:HD3	2.01	0.43
41:CN:108:VAL:HB	41:CN:112:LEU:HD23	1.99	0.43
29:DC:67:PHE:HZ	29:DC:87:ARG:HH12	1.67	0.43
41:DN:100:LYS:HD3	69:DN:306:HOH:O	2.18	0.43
2:AB:100:MET:HA	2:AB:107:VAL:HG21	2.01	0.43
1:BA:79:G:H22	1:BA:90:C:H42	1.64	0.43
31:CA:136:G:H1	31:CA:143:C:N4	2.16	0.43
31:CA:1636:U:H2'	31:CA:1637:A:C8	2.54	0.43
31:CA:1733:G:H2'	31:CA:1734:G:C8	2.53	0.43
55:DA:2026:U:H2'	55:DA:2027:G:O4'	2.18	0.43
55:DA:2636:C:H2'	55:DA:2637:U:C6	2.54	0.43
36:DH:3:VAL:HG12	36:DH:38:PRO:HA	2.01	0.43
1:AA:560:A:H4'	1:AA:561:U:H5''	2.00	0.43
1:AA:663:A:H5'	1:AA:836:G:OP1	2.19	0.43
5:AE:25:VAL:HG21	5:AE:30:ILE:HD11	2.01	0.43
5:AE:57:PRO:O	5:AE:60:ILE:HG13	2.19	0.43
6:AF:3:HIS:CE1	6:AF:65:GLU:HG3	2.53	0.43
42:CO:28:LEU:HD23	42:CO:48:VAL:HG21	2.00	0.43
32:DD:121:THR:HB	32:DD:127:PHE:CD2	2.54	0.43
35:DG:105:LEU:HD22	35:DG:107:LEU:HD11	2.01	0.43
35:DG:118:PRO:HD2	35:DG:121:ILE:HB	2.00	0.43
11:AK:21:ALA:HB2	11:AK:82:LEU:HD13	2.00	0.43
14:BN:13:ARG:HD3	14:BN:59:ARG:O	2.18	0.43
14:BN:69:ARG:HA	14:BN:70:PRO:HD3	1.93	0.43
16:BP:2:VAL:HG13	16:BP:65:ALA:HA	2.01	0.43
18:BR:34:THR:HG22	18:BR:38:LYS:N	2.34	0.43
31:CA:1826:G:C6	31:CA:1827:U:C4	3.06	0.43
43:CP:64:TYR:HB3	43:CP:67:ASN:ND2	2.33	0.43
35:DG:164:TYR:HB2	35:DG:167:GLU:HB2	2.01	0.43
1:AA:1478:U:H2'	1:AA:1479:C:C6	2.54	0.42
1:AA:580:C:H2'	1:AA:581:G:O4'	2.19	0.42
13:AM:12:HIS:HB3	69:AM:204:HOH:O	2.18	0.42
1:AA:107:G:H1	20:AT:6:SER:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1293:C:H2'	1:BA:1294:G:C8	2.54	0.42
1:BA:17:U:H2'	1:BA:18:C:C6	2.54	0.42
1:BA:580:C:H2'	1:BA:581:G:O4'	2.19	0.42
1:BA:663:A:H5'	1:BA:836:G:OP1	2.19	0.42
2:BB:129:LEU:H	2:BB:129:LEU:HG	1.59	0.42
4:BD:192:SER:HB3	4:BD:195:ILE:HD12	2.01	0.42
30:CD:63:PRO:HG3	31:CA:2787:C:H1'	2.01	0.42
39:CL:108:ARG:HA	39:CL:113:MET:HE1	2.02	0.42
31:CA:1651:G:OP1	42:CO:40:LYS:HE3	2.19	0.42
52:CY:11:ARG:HG2	52:CY:12:PRO:HD2	2.00	0.42
55:DA:2895:G:H2'	55:DA:2896:C:C6	2.54	0.42
32:DD:150[A]:MEQ:HG2	69:DA:3422:HOH:O	2.18	0.42
1:AA:108:G:H5''	1:AA:108:G:N3	2.34	0.42
10:AJ:15:HIS:HB3	10:AJ:70:HIS:CE1	2.54	0.42
10:BJ:19:ASP:HA	10:BJ:22:THR:HB	2.01	0.42
31:CA:1681:G:H2'	31:CA:1757:A:N1	2.34	0.42
30:CD:146:ILE:HG21	31:CA:2050:C:O2'	2.18	0.42
31:CA:2273:A:H2'	31:CA:2274:A:C8	2.54	0.42
52:CY:3:ARG:HD2	52:CY:30:LEU:HD22	2.01	0.42
55:DA:1026:G:H2'	55:DA:1027:A:C8	2.55	0.42
55:DA:784:G:H5'	55:DA:785:G:OP1	2.19	0.42
44:DQ:4:ILE:H	44:DQ:4:ILE:HD12	1.83	0.42
4:AD:76:TYR:HE1	4:AD:201:VAL:HG13	1.84	0.42
4:AD:48:LEU:HD21	4:AD:56:ARG:HG3	2.01	0.42
1:BA:1386:G:H2'	1:BA:1387:G:H8	1.83	0.42
1:BA:439:U:H5''	4:BD:121:LYS:HD2	2.02	0.42
5:BE:45:ARG:HE	5:BE:73:ASN:HD21	1.68	0.42
12:BL:36:ARG:HE	12:BL:54:ARG:HH12	1.66	0.42
16:BP:68:SER:HB3	69:BP:101:HOH:O	2.18	0.42
31:CA:2271:G:H2'	31:CA:2272:U:C6	2.54	0.42
27:D0:8:THR:O	27:D0:55:VAL:HA	2.19	0.42
55:DA:2328:A:H2'	55:DA:2329:U:C6	2.54	0.42
34:DF:104:ILE:HG23	34:DF:176:PRO:HD3	2.01	0.42
3:AC:47:LEU:HB3	3:AC:50:ALA:HB3	2.02	0.42
10:AJ:19:ASP:HA	10:AJ:22:THR:HB	2.02	0.42
1:AA:1061:G:H5'	10:AJ:61:ALA:HB2	2.00	0.42
15:AO:2:SER:HB3	15:AO:3:LEU:H	1.76	0.42
17:AQ:16:LYS:O	17:AQ:17:MET:HB2	2.20	0.42
1:BA:1012:A:H61	1:BA:1017:U:H3	1.67	0.42
1:BA:496:A:N3	1:BA:496:A:H2'	2.34	0.42
3:BC:5:VAL:HG21	3:BC:10:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:47:LEU:HB3	3:BC:50:ALA:HB3	2.02	0.42
17:BQ:28:PHE:CD2	17:BQ:37:PHE:HB3	2.54	0.42
31:CA:720:U:H2'	31:CA:721:A:C8	2.54	0.42
36:CH:5:LEU:HD12	36:CH:17:ASP:HB2	2.01	0.42
31:CA:328:U:O3'	49:CV:66:GLN:HG3	2.20	0.42
50:CW:40:ILE:HD12	50:CW:42:LEU:HD21	2.00	0.42
55:DA:2256:G:H21	57:DA:3196:PG4:H31	1.85	0.42
55:DA:2747:G:O6	55:DA:2755:C:H5''	2.19	0.42
28:DB:30:C:H2'	28:DB:31:C:H5'	2.02	0.42
38:DK:36:LEU:O	38:DK:51:GLY:HA3	2.18	0.42
6:AF:26:THR:HG23	6:AF:36:ILE:HG21	2.01	0.42
6:AF:3:HIS:ND1	6:AF:65:GLU:HG3	2.34	0.42
11:AK:13:ARG:HG3	11:AK:14:LYS:H	1.85	0.42
14:AN:6:MET:HE2	14:AN:63:ARG:HH22	1.83	0.42
1:BA:108:G:N3	1:BA:108:G:H5''	2.34	0.42
6:AF:16:GLU:HB3	4:BD:189:SER:HA	2.02	0.42
11:BK:34:ILE:HB	11:BK:74:VAL:HG11	2.00	0.42
15:BO:8:THR:O	15:BO:12:VAL:HG23	2.19	0.42
19:BS:52:HIS:CD2	19:BS:54:GLY:H	2.29	0.42
27:C0:2:ALA:HB1	27:C0:39:GLU:HB3	2.02	0.42
22:C1:12:LYS:HA	22:C1:12:LYS:HD2	1.92	0.42
31:CA:340:A:H2'	31:CA:341:C:O4'	2.19	0.42
26:D5:30:GLU:HG3	26:D5:32:LYS:HB2	2.00	0.42
55:DA:593:U:H2'	55:DA:594:U:C6	2.55	0.42
36:DH:71:LYS:HB3	36:DH:108:VAL:HG22	2.01	0.42
42:DO:55:ALA:HA	42:DO:80:PHE:CE2	2.55	0.42
44:DQ:94:LYS:HE2	55:DA:1754:A:C8	2.55	0.42
49:DV:13:VAL:HG21	49:DV:39:ILE:HG21	2.02	0.42
1:AA:1513:A:H2'	1:AA:1514:G:C8	2.55	0.42
1:AA:412:A:H3'	1:AA:413:G:C5'	2.49	0.42
15:AO:8:THR:O	15:AO:12:VAL:HG23	2.19	0.42
1:BA:1108:G:H5''	3:BC:176:HIS:HD1	1.84	0.42
2:BB:100:MET:HA	2:BB:107:VAL:HG21	2.01	0.42
12:BL:87:VAL:HG11	12:BL:90:LEU:HD22	2.00	0.42
31:CA:1662:U:H3	31:CA:1998:A:H61	1.65	0.42
31:CA:265:A:H4'	31:CA:266:G:OP1	2.19	0.42
55:DA:1101:U:H2'	55:DA:1102:C:C6	2.55	0.42
55:DA:1294:U:H6	55:DA:1294:U:H5''	1.85	0.42
29:DC:30:PHE:HD2	29:DC:33:LEU:HD12	1.85	0.42
32:DD:128:ARG:HG3	69:DA:7855:HOH:O	2.17	0.42
69:DK:301:HOH:O	45:DR:93:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1289:A:H3'	1:AA:1290:G:H8	1.85	0.42
1:AA:17:U:H2'	1:AA:18:C:C6	2.54	0.42
1:AA:815:A:H4'	1:AA:817:C:C4	2.55	0.42
5:AE:13:GLU:HB3	5:AE:39:VAL:HG12	2.01	0.42
3:BC:77:ILE:HA	3:BC:84:VAL:CG2	2.50	0.42
4:BD:91:LEU:HD21	4:BD:195:ILE:HG21	2.02	0.42
3:BC:23:PHE:HD2	10:BJ:97:ASP:HB2	1.85	0.42
12:BL:7:LEU:HD22	12:BL:12:ARG:HG2	2.00	0.42
20:BT:64:LYS:HE3	20:BT:64:LYS:HA	2.01	0.42
31:CA:2498:OMC:HM22	31:CA:2499:C:H5'	2.00	0.42
35:CG:118:PRO:HD2	35:CG:121:ILE:HB	2.01	0.42
41:CN:33:LEU:HD13	41:CN:117:PHE:HB3	2.02	0.42
43:CP:5:SER:HA	43:CP:8:ILE:HD12	2.02	0.42
43:CP:56:LYS:O	43:CP:60:GLU:HB2	2.20	0.42
55:DA:1590:A:H2'	55:DA:1591:A:C8	2.55	0.42
32:DD:55:LYS:HD3	32:DD:60:VAL:HG22	2.01	0.42
54:DI:56:ARG:HB3	54:DI:59:LEU:HB2	2.02	0.42
37:DJ:14:ALA:HB3	37:DJ:17:MET:HB2	2.00	0.42
1:AA:1235:U:H2'	1:AA:1236:A:O4'	2.20	0.42
1:AA:620:C:H2'	1:AA:621:A:O4'	2.20	0.42
1:AA:439:U:H5''	4:AD:121:LYS:HD2	2.02	0.42
14:BN:31:ILE:HG23	14:BN:42:TRP:CZ2	2.51	0.42
14:BN:43:ASN:HA	14:BN:46:LEU:HD12	2.01	0.42
31:CA:1266:G:H5''	47:CT:15:GLN:HE22	1.84	0.42
31:CA:1665:A:H2'	31:CA:1666:G:O4'	2.19	0.42
31:CA:674:G:O2'	33:CE:69:ARG:HD2	2.20	0.42
35:CG:105:LEU:HB2	35:CG:113:VAL:HB	2.01	0.42
40:CM:81:ASP:HA	40:CM:84:LYS:HD2	2.01	0.42
52:CY:45:ARG:HG2	52:CY:46:PHE:N	2.35	0.42
55:DA:1788:C:H6	55:DA:1788:C:O5'	2.03	0.42
45:DR:33:ARG:HD3	69:DA:4039:HOH:O	2.19	0.42
7:BG:51:ALA:HB2	7:BG:58:GLU:HG3	2.02	0.42
12:BL:80:ILE:CD1	12:BL:97:THR:HG22	2.48	0.42
31:CA:593:U:H2'	31:CA:594:U:C6	2.55	0.42
33:CE:105:LEU:HD23	33:CE:108:ILE:HD11	2.01	0.42
55:DA:1847:A:H8	55:DA:1847:A:O5'	2.02	0.42
55:DA:62:U:H5'	58:DA:3206:MPD:H53	2.02	0.42
36:DH:5:LEU:HD12	36:DH:17:ASP:HB2	2.01	0.42
43:DP:41:ALA:HB2	43:DP:48:LEU:HD21	2.02	0.42
1:AA:269:C:H2'	1:AA:270:A:C8	2.55	0.42
1:AA:987:G:H2'	1:AA:988:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:1171:A:H2'	1:BA:1172:C:C6	2.55	0.42
1:BA:429:U:H1'	1:BA:430:A:H5''	2.02	0.42
31:CA:1101:U:H2'	31:CA:1102:C:C6	2.55	0.42
30:CD:186:LEU:HD21	44:CQ:4:ILE:HG21	2.02	0.42
37:CJ:19:ASN:N	37:CJ:20:PRO:HD2	2.34	0.42
55:DA:2117:A:N6	55:DA:2171:A:H61	2.18	0.42
35:DG:74:SER:HA	35:DG:77:ILE:HD12	2.02	0.42
43:DP:68:LYS:HB3	61:DP:201:PEG:H22	2.00	0.42
51:DX:57:HIS:N	51:DX:57:HIS:CD2	2.88	0.42
1:AA:438:U:H5'	4:AD:120:HIS:HB3	2.02	0.41
1:BA:1235:U:H2'	1:BA:1236:A:O4'	2.20	0.41
1:BA:859:G:H2'	1:BA:860:A:C8	2.55	0.41
1:BA:987:G:H2'	1:BA:988:G:H8	1.85	0.41
14:BN:53:ARG:HH21	19:BS:37:ARG:HH22	1.67	0.41
26:C5:36:ARG:HH22	31:CA:2539:C:H4'	1.84	0.41
31:CA:543:G:C8	31:CA:543:G:H5''	2.54	0.41
31:CA:871:U:H2'	31:CA:872:U:C6	2.55	0.41
25:D4:23:LYS:HA	25:D4:48:ALA:O	2.20	0.41
55:DA:720:U:H2'	55:DA:721:A:C8	2.55	0.41
1:AA:1298:U:H3	7:AG:114:LYS:HA	1.85	0.41
8:AH:25:VAL:HG22	8:AH:63:LEU:HD11	2.02	0.41
1:BA:892:A:O2'	1:BA:1415:G:H4'	2.20	0.41
1:BA:438:U:H5'	4:BD:120:HIS:HB3	2.01	0.41
31:CA:141:G:H3'	31:CA:142:A:C8	2.56	0.41
31:CA:70:G:H5''	31:CA:112:U:O2	2.20	0.41
55:DA:1182:G:H2'	55:DA:1183:U:O4'	2.20	0.41
55:DA:1386:C:H2'	55:DA:1387:A:H8	1.85	0.41
55:DA:2051:A:OP2	55:DA:2051:A:H8	2.03	0.41
55:DA:572:A:H5''	55:DA:573:U:OP2	2.20	0.41
35:DG:105:LEU:HB2	35:DG:113:VAL:HB	2.02	0.41
41:DN:18[A]:ARG:HG3	28:DB:90:C:H5''	2.02	0.41
41:DN:41:LEU:CD2	41:DN:125:PRO:HD2	2.49	0.41
1:BA:1377:A:N3	7:BG:2:PRO:HG3	2.35	0.41
3:BC:151:VAL:HG12	3:BC:200:VAL:HG23	2.01	0.41
7:BG:50:LEU:CD1	7:BG:61:ALA:HB1	2.50	0.41
10:BJ:78:GLU:HG2	10:BJ:78:GLU:O	2.20	0.41
27:C0:19:LYS:HE3	31:CA:920:A:OP1	2.21	0.41
29:CC:158:ALA:HB3	31:CA:1820:U:O2'	2.20	0.41
31:CA:668:A:H2'	31:CA:670:A:H62	1.86	0.41
36:CH:78:VAL:HG21	36:CH:103:VAL:HG22	2.02	0.41
27:D0:15:GLY:HA2	55:DA:969:G:O3'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1144:G:H21	1:AA:1146:A:H62	1.68	0.41
9:AI:116:VAL:HG21	10:AJ:62:ARG:HB2	2.03	0.41
11:BK:36:ASP:CG	11:BK:38:GLN:HG2	2.41	0.41
31:CA:2781:A:H5''	31:CA:2782:G:H5'	2.01	0.41
33:CE:75:SER:OG	33:CE:77:ILE:HG12	2.20	0.41
35:CG:105:LEU:HD22	35:CG:107:LEU:HD11	2.02	0.41
35:CG:123:ALA:HB2	35:CG:133:LEU:HD23	2.03	0.41
36:CH:7:ASP:HA	36:CH:15:LEU:HD12	2.02	0.41
24:D3:19:ARG:HD3	55:DA:125:A:OP2	2.20	0.41
55:DA:1604:C:H5'	69:DA:3663:HOH:O	2.20	0.41
55:DA:221:A:N1	55:DA:265:A:O2'	2.51	0.41
59:DA:3187:PUT:H12	69:DA:7225:HOH:O	2.21	0.41
41:DN:18[B]:ARG:HG2	28:DB:91:C:P	2.60	0.41
29:DC:207:LYS:HB2	55:DA:729:G:C5	2.55	0.41
35:DG:12:PRO:HD2	35:DG:15:VAL:HG21	2.03	0.41
1:AA:1001:C:H2'	1:AA:1002:G:C8	2.56	0.41
1:AA:32:A:H2'	1:AA:33:A:C8	2.55	0.41
1:AA:604:G:H2'	1:AA:605:U:O4'	2.20	0.41
2:AB:163:VAL:HG11	2:AB:173:ILE:HD11	2.01	0.41
14:AN:43:ASN:HA	14:AN:46:LEU:HD12	2.02	0.41
17:AQ:45:HIS:HB2	17:AQ:70:THR:O	2.21	0.41
1:BA:1478:U:H2'	1:BA:1479:C:C6	2.56	0.41
1:BA:374:A:H5''	1:BA:452:A:C2	2.56	0.41
1:BA:844:G:H2'	1:BA:844:G:N3	2.35	0.41
1:BA:76:G:H22	1:BA:93:U:H3	1.68	0.41
31:CA:1638:C:H5''	31:CA:2710:C:O2'	2.20	0.41
30:CD:146:ILE:HG12	31:CA:2051:A:H4'	2.02	0.41
31:CA:2845:U:H2'	31:CA:2846:G:O4'	2.21	0.41
31:CA:455:C:HO2'	31:CA:472:A:H2	1.66	0.41
35:CG:164:TYR:HB2	35:CG:167:GLU:HB2	2.01	0.41
50:CW:51:GLN:HB2	50:CW:57:TYR:OH	2.20	0.41
51:DX:18:ALA:HB1	55:DA:2271:G:OP1	2.19	0.41
55:DA:2327:A:H2'	55:DA:2328:A:C8	2.55	0.41
55:DA:352:A:H5''	55:DA:352:A:H8	1.86	0.41
32:DD:125:TRP:CE3	32:DD:160:LYS:HD3	2.55	0.41
37:DJ:19:ASN:N	37:DJ:20:PRO:HD2	2.35	0.41
48:DU:7:LEU:HD13	48:DU:46:ALA:HA	2.02	0.41
1:AA:1377:A:N3	7:AG:2:PRO:HG3	2.35	0.41
1:AA:946:A:H2'	1:AA:947:G:C8	2.56	0.41
31:CA:2016:U:O5'	31:CA:2016:U:H6	2.03	0.41
31:CA:2030:6MZ:N3	31:CA:2499:C:H5''	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:2895:G:H2'	31:CA:2896:C:C6	2.55	0.41
29:CC:266:PHE:H	29:CC:266:PHE:HD1	1.68	0.41
36:CH:71:LYS:HB3	36:CH:108:VAL:HG22	2.02	0.41
36:CH:47:PHE:O	36:CH:51:ARG:HB3	2.21	0.41
38:CK:36:LEU:O	38:CK:51:GLY:HA3	2.20	0.41
55:DA:1730:C:O4'	55:DA:1730:C:O2	2.39	0.41
55:DA:2273:A:H2'	55:DA:2274:A:C8	2.55	0.41
55:DA:2706:A:O5'	55:DA:2706:A:H8	2.03	0.41
55:DA:1831:G:H5'	63:DA:3227:PGE:H62	2.02	0.41
29:DC:177:ARG:HG2	55:DA:1820:U:OP1	2.21	0.41
40:DM:21:ARG:HA	55:DA:811:U:H2'	2.03	0.41
41:DN:17:ASN:O	41:DN:38:ARG:HD3	2.21	0.41
1:AA:721:G:H4'	1:AA:722:G:O4'	2.21	0.41
3:AC:5:VAL:HG21	3:AC:10:ILE:HD13	2.02	0.41
1:AA:1190:G:H5'	3:AC:176:HIS:NE2	2.36	0.41
4:AD:192:SER:HB3	4:AD:195:ILE:HD12	2.02	0.41
5:AE:15:LEU:HA	5:AE:37:THR:HG22	2.02	0.41
3:BC:123:GLN:HB3	3:BC:128:VAL:CG2	2.51	0.41
1:BA:8:A:C6	4:BD:206:LYS:HB3	2.56	0.41
5:BE:106:ILE:HG13	5:BE:123:VAL:O	2.20	0.41
1:BA:266:G:H3'	17:BQ:69:LYS:HB2	2.01	0.41
31:CA:1716:U:H2'	31:CA:1717:A:H8	1.86	0.41
31:CA:2063:C:O2	31:CA:2450:A:N1	2.53	0.41
40:CM:123:ARG:HG3	40:CM:143:GLU:HG3	2.03	0.41
51:CX:51:VAL:HG22	51:CX:82:ILE:HD12	2.02	0.41
55:DA:969:G:H2'	55:DA:970:U:C6	2.54	0.41
16:AP:31:ARG:HA	69:AP:101:HOH:O	2.21	0.41
1:AA:266:G:H3'	17:AQ:69:LYS:HB2	2.02	0.41
1:BA:1144:G:H21	1:BA:1146:A:H62	1.68	0.41
1:BA:269:C:H2'	1:BA:270:A:C8	2.55	0.41
31:CA:1101:U:H2'	31:CA:1102:C:H6	1.86	0.41
31:CA:1847:A:H8	31:CA:1847:A:O5'	2.03	0.41
31:CA:321:U:H5''	33:CE:131:THR:HG23	2.02	0.41
31:CA:35:G:H2'	31:CA:36:G:O4'	2.21	0.41
30:CD:187:LEU:HD21	30:CD:203:VAL:HG11	2.02	0.41
35:CG:52:PHE:N	35:CG:52:PHE:CD2	2.89	0.41
48:DU:1:MET:HG2	55:DA:142:A:H1'	2.03	0.41
55:DA:2243:U:H2'	55:DA:2244:U:C6	2.56	0.41
55:DA:1769:U:H5''	64:DA:3208:SPD:H32	2.02	0.41
48:DU:2:ILE:HG21	48:DU:45:ALA:HB1	2.02	0.41
51:DX:41[A]:ARG:HG2	51:DX:41[A]:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:DY:45:ARG:HG2	52:DY:46:PHE:N	2.36	0.41
1:AA:1171:A:H2'	1:AA:1172:C:C6	2.55	0.41
9:AI:11:ARG:HB3	9:AI:16:ALA:HA	2.02	0.41
12:AL:87:VAL:HG11	12:AL:90:LEU:HD22	2.03	0.41
14:AN:42:TRP:CD1	14:AN:43:ASN:N	2.89	0.41
14:AN:79:LEU:HD22	69:AN:205:HOH:O	2.20	0.41
1:BA:1289:A:H3'	1:BA:1290:G:H8	1.85	0.41
3:BC:138:VAL:HG13	3:BC:149:ILE:HG23	2.02	0.41
1:BA:706:A:H4'	11:BK:31:ILE:HG12	2.03	0.41
31:CA:1072:C:H2'	31:CA:1093:G:O6	2.21	0.41
31:CA:2304:G:H22	31:CA:2312:U:H3	1.69	0.41
31:CA:307:G:N2	31:CA:309:A:H3'	2.34	0.41
55:DA:2291:U:H5''	55:DA:2380:C:O2	2.21	0.41
55:DA:2698:U:H2'	55:DA:2699:C:C6	2.56	0.41
55:DA:68:G:H2'	55:DA:69:C:O4'	2.20	0.41
54:DI:83:ALA:HB2	54:DI:96:PHE:CZ	2.55	0.41
42:DO:28:LEU:HD23	42:DO:48:VAL:HG21	2.01	0.41
51:DX:51:VAL:HG22	51:DX:82:ILE:HD12	2.02	0.41
1:AA:496:A:H2'	1:AA:496:A:N3	2.36	0.41
1:BA:76:G:H1	1:BA:93:U:H3	1.69	0.41
1:BA:1298:U:H3	7:BG:114:LYS:HA	1.86	0.41
19:BS:66:MET:HG2	19:BS:74:PHE:CE2	2.56	0.41
31:CA:1885:A:H2'	31:CA:1886:U:O4'	2.20	0.41
30:CD:121:THR:HB	30:CD:127:PHE:CD2	2.55	0.41
40:CM:19:LEU:HD23	40:CM:31:GLY:O	2.21	0.41
49:CV:72:ILE:HG13	49:CV:72:ILE:H	1.66	0.41
55:DA:2255:G:H21	68:DA:3222:TRS:C1	2.34	0.41
55:DA:2262:U:H4'	55:DA:2328:A:C2	2.56	0.41
55:DA:2886[B]:A:N3	55:DA:2886[B]:A:H2'	2.36	0.41
32:DD:187:LEU:HD21	32:DD:203:VAL:HG11	2.03	0.41
54:DI:129:LEU:HA	54:DI:130:PRO:HD3	1.99	0.41
47:DT:72:THR:CG2	47:DT:108:SER:HB3	2.51	0.41
1:AA:1012:A:H61	1:AA:1017:U:H3	1.67	0.41
1:AA:1492:A:H5'	1:AA:1492:A:C8	2.47	0.41
6:AF:29:ILE:HG23	6:AF:66:ALA:HB2	2.01	0.41
1:AA:1250:A:O3'	9:AI:69:GLY:HA2	2.20	0.41
14:AN:69:ARG:HA	14:AN:70:PRO:HD3	1.92	0.41
6:BF:64:VAL:HG12	6:BF:65:GLU:N	2.36	0.41
31:CA:1587:G:H2'	31:CA:1588:G:H8	1.86	0.41
31:CA:2038:G:H2'	31:CA:2039:U:O4'	2.21	0.41
31:CA:364:C:H2'	31:CA:365:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:CC:105:LEU:HD12	29:CC:105:LEU:N	2.34	0.41
36:CH:27:ARG:HH12	36:CH:38:PRO:HG3	1.86	0.41
39:CL:105:ARG:O	39:CL:108:ARG:HB2	2.19	0.41
45:CR:76:TYR:CZ	45:CR:80:ILE:HG13	2.56	0.41
55:DA:1354:A:H2'	55:DA:1355:G:O4'	2.21	0.41
55:DA:1430:G:H2'	55:DA:1431:A:O4'	2.21	0.41
42:DO:19:ALA:HB2	69:DA:6721:HOH:O	2.20	0.41
43:DP:5:SER:HA	43:DP:8:ILE:HD12	2.02	0.41
1:AA:76:G:H22	1:AA:93:U:H3	1.68	0.40
3:AC:77:ILE:HA	3:AC:84:VAL:CG2	2.51	0.40
1:BA:1001:C:H2'	1:BA:1002:G:C8	2.56	0.40
15:BO:2:SER:HB3	15:BO:3:LEU:H	1.74	0.40
43:DP:1:MET:HB3	43:DP:6:ALA:HB2	2.02	0.40
1:AA:859:G:H2'	1:AA:860:A:C8	2.56	0.40
2:AB:31:ILE:HD13	2:AB:39:HIS:CD2	2.55	0.40
9:AI:57:MET:HG3	9:AI:61:LEU:HG	2.03	0.40
10:AJ:53:ILE:HG13	14:AN:85:ARG:HD2	2.02	0.40
2:BB:41:ILE:HD13	2:BB:202:GLY:HA2	2.03	0.40
4:BD:170:TRP:CD2	4:BD:186:PRO:HB3	2.56	0.40
29:CC:208:ALA:HB2	31:CA:1790:C:H4'	2.04	0.40
31:CA:674:G:H21	33:CE:69:ARG:HH12	1.69	0.40
47:CT:20:VAL:HG11	47:CT:44:ALA:HA	2.03	0.40
55:DA:1093:G:H1'	55:DA:1099:G:H22	1.87	0.40
55:DA:553:G:H2'	55:DA:554:U:O4'	2.20	0.40
29:DC:225:MET:O	29:DC:233:GLY:O	2.40	0.40
41:DN:33:LEU:HD13	41:DN:117:PHE:HB3	2.03	0.40
44:DQ:100:LEU:HD11	44:DQ:110:ILE:HD11	2.03	0.40
44:DQ:10:GLN:HG2	44:DQ:10:GLN:H	1.72	0.40
47:DT:20:VAL:HG11	47:DT:44:ALA:HA	2.02	0.40
1:AA:1508:A:H2'	1:AA:1509:C:O4'	2.22	0.40
1:AA:49:U:O2	1:AA:362:G:H1'	2.20	0.40
1:BA:1081:A:H5'	5:BE:23:LYS:HG3	2.04	0.40
1:BA:1151:A:O2'	1:BA:1152:A:H8	2.03	0.40
13:BM:23:TYR:HD1	13:BM:69:LEU:HD23	1.87	0.40
22:C1:41:HIS:HA	22:C1:49:TYR:OH	2.21	0.40
25:C4:23:LYS:HA	25:C4:48:ALA:O	2.21	0.40
31:CA:2114:A:N6	31:CA:2119:A:H62	2.19	0.40
31:CA:998:C:OP2	45:CR:58:ARG:NH2	2.54	0.40
55:DA:397:U:H6	55:DA:397:U:O5'	2.03	0.40
35:DG:123:ALA:HB2	35:DG:133:LEU:HD23	2.04	0.40
2:AB:41:ILE:HD13	2:AB:202:GLY:HA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AR:52:GLN:HA	18:AR:55:LEU:HD12	2.03	0.40
1:BA:1069:C:O4'	1:BA:1191:A:H2	2.05	0.40
1:BA:1508:A:H2'	1:BA:1509:C:O4'	2.21	0.40
1:BA:946:A:H2'	1:BA:947:G:C8	2.56	0.40
1:BA:1191:A:OP1	3:BC:3:GLN:HB3	2.21	0.40
5:BE:126:LYS:HG2	5:BE:128:TYR:CZ	2.56	0.40
5:BE:13:GLU:HB3	5:BE:39:VAL:HG12	2.03	0.40
11:BK:34:ILE:HG12	11:BK:70:CYS:SG	2.61	0.40
28:CB:14:U:H2'	28:CB:15:A:C2	2.55	0.40
44:CQ:53:ARG:HG2	44:CQ:53:ARG:NH1	2.37	0.40
46:CS:78:ARG:HB2	46:CS:83:TYR:HD1	1.87	0.40
63:D1:102:PGE:H4	69:DT:328:HOH:O	2.21	0.40
55:DA:1716:U:H2'	55:DA:1717:A:H8	1.86	0.40
55:DA:1268:A:C2	55:DA:2013:A:C4	3.09	0.40
55:DA:2188:U:H2'	55:DA:2189:U:C6	2.56	0.40
55:DA:2251:OMG:H1'	55:DA:2251:OMG:HM23	1.87	0.40
55:DA:419:U:H2'	55:DA:420:C:C6	2.57	0.40
55:DA:449:A:H2'	55:DA:450:G:H5'	2.02	0.40
55:DA:572:A:C2	55:DA:2033:A:C2	3.10	0.40
47:DT:90:LYS:HA	55:DA:751:A:H5'	2.02	0.40
33:DE:189:THR:HG21	69:DE:456:HOH:O	2.21	0.40
42:DO:96:ARG:HD2	42:DO:114:GLU:OE1	2.21	0.40
44:DQ:22:PRO:HD3	44:DQ:50:ILE:HD12	2.03	0.40
47:DT:17:VAL:HB	47:DT:76:VAL:HG11	2.04	0.40
7:AG:20:SER:HB3	7:AG:23:LEU:HB2	2.03	0.40
31:CA:2266:A:H4'	31:CA:2267:A:O5'	2.22	0.40
22:C1:38:HIS:CE1	31:CA:2884:U:O4	2.75	0.40
34:CF:36:LEU:HD21	34:CF:91:LEU:CD1	2.52	0.40
40:CM:132:ARG:HG3	40:CM:142:ILE:HD13	2.04	0.40
42:CO:55:ALA:HA	42:CO:80:PHE:CE2	2.56	0.40
49:CV:13:VAL:HG21	49:CV:39:ILE:HG21	2.03	0.40
55:DA:1554:U:H1'	59:DA:3221:PUT:H32	2.04	0.40
55:DA:2849:U:H4'	55:DA:2868:A:C2	2.57	0.40
55:DA:364:C:H2'	55:DA:365:U:C6	2.56	0.40
34:DF:31:VAL:HG23	34:DF:169:LEU:HD21	2.03	0.40
54:DI:29:ASP:HB3	54:DI:106:PHE:HB2	2.02	0.40
52:DY:29:PHE:HB3	55:DA:396:G:H1'	2.04	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	204 (92%)	14 (6%)	4 (2%)	11	42
2	BB	222/224 (99%)	202 (91%)	16 (7%)	4 (2%)	11	42
3	AC	204/206 (99%)	195 (96%)	8 (4%)	1 (0%)	34	74
3	BC	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	19	58
4	AD	203/205 (99%)	193 (95%)	10 (5%)	0	100	100
4	BD	203/205 (99%)	192 (95%)	11 (5%)	0	100	100
5	AE	153/155 (99%)	143 (94%)	9 (6%)	1 (1%)	26	67
5	BE	148/155 (96%)	135 (91%)	10 (7%)	3 (2%)	9	38
6	AF	104/106 (98%)	92 (88%)	12 (12%)	0	100	100
6	BF	98/106 (92%)	82 (84%)	12 (12%)	4 (4%)	3	19
7	AG	149/151 (99%)	135 (91%)	12 (8%)	2 (1%)	15	51
7	BG	149/151 (99%)	138 (93%)	10 (7%)	1 (1%)	26	67
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%)	112 (90%)	12 (10%)	1 (1%)	24	64
9	BI	125/127 (98%)	112 (90%)	12 (10%)	1 (1%)	24	64
10	AJ	97/99 (98%)	90 (93%)	5 (5%)	2 (2%)	9	37
10	BJ	96/99 (97%)	80 (83%)	11 (12%)	5 (5%)	2	14
11	AK	115/117 (98%)	105 (91%)	9 (8%)	1 (1%)	21	61
11	BK	115/117 (98%)	102 (89%)	12 (10%)	1 (1%)	21	61
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
12	BL	120/123 (98%)	115 (96%)	4 (3%)	1 (1%)	24	64
13	AM	112/114 (98%)	97 (87%)	11 (10%)	4 (4%)	4	22
13	BM	112/114 (98%)	95 (85%)	11 (10%)	6 (5%)	2	13
14	AN	98/100 (98%)	91 (93%)	4 (4%)	3 (3%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	BN	98/100 (98%)	93 (95%)	2 (2%)	3 (3%)	5	26
15	AO	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
15	BO	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	16	53
16	AP	80/82 (98%)	67 (84%)	10 (12%)	3 (4%)	4	21
16	BP	80/82 (98%)	63 (79%)	14 (18%)	3 (4%)	4	21
17	AQ	78/80 (98%)	70 (90%)	5 (6%)	3 (4%)	4	21
17	BQ	78/80 (98%)	67 (86%)	7 (9%)	4 (5%)	2	14
18	AR	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
18	BR	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
19	AS	77/79 (98%)	66 (86%)	9 (12%)	2 (3%)	7	30
19	BS	77/79 (98%)	64 (83%)	11 (14%)	2 (3%)	7	30
20	AT	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
20	BT	83/86 (96%)	79 (95%)	2 (2%)	2 (2%)	7	33
21	AU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
21	BU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
22	C1	54/56 (96%)	47 (87%)	3 (6%)	4 (7%)	1	6
22	D1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	3	18
23	D2	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
24	C3	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	C4	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
25	D4	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
26	C5	36/38 (95%)	36 (100%)	0	0	100	100
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	53 (95%)	1 (2%)	2 (4%)	4	22
27	D0	57/58 (98%)	53 (93%)	4 (7%)	0	100	100
29	CC	269/271 (99%)	242 (90%)	21 (8%)	6 (2%)	8	35
29	DC	269/271 (99%)	249 (93%)	18 (7%)	2 (1%)	26	67
30	CD	207/209 (99%)	191 (92%)	16 (8%)	0	100	100
32	DD	206/209 (99%)	197 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	CE	199/201 (99%)	186 (94%)	10 (5%)	3 (2%)	13	47
33	DE	199/201 (99%)	189 (95%)	9 (4%)	1 (0%)	34	74
34	CF	175/177 (99%)	161 (92%)	12 (7%)	2 (1%)	17	56
34	DF	175/177 (99%)	160 (91%)	12 (7%)	3 (2%)	11	43
35	CG	174/176 (99%)	160 (92%)	9 (5%)	5 (3%)	6	27
35	DG	174/176 (99%)	159 (91%)	13 (8%)	2 (1%)	17	56
36	CH	147/149 (99%)	127 (86%)	15 (10%)	5 (3%)	5	23
36	DH	147/149 (99%)	131 (89%)	13 (9%)	3 (2%)	9	38
37	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	5	27
37	DJ	132/134 (98%)	126 (96%)	2 (2%)	4 (3%)	5	27
38	CK	140/142 (99%)	133 (95%)	5 (4%)	2 (1%)	14	49
38	DK	140/142 (99%)	136 (97%)	3 (2%)	1 (1%)	26	67
39	CL	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	11	43
39	DL	121/123 (98%)	115 (95%)	5 (4%)	1 (1%)	24	64
40	CM	142/144 (99%)	131 (92%)	8 (6%)	3 (2%)	9	37
40	DM	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
41	CN	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
41	DN	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
42	CO	118/125 (94%)	110 (93%)	7 (6%)	1 (1%)	24	64
42	DO	123/125 (98%)	115 (94%)	8 (6%)	0	100	100
43	CP	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
43	DP	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
44	CQ	112/114 (98%)	108 (96%)	3 (3%)	1 (1%)	21	61
44	DQ	112/114 (98%)	108 (96%)	3 (3%)	1 (1%)	21	61
45	CR	115/117 (98%)	112 (97%)	2 (2%)	1 (1%)	21	61
45	DR	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
46	CS	101/103 (98%)	90 (89%)	10 (10%)	1 (1%)	19	58
46	DS	101/103 (98%)	95 (94%)	5 (5%)	1 (1%)	19	58
47	CT	108/110 (98%)	102 (94%)	4 (4%)	2 (2%)	10	40
47	DT	108/110 (98%)	106 (98%)	1 (1%)	1 (1%)	21	61
48	CU	91/93 (98%)	85 (93%)	5 (6%)	1 (1%)	17	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	DU	91/93 (98%)	85 (93%)	5 (6%)	1 (1%)	17	56
49	CV	100/102 (98%)	86 (86%)	10 (10%)	4 (4%)	4	19
49	DV	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	9	38
50	CW	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
50	DW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
51	CX	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
51	DX	75/76 (99%)	72 (96%)	3 (4%)	0	100	100
52	CY	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
52	DY	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
53	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11	43
53	DZ	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
54	DI	133/135 (98%)	112 (84%)	15 (11%)	6 (4%)	3	17
All	All	11407/11629 (98%)	10595 (93%)	661 (6%)	151 (1%)	15	51

All (151) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE
5	AE	109	GLY
7	AG	56	LYS
10	AJ	57	VAL
13	AM	5	ALA
14	AN	38	ASP
17	AQ	82	ALA
2	BB	126	PHE
3	BC	61	ALA
6	BF	98	GLU
6	BF	99	ALA
10	BJ	38	GLY
10	BJ	57	VAL
10	BJ	91	ASP
13	BM	5	ALA
13	BM	7	ILE
13	BM	114	LYS
17	BQ	82	ALA
29	CC	108	LYS
29	CC	158	ALA
33	CE	82	GLY

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	CG	46	ALA
35	CG	119	ALA
35	CG	175	LYS
35	CG	176	LYS
36	CH	10	ALA
37	CJ	19	ASN
38	CK	81	ILE
40	CM	29	LYS
49	CV	7	ARG
49	CV	16	GLY
35	DG	46	ALA
36	DH	11	ASN
37	DJ	19	ASN
49	DV	52	LEU
54	DI	91	ALA
9	AI	72	ILE
10	AJ	33	GLY
13	AM	7	ILE
13	AM	105	ASN
17	AQ	16	LYS
17	AQ	17	MET
19	AS	7	LYS
22	C1	44	THR
3	BC	156	ARG
5	BE	103	THR
5	BE	110	ALA
9	BI	72	ILE
12	BL	44	LYS
13	BM	4	ILE
13	BM	105	ASN
14	BN	38	ASP
15	BO	88	ARG
17	BQ	17	MET
17	BQ	71	LYS
19	BS	6	LYS
29	CC	58	HIS
29	CC	233	GLY
29	DC	233	GLY
33	CE	6	LYS
37	CJ	25	GLY
39	CL	35	VAL
40	CM	69	ARG

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Mol	Chain	Res	Type
42	CO	119	SER
44	CQ	105	GLY
46	CS	55	ASP
47	CT	65	ASP
48	CU	89	GLU
49	CV	89	ASP
33	DE	6	LYS
37	DJ	25	GLY
44	DQ	105	GLY
48	DU	89	GLU
49	DV	89	ASP
2	AB	95	ARG
3	AC	156	ARG
11	AK	89	PRO
14	AN	21	PHE
22	C1	25	VAL
22	C1	26	THR
22	C1	27	SER
23	C2	51	GLU
27	C0	14	ILE
2	BB	95	ARG
2	BB	127	ASP
5	BE	24	THR
6	BF	92	THR
7	BG	56	LYS
11	BK	89	PRO
14	BN	21	PHE
16	BP	44	SER
17	BQ	70	THR
29	CC	253	LYS
36	CH	9	VAL
37	CJ	23	PRO
49	CV	17	LYS
37	DJ	23	PRO
39	DL	75	SER
46	DS	44	GLY
54	DI	109	LYS
54	DI	130	PRO
2	AB	125	THR
2	AB	127	ASP
13	AM	47	GLU
16	AP	45	GLU

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Mol	Chain	Res	Type
19	AS	8	GLY
2	BB	125	THR
16	BP	80	LYS
20	BT	5	LYS
35	CG	45	HIS
36	CH	8	LYS
38	CK	25	LEU
39	CL	108	ARG
53	CZ	62	GLY
34	DF	123	ASP
35	DG	45	HIS
54	DI	88	HIS
14	AN	22	ALA
16	AP	31	ARG
27	C0	4	THR
6	BF	94	HIS
10	BJ	36	VAL
14	BN	22	ALA
16	BP	47	GLU
29	CC	261	LYS
29	DC	253	LYS
36	CH	11	ASN
37	CJ	32	GLY
47	CT	60	HIS
37	DJ	32	GLY
38	DK	25	LEU
47	DT	60	HIS
54	DI	108	VAL
7	AG	148	ASN
10	BJ	95	GLY
13	BM	47	GLU
19	BS	8	GLY
20	BT	68	HIS
36	DH	122	LEU
34	CF	176	PRO
34	DF	176	PRO
36	DH	34	GLY
33	CE	83	VAL
36	CH	34	GLY
16	AP	49	GLY
23	C2	5	ILE
45	CR	7	GLY

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Mol	Chain	Res	Type
34	CF	62	GLY
40	CM	87	GLY
34	DF	62	GLY
54	DI	67	THR

### 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%)	168 (90%)	18 (10%)	10	35
2	BB	186/186 (100%)	168 (90%)	18 (10%)	10	35
3	AC	170/170 (100%)	153 (90%)	17 (10%)	9	33
3	BC	170/170 (100%)	160 (94%)	10 (6%)	24	61
4	AD	172/172 (100%)	166 (96%)	6 (4%)	43	79
4	BD	172/172 (100%)	163 (95%)	9 (5%)	29	66
5	AE	118/118 (100%)	100 (85%)	18 (15%)	3	15
5	BE	113/118 (96%)	93 (82%)	20 (18%)	2	11
6	AF	92/92 (100%)	87 (95%)	5 (5%)	27	64
6	BF	87/92 (95%)	78 (90%)	9 (10%)	9	31
7	AG	124/124 (100%)	109 (88%)	15 (12%)	6	24
7	BG	124/124 (100%)	109 (88%)	15 (12%)	6	24
8	AH	104/104 (100%)	92 (88%)	12 (12%)	7	26
8	BH	104/104 (100%)	95 (91%)	9 (9%)	13	41
9	AI	105/105 (100%)	95 (90%)	10 (10%)	11	36
9	BI	105/105 (100%)	94 (90%)	11 (10%)	8	31
10	AJ	87/87 (100%)	79 (91%)	8 (9%)	11	38
10	BJ	86/87 (99%)	76 (88%)	10 (12%)	7	26
11	AK	90/90 (100%)	84 (93%)	6 (7%)	20	55
11	BK	90/90 (100%)	82 (91%)	8 (9%)	12	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	102/102 (100%)	94 (92%)	8 (8%)	16	48
12	BL	102/102 (100%)	91 (89%)	11 (11%)	8	29
13	AM	92/92 (100%)	81 (88%)	11 (12%)	6	24
13	BM	92/92 (100%)	84 (91%)	8 (9%)	13	41
14	AN	83/83 (100%)	80 (96%)	3 (4%)	42	78
14	BN	83/83 (100%)	79 (95%)	4 (5%)	31	70
15	AO	76/76 (100%)	68 (90%)	8 (10%)	8	31
15	BO	76/76 (100%)	67 (88%)	9 (12%)	6	25
16	AP	65/65 (100%)	59 (91%)	6 (9%)	11	38
16	BP	65/65 (100%)	58 (89%)	7 (11%)	8	29
17	AQ	74/74 (100%)	68 (92%)	6 (8%)	15	45
17	BQ	74/74 (100%)	63 (85%)	11 (15%)	4	16
18	AR	48/48 (100%)	43 (90%)	5 (10%)	9	31
18	BR	48/48 (100%)	44 (92%)	4 (8%)	14	44
19	AS	70/70 (100%)	62 (89%)	8 (11%)	7	27
19	BS	70/70 (100%)	63 (90%)	7 (10%)	9	33
20	AT	65/65 (100%)	55 (85%)	10 (15%)	3	15
20	BT	65/65 (100%)	56 (86%)	9 (14%)	4	19
21	AU	48/48 (100%)	47 (98%)	1 (2%)	61	88
21	BU	48/48 (100%)	47 (98%)	1 (2%)	61	88
22	C1	47/47 (100%)	44 (94%)	3 (6%)	22	57
22	D1	47/47 (100%)	46 (98%)	1 (2%)	61	88
23	C2	45/46 (98%)	43 (96%)	2 (4%)	35	73
23	D2	45/46 (98%)	42 (93%)	3 (7%)	20	55
24	C3	38/38 (100%)	35 (92%)	3 (8%)	15	47
24	D3	38/38 (100%)	36 (95%)	2 (5%)	28	65
25	C4	51/51 (100%)	48 (94%)	3 (6%)	24	61
25	D4	51/51 (100%)	48 (94%)	3 (6%)	24	61
26	C5	34/34 (100%)	32 (94%)	2 (6%)	24	61
26	D5	34/34 (100%)	33 (97%)	1 (3%)	50	83
27	C0	48/48 (100%)	42 (88%)	6 (12%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	D0	49/48 (102%)	42 (86%)	7 (14%)	4	18
29	CC	216/216 (100%)	201 (93%)	15 (7%)	19	54
29	DC	216/216 (100%)	207 (96%)	9 (4%)	36	74
30	CD	164/164 (100%)	156 (95%)	8 (5%)	31	69
32	DD	163/163 (100%)	156 (96%)	7 (4%)	35	73
33	CE	165/165 (100%)	149 (90%)	16 (10%)	10	35
33	DE	165/165 (100%)	158 (96%)	7 (4%)	36	74
34	CF	148/148 (100%)	134 (90%)	14 (10%)	11	36
34	DF	148/148 (100%)	134 (90%)	14 (10%)	11	36
35	CG	137/137 (100%)	133 (97%)	4 (3%)	50	83
35	DG	137/137 (100%)	132 (96%)	5 (4%)	42	78
36	CH	114/114 (100%)	103 (90%)	11 (10%)	10	36
36	DH	114/114 (100%)	104 (91%)	10 (9%)	12	41
37	CJ	104/104 (100%)	98 (94%)	6 (6%)	25	62
37	DJ	104/104 (100%)	98 (94%)	6 (6%)	25	62
38	CK	116/116 (100%)	113 (97%)	3 (3%)	54	84
38	DK	116/116 (100%)	112 (97%)	4 (3%)	44	80
39	CL	103/104 (99%)	96 (93%)	7 (7%)	20	54
39	DL	104/104 (100%)	96 (92%)	8 (8%)	16	48
40	CM	103/103 (100%)	94 (91%)	9 (9%)	13	41
40	DM	103/103 (100%)	97 (94%)	6 (6%)	25	62
41	CN	108/108 (100%)	101 (94%)	7 (6%)	21	56
41	DN	109/108 (101%)	103 (94%)	6 (6%)	27	64
42	CO	100/102 (98%)	91 (91%)	9 (9%)	12	40
42	DO	102/102 (100%)	95 (93%)	7 (7%)	19	54
43	CP	86/87 (99%)	79 (92%)	7 (8%)	15	45
43	DP	87/87 (100%)	79 (91%)	8 (9%)	11	38
44	CQ	99/99 (100%)	91 (92%)	8 (8%)	15	45
44	DQ	99/99 (100%)	93 (94%)	6 (6%)	23	59
45	CR	89/89 (100%)	83 (93%)	6 (7%)	20	55
45	DR	89/89 (100%)	85 (96%)	4 (4%)	34	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	CS	84/84 (100%)	81 (96%)	3 (4%)	42	78
46	DS	84/84 (100%)	82 (98%)	2 (2%)	57	86
47	CT	93/93 (100%)	88 (95%)	5 (5%)	27	64
47	DT	93/93 (100%)	91 (98%)	2 (2%)	60	87
48	CU	80/80 (100%)	72 (90%)	8 (10%)	9	33
48	DU	80/80 (100%)	74 (92%)	6 (8%)	17	49
49	CV	83/83 (100%)	77 (93%)	6 (7%)	18	51
49	DV	83/83 (100%)	80 (96%)	3 (4%)	42	78
50	CW	78/78 (100%)	73 (94%)	5 (6%)	22	57
50	DW	78/78 (100%)	75 (96%)	3 (4%)	40	77
51	CX	56/58 (97%)	50 (89%)	6 (11%)	8	29
51	DX	58/58 (100%)	49 (84%)	9 (16%)	3	14
52	CY	67/67 (100%)	62 (92%)	5 (8%)	17	49
52	DY	67/67 (100%)	62 (92%)	5 (8%)	17	49
53	CZ	54/54 (100%)	51 (94%)	3 (6%)	26	63
53	DZ	54/54 (100%)	53 (98%)	1 (2%)	65	89
54	DI	103/103 (100%)	94 (91%)	9 (9%)	13	41
All	All	9461/9478 (100%)	8736 (92%)	725 (8%)	16	48

All (725) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AB	8	ASP
2	AB	23	TRP
2	AB	44	GLU
2	AB	70	VAL
2	AB	73	LYS
2	AB	93	ASN
2	AB	105	LYS
2	AB	117	LEU
2	AB	125	THR
2	AB	129	LEU
2	AB	130	THR
2	AB	135	LEU
2	AB	161	LEU
2	AB	167	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	AB	168	HIS
2	AB	190	ASN
2	AB	205	ASP
2	AB	207	ILE
3	AC	23	PHE
3	AC	28	GLU
3	AC	33	LEU
3	AC	38	LYS
3	AC	55	ILE
3	AC	75	ILE
3	AC	85	GLU
3	AC	107	ARG
3	AC	110	GLU
3	AC	121	THR
3	AC	128	VAL
3	AC	144	LEU
3	AC	161	GLU
3	AC	168	TYR
3	AC	178	LEU
3	AC	185	ASN
3	AC	207	ILE
4	AD	17	THR
4	AD	22	LYS
4	AD	26	ARG
4	AD	44	ARG
4	AD	143	VAL
4	AD	194	ASP
5	AE	11	LEU
5	AE	14	LYS
5	AE	46	VAL
5	AE	69	ARG
5	AE	74	VAL
5	AE	76	LEU
5	AE	78	ASN
5	AE	82	GLN
5	AE	94	VAL
5	AE	100	SER
5	AE	101	GLU
5	AE	123	VAL
5	AE	124	LEU
5	AE	126	LYS
5	AE	134	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	AE	142	ASP
5	AE	162	GLU
5	AE	164	ILE
6	AF	36	ILE
6	AF	39	LEU
6	AF	69	GLU
6	AF	71	ILE
6	AF	93	LYS
7	AG	11	LYS
7	AG	13	LEU
7	AG	18	PHE
7	AG	22	LEU
7	AG	59	LEU
7	AG	63	GLU
7	AG	89	VAL
7	AG	95	ARG
7	AG	109	ARG
7	AG	120	LEU
7	AG	124	LEU
7	AG	131	LYS
7	AG	133	THR
7	AG	140	ASP
7	AG	146	GLU
8	AH	3	MET
8	AH	51	VAL
8	AH	54	ASP
8	AH	55	THR
8	AH	60	GLU
8	AH	76	GLN
8	AH	77	ARG
8	AH	80	ARG
8	AH	83	LEU
8	AH	90	ASP
8	AH	96	MET
8	AH	107	SER
9	AI	9	THR
9	AI	11	ARG
9	AI	46	MET
9	AI	57	MET
9	AI	61	LEU
9	AI	63	LEU
9	AI	66	THR

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Mol	Chain	Res	Type
9	AI	89	GLU
9	AI	96	SER
9	AI	99	ARG
10	AJ	6	ILE
10	AJ	8	ILE
10	AJ	16	ARG
10	AJ	19	ASP
10	AJ	63	ASP
10	AJ	69	THR
10	AJ	89	ARG
10	AJ	90	LEU
11	AK	16	VAL
11	AK	22	HIS
11	AK	23	ILE
11	AK	65	VAL
11	AK	74	VAL
11	AK	129	VAL
12	AL	24	LEU
12	AL	40	THR
12	AL	55	VAL
12	AL	74	LEU
12	AL	88	LYS
12	AL	90	LEU
12	AL	110	ARG
12	AL	121	ARG
13	AM	7	ILE
13	AM	8	ASN
13	AM	13	LYS
13	AM	17	ILE
13	AM	27	LYS
13	AM	30	SER
13	AM	48	LEU
13	AM	58	ASP
13	AM	63	PHE
13	AM	71	ARG
13	AM	109	ARG
14	AN	59	ARG
14	AN	80	SER
14	AN	100	SER
15	AO	2	SER
15	AO	4	SER
15	AO	24	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	AO	40	GLN
15	AO	62	GLN
15	AO	70	LEU
15	AO	88	ARG
15	AO	89	ARG
16	AP	18	GLN
16	AP	20	VAL
16	AP	33	ILE
16	AP	36	VAL
16	AP	47	GLU
16	AP	48	GLU
17	AQ	5	ILE
17	AQ	21	ILE
17	AQ	33	ILE
17	AQ	38	ILE
17	AQ	40	ARG
17	AQ	75	LEU
18	AR	20	GLU
18	AR	33	ILE
18	AR	36	SER
18	AR	47	THR
18	AR	71	THR
19	AS	5	LEU
19	AS	7	LYS
19	AS	12	ASP
19	AS	13	LEU
19	AS	27	ASP
19	AS	37	ARG
19	AS	52	HIS
19	AS	63	THR
20	AT	5	LYS
20	AT	6	SER
20	AT	12	ILE
20	AT	23	SER
20	AT	27	MET
20	AT	43	ASP
20	AT	44	LYS
20	AT	64	LYS
20	AT	66	LEU
20	AT	84	ASN
21	AU	56	HIS
22	C1	10	ARG

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Mol	Chain	Res	Type
22	C1	23	THR
22	C1	26	THR
23	C2	5	ILE
23	C2	47	VAL
24	C3	1	MET
24	C3	8	SER
24	C3	46	LYS
25	C4	31	HIS
25	C4	52	LYS
25	C4	55	LEU
26	C5	26	ILE
26	C5	34	LYS
27	C0	3	LYS
27	C0	4	THR
27	C0	5	ILE
27	C0	10	THR
27	C0	36	VAL
27	C0	59	GLU
2	BB	8	ASP
2	BB	23	TRP
2	BB	44	GLU
2	BB	70	VAL
2	BB	73	LYS
2	BB	93	ASN
2	BB	105	LYS
2	BB	117	LEU
2	BB	125	THR
2	BB	129	LEU
2	BB	130	THR
2	BB	135	LEU
2	BB	161	LEU
2	BB	167	ASP
2	BB	168	HIS
2	BB	190	ASN
2	BB	205	ASP
2	BB	207	ILE
3	BC	28	GLU
3	BC	33	LEU
3	BC	107	ARG
3	BC	121	THR
3	BC	144	LEU
3	BC	152	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	BC	161	GLU
3	BC	168	TYR
3	BC	185	ASN
3	BC	207	ILE
4	BD	17	THR
4	BD	22	LYS
4	BD	26	ARG
4	BD	44	ARG
4	BD	47	ARG
4	BD	143	VAL
4	BD	153	SER
4	BD	194	ASP
4	BD	206	LYS
5	BE	11	LEU
5	BE	14	LYS
5	BE	24	THR
5	BE	45	ARG
5	BE	46	VAL
5	BE	69	ARG
5	BE	76	LEU
5	BE	81	LEU
5	BE	82	GLN
5	BE	88	VAL
5	BE	94	VAL
5	BE	103	THR
5	BE	114	VAL
5	BE	115	LEU
5	BE	123	VAL
5	BE	124	LEU
5	BE	126	LYS
5	BE	142	ASP
5	BE	157	ARG
5	BE	159	LYS
6	BF	14	GLN
6	BF	36	ILE
6	BF	39	LEU
6	BF	53	LYS
6	BF	68	GLN
6	BF	69	GLU
6	BF	71	ILE
6	BF	79	ARG
6	BF	93	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	BG	4	ARG
7	BG	5	ARG
7	BG	10	ARG
7	BG	18	PHE
7	BG	22	LEU
7	BG	50	LEU
7	BG	59	LEU
7	BG	63	GLU
7	BG	95	ARG
7	BG	109	ARG
7	BG	120	LEU
7	BG	124	LEU
7	BG	131	LYS
7	BG	133	THR
7	BG	146	GLU
8	BH	3	MET
8	BH	60	GLU
8	BH	76	GLN
8	BH	77	ARG
8	BH	80	ARG
8	BH	83	LEU
8	BH	90	ASP
8	BH	96	MET
8	BH	107	SER
9	BI	9	THR
9	BI	11	ARG
9	BI	46	MET
9	BI	57	MET
9	BI	61	LEU
9	BI	63	LEU
9	BI	66	THR
9	BI	89	GLU
9	BI	96	SER
9	BI	99	ARG
9	BI	110	GLN
10	BJ	5	ARG
10	BJ	6	ILE
10	BJ	16	ARG
10	BJ	19	ASP
10	BJ	59	LYS
10	BJ	63	ASP
10	BJ	69	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	BJ	78	GLU
10	BJ	89	ARG
10	BJ	90	LEU
11	BK	16	VAL
11	BK	18	ASP
11	BK	23	ILE
11	BK	31	ILE
11	BK	38	GLN
11	BK	65	VAL
11	BK	72	ASP
11	BK	129	VAL
12	BL	24	LEU
12	BL	44	LYS
12	BL	50	ARG
12	BL	55	VAL
12	BL	58	THR
12	BL	74	LEU
12	BL	82	ILE
12	BL	88	LYS
12	BL	90	LEU
12	BL	110	ARG
12	BL	121	ARG
13	BM	11	ASP
13	BM	16	VAL
13	BM	17	ILE
13	BM	27	LYS
13	BM	30	SER
13	BM	41	GLU
13	BM	48	LEU
13	BM	109	ARG
14	BN	26	GLU
14	BN	59	ARG
14	BN	80	SER
14	BN	100	SER
15	BO	2	SER
15	BO	4	SER
15	BO	24	SER
15	BO	40	GLN
15	BO	62	GLN
15	BO	64	ARG
15	BO	70	LEU
15	BO	87	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	BO	88	ARG
16	BP	18	GLN
16	BP	20	VAL
16	BP	33	ILE
16	BP	36	VAL
16	BP	46	LYS
16	BP	47	GLU
16	BP	48	GLU
17	BQ	16	LYS
17	BQ	17	MET
17	BQ	20	SER
17	BQ	21	ILE
17	BQ	26	GLU
17	BQ	28	PHE
17	BQ	33	ILE
17	BQ	38	ILE
17	BQ	40	ARG
17	BQ	67	LEU
17	BQ	75	LEU
18	BR	33	ILE
18	BR	36	SER
18	BR	47	THR
18	BR	71	THR
19	BS	6	LYS
19	BS	12	ASP
19	BS	13	LEU
19	BS	37	ARG
19	BS	52	HIS
19	BS	63	THR
19	BS	74	PHE
20	BT	5	LYS
20	BT	12	ILE
20	BT	43	ASP
20	BT	54	MET
20	BT	64	LYS
20	BT	66	LEU
20	BT	67	ILE
20	BT	69	LYS
20	BT	86	LEU
21	BU	56	HIS
22	D1	23	THR
23	D2	5	ILE

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Mol	Chain	Res	Type
23	D2	47	VAL
23	D2	48	ILE
24	D3	1	MET
24	D3	8	SER
25	D4	31	HIS
25	D4	52	LYS
25	D4	55	LEU
26	D5	26	ILE
27	D0	3[A]	LYS
27	D0	3[B]	LYS
27	D0	10	THR
27	D0	25	LEU
27	D0	36	VAL
27	D0	58	GLU
27	D0	59	GLU
29	CC	23	GLU
29	CC	43	ARG
29	CC	59	LYS
29	CC	97	LYS
29	CC	118	SER
29	CC	130	LEU
29	CC	133	ARG
29	CC	156	ARG
29	CC	157	SER
29	CC	168	ASP
29	CC	195	VAL
29	CC	204	VAL
29	CC	205	LEU
29	CC	236	GLU
29	CC	266	PHE
30	CD	4	LEU
30	CD	18	ASP
30	CD	52	THR
30	CD	89	GLU
30	CD	92	VAL
30	CD	95	SER
30	CD	137	SER
30	CD	183	GLU
29	DC	23	GLU
29	DC	59	LYS
29	DC	70	ASN
29	DC	97	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
29	DC	118	SER
29	DC	130	LEU
29	DC	133	ARG
29	DC	156	ARG
29	DC	168	ASP
32	DD	18	ASP
32	DD	52	THR
32	DD	86	GLU
32	DD	89	GLU
32	DD	92	VAL
32	DD	95	SER
32	DD	183	GLU
33	CE	7	ASP
33	CE	12	LEU
33	CE	25	GLU
33	CE	40	ARG
33	CE	44	ARG
33	CE	73	ILE
33	CE	78	TRP
33	CE	83	VAL
33	CE	107	SER
33	CE	122	GLU
33	CE	127	GLU
33	CE	149	ILE
33	CE	152	GLU
33	CE	171	ASP
33	CE	179	SER
33	CE	189	THR
34	CF	27	GLN
34	CF	35	THR
34	CF	36	LEU
34	CF	49	LEU
34	CF	66	LEU
34	CF	72	LYS
34	CF	94	GLU
34	CF	117	LEU
34	CF	123	ASP
34	CF	134	GLU
34	CF	141	ILE
34	CF	149	VAL
34	CF	152	LEU
34	CF	174	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
35	CG	11	VAL
35	CG	18	LYS
35	CG	72	LEU
35	CG	155	GLU
36	CH	7	ASP
36	CH	15	LEU
36	CH	21	VAL
36	CH	50	ARG
36	CH	51	ARG
36	CH	53	GLU
36	CH	54	LEU
36	CH	55	GLU
36	CH	58	LEU
36	CH	89	LYS
36	CH	112	LYS
37	CJ	13	VAL
37	CJ	28	LEU
37	CJ	35	ILE
37	CJ	53	LEU
37	CJ	55	ILE
37	CJ	113	LYS
38	CK	11	VAL
38	CK	124	VAL
38	CK	142	ILE
39	CL	21	CYS
39	CL	32	TYR
39	CL	49	ARG
39	CL	58	LEU
39	CL	70	ARG
39	CL	89	ASN
39	CL	108	ARG
40	CM	2	ARG
40	CM	42	SER
40	CM	94	THR
40	CM	99	ASN
40	CM	100	ILE
40	CM	103	ILE
40	CM	107	PHE
40	CM	120	VAL
40	CM	125	LEU
41	CN	41	LEU
41	CN	59	ARG

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Mol	Chain	Res	Type
41	CN	75	GLU
41	CN	78	LEU
41	CN	88	ASN
41	CN	100	LYS
41	CN	115	GLU
42	CO	2	ARG
42	CO	6	SER
42	CO	14	SER
42	CO	18	GLN
42	CO	22	ARG
42	CO	51	LEU
42	CO	76	VAL
42	CO	94	TYR
42	CO	95	THR
43	CP	3	LYS
43	CP	25	ARG
43	CP	28	VAL
43	CP	31	THR
43	CP	38	GLN
43	CP	48	LEU
43	CP	78	VAL
44	CQ	7	GLN
44	CQ	10	GLN
44	CQ	26	VAL
44	CQ	39	ARG
44	CQ	40	LEU
44	CQ	63	LYS
44	CQ	65	SER
44	CQ	114	LEU
45	CR	5	LYS
45	CR	9	ILE
45	CR	22	LYS
45	CR	51	ARG
45	CR	52	GLN
45	CR	112	LYS
46	CS	29	THR
46	CS	45	GLU
46	CS	46	GLU
47	CT	7	HIS
47	CT	29	VAL
47	CT	86	MET
47	CT	99	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
47	CT	109	ASP
48	CU	1	MET
48	CU	2	ILE
48	CU	3	ARG
48	CU	18	GLU
48	CU	30	ILE
48	CU	49	LYS
48	CU	69	ARG
48	CU	73	ARG
49	CV	9	ASP
49	CV	29	LEU
49	CV	52	LEU
49	CV	61	LYS
49	CV	81	ASP
49	CV	98	SER
50	CW	1	MET
50	CW	7	GLU
50	CW	10	LYS
50	CW	14	LYS
50	CW	66	ASP
51	CX	38	VAL
51	CX	39	ARG
51	CX	62	LYS
51	CX	70	GLU
51	CX	77	ARG
51	CX	82	ILE
52	CY	2	SER
52	CY	35	SER
52	CY	44	LYS
52	CY	48	THR
52	CY	66	THR
53	CZ	18	LEU
53	CZ	22	LEU
53	CZ	58	ASN
33	DE	12	LEU
33	DE	107	SER
33	DE	122	GLU
33	DE	127	GLU
33	DE	150	THR
33	DE	179	SER
33	DE	189	THR
34	DF	10	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
34	DF	18	THR
34	DF	27	GLN
34	DF	35	THR
34	DF	49	LEU
34	DF	66	LEU
34	DF	72	LYS
34	DF	94	GLU
34	DF	117	LEU
34	DF	141	ILE
34	DF	149	VAL
34	DF	152	LEU
34	DF	174	ASP
34	DF	178	ARG
35	DG	3	ARG
35	DG	18	LYS
35	DG	30	ASN
35	DG	72	LEU
35	DG	155	GLU
36	DH	7	ASP
36	DH	15	LEU
36	DH	21	VAL
36	DH	50	ARG
36	DH	53	GLU
36	DH	54	LEU
36	DH	58	LEU
36	DH	89	LYS
36	DH	112	LYS
36	DH	116	ARG
37	DJ	13	VAL
37	DJ	28	LEU
37	DJ	35	ILE
37	DJ	53	LEU
37	DJ	55	ILE
37	DJ	113	LYS
38	DK	1	MET
38	DK	11	VAL
38	DK	124	VAL
38	DK	142	ILE
39	DL	21	CYS
39	DL	32	TYR
39	DL	58	LEU
39	DL	70	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	DL	89	ASN
39	DL	108	ARG
39	DL	110	GLU
39	DL	123	LEU
40	DM	2	ARG
40	DM	94	THR
40	DM	103	ILE
40	DM	107	PHE
40	DM	120	VAL
40	DM	125	LEU
41	DN	6	ARG
41	DN	75	GLU
41	DN	78	LEU
41	DN	88	ASN
41	DN	100	LYS
41	DN	115	GLU
42	DO	2	ARG
42	DO	6	SER
42	DO	14	SER
42	DO	18	GLN
42	DO	22	ARG
42	DO	42	LYS
42	DO	76	VAL
43	DP	1	MET
43	DP	2	ASP
43	DP	3	LYS
43	DP	25	ARG
43	DP	28	VAL
43	DP	31	THR
43	DP	49	VAL
43	DP	78	VAL
44	DQ	7	GLN
44	DQ	10	GLN
44	DQ	26	VAL
44	DQ	40	LEU
44	DQ	63	LYS
44	DQ	65	SER
45	DR	5	LYS
45	DR	9	ILE
45	DR	51	ARG
45	DR	112	LYS
46	DS	29	THR

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Mol	Chain	Res	Type
46	DS	38	VAL
47	DT	86	MET
47	DT	109	ASP
48	DU	1	MET
48	DU	3	ARG
48	DU	16	VAL
48	DU	24	MET
48	DU	33	LYS
48	DU	69	ARG
49	DV	29	LEU
49	DV	52	LEU
49	DV	61	LYS
50	DW	7	GLU
50	DW	53	LYS
50	DW	66	ASP
51	DX	11	ARG
51	DX	38	VAL
51	DX	39	ARG
51	DX	41[A]	ARG
51	DX	41[B]	ARG
51	DX	62	LYS
51	DX	70	GLU
51	DX	77	ARG
51	DX	82	ILE
52	DY	2	SER
52	DY	35	SER
52	DY	44	LYS
52	DY	66	THR
52	DY	71	LEU
53	DZ	22	LEU
54	DI	6	GLN
54	DI	23	LEU
54	DI	47	GLU
54	DI	53	ARG
54	DI	64	VAL
54	DI	67	THR
54	DI	107	GLU
54	DI	117	LEU
54	DI	123	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
2	AB	39	HIS
2	AB	93	ASN
2	AB	94	HIS
2	AB	120	GLN
2	AB	177	ASN
2	AB	178	ASN
3	AC	139	GLN
4	AD	136	GLN
5	AE	89	HIS
6	AF	63	ASN
16	AP	26	ASN
17	AQ	45	HIS
19	AS	57	HIS
20	AT	13	GLN
20	AT	52	ASN
2	BB	39	HIS
2	BB	93	ASN
2	BB	94	HIS
2	BB	120	GLN
2	BB	177	ASN
2	BB	178	ASN
3	BC	139	GLN
5	BE	70	ASN
5	BE	73	ASN
14	BN	66	GLN
16	BP	26	ASN
17	BQ	45	HIS
20	BT	13	GLN
20	BT	48	GLN
20	BT	52	ASN
20	BT	78	ASN
32	DD	167	ASN
34	CF	27	GLN
35	CG	38	ASN
36	CH	135	HIS
37	CJ	43	ASN
37	CJ	94	ASN
43	CP	29	HIS
45	CR	20	GLN
46	CS	12	HIS
47	CT	15	GLN
49	CV	74	ASN
53	CZ	45	GLN

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Mol	Chain	Res	Type
35	DG	101	ASN
35	DG	116	GLN
36	DH	135	HIS
37	DJ	43	ASN
37	DJ	94	ASN
49	DV	54	GLN
54	DI	122	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	256 (16%)	35 (2%)
1	BA	1529/1534 (99%)	259 (16%)	39 (2%)
28	CB	117/120 (97%)	12 (10%)	0
28	DB	119/120 (99%)	11 (9%)	0
31	CA	2892/2904 (99%)	488 (16%)	79 (2%)
55	DA	2880/2904 (99%)	423 (14%)	63 (2%)
All	All	9067/9116 (99%)	1449 (15%)	216 (2%)

All (1449) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G
1	AA	47	C
1	AA	48	C
1	AA	50	A
1	AA	51	A
1	AA	52	C
1	AA	69	G
1	AA	70	U
1	AA	71	A
1	AA	72	A
1	AA	74	A
1	AA	80	A
1	AA	81	A

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Mol	Chain	Res	Type
1	AA	82	G
1	AA	83	C
1	AA	84	U
1	AA	85	U
1	AA	86	G
1	AA	88	U
1	AA	89	U
1	AA	90	C
1	AA	94	G
1	AA	95	C
1	AA	108	G
1	AA	120	A
1	AA	130	A
1	AA	131	A
1	AA	141	G
1	AA	144	G
1	AA	149	A
1	AA	159	G
1	AA	163	C
1	AA	166	U
1	AA	168	G
1	AA	177	G
1	AA	197	A
1	AA	200	G
1	AA	205	A
1	AA	210	C
1	AA	211	G
1	AA	212	G
1	AA	226	G
1	AA	240	G
1	AA	245	U
1	AA	247	G
1	AA	250	A
1	AA	251	G
1	AA	262	A
1	AA	264	C
1	AA	266	G
1	AA	267	C
1	AA	281	G
1	AA	289	G
1	AA	306	A
1	AA	321	A

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Mol	Chain	Res	Type
1	AA	328	C
1	AA	329	A
1	AA	330	C
1	AA	332	G
1	AA	346	G
1	AA	352	C
1	AA	354	G
1	AA	367	U
1	AA	372	C
1	AA	373	A
1	AA	382	A
1	AA	384	G
1	AA	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	438	U
1	AA	439	U
1	AA	457	G
1	AA	458	U
1	AA	466	A
1	AA	467	U
1	AA	468	A
1	AA	474	G
1	AA	479	U
1	AA	481	G
1	AA	484	G
1	AA	486	U
1	AA	495	A
1	AA	496	A
1	AA	511	C
1	AA	518	C
1	AA	524	G
1	AA	527	G7M
1	AA	532	A
1	AA	533	A

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Mol	Chain	Res	Type
1	AA	547	A
1	AA	559	A
1	AA	562	U
1	AA	564	C
1	AA	568	G
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	577	G
1	AA	579	A
1	AA	633	G
1	AA	639	G
1	AA	650	G
1	AA	653	U
1	AA	661	G
1	AA	665	A
1	AA	703	G
1	AA	721	G
1	AA	723	U
1	AA	734	G
1	AA	748	G
1	AA	755	G
1	AA	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	839	C
1	AA	841	C
1	AA	842	U
1	AA	843	U
1	AA	844	G
1	AA	845	A
1	AA	873	A
1	AA	914	A
1	AA	926	G
1	AA	927	G
1	AA	934	C

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Mol	Chain	Res	Type
1	AA	942	G
1	AA	960	U
1	AA	966	2MG
1	AA	969	A
1	AA	971	G
1	AA	975	A
1	AA	976	G
1	AA	977	A
1	AA	992	U
1	AA	993	G
1	AA	996	A
1	AA	1004	A
1	AA	1005	A
1	AA	1009	U
1	AA	1015	G
1	AA	1019	A
1	AA	1026	G
1	AA	1027	C
1	AA	1030	U
1	AA	1031	C
1	AA	1032	G
1	AA	1033	G
1	AA	1036	A
1	AA	1037	C
1	AA	1043	G
1	AA	1052	G
1	AA	1053	G
1	AA	1054	C
1	AA	1065	U
1	AA	1066	C
1	AA	1070	U
1	AA	1086	U
1	AA	1094	G
1	AA	1095	U
1	AA	1101	A
1	AA	1124	G
1	AA	1125	U
1	AA	1127	G
1	AA	1132	C
1	AA	1133	G
1	AA	1136	C
1	AA	1137	C

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Mol	Chain	Res	Type
1	AA	1138	G
1	AA	1139	G
1	AA	1140	C
1	AA	1141	C
1	AA	1143	G
1	AA	1145	A
1	AA	1152	A
1	AA	1158	C
1	AA	1159	U
1	AA	1160	G
1	AA	1168	U
1	AA	1184	G
1	AA	1193	G
1	AA	1196	A
1	AA	1197	A
1	AA	1200	C
1	AA	1202	U
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1215	G
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	1296	C
1	AA	1300	G
1	AA	1302	C
1	AA	1305	G
1	AA	1312	G
1	AA	1317	C
1	AA	1318	A
1	AA	1320	C
1	AA	1323	G
1	AA	1346	A

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Mol	Chain	Res	Type
1	AA	1353	G
1	AA	1363	A
1	AA	1370	G
1	AA	1379	G
1	AA	1381	U
1	AA	1429	A
1	AA	1432	G
1	AA	1441	A
1	AA	1442	G
1	AA	1446	A
1	AA	1447	A
1	AA	1448	C
1	AA	1451	U
1	AA	1452	C
1	AA	1453	G
1	AA	1475	G
1	AA	1487	G
1	AA	1492	A
1	AA	1497	G
1	AA	1503	A
1	AA	1506	U
1	AA	1507	A
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1533	C
1	AA	1534	A
1	BA	4	U
1	BA	5	U
1	BA	6	G
1	BA	9	G
1	BA	22	G
1	BA	32	A
1	BA	39	G
1	BA	47	C
1	BA	48	C
1	BA	50	A
1	BA	51	A
1	BA	52	C
1	BA	69	G
1	BA	70	U
1	BA	71	A

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Mol	Chain	Res	Type
1	BA	72	A
1	BA	74	A
1	BA	82	G
1	BA	83	C
1	BA	84	U
1	BA	85	U
1	BA	87	C
1	BA	88	U
1	BA	89	U
1	BA	90	C
1	BA	94	G
1	BA	95	C
1	BA	108	G
1	BA	120	A
1	BA	130	A
1	BA	131	A
1	BA	141	G
1	BA	144	G
1	BA	149	A
1	BA	159	G
1	BA	163	C
1	BA	166	U
1	BA	168	G
1	BA	177	G
1	BA	197	A
1	BA	200	G
1	BA	205	A
1	BA	210	C
1	BA	211	G
1	BA	212	G
1	BA	226	G
1	BA	240	G
1	BA	245	U
1	BA	247	G
1	BA	250	A
1	BA	251	G
1	BA	262	A
1	BA	264	C
1	BA	266	G
1	BA	267	C
1	BA	281	G
1	BA	289	G

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Mol	Chain	Res	Type
1	BA	306	A
1	BA	321	A
1	BA	328	C
1	BA	329	A
1	BA	330	C
1	BA	332	G
1	BA	346	G
1	BA	352	C
1	BA	354	G
1	BA	367	U
1	BA	372	C
1	BA	373	A
1	BA	382	A
1	BA	384	G
1	BA	406	G
1	BA	411	A
1	BA	412	A
1	BA	413	G
1	BA	421	U
1	BA	422	C
1	BA	424	G
1	BA	429	U
1	BA	430	A
1	BA	438	U
1	BA	439	U
1	BA	451	A
1	BA	457	G
1	BA	458	U
1	BA	467	U
1	BA	468	A
1	BA	474	G
1	BA	481	G
1	BA	484	G
1	BA	486	U
1	BA	495	A
1	BA	496	A
1	BA	511	C
1	BA	518	C
1	BA	524	G
1	BA	527	G7M
1	BA	532	A
1	BA	533	A

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Mol	Chain	Res	Type
1	BA	547	A
1	BA	559	A
1	BA	560	A
1	BA	561	U
1	BA	562	U
1	BA	564	C
1	BA	568	G
1	BA	572	A
1	BA	573	A
1	BA	576	C
1	BA	577	G
1	BA	579	A
1	BA	633	G
1	BA	639	G
1	BA	650	G
1	BA	653	U
1	BA	661	G
1	BA	665	A
1	BA	703	G
1	BA	721	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	873	A

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Mol	Chain	Res	Type
1	BA	914	A
1	BA	926	G
1	BA	927	G
1	BA	934	C
1	BA	942	G
1	BA	960	U
1	BA	963	G
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	992	U
1	BA	993	G
1	BA	996	A
1	BA	1004	A
1	BA	1005	A
1	BA	1008	U
1	BA	1009	U
1	BA	1015	G
1	BA	1019	A
1	BA	1026	G
1	BA	1027	C
1	BA	1030	U
1	BA	1031	C
1	BA	1032	G
1	BA	1033	G
1	BA	1036	A
1	BA	1037	C
1	BA	1043	G
1	BA	1052	G
1	BA	1053	G
1	BA	1054	C
1	BA	1065	U
1	BA	1066	C
1	BA	1070	U
1	BA	1086	U
1	BA	1094	G
1	BA	1095	U
1	BA	1101	A
1	BA	1124	G

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Mol	Chain	Res	Type
1	BA	1125	U
1	BA	1127	G
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	1143	G
1	BA	1145	A
1	BA	1152	A
1	BA	1159	U
1	BA	1160	G
1	BA	1168	U
1	BA	1193	G
1	BA	1196	A
1	BA	1197	A
1	BA	1200	C
1	BA	1202	U
1	BA	1212	U
1	BA	1213	A
1	BA	1214	C
1	BA	1215	G
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	1258	G
1	BA	1260	G
1	BA	1261	A
1	BA	1280	A
1	BA	1281	C
1	BA	1286	U
1	BA	1287	A
1	BA	1296	C
1	BA	1300	G
1	BA	1302	C
1	BA	1305	G

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Mol	Chain	Res	Type
1	BA	1312	G
1	BA	1317	C
1	BA	1318	A
1	BA	1320	C
1	BA	1323	G
1	BA	1346	A
1	BA	1353	G
1	BA	1362	A
1	BA	1363	A
1	BA	1370	G
1	BA	1379	G
1	BA	1381	U
1	BA	1429	A
1	BA	1432	G
1	BA	1441	A
1	BA	1442	G
1	BA	1446	A
1	BA	1447	A
1	BA	1448	C
1	BA	1451	U
1	BA	1452	C
1	BA	1453	G
1	BA	1475	G
1	BA	1487	G
1	BA	1493	A
1	BA	1497	G
1	BA	1503	A
1	BA	1506	U
1	BA	1507	A
1	BA	1517	G
1	BA	1529	G
1	BA	1530	G
1	BA	1533	C
1	BA	1534	A
28	CB	9	G
28	CB	25	U
28	CB	35	C
28	CB	44	G
28	CB	56	G
28	CB	57	A
28	CB	67	G
28	CB	88	C

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Mol	Chain	Res	Type
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	71	A
31	CA	74	A
31	CA	75	G
31	CA	83	A
31	CA	84	A
31	CA	86	G
31	CA	102	U
31	CA	118	A
31	CA	119	A
31	CA	120	U
31	CA	125	A
31	CA	138	U
31	CA	139	U
31	CA	140	C
31	CA	141	G
31	CA	142	A
31	CA	165	A
31	CA	177	G
31	CA	178	G
31	CA	188	G
31	CA	196	A
31	CA	197	A
31	CA	199	A
31	CA	200	U
31	CA	215	G
31	CA	216	A
31	CA	221	A
31	CA	222	A
31	CA	226	A
31	CA	248	G

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Mol	Chain	Res	Type
31	CA	264	C
31	CA	265	A
31	CA	266	G
31	CA	272	A
31	CA	276	U
31	CA	277	G
31	CA	278	A
31	CA	279	A
31	CA	285	G
31	CA	310	A
31	CA	311	A
31	CA	324	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	386	G
31	CA	399	U
31	CA	404	A
31	CA	405	U
31	CA	411	G
31	CA	412	A
31	CA	420	C
31	CA	424	G
31	CA	451	U
31	CA	455	C
31	CA	456	C
31	CA	457	A
31	CA	459	U
31	CA	481	G
31	CA	491	G
31	CA	501	A
31	CA	503	A
31	CA	504	A
31	CA	505	A
31	CA	508	A
31	CA	517	C

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Mol	Chain	Res	Type
31	CA	527	C
31	CA	528	A
31	CA	532	A
31	CA	538	A
31	CA	543	G
31	CA	544	C
31	CA	545	U
31	CA	546	U
31	CA	547	A
31	CA	549	G
31	CA	550	C
31	CA	551	G
31	CA	556	A
31	CA	557	C
31	CA	563	A
31	CA	573	U
31	CA	575	A
31	CA	586	A
31	CA	603	A
31	CA	613	A
31	CA	614	A
31	CA	622	G
31	CA	627	A
31	CA	632	A
31	CA	637	A
31	CA	645	C
31	CA	647	G
31	CA	653	U
31	CA	654	A
31	CA	655	A
31	CA	684	G
31	CA	685	A
31	CA	686	U
31	CA	695	G
31	CA	696	G
31	CA	717	C
31	CA	723	C
31	CA	730	A
31	CA	740	C
31	CA	747	5MU
31	CA	763	G
31	CA	764	A

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Mol	Chain	Res	Type
31	CA	765	C
31	CA	775	G
31	CA	776	G
31	CA	782	A
31	CA	784	G
31	CA	785	G
31	CA	792	A
31	CA	802	A
31	CA	805	G
31	CA	812	C
31	CA	819	A
31	CA	827	U
31	CA	828	U
31	CA	845	A
31	CA	846	U
31	CA	847	U
31	CA	858	G
31	CA	859	G
31	CA	878	A
31	CA	882	G
31	CA	893	C
31	CA	896	A
31	CA	897	C
31	CA	907	G
31	CA	910	A
31	CA	931	U
31	CA	932	U
31	CA	941	A
31	CA	946	C
31	CA	953	G
31	CA	961	C
31	CA	974	G
31	CA	983	A
31	CA	984	A
31	CA	985	C
31	CA	995	C
31	CA	996	A
31	CA	1005	C
31	CA	1012	U
31	CA	1013	C
31	CA	1022	G
31	CA	1025	G

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Mol	Chain	Res	Type
31	CA	1026	G
31	CA	1033	U
31	CA	1040	A
31	CA	1045	C
31	CA	1046	A
31	CA	1047	G
31	CA	1061	U
31	CA	1062	G
31	CA	1068	G
31	CA	1070	A
31	CA	1073	A
31	CA	1083	U
31	CA	1088	A
31	CA	1089	A
31	CA	1090	A
31	CA	1096	A
31	CA	1111	A
31	CA	1112	G
31	CA	1119	U
31	CA	1122	G
31	CA	1128	G
31	CA	1129	A
31	CA	1132	U
31	CA	1133	A
31	CA	1134	A
31	CA	1135	C
31	CA	1136	G
31	CA	1142	A
31	CA	1156	A
31	CA	1168	G
31	CA	1169	A
31	CA	1175	A
31	CA	1176	U
31	CA	1177	G
31	CA	1179	G
31	CA	1180	U
31	CA	1186	G
31	CA	1206	G
31	CA	1212	G
31	CA	1218	G
31	CA	1227	G
31	CA	1236	G

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Mol	Chain	Res	Type
31	CA	1238	G
31	CA	1247	A
31	CA	1248	G
31	CA	1253	A
31	CA	1256	G
31	CA	1262	A
31	CA	1266	G
31	CA	1269	A
31	CA	1271	G
31	CA	1272	A
31	CA	1273	U
31	CA	1300	G
31	CA	1301	A
31	CA	1321	A
31	CA	1329	U
31	CA	1330	C
31	CA	1344	U
31	CA	1352	U
31	CA	1360	G
31	CA	1365	A
31	CA	1376	C
31	CA	1379	U
31	CA	1380	G
31	CA	1383	A
31	CA	1416	G
31	CA	1417	C
31	CA	1420	A
31	CA	1428	C
31	CA	1452	G
31	CA	1453	A
31	CA	1460	U
31	CA	1478	G
31	CA	1482	G
31	CA	1490	A
31	CA	1491	G
31	CA	1493	C
31	CA	1494	A
31	CA	1497	U
31	CA	1504	A
31	CA	1509	A
31	CA	1510	G
31	CA	1515	A

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Mol	Chain	Res	Type
31	CA	1523	U
31	CA	1529	G
31	CA	1532	A
31	CA	1533	C
31	CA	1534	U
31	CA	1535	A
31	CA	1536	C
31	CA	1537	G
31	CA	1554	U
31	CA	1565	C
31	CA	1567	G
31	CA	1568	G
31	CA	1569	A
31	CA	1578	U
31	CA	1583	A
31	CA	1585	C
31	CA	1607	C
31	CA	1608	A
31	CA	1616	A
31	CA	1647	U
31	CA	1648	U
31	CA	1649	G
31	CA	1654	A
31	CA	1668	A
31	CA	1674	G
31	CA	1675	C
31	CA	1715	G
31	CA	1729	U
31	CA	1730	C
31	CA	1738	G
31	CA	1744	A
31	CA	1750	G
31	CA	1754	A
31	CA	1764	C
31	CA	1773	A
31	CA	1782	U
31	CA	1787	A
31	CA	1791	A
31	CA	1800	C
31	CA	1801	A
31	CA	1808	A
31	CA	1812	U

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Mol	Chain	Res	Type
31	CA	1816	C
31	CA	1822	C
31	CA	1828	G
31	CA	1829	A
31	CA	1870	C
31	CA	1871	A
31	CA	1872	A
31	CA	1873	G
31	CA	1882	U
31	CA	1900	A
31	CA	1901	A
31	CA	1903	G
31	CA	1906	G
31	CA	1907	G
31	CA	1914	C
31	CA	1929	G
31	CA	1930	G
31	CA	1931	U
31	CA	1933	G
31	CA	1937	A
31	CA	1938	A
31	CA	1945	G
31	CA	1955	U
31	CA	1967	C
31	CA	1970	A
31	CA	1972	G
31	CA	1991	U
31	CA	1992	G
31	CA	1993	U
31	CA	1997	C
31	CA	2022	U
31	CA	2023	C
31	CA	2027	G
31	CA	2033	A
31	CA	2035	G
31	CA	2036	C
31	CA	2043	C
31	CA	2046	G
31	CA	2049	G
31	CA	2055	C
31	CA	2056	G
31	CA	2060	A

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Mol	Chain	Res	Type
31	CA	2061	G
31	CA	2062	A
31	CA	2069	G7M
31	CA	2072	C
31	CA	2092	U
31	CA	2093	G
31	CA	2095	A
31	CA	2107	G
31	CA	2110	G
31	CA	2111	U
31	CA	2112	G
31	CA	2113	U
31	CA	2114	A
31	CA	2115	G
31	CA	2117	A
31	CA	2118	U
31	CA	2119	A
31	CA	2120	G
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	2136	G
31	CA	2146	C
31	CA	2147	A
31	CA	2157	G
31	CA	2158	A
31	CA	2159	G
31	CA	2162	G
31	CA	2164	C
31	CA	2165	C
31	CA	2171	A
31	CA	2172	U
31	CA	2173	A
31	CA	2174	C
31	CA	2183	A
31	CA	2190	G

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Mol	Chain	Res	Type
31	CA	2198	A
31	CA	2203	U
31	CA	2204	G
31	CA	2211	A
31	CA	2225	A
31	CA	2226	C
31	CA	2238	G
31	CA	2239	G
31	CA	2259	U
31	CA	2268	A
31	CA	2278	A
31	CA	2280	G
31	CA	2282	G
31	CA	2283	C
31	CA	2286	G
31	CA	2287	A
31	CA	2305	U
31	CA	2311	A
31	CA	2322	A
31	CA	2324	U
31	CA	2325	G
31	CA	2326	C
31	CA	2327	A
31	CA	2333	A
31	CA	2334	U
31	CA	2335	A
31	CA	2345	G
31	CA	2347	C
31	CA	2350	C
31	CA	2354	C
31	CA	2358	A
31	CA	2361	G
31	CA	2383	G
31	CA	2385	C
31	CA	2402	U
31	CA	2403	C
31	CA	2406	A
31	CA	2410	G
31	CA	2424	C
31	CA	2425	A
31	CA	2426	A
31	CA	2429	G

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Mol	Chain	Res	Type
31	CA	2430	A
31	CA	2435	A
31	CA	2441	U
31	CA	2448	A
31	CA	2465	C
31	CA	2474	U
31	CA	2476	A
31	CA	2482	A
31	CA	2491	U
31	CA	2502	G
31	CA	2504	PSU
31	CA	2505	G
31	CA	2518	A
31	CA	2520	C
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	2578	G
31	CA	2582	G
31	CA	2585	U
31	CA	2602	A
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	2693	G
31	CA	2714	G
31	CA	2718	G
31	CA	2719	G
31	CA	2726	A

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Mol	Chain	Res	Type
31	CA	2744	G
31	CA	2748	A
31	CA	2765	A
31	CA	2777	G
31	CA	2778	A
31	CA	2779	U
31	CA	2780	G
31	CA	2791	G
31	CA	2792	A
31	CA	2794	C
31	CA	2799	A
31	CA	2803	G
31	CA	2811	G
31	CA	2813	A
31	CA	2818	U
31	CA	2820	A
31	CA	2821	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	2868	A
31	CA	2883	A
31	CA	2886	A
31	CA	2893	A
31	CA	2894	G
31	CA	2901	C
31	CA	2904	U
28	DB	9	G
28	DB	25	U
28	DB	35	C
28	DB	44	G
28	DB	56	G
28	DB	57	A
28	DB	67	G
28	DB	88	C
28	DB	89	U
28	DB	90	C
28	DB	109	A
55	DA	10	A

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Mol	Chain	Res	Type
55	DA	12	U
55	DA	13	A
55	DA	14	A
55	DA	15	G
55	DA	34	U
55	DA	42	A
55	DA	46	G
55	DA	71	A
55	DA	74	A
55	DA	75	G
55	DA	84	A
55	DA	86	G
55	DA	101	A
55	DA	102	U
55	DA	118	A
55	DA	119	A
55	DA	120	U
55	DA	125	A
55	DA	138	U
55	DA	139	U
55	DA	140	C
55	DA	141	G
55	DA	142	A
55	DA	165	A
55	DA	196	A
55	DA	199	A
55	DA	200	U
55	DA	216	A
55	DA	221	A
55	DA	222	A
55	DA	226	A
55	DA	227	A
55	DA	248	G
55	DA	264	C
55	DA	265	A
55	DA	266	G
55	DA	272	A
55	DA	276	U
55	DA	277	G
55	DA	278	A
55	DA	279	A
55	DA	285	G

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Mol	Chain	Res	Type
55	DA	302	C
55	DA	310	A
55	DA	311	A
55	DA	324	A
55	DA	329	G
55	DA	330	A
55	DA	343	C
55	DA	352	A
55	DA	353	C
55	DA	362	A
55	DA	370	G
55	DA	372	G
55	DA	385	C
55	DA	386	G
55	DA	389	G
55	DA	399	U
55	DA	411	G
55	DA	412	A
55	DA	420	C
55	DA	424	G
55	DA	454	A
55	DA	481	G
55	DA	491	G
55	DA	503	A
55	DA	504	A
55	DA	505	A
55	DA	508	A
55	DA	528	A
55	DA	531	C
55	DA	532	A
55	DA	533	G
55	DA	543	G
55	DA	544	C
55	DA	545	U
55	DA	546	U
55	DA	547	A
55	DA	549	G
55	DA	550	C
55	DA	551	G
55	DA	563	A
55	DA	573	U
55	DA	575	A

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Mol	Chain	Res	Type
55	DA	586	A
55	DA	603	A
55	DA	613	A
55	DA	614	A
55	DA	615	U
55	DA	627	A
55	DA	637	A
55	DA	645	C
55	DA	647	G
55	DA	653	U
55	DA	654	A
55	DA	655	A
55	DA	686	U
55	DA	717	C
55	DA	723	C
55	DA	730	A
55	DA	738	G
55	DA	747	5MU
55	DA	763	G
55	DA	775	G
55	DA	776	G
55	DA	782	A
55	DA	784	G
55	DA	785	G
55	DA	790	U
55	DA	805	G
55	DA	812	C
55	DA	827	U
55	DA	828	U
55	DA	858	G
55	DA	859	G
55	DA	860	U
55	DA	866	A
55	DA	878	A
55	DA	882	G
55	DA	885	C
55	DA	893	C
55	DA	896	A
55	DA	897	C
55	DA	907	G
55	DA	910	A
55	DA	914	G

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Mol	Chain	Res	Type
55	DA	915	C
55	DA	931	U
55	DA	932	U
55	DA	946	C
55	DA	953	G
55	DA	957	C
55	DA	961	C
55	DA	974	G
55	DA	983	A
55	DA	984	A
55	DA	985	C
55	DA	996	A
55	DA	1005	C
55	DA	1012	U
55	DA	1013	C
55	DA	1022	G
55	DA	1026	G
55	DA	1033	U
55	DA	1040	A
55	DA	1047	G
55	DA	1061	U
55	DA	1062	G
55	DA	1068	G
55	DA	1070	A
55	DA	1073	A
55	DA	1083	U
55	DA	1088	A
55	DA	1089	A
55	DA	1090	A
55	DA	1096	A
55	DA	1112	G
55	DA	1119	U
55	DA	1128	G
55	DA	1129	A
55	DA	1132	U
55	DA	1133	A
55	DA	1134	A
55	DA	1135	C
55	DA	1136	G
55	DA	1142	A
55	DA	1156	A
55	DA	1168	G

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Mol	Chain	Res	Type
55	DA	1171	G
55	DA	1172	C
55	DA	1174	U
55	DA	1176	U
55	DA	1177	G
55	DA	1206	G
55	DA	1212	G
55	DA	1218	G
55	DA	1227	G
55	DA	1236	G
55	DA	1238	G
55	DA	1253	A
55	DA	1256	G
55	DA	1271	G
55	DA	1272	A
55	DA	1273	U
55	DA	1300	G
55	DA	1301	A
55	DA	1302	A
55	DA	1321	A
55	DA	1329	U
55	DA	1352	U
55	DA	1360	G
55	DA	1365	A
55	DA	1379	U
55	DA	1380	G
55	DA	1383	A
55	DA	1416	G
55	DA	1417	C
55	DA	1420	A
55	DA	1427	A
55	DA	1428	C
55	DA	1435	G
55	DA	1452	G
55	DA	1453	A
55	DA	1460	U
55	DA	1478	G
55	DA	1482	G
55	DA	1490	A
55	DA	1491	G
55	DA	1493	C
55	DA	1494	A

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Mol	Chain	Res	Type
55	DA	1497	U
55	DA	1504	A
55	DA	1508	A
55	DA	1509	A
55	DA	1510	G
55	DA	1515	A
55	DA	1523	U
55	DA	1529	G
55	DA	1532	A
55	DA	1533	C
55	DA	1534	U
55	DA	1535	A
55	DA	1536	C
55	DA	1537	G
55	DA	1554	U
55	DA	1569	A
55	DA	1578	U
55	DA	1583	A
55	DA	1585	C
55	DA	1607	C
55	DA	1608	A
55	DA	1609	A
55	DA	1647	U
55	DA	1648	U
55	DA	1649	G
55	DA	1674	G
55	DA	1715	G
55	DA	1729	U
55	DA	1730	C
55	DA	1738	G
55	DA	1744	A
55	DA	1750	G
55	DA	1754	A
55	DA	1764	C
55	DA	1773	A
55	DA	1782	U
55	DA	1800	C
55	DA	1801	A
55	DA	1808	A
55	DA	1812	U
55	DA	1816	C
55	DA	1828	G

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Mol	Chain	Res	Type
55	DA	1829	A
55	DA	1870	C
55	DA	1871	A
55	DA	1872	A
55	DA	1873	G
55	DA	1882	U
55	DA	1900	A
55	DA	1906	G
55	DA	1907	G
55	DA	1913	A
55	DA	1914	C
55	DA	1929	G
55	DA	1930	G
55	DA	1931	U
55	DA	1932	A
55	DA	1937	A
55	DA	1938	A
55	DA	1945	G
55	DA	1955	U
55	DA	1965	C
55	DA	1967	C
55	DA	1970	A
55	DA	1972	G
55	DA	1991	U
55	DA	1993	U
55	DA	1997	C
55	DA	2023	C
55	DA	2031	A
55	DA	2033	A
55	DA	2043	C
55	DA	2055	C
55	DA	2056	G
55	DA	2058	A
55	DA	2060	A
55	DA	2061	G
55	DA	2062	A
55	DA	2069	G7M
55	DA	2093	G
55	DA	2097	A
55	DA	2105	U
55	DA	2107	G
55	DA	2111	U

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Mol	Chain	Res	Type
55	DA	2112	G
55	DA	2113	U
55	DA	2116	G
55	DA	2117	A
55	DA	2118	U
55	DA	2119	A
55	DA	2120	G
55	DA	2123	G
55	DA	2125	G
55	DA	2126	A
55	DA	2127	G
55	DA	2128	G
55	DA	2131	U
55	DA	2132	U
55	DA	2133	G
55	DA	2134	A
55	DA	2135	A
55	DA	2145	C
55	DA	2146	C
55	DA	2148	G
55	DA	2158	A
55	DA	2159	G
55	DA	2160	C
55	DA	2161	C
55	DA	2162	G
55	DA	2163	A
55	DA	2164	C
55	DA	2165	C
55	DA	2167	U
55	DA	2168	G
55	DA	2169	A
55	DA	2170	A
55	DA	2171	A
55	DA	2172	U
55	DA	2173	A
55	DA	2178	C
55	DA	2179	C
55	DA	2181	U
55	DA	2183	A
55	DA	2185	U
55	DA	2186	G
55	DA	2190	G

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Mol	Chain	Res	Type
55	DA	2198	A
55	DA	2203	U
55	DA	2204	G
55	DA	2211	A
55	DA	2225	A
55	DA	2238	G
55	DA	2239	G
55	DA	2268	A
55	DA	2278	A
55	DA	2280	G
55	DA	2283	C
55	DA	2287	A
55	DA	2305	U
55	DA	2308	G
55	DA	2322	A
55	DA	2324	U
55	DA	2325	G
55	DA	2327	A
55	DA	2333	A
55	DA	2334	U
55	DA	2335	A
55	DA	2345	G
55	DA	2347	C
55	DA	2350	C
55	DA	2383	G
55	DA	2385	C
55	DA	2402	U
55	DA	2406	A
55	DA	2407	A
55	DA	2424	C
55	DA	2425	A
55	DA	2435	A
55	DA	2441	U
55	DA	2448	A
55	DA	2474	U
55	DA	2476	A
55	DA	2480	C
55	DA	2491	U
55	DA	2502	G
55	DA	2504	PSU
55	DA	2505	G
55	DA	2518	A

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Mol	Chain	Res	Type
55	DA	2520	C
55	DA	2529	G
55	DA	2535	G
55	DA	2547	A
55	DA	2556	C
55	DA	2566	A
55	DA	2567	G
55	DA	2573	C
55	DA	2585	U
55	DA	2602	A
55	DA	2603	G
55	DA	2609	U
55	DA	2613	U
55	DA	2629	U
55	DA	2630	G
55	DA	2661	G
55	DA	2663	G
55	DA	2689	U
55	DA	2690	U
55	DA	2714	G
55	DA	2726	A
55	DA	2744	G
55	DA	2748	A
55	DA	2765	A
55	DA	2777	G
55	DA	2778	A
55	DA	2779	U
55	DA	2780	G
55	DA	2791	G
55	DA	2792	A
55	DA	2798	U
55	DA	2799	A
55	DA	2803	G
55	DA	2813	A
55	DA	2818	U
55	DA	2820	A
55	DA	2821	A
55	DA	2826	A
55	DA	2835	A
55	DA	2861	U
55	DA	2867	G
55	DA	2883	A

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Mol	Chain	Res	Type
55	DA	2891	U
55	DA	2901	C

All (216) 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	94	G
1	AA	209	U
1	AA	305	G
1	AA	367	U
1	AA	372	C
1	AA	413	G
1	AA	422	C
1	AA	429	U
1	AA	438	U
1	AA	653	U
1	AA	702	A
1	AA	733	G
1	AA	793	U
1	AA	841	C
1	AA	884	U
1	AA	992	U
1	AA	1086	U
1	AA	1129	C
1	AA	1136	C
1	AA	1137	C
1	AA	1139	G
1	AA	1140	C
1	AA	1225	A
1	AA	1239	A
1	AA	1281	C
1	AA	1297	G
1	AA	1299	A
1	AA	1301	U
1	AA	1432	G
1	AA	1447	A
1	AA	1452	C
1	BA	5	U

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Mol	Chain	Res	Type
1	BA	70	U
1	BA	89	U
1	BA	94	G
1	BA	183	C
1	BA	209	U
1	BA	246	A
1	BA	305	G
1	BA	372	C
1	BA	422	C
1	BA	429	U
1	BA	438	U
1	BA	559	A
1	BA	560	A
1	BA	561	U
1	BA	653	U
1	BA	702	A
1	BA	733	G
1	BA	793	U
1	BA	842	U
1	BA	844	G
1	BA	884	U
1	BA	992	U
1	BA	1086	U
1	BA	1129	C
1	BA	1136	C
1	BA	1137	C
1	BA	1139	G
1	BA	1140	C
1	BA	1225	A
1	BA	1281	C
1	BA	1297	G
1	BA	1299	A
1	BA	1301	U
1	BA	1362	A
1	BA	1432	G
1	BA	1447	A
1	BA	1452	C
1	BA	1493	A
31	CA	125	A
31	CA	138	U
31	CA	139	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	271	G
31	CA	278	A
31	CA	310	A
31	CA	371	A
31	CA	403	U
31	CA	404	A
31	CA	411	G
31	CA	455	C
31	CA	503	A
31	CA	527	C
31	CA	555	G
31	CA	685	A
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	1061	U
31	CA	1069	A
31	CA	1070	A
31	CA	1088	A
31	CA	1089	A
31	CA	1111	A
31	CA	1128	G
31	CA	1133	A
31	CA	1141	U
31	CA	1253	A
31	CA	1286	A
31	CA	1288	G
31	CA	1300	G
31	CA	1324	G
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

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Mol	Chain	Res	Type
31	CA	1536	C
31	CA	1567	G
31	CA	1607	C
31	CA	1647	U
31	CA	1818	U
31	CA	1870	C
31	CA	1900	A
31	CA	1913	A
31	CA	2035	G
31	CA	2062	A
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	2238	G
31	CA	2275	C
31	CA	2282	G
31	CA	2286	G
31	CA	2324	U
31	CA	2326	C
31	CA	2423	U
31	CA	2425	A
31	CA	2581	G
31	CA	2680	U
31	CA	2779	U
31	CA	2820	A
31	CA	2849	U
31	CA	2867	G
31	CA	2873	A
31	CA	2893	A
55	DA	125	A
55	DA	138	U
55	DA	141	G
55	DA	196	A
55	DA	199	A
55	DA	271	G
55	DA	278	A
55	DA	310	A
55	DA	371	A

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Mol	Chain	Res	Type
55	DA	403	U
55	DA	503	A
55	DA	627	A
55	DA	764	A
55	DA	784	G
55	DA	961	C
55	DA	984	A
55	DA	1061	U
55	DA	1069	A
55	DA	1070	A
55	DA	1088	A
55	DA	1089	A
55	DA	1128	G
55	DA	1133	A
55	DA	1141	U
55	DA	1142	A
55	DA	1171	G
55	DA	1286	A
55	DA	1300	G
55	DA	1301	A
55	DA	1320	C
55	DA	1490	A
55	DA	1497	U
55	DA	1509	A
55	DA	1535	A
55	DA	1565	C
55	DA	1607	C
55	DA	1609	A
55	DA	1647	U
55	DA	1870	C
55	DA	1900	A
55	DA	2062	A
55	DA	2097	A
55	DA	2116	G
55	DA	2119	A
55	DA	2127	G
55	DA	2146	C
55	DA	2157	G
55	DA	2158	A
55	DA	2162	G
55	DA	2164	C
55	DA	2238	G

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Mol	Chain	Res	Type
55	DA	2275	C
55	DA	2282	G
55	DA	2286	G
55	DA	2311	A
55	DA	2324	U
55	DA	2406	A
55	DA	2423	U
55	DA	2585	U
55	DA	2779	U
55	DA	2798	U
55	DA	2820	A
55	DA	2873	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	2MG	AA	1207	1	18,26,27	1.06	1 (5%)	21,38,41	2.46	4 (19%)
1	4OC	AA	1402	1	15,23,24	0.79	1 (6%)	21,32,35	1.18	2 (9%)
1	5MC	AA	1407	1	14,22,23	0.84	1 (7%)	17,32,35	0.76	1 (5%)
1	UR3	AA	1498	1	13,22,23	1.04	1 (7%)	18,32,35	0.58	0
1	2MG	AA	1516	1	18,26,27	1.22	2 (11%)	21,38,41	2.39	3 (14%)
1	MA6	AA	1518	1	18,26,27	0.68	0	15,38,41	0.61	0
1	MA6	AA	1519	1	18,26,27	0.85	1 (5%)	15,38,41	0.64	0
1	PSU	AA	516	1,56	15,21,22	1.26	2 (13%)	16,30,33	3.48	2 (12%)
1	G7M	AA	527	1	18,26,27	1.10	2 (11%)	21,39,42	3.43	5 (23%)
1	2MG	AA	966	1	18,26,27	1.12	1 (5%)	21,38,41	2.49	3 (14%)
1	5MC	AA	967	1	14,22,23	0.82	0	17,32,35	0.64	1 (5%)
12	D2T	AL	89	12	4,9,10	0.55	0	4,11,13	1.70	1 (25%)
1	2MG	BA	1207	1	18,26,27	1.13	2 (11%)	21,38,41	2.50	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4OC	BA	1402	1	15,23,24	0.76	0	21,32,35	1.17	2 (9%)
1	5MC	BA	1407	1	14,22,23	0.91	1 (7%)	17,32,35	0.74	1 (5%)
1	UR3	BA	1498	1	13,22,23	0.98	1 (7%)	18,32,35	0.55	0
1	2MG	BA	1516	1	18,26,27	1.15	2 (11%)	21,38,41	2.39	3 (14%)
1	MA6	BA	1518	1	18,26,27	0.65	0	15,38,41	0.53	0
1	MA6	BA	1519	1	18,26,27	0.82	0	15,38,41	0.64	0
1	PSU	BA	516	1	15,21,22	1.23	2 (13%)	16,30,33	3.48	2 (12%)
1	G7M	BA	527	1	18,26,27	1.04	1 (5%)	21,39,42	3.54	6 (28%)
1	2MG	BA	966	1	18,26,27	1.07	1 (5%)	21,38,41	2.54	4 (19%)
1	5MC	BA	967	1	14,22,23	0.80	0	17,32,35	0.68	1 (5%)
12	D2T	BL	89	12	4,9,10	0.60	0	4,11,13	1.72	1 (25%)
31	6MZ	CA	1618	31	17,25,26	0.82	1 (5%)	15,36,39	0.81	1 (6%)
31	2MG	CA	1835	31	18,26,27	1.13	1 (5%)	21,38,41	2.44	4 (19%)
31	PSU	CA	1911	31	15,21,22	1.16	2 (13%)	16,30,33	3.48	1 (6%)
31	3TD	CA	1915	31	15,22,23	1.11	2 (13%)	17,32,35	1.01	1 (5%)
31	PSU	CA	1917	31	15,21,22	1.11	2 (13%)	16,30,33	3.49	1 (6%)
31	5MU	CA	1939	31	13,22,23	1.10	1 (7%)	16,32,35	4.75	3 (18%)
31	5MC	CA	1962	31	14,22,23	0.85	1 (7%)	17,32,35	0.67	1 (5%)
31	6MZ	CA	2030	31	17,25,26	0.84	0	15,36,39	0.93	1 (6%)
31	G7M	CA	2069	31	18,26,27	0.90	1 (5%)	21,39,42	3.62	6 (28%)
31	OMG	CA	2251	31	18,26,27	1.10	1 (5%)	21,38,41	2.74	4 (19%)
31	2MG	CA	2445	31	18,26,27	1.16	2 (11%)	21,38,41	2.62	4 (19%)
31	PSU	CA	2457	31	15,21,22	1.30	2 (13%)	16,30,33	3.46	2 (12%)
31	OMC	CA	2498	31,56	15,22,23	0.79	1 (6%)	20,31,34	0.47	0
31	2MA	CA	2503	31	17,25,26	0.89	1 (5%)	18,37,40	1.15	2 (11%)
31	PSU	CA	2504	31	15,21,22	1.18	2 (13%)	16,30,33	3.41	1 (6%)
31	OMU	CA	2552	31	14,22,23	1.17	2 (14%)	19,31,34	2.92	2 (10%)
31	PSU	CA	2580	31	15,21,22	1.21	3 (20%)	16,30,33	3.59	3 (18%)
31	PSU	CA	2605	31	15,21,22	1.26	2 (13%)	16,30,33	3.55	3 (18%)
31	1MG	CA	745	31	17,26,27	1.17	2 (11%)	19,39,42	1.08	2 (10%)
31	PSU	CA	746	31,56	15,21,22	1.30	3 (20%)	16,30,33	3.45	2 (12%)
31	5MU	CA	747	31	13,22,23	1.06	2 (15%)	16,32,35	4.77	3 (18%)
31	PSU	CA	955	31	15,21,22	1.13	2 (13%)	16,30,33	3.48	1 (6%)
41	4D4	CN	81	41	7,11,12	0.64	0	5,13,15	0.83	0
55	6MZ	DA	1618	55	17,25,26	0.91	1 (5%)	15,36,39	0.68	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
55	2MG	DA	1835	55	18,26,27	0.99	1 (5%)	21,38,41	2.46	4 (19%)
55	PSU	DA	1911	55	15,21,22	1.19	2 (13%)	16,30,33	3.45	1 (6%)
55	3TD	DA	1915	55	15,22,23	1.09	2 (13%)	17,32,35	1.07	2 (11%)
55	PSU	DA	1917	55	15,21,22	1.22	2 (13%)	16,30,33	3.53	1 (6%)
55	5MU	DA	1939	55	13,22,23	1.45	3 (23%)	16,32,35	4.71	3 (18%)
55	5MC	DA	1962	55	14,22,23	0.96	1 (7%)	17,32,35	0.70	1 (5%)
55	6MZ	DA	2030	55	17,25,26	1.27	2 (11%)	15,36,39	0.87	1 (6%)
55	G7M	DA	2069	55	18,26,27	0.94	1 (5%)	21,39,42	3.20	5 (23%)
55	OMG	DA	2251	55	18,26,27	0.98	1 (5%)	21,38,41	2.64	4 (19%)
55	2MG	DA	2445	55	18,26,27	1.40	2 (11%)	21,38,41	2.53	4 (19%)
55	H2U	DA	2449	55	17,21,22	0.36	0	23,30,33	0.45	0
55	PSU	DA	2457	55	15,21,22	1.52	3 (20%)	16,30,33	3.50	2 (12%)
55	OMC	DA	2498	55,56	15,22,23	0.96	1 (6%)	20,31,34	0.58	0
55	2MA	DA	2503	55,56	17,25,26	0.93	1 (5%)	18,37,40	1.37	4 (22%)
55	PSU	DA	2504	55	15,21,22	1.24	2 (13%)	16,30,33	3.46	1 (6%)
55	OMU	DA	2552	55	14,22,23	1.12	2 (14%)	19,31,34	2.90	2 (10%)
55	PSU	DA	2580	55	15,21,22	1.55	5 (33%)	16,30,33	3.52	2 (12%)
55	PSU	DA	2604	55	15,21,22	1.77	5 (33%)	16,30,33	3.56	2 (12%)
55	PSU	DA	2605	55	15,21,22	1.35	3 (20%)	16,30,33	3.56	2 (12%)
55	1MG	DA	745	55	17,26,27	0.96	0	19,39,42	1.04	2 (10%)
55	PSU	DA	746	55,56	15,21,22	1.62	4 (26%)	16,30,33	3.56	2 (12%)
55	5MU	DA	747	55	13,22,23	1.15	2 (15%)	16,32,35	4.74	2 (12%)
55	PSU	DA	955	55	15,21,22	1.44	3 (20%)	16,30,33	3.46	1 (6%)
32	MEQ	DD	150[A]	32	7,9,10	0.46	0	8,10,12	1.32	2 (25%)
32	MEQ	DD	150[B]	32	7,9,10	1.17	1 (14%)	8,10,12	1.71	3 (37%)
41	4D4	DN	81[A]	-	7,11,12	0.87	0	5,13,15	0.90	0
41	4D4	DN	81[B]	-	7,11,12	1.08	1 (14%)	5,13,15	0.80	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	AA	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	AA	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	AA	516	1,56	-	0/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	0/3/25/26	0/3/3/3
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
1	5MC	AA	967	1	-	0/3/25/26	0/2/2/2
12	D2T	AL	89	12	-	0/2/12/14	0/0/0/0
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	BA	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	BA	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	BA	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	BA	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	BA	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
1	G7M	BA	527	1	-	0/3/25/26	0/3/3/3
1	2MG	BA	966	1	-	0/5/27/28	0/3/3/3
1	5MC	BA	967	1	-	0/3/25/26	0/2/2/2
12	D2T	BL	89	12	-	0/2/12/14	0/0/0/0
31	6MZ	CA	1618	31	-	0/5/27/28	0/3/3/3
31	2MG	CA	1835	31	-	0/5/27/28	0/3/3/3
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
31	5MU	CA	1939	31	-	0/3/25/26	0/2/2/2
31	5MC	CA	1962	31	-	0/3/25/26	0/2/2/2
31	6MZ	CA	2030	31	-	0/5/27/28	0/3/3/3
31	G7M	CA	2069	31	-	0/3/25/26	0/3/3/3
31	OMG	CA	2251	31	-	0/5/27/28	0/3/3/3
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
31	OMC	CA	2498	31,56	-	0/5/27/28	0/2/2/2
31	2MA	CA	2503	31	-	0/3/25/26	0/3/3/3
31	PSU	CA	2504	31	-	0/7/25/26	0/2/2/2
31	OMU	CA	2552	31	-	0/5/27/28	0/2/2/2
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
31	PSU	CA	746	31,56	-	0/7/25/26	0/2/2/2
31	5MU	CA	747	31	-	0/3/25/26	0/2/2/2

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

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	2604	PSU	C5-C1'	-3.68	1.49	1.52
55	DA	746	PSU	O4'-C1'	-3.67	1.38	1.44
55	DA	2030	6MZ	C2'-C1'	-3.22	1.48	1.53
55	DA	2457	PSU	C5-C1'	-3.20	1.49	1.52
55	DA	955	PSU	C2'-C1'	-3.08	1.50	1.53
55	DA	1939	5MU	C2'-C1'	-3.03	1.48	1.53
55	DA	2030	6MZ	O4'-C1'	-2.92	1.37	1.41
55	DA	2605	PSU	C2'-C1'	-2.77	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	2503	2MA	C8-N7	-2.57	1.29	1.34
55	DA	2580	PSU	C5-C1'	-2.48	1.50	1.52
55	DA	2580	PSU	C6-C5	-2.42	1.35	1.38
55	DA	2604	PSU	C2'-C1'	-2.35	1.51	1.53
55	DA	2604	PSU	C6-C5	-2.27	1.35	1.38
31	CA	2503	2MA	C8-N7	-2.27	1.30	1.34
55	DA	2457	PSU	C6-C5	-2.24	1.35	1.38
55	DA	955	PSU	C6-C5	-2.23	1.35	1.38
55	DA	2504	PSU	C6-C5	-2.21	1.35	1.38
55	DA	746	PSU	C6-C5	-2.21	1.35	1.38
55	DA	2604	PSU	O3'-C3'	-2.21	1.37	1.43
31	CA	1915	3TD	C6-C5	-2.21	1.35	1.38
31	CA	955	PSU	C6-C5	-2.20	1.35	1.38
55	DA	1911	PSU	C6-C5	-2.20	1.35	1.38
1	BA	1407	5MC	C6-C5	-2.20	1.34	1.40
1	AA	1407	5MC	C6-C5	-2.19	1.34	1.40
1	AA	516	PSU	C6-C5	-2.16	1.35	1.38
1	AA	527	G7M	O3'-C3'	-2.16	1.37	1.43
31	CA	2504	PSU	C6-C5	-2.15	1.35	1.38
31	CA	1917	PSU	C6-C5	-2.15	1.35	1.38
31	CA	2457	PSU	C6-C5	-2.13	1.35	1.38
31	CA	2580	PSU	O4'-C1'	-2.11	1.41	1.44
55	DA	2580	PSU	O4'-C1'	-2.11	1.41	1.44
55	DA	747	5MU	C6-C5	-2.10	1.34	1.40
55	DA	2580	PSU	C2'-C1'	-2.10	1.51	1.53
55	DA	1962	5MC	C6-C5	-2.10	1.34	1.40
55	DA	2605	PSU	C6-C5	-2.09	1.35	1.38
55	DA	1915	3TD	C6-C5	-2.07	1.35	1.38
31	CA	1618	6MZ	C8-N7	-2.07	1.30	1.34
1	BA	516	PSU	C6-C5	-2.07	1.35	1.38
31	CA	2580	PSU	C6-C5	-2.07	1.35	1.38
55	DA	746	PSU	C2'-C1'	-2.06	1.51	1.53
55	DA	1917	PSU	C6-C5	-2.06	1.35	1.38
31	CA	2605	PSU	C6-C5	-2.05	1.35	1.38
31	CA	746	PSU	O4'-C1'	-2.05	1.41	1.44
31	CA	1911	PSU	C6-C5	-2.05	1.35	1.38
55	DA	1939	5MU	C6-C5	-2.04	1.34	1.40
31	CA	746	PSU	C6-C5	-2.03	1.35	1.38
1	AA	1519	MA6	O3'-C3'	-2.03	1.38	1.43
31	CA	1962	5MC	C6-C5	-2.03	1.34	1.40
55	DA	1618	6MZ	C8-N7	-2.02	1.30	1.34
31	CA	747	5MU	C6-C5	-2.01	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	745	1MG	C6-N1	2.00	1.41	1.38
1	AA	1402	4OC	C6-N1	2.02	1.38	1.35
31	CA	2498	OMC	C6-N1	2.02	1.38	1.35
55	DA	2552	OMU	C6-N1	2.02	1.38	1.35
31	CA	2445	2MG	C6-C5	2.09	1.45	1.41
1	BA	1207	2MG	C6-C5	2.16	1.45	1.41
31	CA	2552	OMU	C6-N1	2.24	1.38	1.35
55	DA	1915	3TD	C4-N3	2.27	1.41	1.38
55	DA	2498	OMC	C6-N1	2.32	1.38	1.35
31	CA	1915	3TD	C4-N3	2.39	1.41	1.38
1	BA	1498	UR3	C4-N3	2.51	1.42	1.38
41	DN	81[B]	4D4	CB-CA	2.51	1.58	1.54
1	AA	1498	UR3	C4-N3	2.58	1.42	1.38
1	BA	1516	2MG	C6-C5	2.63	1.46	1.41
55	DA	1835	2MG	C6-N1	2.77	1.38	1.33
1	AA	1516	2MG	C6-C5	2.79	1.46	1.41
55	DA	2605	PSU	C4-N3	2.92	1.38	1.33
31	CA	2069	G7M	C6-N1	2.96	1.38	1.33
55	DA	2445	2MG	C6-N1	2.97	1.38	1.33
55	DA	2552	OMU	C4-N3	2.97	1.38	1.33
32	DD	150[B]	MEQ	CB-CA	2.97	1.57	1.53
55	DA	2445	2MG	C6-C5	3.02	1.47	1.41
55	DA	2604	PSU	C4-N3	3.05	1.38	1.33
1	AA	527	G7M	C6-N1	3.06	1.38	1.33
55	DA	2069	G7M	C6-N1	3.09	1.38	1.33
31	CA	747	5MU	C4-N3	3.09	1.38	1.33
31	CA	1939	5MU	C4-N3	3.10	1.38	1.33
55	DA	2251	OMG	C6-N1	3.11	1.38	1.33
55	DA	1939	5MU	C4-N3	3.12	1.38	1.33
55	DA	955	PSU	C4-N3	3.14	1.38	1.33
31	CA	2251	OMG	C6-N1	3.15	1.38	1.33
31	CA	2580	PSU	C4-N3	3.16	1.38	1.33
1	BA	527	G7M	C6-N1	3.18	1.38	1.33
55	DA	747	5MU	C4-N3	3.20	1.38	1.33
31	CA	1917	PSU	C4-N3	3.23	1.38	1.33
1	BA	1516	2MG	C6-N1	3.23	1.38	1.33
55	DA	1911	PSU	C4-N3	3.23	1.38	1.33
31	CA	955	PSU	C4-N3	3.24	1.38	1.33
31	CA	2605	PSU	C4-N3	3.25	1.38	1.33
55	DA	2580	PSU	C4-N3	3.25	1.38	1.33
31	CA	2445	2MG	C6-N1	3.25	1.38	1.33
1	BA	966	2MG	C6-N1	3.25	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	1917	PSU	C4-N3	3.25	1.38	1.33
31	CA	2552	OMU	C4-N3	3.26	1.38	1.33
1	BA	516	PSU	C4-N3	3.29	1.39	1.33
31	CA	1911	PSU	C4-N3	3.31	1.39	1.33
31	CA	1835	2MG	C6-N1	3.31	1.39	1.33
55	DA	746	PSU	C4-N3	3.32	1.39	1.33
55	DA	2504	PSU	C4-N3	3.34	1.39	1.33
1	AA	1207	2MG	C6-N1	3.34	1.39	1.33
1	BA	1207	2MG	C6-N1	3.35	1.39	1.33
31	CA	2457	PSU	C4-N3	3.37	1.39	1.33
31	CA	745	1MG	C6-C5	3.39	1.47	1.40
31	CA	2504	PSU	C4-N3	3.45	1.39	1.33
1	AA	1516	2MG	C6-N1	3.45	1.39	1.33
31	CA	746	PSU	C4-N3	3.46	1.39	1.33
1	AA	966	2MG	C6-N1	3.48	1.39	1.33
1	AA	516	PSU	C4-N3	3.49	1.39	1.33
55	DA	2457	PSU	C4-N3	3.51	1.39	1.33

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	747	5MU	C5-C4-N3	-12.23	115.08	125.35
55	DA	1939	5MU	C5-C4-N3	-12.12	115.17	125.35
31	CA	747	5MU	C5-C4-N3	-12.12	115.18	125.35
31	CA	1939	5MU	C5-C4-N3	-11.92	115.34	125.35
31	CA	2069	G7M	C5-C6-N1	-10.25	110.12	123.52
1	AA	527	G7M	C5-C6-N1	-10.13	110.28	123.52
55	DA	2069	G7M	C5-C6-N1	-9.94	110.53	123.52
1	BA	527	G7M	C5-C6-N1	-9.87	110.62	123.52
31	CA	2069	G7M	C6-C5-C4	-9.12	110.44	120.86
31	CA	2445	2MG	C5-C6-N1	-8.80	112.02	123.52
1	BA	966	2MG	C5-C6-N1	-8.62	112.25	123.52
31	CA	2251	OMG	C5-C6-N1	-8.54	112.36	123.52
55	DA	2445	2MG	C5-C6-N1	-8.50	112.41	123.52
1	AA	966	2MG	C5-C6-N1	-8.47	112.44	123.52
1	BA	527	G7M	C6-C5-C4	-8.36	111.31	120.86
55	DA	2251	OMG	C5-C6-N1	-8.35	112.60	123.52
1	BA	1207	2MG	C5-C6-N1	-8.32	112.65	123.52
1	AA	1207	2MG	C5-C6-N1	-8.28	112.70	123.52
31	CA	1835	2MG	C5-C6-N1	-8.27	112.72	123.52
55	DA	1835	2MG	C5-C6-N1	-8.26	112.73	123.52
1	BA	1516	2MG	C5-C6-N1	-8.10	112.94	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1516	2MG	C5-C6-N1	-7.98	113.09	123.52
1	AA	527	G7M	C6-C5-C4	-7.18	112.66	120.86
55	DA	2069	G7M	C6-C5-C4	-4.22	116.04	120.86
31	CA	2069	G7M	N3-C2-N1	-4.05	122.04	127.56
1	BA	527	G7M	N3-C2-N1	-4.02	122.08	127.56
1	AA	527	G7M	N3-C2-N1	-3.68	122.54	127.56
31	CA	2552	OMU	C5-C4-N3	-3.47	114.76	123.28
55	DA	2069	G7M	N3-C2-N1	-3.46	122.86	127.56
55	DA	746	PSU	C4-C5-C1'	-3.43	115.45	121.22
55	DA	2552	OMU	C5-C4-N3	-3.42	114.89	123.28
31	CA	745	1MG	C6-C5-C4	-3.39	117.51	119.93
55	DA	2251	OMG	N3-C2-N1	-3.36	122.98	127.56
1	AA	1516	2MG	C6-C5-C4	-3.11	117.31	120.86
31	CA	2251	OMG	N3-C2-N1	-3.00	123.47	127.56
55	DA	1915	3TD	C5-C4-N3	-2.99	116.21	118.65
55	DA	2604	PSU	C4-C5-C1'	-2.99	116.18	121.22
31	CA	1915	3TD	C5-C4-N3	-2.92	116.27	118.65
1	BA	1516	2MG	C6-C5-C4	-2.92	117.52	120.86
55	DA	745	1MG	C6-C5-C4	-2.87	117.88	119.93
32	DD	150[B]	MEQ	O-C-CA	-2.80	118.20	125.72
1	BA	1207	2MG	C6-C5-C4	-2.79	117.67	120.86
1	AA	966	2MG	C6-C5-C4	-2.78	117.67	120.86
55	DA	2445	2MG	C6-C5-C4	-2.71	117.76	120.86
1	AA	1207	2MG	C6-C5-C4	-2.61	117.87	120.86
31	CA	2251	OMG	C6-C5-C4	-2.57	117.92	120.86
31	CA	1835	2MG	C6-C5-C4	-2.57	117.92	120.86
32	DD	150[A]	MEQ	O-C-CA	-2.55	118.88	125.72
55	DA	2605	PSU	C4-C5-C1'	-2.51	116.99	121.22
1	BA	527	G7M	C1'-N9-C4	-2.48	124.04	126.81
31	CA	2445	2MG	C6-C5-C4	-2.47	118.04	120.86
31	CA	2605	PSU	C4-C5-C1'	-2.43	117.12	121.22
32	DD	150[A]	MEQ	CG-CB-CA	-2.40	108.58	114.03
55	DA	1835	2MG	C6-C5-C4	-2.39	118.13	120.86
55	DA	745	1MG	C5-C6-N1	-2.38	115.23	118.35
1	BA	966	2MG	C6-C5-C4	-2.31	118.22	120.86
31	CA	745	1MG	C5-C6-N1	-2.30	115.33	118.35
55	DA	2251	OMG	C6-C5-C4	-2.17	118.38	120.86
31	CA	2069	G7M	C1'-N9-C4	-2.10	124.47	126.81
31	CA	746	PSU	C4-C5-C1'	-2.00	117.84	121.22
55	DA	2503	2MA	N3-C2-N1	-2.00	121.67	125.60
55	DA	1618	6MZ	C2-N1-C6	2.00	117.91	116.47
1	AA	516	PSU	O4'-C1'-C2'	2.01	106.87	104.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	2457	PSU	O4'-C1'-C2'	2.02	106.88	104.69
31	CA	2605	PSU	O4'-C1'-C2'	2.02	106.88	104.69
31	CA	2580	PSU	C3'-C2'-C1'	2.06	104.15	101.71
31	CA	2457	PSU	O4'-C1'-C2'	2.07	106.93	104.69
55	DA	1939	5MU	C5M-C5-C6	2.08	122.84	118.63
1	BA	516	PSU	O4'-C1'-C2'	2.09	106.94	104.69
55	DA	1915	3TD	O4'-C1'-C2'	2.11	106.97	104.69
31	CA	747	5MU	C5M-C5-C6	2.15	122.99	118.63
1	BA	1407	5MC	CM5-C5-C6	2.15	122.99	118.63
31	CA	1835	2MG	N2-C2-N3	2.15	119.44	116.94
1	AA	967	5MC	CM5-C5-C6	2.15	123.00	118.63
55	DA	2503	2MA	CM2-C2-N3	2.21	120.99	117.22
31	CA	1939	5MU	C5M-C5-C6	2.24	123.17	118.63
1	AA	1407	5MC	CM5-C5-C6	2.24	123.18	118.63
1	BA	967	5MC	CM5-C5-C6	2.28	123.25	118.63
31	CA	1962	5MC	CM5-C5-C6	2.28	123.26	118.63
1	AA	1207	2MG	N2-C2-N3	2.30	119.62	116.94
32	DD	150[B]	MEQ	CG-CB-CA	2.31	119.29	114.03
31	CA	2445	2MG	N2-C2-N3	2.31	119.63	116.94
31	CA	2503	2MA	C2-N3-C4	2.35	116.42	115.29
1	BA	1207	2MG	N2-C2-N3	2.37	119.69	116.94
55	DA	1962	5MC	CM5-C5-C6	2.37	123.44	118.63
12	AL	89	D2T	C-CA-N	2.38	115.22	109.95
31	CA	1618	6MZ	C2-N1-C6	2.44	118.22	116.47
1	BA	966	2MG	N2-C2-N3	2.45	119.79	116.94
55	DA	1835	2MG	N2-C2-N3	2.46	119.80	116.94
1	BA	1402	4OC	CM4-N4-C4	2.58	125.05	122.87
55	DA	2445	2MG	N2-C2-N3	2.58	119.94	116.94
32	DD	150[B]	MEQ	CB-CA-N	2.62	117.90	110.54
1	AA	1402	4OC	CM4-N4-C4	2.68	125.13	122.87
12	BL	89	D2T	C-CA-N	2.70	115.92	109.95
31	CA	2030	6MZ	C2-N1-C6	2.78	118.47	116.47
31	CA	2503	2MA	C1'-N9-C4	2.83	129.96	126.81
55	DA	2030	6MZ	C2-N1-C6	2.98	118.61	116.47
55	DA	2580	PSU	O4'-C1'-C2'	2.98	107.91	104.69
31	CA	2580	PSU	O4'-C1'-C2'	3.08	108.02	104.69
55	DA	2503	2MA	C1'-N9-C4	3.13	130.30	126.81
55	DA	2503	2MA	C2-N3-C4	3.48	116.96	115.29
31	CA	2069	G7M	O4'-C1'-N9	3.48	114.69	108.11
1	AA	1402	4OC	C2-N3-C4	3.95	120.46	115.43
1	BA	1402	4OC	C2-N3-C4	3.97	120.48	115.43
1	AA	527	G7M	O4'-C1'-N9	4.40	116.42	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	DA	2069	G7M	O4'-C1'-N9	4.49	116.59	108.11
1	BA	527	G7M	O4'-C1'-N9	4.86	117.29	108.11
1	AA	1516	2MG	C6-N1-C2	5.91	123.71	115.24
1	BA	1516	2MG	C6-N1-C2	5.98	123.80	115.24
31	CA	1835	2MG	C6-N1-C2	6.20	124.12	115.24
1	AA	1207	2MG	C6-N1-C2	6.27	124.22	115.24
55	DA	1835	2MG	C6-N1-C2	6.32	124.28	115.24
1	BA	1207	2MG	C6-N1-C2	6.34	124.32	115.24
55	DA	2445	2MG	C6-N1-C2	6.35	124.33	115.24
1	AA	966	2MG	C6-N1-C2	6.36	124.35	115.24
1	BA	966	2MG	C6-N1-C2	6.50	124.54	115.24
31	CA	2069	G7M	C6-N1-C2	6.77	123.81	115.88
31	CA	2445	2MG	C6-N1-C2	6.79	124.97	115.24
1	BA	527	G7M	C6-N1-C2	6.81	123.86	115.88
1	AA	527	G7M	C6-N1-C2	7.26	124.39	115.88
55	DA	2251	OMG	C6-N1-C2	7.64	124.83	115.88
55	DA	2069	G7M	C6-N1-C2	7.81	125.04	115.88
31	CA	2251	OMG	C6-N1-C2	8.03	125.30	115.88
55	DA	2552	OMU	C4-N3-C2	12.04	126.89	114.21
31	CA	2552	OMU	C4-N3-C2	12.11	126.96	114.21
31	CA	2504	PSU	C4-N3-C2	13.39	126.33	115.16
55	DA	955	PSU	C4-N3-C2	13.43	126.36	115.16
31	CA	2457	PSU	C4-N3-C2	13.45	126.38	115.16
55	DA	2604	PSU	C4-N3-C2	13.45	126.38	115.16
55	DA	2580	PSU	C4-N3-C2	13.46	126.39	115.16
55	DA	1911	PSU	C4-N3-C2	13.46	126.39	115.16
31	CA	955	PSU	C4-N3-C2	13.46	126.39	115.16
31	CA	746	PSU	C4-N3-C2	13.50	126.43	115.16
1	BA	516	PSU	C4-N3-C2	13.51	126.43	115.16
55	DA	2457	PSU	C4-N3-C2	13.51	126.43	115.16
1	AA	516	PSU	C4-N3-C2	13.52	126.44	115.16
31	CA	1911	PSU	C4-N3-C2	13.52	126.44	115.16
31	CA	2605	PSU	C4-N3-C2	13.53	126.45	115.16
31	CA	2580	PSU	C4-N3-C2	13.54	126.45	115.16
55	DA	2605	PSU	C4-N3-C2	13.57	126.48	115.16
55	DA	2504	PSU	C4-N3-C2	13.62	126.52	115.16
55	DA	746	PSU	C4-N3-C2	13.62	126.53	115.16
31	CA	1917	PSU	C4-N3-C2	13.68	126.57	115.16
55	DA	1917	PSU	C4-N3-C2	13.78	126.66	115.16
55	DA	1939	5MU	C4-N3-C2	14.13	126.95	115.16
55	DA	747	5MU	C4-N3-C2	14.26	127.06	115.16
31	CA	1939	5MU	C4-N3-C2	14.50	127.26	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
31	CA	747	5MU	C4-N3-C2	14.51	127.27	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1518	MA6	2	0
1	AA	1519	MA6	2	0
1	BA	1518	MA6	2	0
1	BA	1519	MA6	2	0
31	CA	2030	6MZ	2	0
31	CA	2251	OMG	1	0
31	CA	2498	OMC	1	0
31	CA	2503	2MA	1	0
31	CA	747	5MU	1	0
55	DA	2030	6MZ	2	0
55	DA	2251	OMG	1	0
55	DA	747	5MU	1	0
32	DD	150[A]	MEQ	2	0
32	DD	150[B]	MEQ	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 552 ligands modelled in this entry, 472 are monoatomic - leaving 80 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	PG4	AA	1670	-	12,12,12	0.37	0	11,11,11	0.34	0
58	MPD	AA	1671	-	6,7,7	0.39	0	6,10,10	0.40	0
59	PUT	AA	1672	-	5,5,5	0.29	0	4,4,4	0.18	0
59	PUT	AA	1673	-	5,5,5	0.18	0	4,4,4	0.18	0
59	PUT	AA	1674	-	5,5,5	0.22	0	4,4,4	0.15	0
59	PUT	AA	1675	-	5,5,5	0.25	0	4,4,4	0.10	0
58	MPD	AA	1676	-	6,7,7	0.46	0	6,10,10	0.18	0
61	PEG	AL	201	-	6,6,6	0.28	0	5,5,5	0.22	0
57	PG4	BA	1642	-	12,12,12	0.35	0	11,11,11	0.25	0
62	EDO	D1	101	-	3,3,3	0.59	0	2,2,2	0.25	0
63	PGE	D1	102	-	9,9,9	0.29	0	8,8,8	0.24	0
61	PEG	D1	103	-	6,6,6	0.30	0	5,5,5	0.15	0
63	PGE	D3	101	-	9,9,9	0.32	0	8,8,8	0.29	0
61	PEG	D3	102	-	6,6,6	0.51	0	5,5,5	0.37	0
62	EDO	DA	3002	-	3,3,3	0.66	0	2,2,2	0.19	0
62	EDO	DA	3003	-	3,3,3	0.61	0	2,2,2	0.33	0
58	MPD	DA	3004	-	6,7,7	0.46	0	6,10,10	0.13	0
62	EDO	DA	3005	-	3,3,3	0.55	0	2,2,2	0.36	0
64	SPD	DA	3186	-	9,9,9	0.21	0	8,8,8	0.17	0
59	PUT	DA	3187	-	5,5,5	0.48	0	4,4,4	0.26	0
65	1PE	DA	3188	-	15,15,15	0.21	0	14,14,14	0.30	0
63	PGE	DA	3189	-	9,9,9	0.43	0	8,8,8	0.28	0
64	SPD	DA	3190	-	9,9,9	0.16	0	8,8,8	0.19	0
59	PUT	DA	3191	-	5,5,5	0.14	0	4,4,4	0.21	0
59	PUT	DA	3192	-	5,5,5	0.40	0	4,4,4	0.41	0
58	MPD	DA	3193	-	6,7,7	0.31	0	6,10,10	0.44	0
66	ACY	DA	3194	-	0,3,3	0.00	-	0,3,3	0.00	-
58	MPD	DA	3195	-	6,7,7	0.38	0	6,10,10	0.49	0
57	PG4	DA	3196	-	12,12,12	0.39	0	11,11,11	0.29	0
62	EDO	DA	3197	-	3,3,3	1.02	0	2,2,2	0.32	0
59	PUT	DA	3198	-	5,5,5	0.27	0	4,4,4	0.21	0
66	ACY	DA	3199	-	0,3,3	0.00	-	0,3,3	0.00	-
62	EDO	DA	3200	-	3,3,3	0.71	0	2,2,2	0.14	0
62	EDO	DA	3201	-	3,3,3	0.50	0	2,2,2	0.52	0
61	PEG	DA	3202	-	6,6,6	0.24	0	5,5,5	0.14	0
61	PEG	DA	3203	-	6,6,6	0.32	0	5,5,5	0.17	0
66	ACY	DA	3204	-	0,3,3	0.00	-	0,3,3	0.00	-
65	1PE	DA	3205	-	15,15,15	0.42	0	14,14,14	0.50	0
58	MPD	DA	3206	-	6,7,7	0.72	0	6,10,10	0.58	0
59	PUT	DA	3207	-	5,5,5	0.25	0	4,4,4	0.20	0
64	SPD	DA	3208	-	9,9,9	0.22	0	8,8,8	0.19	0
58	MPD	DA	3209	-	6,7,7	0.50	0	6,10,10	0.51	0
62	EDO	DA	3210	-	3,3,3	0.63	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
62	EDO	DA	3211	-	3,3,3	0.65	0	2,2,2	0.25	0
58	MPD	DA	3212	-	6,7,7	0.49	0	6,10,10	0.39	0
67	GUN	DA	3213	-	9,12,12	1.73	2 (22%)	7,17,17	4.84	5 (71%)
59	PUT	DA	3214	-	5,5,5	0.27	0	4,4,4	0.10	0
59	PUT	DA	3215	-	5,5,5	0.30	0	4,4,4	0.20	0
63	PGE	DA	3216	-	9,9,9	0.31	0	8,8,8	0.34	0
62	EDO	DA	3217	-	3,3,3	0.61	0	2,2,2	0.33	0
57	PG4	DA	3218	-	12,12,12	0.21	0	11,11,11	0.25	0
63	PGE	DA	3219	-	9,9,9	0.23	0	8,8,8	0.26	0
61	PEG	DA	3220	-	6,6,6	0.22	0	5,5,5	0.04	0
59	PUT	DA	3221	-	5,5,5	0.19	0	4,4,4	0.15	0
68	TRS	DA	3222	-	7,7,7	0.55	0	9,9,9	0.44	0
59	PUT	DA	3223	-	5,5,5	0.31	0	4,4,4	0.20	0
59	PUT	DA	3224	-	5,5,5	0.48	0	4,4,4	0.64	0
59	PUT	DA	3225	-	5,5,5	0.29	0	4,4,4	0.24	0
64	SPD	DA	3226	-	9,9,9	0.36	0	8,8,8	0.45	0
63	PGE	DA	3227	-	9,9,9	0.20	0	8,8,8	0.23	0
61	PEG	DA	3228	-	6,6,6	0.43	0	5,5,5	0.30	0
61	PEG	DA	3229	-	6,6,6	0.40	0	5,5,5	0.21	0
62	EDO	DB	210	-	3,3,3	0.65	0	2,2,2	0.05	0
62	EDO	DB	211	-	3,3,3	0.69	0	2,2,2	0.09	0
63	PGE	DD	301	-	9,9,9	0.20	0	8,8,8	0.16	0
58	MPD	DE	301	-	6,7,7	0.43	0	6,10,10	0.47	0
58	MPD	DE	302	-	6,7,7	0.59	0	6,10,10	0.27	0
58	MPD	DK	201	-	6,7,7	0.44	0	6,10,10	0.26	0
61	PEG	DL	201	-	6,6,6	0.20	0	5,5,5	0.13	0
59	PUT	DM	201	-	5,5,5	0.20	0	4,4,4	0.24	0
58	MPD	DN	201	-	6,7,7	0.71	0	6,10,10	0.57	0
61	PEG	DP	201	-	6,6,6	0.31	0	5,5,5	0.12	0
61	PEG	DQ	201	-	6,6,6	0.36	0	5,5,5	0.27	0
57	PG4	DQ	202	-	12,12,12	0.30	0	11,11,11	0.24	0
57	PG4	DR	202	-	12,12,12	0.33	0	11,11,11	0.34	0
63	PGE	DS	201	-	9,9,9	0.40	0	8,8,8	0.31	0
57	PG4	DS	202	-	12,12,12	0.40	0	11,11,11	0.31	0
58	MPD	DS	203	-	6,7,7	0.37	0	6,10,10	0.43	0
58	MPD	DT	201	-	6,7,7	0.44	0	6,10,10	0.45	0
63	PGE	DU	101	-	9,9,9	0.31	0	8,8,8	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PG4	AA	1670	-	-	0/10/10/10	0/0/0/0
58	MPD	AA	1671	-	-	0/5/5/5	0/0/0/0
59	PUT	AA	1672	-	-	0/3/3/3	0/0/0/0
59	PUT	AA	1673	-	-	0/3/3/3	0/0/0/0
59	PUT	AA	1674	-	-	0/3/3/3	0/0/0/0
59	PUT	AA	1675	-	-	0/3/3/3	0/0/0/0
58	MPD	AA	1676	-	-	0/5/5/5	0/0/0/0
61	PEG	AL	201	-	-	0/4/4/4	0/0/0/0
57	PG4	BA	1642	-	-	0/10/10/10	0/0/0/0
62	EDO	D1	101	-	-	0/1/1/1	0/0/0/0
63	PGE	D1	102	-	-	0/7/7/7	0/0/0/0
61	PEG	D1	103	-	-	0/4/4/4	0/0/0/0
63	PGE	D3	101	-	-	0/7/7/7	0/0/0/0
61	PEG	D3	102	-	-	0/4/4/4	0/0/0/0
62	EDO	DA	3002	-	-	0/1/1/1	0/0/0/0
62	EDO	DA	3003	-	-	0/1/1/1	0/0/0/0
58	MPD	DA	3004	-	-	0/5/5/5	0/0/0/0
62	EDO	DA	3005	-	-	0/1/1/1	0/0/0/0
64	SPD	DA	3186	-	-	0/7/7/7	0/0/0/0
59	PUT	DA	3187	-	-	0/3/3/3	0/0/0/0
65	1PE	DA	3188	-	-	0/13/13/13	0/0/0/0
63	PGE	DA	3189	-	-	0/7/7/7	0/0/0/0
64	SPD	DA	3190	-	-	0/7/7/7	0/0/0/0
59	PUT	DA	3191	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3192	-	-	0/3/3/3	0/0/0/0
58	MPD	DA	3193	-	-	0/5/5/5	0/0/0/0
66	ACY	DA	3194	-	-	0/0/0/0	0/0/0/0
58	MPD	DA	3195	-	-	0/5/5/5	0/0/0/0
57	PG4	DA	3196	-	-	0/10/10/10	0/0/0/0
62	EDO	DA	3197	-	-	0/1/1/1	0/0/0/0
59	PUT	DA	3198	-	-	0/3/3/3	0/0/0/0
66	ACY	DA	3199	-	-	0/0/0/0	0/0/0/0
62	EDO	DA	3200	-	-	0/1/1/1	0/0/0/0
62	EDO	DA	3201	-	-	0/1/1/1	0/0/0/0
61	PEG	DA	3202	-	-	0/4/4/4	0/0/0/0
61	PEG	DA	3203	-	-	0/4/4/4	0/0/0/0
66	ACY	DA	3204	-	-	0/0/0/0	0/0/0/0
65	1PE	DA	3205	-	-	0/13/13/13	0/0/0/0
58	MPD	DA	3206	-	-	0/5/5/5	0/0/0/0
59	PUT	DA	3207	-	-	0/3/3/3	0/0/0/0
64	SPD	DA	3208	-	-	0/7/7/7	0/0/0/0
58	MPD	DA	3209	-	-	0/5/5/5	0/0/0/0
62	EDO	DA	3210	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	EDO	DA	3211	-	-	0/1/1/1	0/0/0/0
58	MPD	DA	3212	-	-	0/5/5/5	0/0/0/0
67	GUN	DA	3213	-	-	0/0/0/0	0/2/2/2
59	PUT	DA	3214	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3215	-	-	0/3/3/3	0/0/0/0
63	PGE	DA	3216	-	-	0/7/7/7	0/0/0/0
62	EDO	DA	3217	-	-	0/1/1/1	0/0/0/0
57	PG4	DA	3218	-	-	0/10/10/10	0/0/0/0
63	PGE	DA	3219	-	-	0/7/7/7	0/0/0/0
61	PEG	DA	3220	-	-	0/4/4/4	0/0/0/0
59	PUT	DA	3221	-	-	0/3/3/3	0/0/0/0
68	TRS	DA	3222	-	-	0/9/9/9	0/0/0/0
59	PUT	DA	3223	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3224	-	-	0/3/3/3	0/0/0/0
59	PUT	DA	3225	-	-	0/3/3/3	0/0/0/0
64	SPD	DA	3226	-	-	0/7/7/7	0/0/0/0
63	PGE	DA	3227	-	-	0/7/7/7	0/0/0/0
61	PEG	DA	3228	-	-	0/4/4/4	0/0/0/0
61	PEG	DA	3229	-	-	0/4/4/4	0/0/0/0
62	EDO	DB	210	-	-	0/1/1/1	0/0/0/0
62	EDO	DB	211	-	-	0/1/1/1	0/0/0/0
63	PGE	DD	301	-	-	0/7/7/7	0/0/0/0
58	MPD	DE	301	-	-	0/5/5/5	0/0/0/0
58	MPD	DE	302	-	-	0/5/5/5	0/0/0/0
58	MPD	DK	201	-	-	0/5/5/5	0/0/0/0
61	PEG	DL	201	-	-	0/4/4/4	0/0/0/0
59	PUT	DM	201	-	-	0/3/3/3	0/0/0/0
58	MPD	DN	201	-	-	0/5/5/5	0/0/0/0
61	PEG	DP	201	-	-	0/4/4/4	0/0/0/0
61	PEG	DQ	201	-	-	0/4/4/4	0/0/0/0
57	PG4	DQ	202	-	-	0/10/10/10	0/0/0/0
57	PG4	DR	202	-	-	0/10/10/10	0/0/0/0
63	PGE	DS	201	-	-	0/7/7/7	0/0/0/0
57	PG4	DS	202	-	-	0/10/10/10	0/0/0/0
58	MPD	DS	203	-	-	0/5/5/5	0/0/0/0
58	MPD	DT	201	-	-	0/5/5/5	0/0/0/0
63	PGE	DU	101	-	-	0/7/7/7	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	DA	3213	GUN	C6-N1	3.31	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	DA	3213	GUN	C6-C5	3.58	1.48	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	DA	3213	GUN	C5-C6-N1	-8.61	112.26	123.52
67	DA	3213	GUN	C5-C4-N9	-3.26	105.35	111.12
67	DA	3213	GUN	C6-C5-C4	-2.91	117.53	120.86
67	DA	3213	GUN	N3-C2-N1	-2.83	123.71	127.56
67	DA	3213	GUN	C6-N1-C2	7.82	125.04	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

30 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	1670	PG4	1	0
58	AA	1671	MPD	2	0
57	BA	1642	PG4	1	0
63	D1	102	PGE	3	0
61	D1	103	PEG	1	0
61	D3	102	PEG	2	0
59	DA	3187	PUT	1	0
65	DA	3188	1PE	1	0
58	DA	3195	MPD	1	0
57	DA	3196	PG4	1	0
62	DA	3197	EDO	2	0
62	DA	3201	EDO	1	0
58	DA	3206	MPD	2	0
64	DA	3208	SPD	1	0
58	DA	3209	MPD	1	0
63	DA	3216	PGE	1	0
57	DA	3218	PG4	1	0
59	DA	3221	PUT	1	0
68	DA	3222	TRS	2	0
59	DA	3224	PUT	2	0
64	DA	3226	SPD	1	0
63	DA	3227	PGE	3	0
62	DB	211	EDO	1	0
61	DP	201	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	DQ	201	PEG	1	0
57	DQ	202	PG4	1	0
57	DR	202	PG4	3	0
57	DS	202	PG4	1	0
58	DS	203	MPD	3	0
63	DU	101	PGE	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1523/1534 (99%)	-0.01	32 (2%) 67 37	37, 95, 237, 293	0
1	BA	1522/1534 (99%)	0.48	146 (9%) 10 4	58, 133, 255, 272	0
2	AB	224/224 (100%)	0.49	15 (6%) 21 7	76, 123, 192, 236	0
2	BB	224/224 (100%)	0.71	35 (15%) 3 1	101, 145, 205, 239	0
3	AC	206/206 (100%)	-0.12	3 (1%) 76 49	65, 93, 121, 147	0
3	BC	206/206 (100%)	0.19	7 (3%) 49 21	86, 121, 150, 169	0
4	AD	205/205 (100%)	-0.20	1 (0%) 91 77	69, 97, 128, 136	0
4	BD	205/205 (100%)	-0.19	0 100 100	68, 101, 127, 138	0
5	AE	155/155 (100%)	-0.19	1 (0%) 90 74	60, 84, 120, 175	0
5	BE	150/155 (96%)	0.28	6 (4%) 42 18	72, 106, 138, 202	0
6	AF	106/106 (100%)	0.11	7 (6%) 22 7	69, 103, 126, 144	0
6	BF	100/106 (94%)	0.46	4 (4%) 42 18	82, 115, 140, 149	0
7	AG	151/151 (100%)	0.92	26 (17%) 2 1	106, 150, 177, 189	0
7	BG	151/151 (100%)	1.89	65 (43%) 0 0	137, 190, 215, 221	0
8	AH	129/129 (100%)	0.04	4 (3%) 52 24	68, 91, 119, 130	0
8	BH	129/129 (100%)	0.11	5 (3%) 43 18	98, 126, 151, 161	0
9	AI	127/127 (100%)	1.06	25 (19%) 1 1	75, 144, 180, 187	0
9	BI	127/127 (100%)	1.20	30 (23%) 1 0	111, 162, 195, 202	0
10	AJ	99/99 (100%)	0.46	10 (10%) 9 3	82, 112, 142, 147	0
10	BJ	98/99 (98%)	2.21	44 (44%) 0 0	111, 152, 181, 187	0
11	AK	117/117 (100%)	0.38	6 (5%) 32 13	54, 104, 138, 152	0
11	BK	117/117 (100%)	0.11	3 (2%) 59 29	62, 97, 134, 165	0
12	AL	122/123 (99%)	-0.05	1 (0%) 87 68	48, 65, 106, 141	0
12	BL	122/123 (99%)	0.65	10 (8%) 14 5	82, 102, 129, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	114/114 (100%)	1.82	39 (34%) 0 0	126, 159, 182, 189	0
13	BM	114/114 (100%)	2.76	74 (64%) 0 0	187, 224, 236, 244	0
14	AN	100/100 (100%)	0.60	7 (7%) 19 7	72, 110, 177, 184	0
14	BN	100/100 (100%)	1.50	33 (33%) 0 0	107, 167, 215, 218	0
15	AO	88/88 (100%)	0.04	1 (1%) 82 58	63, 91, 115, 142	0
15	BO	88/88 (100%)	0.68	10 (11%) 7 2	84, 114, 143, 156	0
16	AP	82/82 (100%)	0.54	7 (8%) 13 4	68, 85, 126, 145	0
16	BP	82/82 (100%)	1.78	28 (34%) 0 0	100, 125, 161, 175	0
17	AQ	80/80 (100%)	0.01	2 (2%) 61 30	63, 87, 116, 138	0
17	BQ	80/80 (100%)	1.11	21 (26%) 1 0	101, 142, 165, 173	0
18	AR	55/55 (100%)	0.93	9 (16%) 2 1	73, 97, 142, 174	0
18	BR	55/55 (100%)	0.10	2 (3%) 46 20	67, 90, 125, 166	0
19	AS	79/79 (100%)	1.24	17 (21%) 1 0	138, 162, 179, 182	0
19	BS	79/79 (100%)	2.25	39 (49%) 0 0	197, 221, 238, 243	0
20	AT	86/86 (100%)	-0.04	1 (1%) 81 55	63, 85, 116, 128	0
20	BT	85/86 (98%)	2.02	37 (43%) 0 0	110, 143, 164, 169	0
21	AU	56/56 (100%)	0.13	1 (1%) 71 43	75, 113, 153, 163	0
21	BU	56/56 (100%)	0.25	1 (1%) 71 43	69, 94, 123, 138	0
22	C1	56/56 (100%)	1.44	17 (30%) 1 0	93, 155, 176, 188	0
22	D1	56/56 (100%)	-0.48	0 100 100	21, 45, 74, 114	0
23	C2	50/51 (98%)	2.22	22 (44%) 0 0	150, 178, 190, 205	0
23	D2	51/51 (100%)	0.02	0 100 100	47, 63, 89, 108	0
24	C3	46/46 (100%)	1.79	18 (39%) 0 0	100, 132, 149, 173	0
24	D3	46/46 (100%)	-0.29	0 100 100	25, 35, 54, 118	0
25	C4	64/64 (100%)	0.69	7 (10%) 7 3	95, 116, 139, 151	0
25	D4	64/64 (100%)	-0.34	0 100 100	29, 39, 57, 68	0
26	C5	38/38 (100%)	0.57	4 (10%) 8 3	97, 115, 133, 149	0
26	D5	38/38 (100%)	-0.28	0 100 100	32, 45, 71, 83	0
27	C0	58/58 (100%)	1.46	19 (32%) 0 0	99, 121, 149, 157	0
27	D0	58/58 (100%)	-0.51	0 100 100	23, 34, 54, 88	0
28	CB	118/120 (98%)	0.75	16 (13%) 4 1	104, 167, 221, 231	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DB	120/120 (100%)	-0.32	0 100 100	28, 53, 86, 134	0
29	CC	271/271 (100%)	0.25	9 (3%) 50 22	76, 98, 120, 132	0
29	DC	271/271 (100%)	-0.36	1 (0%) 93 80	23, 52, 80, 100	0
30	CD	209/209 (100%)	1.10	50 (23%) 1 0	88, 118, 149, 165	0
31	CA	2876/2904 (99%)	0.62	284 (9%) 9 3	65, 132, 252, 292	0
32	DD	208/209 (99%)	-0.49	0 100 100	18, 38, 71, 100	0
33	CE	201/201 (100%)	1.06	40 (19%) 1 0	88, 159, 186, 195	0
33	DE	201/201 (100%)	-0.41	1 (0%) 91 77	20, 52, 98, 127	0
34	CF	177/177 (100%)	2.64	107 (60%) 0 0	186, 212, 225, 231	0
34	DF	177/177 (100%)	-0.11	0 100 100	45, 78, 126, 139	0
35	CG	176/176 (100%)	2.46	93 (52%) 0 0	138, 164, 187, 198	0
35	DG	176/176 (100%)	-0.13	2 (1%) 82 58	45, 74, 105, 131	0
36	CH	149/149 (100%)	1.15	33 (22%) 1 0	81, 148, 176, 186	0
36	DH	149/149 (100%)	0.92	28 (18%) 2 1	60, 158, 195, 208	0
37	CJ	134/134 (100%)	4.62	106 (79%) 0 0	237, 258, 270, 275	0
37	DJ	134/134 (100%)	3.61	84 (62%) 0 0	204, 238, 246, 254	0
38	CK	142/142 (100%)	0.38	5 (3%) 48 21	91, 108, 135, 150	0
38	DK	142/142 (100%)	-0.50	0 100 100	18, 36, 58, 94	0
39	CL	122/123 (99%)	0.42	9 (7%) 17 6	91, 114, 148, 163	0
39	DL	123/123 (100%)	-0.48	0 100 100	29, 43, 72, 106	0
40	CM	144/144 (100%)	1.63	48 (33%) 0 0	87, 146, 186, 214	0
40	DM	144/144 (100%)	-0.37	0 100 100	19, 50, 81, 115	0
41	CN	135/136 (99%)	0.45	8 (5%) 26 10	75, 113, 134, 162	0
41	DN	135/136 (99%)	-0.58	0 100 100	25, 39, 68, 99	0
42	CO	120/125 (96%)	0.77	13 (10%) 8 3	107, 124, 146, 197	0
42	DO	125/125 (100%)	-0.37	1 (0%) 87 68	23, 37, 73, 145	0
43	CP	116/117 (99%)	2.38	65 (56%) 0 0	132, 154, 173, 181	0
43	DP	117/117 (100%)	-0.22	0 100 100	36, 54, 81, 96	0
44	CQ	114/114 (100%)	1.27	24 (21%) 1 0	110, 127, 146, 168	0
44	DQ	114/114 (100%)	-0.38	1 (0%) 85 64	28, 50, 84, 119	0
45	CR	117/117 (100%)	0.57	11 (9%) 11 4	76, 107, 129, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	DR	117/117 (100%)	-0.44	1 (0%) 85 64	15, 30, 49, 85	0
46	CS	103/103 (100%)	1.62	37 (35%) 0 0	94, 127, 152, 164	0
46	DS	103/103 (100%)	-0.56	0 100 100	21, 41, 70, 99	0
47	CT	110/110 (100%)	0.72	16 (14%) 3 1	99, 123, 157, 176	0
47	DT	110/110 (100%)	-0.50	0 100 100	17, 32, 61, 114	0
48	CU	93/93 (100%)	1.67	35 (37%) 0 0	129, 147, 176, 181	0
48	DU	93/93 (100%)	-0.05	2 (2%) 65 35	31, 52, 115, 130	0
49	CV	102/102 (100%)	2.88	57 (55%) 0 0	148, 166, 201, 204	0
49	DV	102/102 (100%)	-0.28	1 (0%) 84 61	40, 62, 97, 129	0
50	CW	94/94 (100%)	0.98	15 (15%) 3 1	114, 140, 159, 164	0
50	DW	94/94 (100%)	-0.50	1 (1%) 82 58	31, 52, 84, 96	0
51	CX	75/76 (98%)	1.07	19 (25%) 1 0	92, 120, 134, 183	0
51	DX	76/76 (100%)	-0.51	1 (1%) 79 53	24, 39, 67, 116	0
52	CY	77/77 (100%)	0.39	4 (5%) 31 12	78, 117, 147, 166	0
52	DY	77/77 (100%)	-0.35	0 100 100	32, 53, 93, 111	0
53	CZ	62/62 (100%)	1.92	28 (45%) 0 0	133, 169, 183, 190	0
53	DZ	62/62 (100%)	0.16	1 (1%) 74 47	42, 70, 110, 138	0
54	DI	135/135 (100%)	1.56	38 (28%) 1 0	81, 152, 215, 229	1 (0%)
55	DA	2873/2904 (98%)	-0.03	89 (3%) 52 24	19, 44, 227, 299	0
All	All	20634/20745 (99%)	0.48	2286 (11%) 7 2	15, 106, 233, 299	1 (0%)

All (2286) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	DJ	135	SER	21.3
37	DJ	54	PRO	17.4
37	CJ	13	VAL	17.1
31	CA	2172	U	16.1
37	CJ	59	ILE	15.3
37	CJ	23	PRO	13.2
37	CJ	57	VAL	13.2
37	CJ	9	VAL	13.0
31	CA	1067	A	13.0
37	CJ	11	LEU	12.8
31	CA	1068	G	12.5

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Mol	Chain	Res	Type	RSRZ
37	CJ	69	PHE	12.3
37	DJ	53	LEU	11.9
37	CJ	54	PRO	11.0
37	CJ	12	GLN	10.9
37	CJ	53	LEU	10.7
55	DA	2120	G	10.6
37	DJ	96	ASP	10.6
37	DJ	94	ASN	10.6
37	CJ	87	LYS	10.5
46	CS	50	GLY	10.5
37	CJ	75	PRO	10.5
37	CJ	21	SER	10.2
54	DI	131	THR	10.2
37	DJ	67	PHE	9.9
37	DJ	23	PRO	9.9
31	CA	1537	G	9.7
49	CV	20	GLY	9.6
37	CJ	14	ALA	9.6
44	CQ	115	ASN	9.5
37	DJ	133	ALA	9.3
55	DA	2163	A	9.2
1	BA	82	G	9.1
37	DJ	79	LEU	9.1
37	CJ	56	PRO	9.0
31	CA	2174	C	8.9
23	C2	18	GLY	8.9
37	CJ	20	PRO	8.9
31	CA	2402	U	8.9
31	CA	2173	A	8.9
9	BI	128	SER	8.8
40	CM	81	ASP	8.8
35	CG	33	LEU	8.8
14	BN	35	ASN	8.7
37	CJ	17	MET	8.7
19	BS	4	SER	8.6
54	DI	128	THR	8.6
31	CA	2126	A	8.4
37	DJ	138	LEU	8.4
10	BJ	76	ILE	8.4
54	DI	130	PRO	8.4
1	BA	1030	U	8.4
37	DJ	24	VAL	8.4

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Mol	Chain	Res	Type	RSRZ
1	BA	211	G	8.2
34	CF	153	ASP	8.2
35	CG	103	ILE	8.2
37	DJ	55	ILE	8.2
2	AB	123	ASP	8.2
1	AA	844	G	8.2
55	DA	884	U	8.1
55	DA	1065	U	8.1
37	DJ	13	VAL	8.1
49	CV	32	GLY	8.0
35	CG	105	LEU	8.0
37	DJ	76	ALA	8.0
55	DA	1064	C	8.0
34	CF	176	PRO	8.0
37	CJ	120	ALA	8.0
51	CX	54	GLY	7.9
10	BJ	74	VAL	7.9
37	CJ	22	PRO	7.9
37	CJ	89	GLY	7.8
37	CJ	118	THR	7.8
37	DJ	66	SER	7.8
35	CG	32	GLU	7.8
49	CV	80	ALA	7.8
49	CV	29	LEU	7.8
37	CJ	60	THR	7.7
37	DJ	88	SER	7.7
1	AA	1030	U	7.7
49	CV	33	LYS	7.7
37	CJ	126	THR	7.6
49	CV	89	ASP	7.6
13	BM	10	PRO	7.6
1	AA	86	G	7.6
31	CA	1087	G	7.6
55	DA	2125	G	7.5
19	BS	74	PHE	7.5
37	DJ	137	GLY	7.5
55	DA	892	A	7.5
37	CJ	82	LYS	7.5
17	BQ	70	THR	7.5
13	BM	95	LEU	7.4
16	BP	16	PHE	7.4
55	DA	2124	G	7.4

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Mol	Chain	Res	Type	RSRZ
37	CJ	121	ASP	7.4
37	DJ	132	THR	7.3
20	BT	4	ILE	7.3
10	BJ	75	ASP	7.3
31	CA	1104	C	7.2
37	CJ	90	SER	7.2
40	CM	114	GLY	7.2
31	CA	1103	A	7.2
35	CG	111	HIS	7.2
37	CJ	47	ASP	7.2
13	AM	24	GLY	7.1
35	CG	84	THR	7.1
37	CJ	61	VAL	7.1
55	DA	881	G	7.1
34	CF	116	GLY	7.0
37	CJ	80	LEU	7.0
49	CV	79	LYS	7.0
55	DA	2127	G	7.0
9	AI	130	ARG	7.0
37	CJ	68	THR	7.0
37	CJ	76	ALA	7.0
31	CA	2163	A	6.9
34	CF	132	VAL	6.9
43	CP	51	ALA	6.9
49	CV	31	SER	6.9
14	AN	21	PHE	6.9
31	CA	2125	G	6.9
31	CA	1175	A	6.9
31	CA	1066	U	6.9
19	BS	49	ILE	6.8
55	DA	2110	G	6.8
37	DJ	78	VAL	6.8
16	BP	17	TYR	6.8
37	DJ	98	VAL	6.8
55	DA	1172	C	6.8
31	CA	1057	A	6.8
49	CV	13	VAL	6.8
37	DJ	68	THR	6.7
49	CV	3	ALA	6.7
37	DJ	114	ALA	6.7
37	DJ	80	LEU	6.7
34	CF	154	ILE	6.7

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Mol	Chain	Res	Type	RSRZ
13	BM	65	VAL	6.7
35	CG	106	SER	6.7
34	CF	152	LEU	6.7
37	DJ	69	PHE	6.7
7	BG	62	PHE	6.7
34	CF	40	VAL	6.7
31	CA	2127	G	6.7
13	AM	64	VAL	6.7
10	BJ	39	PRO	6.6
20	BT	3	ASN	6.6
31	CA	75	G	6.6
31	CA	329	G	6.6
13	AM	13	LYS	6.5
31	CA	2120	G	6.5
34	CF	175	PHE	6.5
48	CU	57	VAL	6.5
31	CA	2171	A	6.5
37	DJ	12	GLN	6.5
13	AM	33	ILE	6.4
43	CP	53	THR	6.4
19	BS	60	VAL	6.4
36	CH	11	ASN	6.4
34	CF	85	ILE	6.4
13	BM	96	PRO	6.4
31	CA	1084	A	6.4
55	DA	2172	U	6.4
34	CF	36	LEU	6.4
34	CF	136	ILE	6.3
10	BJ	40	ILE	6.3
55	DA	2121	G	6.3
10	BJ	102	LEU	6.3
7	BG	4	ARG	6.3
49	CV	30	SER	6.3
49	CV	78	GLY	6.3
1	BA	94	G	6.2
37	CJ	79	LEU	6.2
31	CA	331	C	6.2
31	CA	1065	U	6.2
19	BS	39	THR	6.2
55	DA	882	G	6.2
10	BJ	25	ILE	6.2
37	CJ	74	PRO	6.2

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Mol	Chain	Res	Type	RSRZ
31	CA	2119	A	6.2
55	DA	1067	A	6.2
23	C2	16	GLY	6.2
37	DJ	19	ASN	6.1
10	BJ	26	VAL	6.1
1	AA	87	C	6.1
31	CA	1056	G	6.1
34	CF	135	GLN	6.1
35	CG	110	SER	6.1
37	DJ	20	PRO	6.1
35	CG	82	GLY	6.1
37	CJ	88	SER	6.0
10	BJ	77	VAL	6.0
55	DA	879	G	6.0
34	CF	65	PRO	6.0
13	AM	30	SER	6.0
37	DJ	93	PRO	6.0
13	BM	2	ALA	6.0
23	C2	45	GLN	6.0
31	CA	2161	C	6.0
37	DJ	99	GLY	6.0
14	BN	31	ILE	6.0
37	DJ	134	ARG	6.0
43	CP	65	THR	6.0
9	AI	32	GLN	6.0
1	BA	1236	A	5.9
31	CA	2128	G	6.0
19	BS	24	GLU	5.9
55	DA	883	G	5.9
43	CP	64	TYR	5.9
49	CV	36	VAL	5.9
37	CJ	28	LEU	5.9
35	CG	30	ASN	5.9
35	CG	121	ILE	5.9
46	CS	96	VAL	5.9
31	CA	549	G	5.9
7	BG	151	PHE	5.8
34	CF	144	ASP	5.8
7	BG	116	MET	5.8
55	DA	2111	U	5.8
30	CD	26	VAL	5.8
34	CF	34	ILE	5.8

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Mol	Chain	Res	Type	RSRZ
13	AM	19	LEU	5.8
31	CA	2164	C	5.8
10	BJ	8	ILE	5.8
19	BS	3	ARG	5.8
31	CA	2116	G	5.7
43	CP	34	HIS	5.7
16	BP	57	ILE	5.7
55	DA	880	G	5.7
54	DI	134	GLU	5.7
34	CF	128	TYR	5.7
37	CJ	86	ILE	5.7
37	CJ	119	GLY	5.7
35	CG	148	LEU	5.7
31	CA	2110	G	5.7
35	CG	83	PHE	5.7
37	DJ	28	LEU	5.7
55	DA	896	A	5.6
35	CG	31	GLY	5.6
37	CJ	58	VAL	5.6
34	CF	174	ASP	5.6
16	BP	11	ALA	5.6
37	CJ	52	GLY	5.6
43	CP	52	SER	5.6
1	AA	1032	G	5.6
14	BN	33	ASP	5.6
53	CZ	45	GLN	5.6
18	BR	20	GLU	5.6
51	CX	52	GLY	5.6
35	CG	80	THR	5.6
55	DA	1068	G	5.6
40	CM	82	LEU	5.6
55	DA	2167	U	5.5
31	CA	318	C	5.5
55	DA	2174	C	5.5
37	CJ	8	TYR	5.5
34	CF	156	ILE	5.5
23	C2	43	VAL	5.5
55	DA	885	C	5.5
1	BA	85	U	5.5
43	CP	24	THR	5.5
16	BP	39	PHE	5.5
37	DJ	38	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
55	DA	2175	C	5.5
40	CM	79	LEU	5.5
34	CF	130	MET	5.5
7	BG	148	ASN	5.5
31	CA	1086	A	5.5
55	DA	1077	A	5.5
43	CP	35	ILE	5.4
55	DA	2126	A	5.4
7	BG	123	GLU	5.4
49	CV	5	ILE	5.4
35	CG	104	ASN	5.4
43	CP	26	LEU	5.4
43	CP	40	ILE	5.4
43	CP	63	LYS	5.4
31	CA	2123	G	5.4
9	AI	20	PHE	5.4
20	BT	77	ALA	5.4
46	CS	20	VAL	5.4
55	DA	2162	G	5.4
35	CG	2	SER	5.4
37	CJ	29	GLY	5.4
31	CA	1095	A	5.4
10	BJ	38	GLY	5.3
31	CA	2802	G	5.3
1	BA	84	U	5.3
34	CF	157	THR	5.3
37	CJ	46	THR	5.3
35	CG	117	LEU	5.3
49	CV	15	THR	5.3
49	CV	88	GLU	5.3
16	BP	52	LEU	5.3
31	CA	1083	U	5.3
14	BN	36	ALA	5.3
34	CF	106	ILE	5.3
40	CM	144	GLU	5.3
31	CA	878	A	5.3
37	DJ	11	LEU	5.3
13	BM	97	VAL	5.3
7	BG	5	ARG	5.3
55	DA	1062	G	5.3
55	DA	2123	G	5.3
37	CJ	71	THR	5.3

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Mol	Chain	Res	Type	RSRZ
10	BJ	42	LEU	5.3
31	CA	931	U	5.3
55	DA	2109	U	5.3
1	BA	1314	C	5.2
54	DI	136	ILE	5.2
20	BT	60	ARG	5.2
7	BG	8	GLY	5.2
18	AR	20	GLU	5.2
31	CA	1105	U	5.2
44	CQ	91	ALA	5.2
1	BA	1032	G	5.2
10	BJ	73	LEU	5.2
47	CT	43	ALA	5.2
49	CV	40	ASN	5.2
31	CA	1536	C	5.2
37	CJ	115	ALA	5.2
54	DI	132	TYR	5.2
43	CP	78	VAL	5.2
13	BM	99	GLY	5.2
14	BN	39	GLU	5.2
31	CA	2162	G	5.2
31	CA	330	A	5.2
49	CV	35	ILE	5.2
37	DJ	22	PRO	5.2
55	DA	2116	G	5.2
13	BM	29	ARG	5.2
55	DA	1063	G	5.2
31	CA	1085	A	5.1
31	CA	2666	C	5.1
9	BI	16	ALA	5.1
13	BM	25	VAL	5.1
44	CQ	111	LYS	5.1
43	CP	58	ILE	5.1
46	CS	27	ILE	5.1
2	BB	34	ALA	5.1
48	DU	1	MET	5.1
13	BM	41	GLU	5.1
33	CE	144	GLU	5.1
44	CQ	85	SER	5.1
14	BN	60	GLN	5.1
49	CV	6	ARG	5.1
40	CM	89	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
31	CA	1210	G	5.0
35	CG	102	VAL	5.0
35	CG	151	TYR	5.0
37	CJ	24	VAL	5.0
7	BG	43	VAL	5.0
7	AG	61	ALA	5.0
31	CA	2170	A	5.0
13	BM	47	GLU	5.0
24	C3	32	ALA	5.0
14	BN	30	ILE	5.0
37	CJ	129	ILE	5.0
30	CD	6	GLY	5.0
7	AG	6	VAL	5.0
34	CF	35	THR	5.0
13	BM	56	LEU	5.0
35	CG	112	PRO	5.0
53	CZ	42	LEU	5.0
1	BA	202	G	5.0
13	AM	7	ILE	5.0
23	C2	47	VAL	5.0
19	BS	80	TYR	5.0
37	DJ	42	PHE	5.0
53	CZ	15	ASN	5.0
13	BM	48	LEU	4.9
10	BJ	41	PRO	4.9
40	CM	80	SER	4.9
13	BM	17	ILE	4.9
37	DJ	59	ILE	4.9
33	CE	124	PHE	4.9
13	BM	60	VAL	4.9
9	BI	7	TYR	4.9
9	BI	38	TYR	4.9
34	CF	32	GLU	4.9
49	CV	28	VAL	4.9
19	BS	29	LYS	4.9
43	CP	66	GLY	4.9
37	CJ	122	ILE	4.9
40	CM	101	ILE	4.9
23	C2	52	ALA	4.9
1	BA	4	U	4.8
34	CF	117	LEU	4.8
54	DI	96	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
26	C5	38	GLY	4.8
22	C1	11	SER	4.8
55	DA	1078	U	4.8
12	AL	124	ALA	4.8
53	CZ	49	ASP	4.8
34	CF	105	THR	4.8
49	CV	87	PHE	4.8
49	CV	75	ALA	4.8
44	CQ	8	LEU	4.8
14	AN	23	LYS	4.8
10	AJ	35	GLN	4.8
31	CA	1071	G	4.8
31	CA	2169	A	4.8
27	C0	56	LYS	4.8
50	CW	48	MET	4.8
13	BM	39	ILE	4.8
7	BG	152	ALA	4.8
1	BA	203	G	4.8
1	BA	1302	C	4.8
30	CD	186	LEU	4.8
13	AM	43	VAL	4.7
49	CV	77	THR	4.7
31	CA	1090	A	4.7
49	CV	83	VAL	4.7
54	DI	104	ALA	4.7
17	BQ	45	HIS	4.7
37	DJ	136	MET	4.7
43	CP	37	ALA	4.7
9	BI	130	ARG	4.7
40	CM	10	GLU	4.7
7	AG	5	ARG	4.7
31	CA	1535	A	4.7
31	CA	1094	U	4.7
20	BT	36	TYR	4.7
13	BM	30	SER	4.7
37	CJ	67	PHE	4.7
13	BM	40	ALA	4.6
53	CZ	63	ALA	4.6
31	CA	2121	G	4.6
1	BA	209	U	4.6
43	CP	38	GLN	4.6
37	CJ	33	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
37	CJ	45	LYS	4.6
7	BG	42	ILE	4.6
20	BT	76	LYS	4.6
34	CF	158	THR	4.6
24	C3	35	ARG	4.6
48	CU	43	ILE	4.6
37	CJ	98	VAL	4.6
13	BM	115	PRO	4.6
37	CJ	132	THR	4.6
48	CU	56	GLU	4.6
1	AA	84	U	4.6
31	CA	1863	G	4.5
37	DJ	92	LYS	4.5
54	DI	133	GLU	4.5
54	DI	129	LEU	4.5
7	BG	144	MET	4.5
1	BA	1296	C	4.5
35	CG	75	MET	4.5
36	DH	137	GLU	4.5
14	BN	21	PHE	4.5
34	CF	67	ILE	4.5
1	AA	1031	C	4.5
7	AG	8	GLY	4.5
35	CG	131	ILE	4.5
55	DA	2168	G	4.5
16	BP	42	ILE	4.5
37	CJ	38	PHE	4.5
51	CX	53	CYS	4.5
20	BT	52	ASN	4.5
14	BN	49	GLN	4.5
31	CA	2124	G	4.5
17	BQ	63	GLU	4.4
34	CF	113	ASP	4.4
37	CJ	116	ASP	4.4
37	CJ	99	GLY	4.4
10	BJ	37	ARG	4.4
35	CG	96	ALA	4.4
37	CJ	55	ILE	4.4
40	CM	100	ILE	4.4
34	CF	138	PHE	4.4
34	CF	93	GLY	4.4
37	CJ	62	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
35	CG	10	VAL	4.4
54	DI	55	VAL	4.4
10	BJ	91	ASP	4.4
22	C1	55	ILE	4.4
2	BB	130	THR	4.4
54	DI	94	ARG	4.4
34	CF	111	ILE	4.4
13	BM	42	ASP	4.4
31	CA	88	G	4.4
2	BB	35	ARG	4.4
12	BL	124	ALA	4.4
1	BA	83	C	4.4
31	CA	1167	C	4.4
7	AG	62	PHE	4.4
13	BM	4	ILE	4.4
53	CZ	40	SER	4.4
40	CM	78	ARG	4.4
37	DJ	87	LYS	4.3
9	BI	4	ASN	4.3
31	CA	312	G	4.3
44	CQ	9	GLU	4.3
7	AG	112	GLY	4.3
35	CG	26	ILE	4.3
43	CP	36	TYR	4.3
7	AG	58	GLU	4.3
2	BB	33	GLY	4.3
37	CJ	31	GLN	4.3
49	CV	12	ILE	4.3
7	BG	72	THR	4.3
49	CV	19	LYS	4.3
36	DH	67	ALA	4.3
13	AM	99	GLY	4.3
16	BP	41	PRO	4.3
20	BT	59	ASP	4.3
23	C2	48	ILE	4.3
37	DJ	95	LYS	4.3
41	CN	136	MET	4.3
30	CD	4	LEU	4.3
21	AU	2	PRO	4.3
37	CJ	51	LYS	4.3
9	BI	5	GLN	4.3
12	BL	70	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
10	BJ	6	ILE	4.3
1	BA	983	A	4.3
7	AG	4	ARG	4.3
55	DA	1060	U	4.3
46	CS	32	THR	4.3
35	CG	40	ALA	4.3
20	BT	75	HIS	4.3
44	CQ	84	ILE	4.3
44	CQ	12	GLN	4.3
7	BG	16	PRO	4.3
31	CA	103	A	4.2
15	BO	89	ARG	4.2
1	BA	1024	G	4.2
10	AJ	75	ASP	4.2
36	DH	94	ILE	4.2
43	CP	92	PHE	4.2
34	CF	102	ARG	4.2
23	C2	24	THR	4.2
43	CP	117	PHE	4.2
1	BA	470	C	4.2
20	BT	72	ALA	4.2
37	CJ	78	VAL	4.2
34	CF	129	SER	4.2
34	CF	94	GLU	4.2
9	AI	22	LYS	4.2
7	BG	120	LEU	4.2
31	CA	2803	G	4.2
53	CZ	37	LEU	4.2
1	BA	1031	C	4.2
46	CS	63	VAL	4.2
19	BS	76	PRO	4.2
10	BJ	7	ARG	4.2
48	CU	15	HIS	4.2
37	CJ	42	PHE	4.2
37	CJ	95	LYS	4.2
50	CW	94	ALA	4.2
9	BI	32	GLN	4.1
31	CA	613	A	4.1
13	AM	23	TYR	4.1
34	CF	95	ARG	4.1
16	BP	53	ASP	4.1
54	DI	38	MET	4.1

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Mol	Chain	Res	Type	RSRZ
55	DA	2173	A	4.1
16	AP	47	GLU	4.1
40	CM	8	PRO	4.1
53	CZ	41	HIS	4.1
19	BS	31	LEU	4.1
49	CV	51	ALA	4.1
13	AM	16	VAL	4.1
55	DA	893	C	4.1
30	CD	179	ARG	4.1
7	BG	48	GLU	4.1
34	CF	151	GLY	4.1
35	CG	81	GLU	4.1
31	CA	1061	U	4.1
40	CM	92	LEU	4.1
10	BJ	90	LEU	4.1
34	CF	97	TRP	4.1
1	AA	88	U	4.1
31	CA	546	U	4.1
7	BG	129	GLU	4.1
34	CF	83	TYR	4.1
14	BN	55	SER	4.1
37	CJ	26	PRO	4.1
38	CK	142	ILE	4.1
35	CG	166	ASP	4.1
49	CV	81	ASP	4.1
34	CF	86	GLY	4.1
43	CP	33	ARG	4.1
55	DA	2166	U	4.1
2	BB	9	MET	4.1
17	BQ	73	TRP	4.1
13	AM	5	ALA	4.1
54	DI	121	SER	4.1
7	BG	52	GLN	4.1
55	DA	1088	A	4.1
40	CM	118	THR	4.0
35	CG	86	LYS	4.0
11	AK	19	GLY	4.0
31	CA	2797	U	4.0
20	BT	35	VAL	4.0
46	CS	7	SER	4.0
43	CP	39	VAL	4.0
54	DI	135	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	BA	1034	G	4.0
55	DA	1087	G	4.0
49	CV	4	LYS	4.0
37	DJ	115	ALA	4.0
14	BN	27	LEU	4.0
20	BT	24	ARG	4.0
23	C2	31	PRO	4.0
40	CM	126	ARG	4.0
27	C0	43	ALA	4.0
34	CF	38	MET	4.0
31	CA	2667	C	4.0
1	BA	80	A	4.0
1	BA	81	A	4.0
31	CA	2665	A	4.0
31	CA	879	G	4.0
55	DA	1731	G	4.0
7	BG	88	PRO	4.0
48	CU	16	VAL	4.0
33	CE	172	ALA	4.0
1	BA	208	U	4.0
13	AM	32	ALA	4.0
19	BS	66	MET	4.0
9	BI	129	LYS	4.0
37	DJ	100	LYS	4.0
1	BA	68	G	4.0
37	DJ	110	ALA	4.0
35	CG	116	GLN	4.0
36	DH	87	GLU	4.0
31	CA	12	U	4.0
31	CA	138	U	4.0
1	BA	469	C	4.0
43	CP	54	VAL	4.0
55	DA	1072	C	4.0
7	AG	50	LEU	4.0
46	CS	95	ASP	4.0
7	BG	145	ALA	4.0
7	BG	6	VAL	3.9
10	BJ	10	LEU	3.9
24	C3	31	LEU	3.9
34	CF	131	GLY	3.9
31	CA	1106	G	3.9
43	CP	62	LEU	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
37	CJ	96	ASP	3.9
31	CA	311	A	3.9
35	CG	132	VAL	3.9
27	C0	8	THR	3.9
31	CA	1064	C	3.9
1	AA	82	G	3.9
33	CE	33	VAL	3.9
34	CF	112	ARG	3.9
22	C1	15	MET	3.9
36	CH	140	ALA	3.9
2	BB	213	TYR	3.9
14	BN	40	ASP	3.9
13	BM	21	SER	3.9
34	CF	143	TYR	3.9
37	CJ	113	LYS	3.9
30	CD	25	THR	3.9
13	BM	31	LYS	3.9
1	BA	844	G	3.9
7	BG	109	ARG	3.9
40	CM	132	ARG	3.9
13	BM	100	GLN	3.9
37	CJ	18	ALA	3.9
37	CJ	83	ALA	3.9
43	CP	41	ALA	3.9
35	CG	76	VAL	3.9
13	BM	105	ASN	3.9
55	DA	1066	U	3.9
33	CE	8	ALA	3.9
13	BM	16	VAL	3.9
37	CJ	32	GLY	3.9
49	CV	84	GLY	3.9
19	BS	37	ARG	3.9
23	C2	35	GLU	3.9
37	CJ	73	THR	3.9
44	CQ	2	SER	3.9
37	DJ	131	GLY	3.9
7	AG	7	ILE	3.9
37	DJ	36	MET	3.9
35	CG	136	ALA	3.9
34	CF	31	VAL	3.9
53	CZ	29	ARG	3.9
19	BS	59	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
33	CE	190	ALA	3.9
49	CV	27	ASN	3.9
24	C3	42	LEU	3.8
53	CZ	33	ALA	3.9
20	BT	48	GLN	3.8
1	BA	1242	G	3.8
9	AI	21	ILE	3.8
51	CX	63	ALA	3.8
31	CA	262	A	3.8
50	CW	11	GLU	3.8
37	DJ	21	SER	3.8
13	AM	25	VAL	3.8
51	CX	85	GLU	3.8
31	CA	267	C	3.8
13	BM	23	TYR	3.8
33	CE	30	GLN	3.8
37	CJ	10	LYS	3.8
40	CM	133	ALA	3.8
37	DJ	89	GLY	3.8
36	DH	99	ILE	3.8
13	BM	37	ALA	3.8
1	BA	632	U	3.8
26	C5	10	LEU	3.8
43	CP	115	LEU	3.8
7	BG	71	PRO	3.8
31	CA	356	G	3.8
55	DA	2128	G	3.8
31	CA	892	A	3.8
37	CJ	43	ASN	3.8
43	CP	67	ASN	3.8
2	BB	131	LYS	3.8
1	BA	134	G	3.8
28	CB	51	G	3.8
37	CJ	138	LEU	3.8
10	BJ	19	ASP	3.8
19	AS	56	GLN	3.8
20	BT	53	GLU	3.8
9	BI	67	VAL	3.8
31	CA	1538	G	3.8
7	AG	109	ARG	3.8
30	CD	77	ARG	3.8
9	BI	66	THR	3.8

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Mol	Chain	Res	Type	RSRZ
13	BM	85	CYS	3.8
24	C3	30	VAL	3.8
35	CG	113	VAL	3.8
13	BM	32	ALA	3.7
34	CF	170	LEU	3.7
5	BE	91	GLY	3.7
55	DA	2165	C	3.7
17	BQ	53	CYS	3.7
40	CM	77	ILE	3.7
37	CJ	91	GLY	3.7
35	CG	27	LYS	3.7
14	BN	37	SER	3.7
13	BM	103	LYS	3.7
20	BT	49	LYS	3.7
49	CV	39	ILE	3.7
55	DA	654	A	3.7
31	CA	1049	C	3.7
6	BF	8	PHE	3.7
1	AA	81	A	3.7
40	CM	120	VAL	3.7
48	CU	55	VAL	3.7
48	CU	85	VAL	3.7
31	CA	76	C	3.7
34	CF	23	ASN	3.7
13	AM	58	ASP	3.7
55	DA	138	U	3.7
19	BS	48	THR	3.7
53	CZ	17	GLU	3.7
31	CA	74	A	3.7
55	DA	897	C	3.7
20	BT	56	PRO	3.7
30	CD	200	ASP	3.7
31	CA	2168	G	3.7
37	CJ	84	ALA	3.7
34	CF	60	ILE	3.7
36	CH	132	PHE	3.7
19	AS	77	THR	3.7
55	DA	1089	A	3.7
34	CF	139	PRO	3.7
47	CT	97	LEU	3.7
2	BB	40	ILE	3.7
34	CF	173	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
15	BO	22	THR	3.6
44	CQ	110	ILE	3.6
19	BS	56	GLN	3.6
48	CU	87	LEU	3.6
1	BA	472	U	3.6
10	BJ	72	ARG	3.6
49	CV	50	PRO	3.6
43	CP	46	GLU	3.6
31	CA	877	A	3.6
31	CA	1069	A	3.6
2	BB	201	PRO	3.6
1	BA	121	U	3.6
16	BP	60	TRP	3.6
49	CV	21	LYS	3.6
35	CG	73	ASN	3.6
13	BM	9	ILE	3.6
31	CA	846	U	3.6
13	BM	101	ARG	3.6
35	CG	115	HIS	3.6
22	C1	36	GLU	3.6
31	CA	1238	G	3.6
31	CA	2410	G	3.6
23	C2	21	TYR	3.6
13	BM	49	SER	3.6
14	BN	32	SER	3.6
24	C3	28	ARG	3.6
36	DH	93	SER	3.6
9	BI	58	VAL	3.6
33	CE	119	ILE	3.6
13	BM	24	GLY	3.6
7	AG	54	SER	3.6
19	AS	74	PHE	3.6
31	CA	1211	C	3.6
33	CE	7	ASP	3.6
1	BA	191	G	3.6
1	BA	1026	G	3.6
31	CA	1107	G	3.6
35	CG	152	ARG	3.6
46	CS	35	PHE	3.6
19	BS	12	ASP	3.6
48	CU	60	THR	3.6
12	BL	48	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
37	CJ	44	ALA	3.6
37	DJ	10	LYS	3.6
55	DA	878	A	3.6
17	BQ	46	VAL	3.6
13	BM	108	THR	3.6
9	BI	90	TYR	3.6
54	DI	106	PHE	3.5
31	CA	896	A	3.5
45	CR	81	ASN	3.5
13	BM	34	LEU	3.5
33	CE	143	LEU	3.5
35	CG	94	TYR	3.5
13	BM	19	LEU	3.5
20	BT	8	LYS	3.5
35	CG	108	GLY	3.5
23	C2	40	ASP	3.5
31	CA	1870	C	3.5
31	CA	1111	A	3.5
7	AG	42	ILE	3.5
14	BN	53	ARG	3.5
1	BA	1033	G	3.5
31	CA	431	U	3.5
35	CG	97	ALA	3.5
49	CV	95	PHE	3.5
47	CT	94	ASP	3.5
2	BB	14	VAL	3.5
13	BM	22	ILE	3.5
25	C4	61	CYS	3.5
35	CG	162	VAL	3.5
10	BJ	87	LEU	3.5
2	BB	206	ALA	3.5
2	BB	82	ASP	3.5
31	CA	1731	G	3.5
31	CA	1048	A	3.5
49	CV	18	ASP	3.5
10	BJ	35	GLN	3.5
46	CS	49	ILE	3.5
31	CA	1046	A	3.5
1	BA	218	U	3.5
24	C3	33	ARG	3.5
40	CM	1	MET	3.5
9	AI	6	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
10	BJ	81	GLU	3.5
34	CF	155	THR	3.5
37	CJ	128	SER	3.5
37	DJ	128	SER	3.5
30	CD	180	VAL	3.5
35	CG	24	ILE	3.5
31	CA	2129	C	3.5
55	DA	1071	G	3.5
23	C2	37	LYS	3.5
30	CD	1	MET	3.5
13	BM	5	ALA	3.5
31	CA	316	C	3.4
1	BA	1241	G	3.4
30	CD	188	LEU	3.4
31	CA	317	G	3.4
54	DI	80	THR	3.4
37	DJ	40	LYS	3.4
30	CD	45	TYR	3.4
34	CF	142	ASP	3.4
7	BG	41	SER	3.4
27	C0	29	LEU	3.4
27	C0	47	MET	3.4
27	C0	39	GLU	3.4
40	CM	113	ALA	3.4
2	BB	37	LYS	3.4
13	AM	29	ARG	3.4
54	DI	103	ASN	3.4
9	BI	127	PHE	3.4
2	BB	135	LEU	3.4
35	CG	133	LEU	3.4
11	AK	81	ASN	3.4
51	CX	60	PHE	3.4
47	CT	5	ALA	3.4
10	AJ	74	VAL	3.4
35	CG	141	ILE	3.4
55	DA	2171	A	3.4
35	CG	85	LYS	3.4
40	CM	115	GLU	3.4
1	AA	85	U	3.4
10	BJ	21	ALA	3.4
18	AR	32	TYR	3.4
34	CF	114	PHE	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
30	CD	42	ASN	3.4
37	CJ	19	ASN	3.4
44	CQ	34	GLU	3.4
9	BI	9	THR	3.4
19	BS	40	ILE	3.4
24	C3	18	PHE	3.4
13	AM	8	ASN	3.4
37	CJ	139	VAL	3.4
35	CG	109	PHE	3.4
36	CH	18	GLN	3.4
43	CP	99	TYR	3.4
19	BS	61	PHE	3.4
43	CP	69	ASP	3.4
49	CV	14	LEU	3.4
33	CE	183	PHE	3.4
14	AN	47	LYS	3.4
20	BT	50	ALA	3.4
1	BA	1038	C	3.4
31	CA	313	G	3.4
48	CU	35	ALA	3.4
31	CA	1868	C	3.4
55	DA	1074	G	3.4
55	DA	2161	C	3.4
37	DJ	25	GLY	3.4
1	BA	325	A	3.4
31	CA	1089	A	3.4
31	CA	1169	A	3.4
34	CF	110	ARG	3.4
40	CM	90	VAL	3.4
49	CV	70	VAL	3.4
10	BJ	24	GLU	3.4
13	BM	50	GLU	3.4
31	CA	183	C	3.4
36	DH	95	GLY	3.4
13	BM	112	PRO	3.3
27	C0	2	ALA	3.3
30	CD	209	ALA	3.3
31	CA	309	A	3.3
8	AH	121	LEU	3.3
13	BM	12	HIS	3.3
9	AI	39	PHE	3.3
30	CD	76	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
48	CU	37	ASP	3.3
37	DJ	58	VAL	3.3
28	CB	97	C	3.3
35	CG	59	ALA	3.3
34	CF	80	ARG	3.3
30	CD	43	ASP	3.3
46	CS	31	GLU	3.3
10	AJ	6	ILE	3.3
30	CD	10	GLY	3.3
13	AM	63	PHE	3.3
9	AI	17	ALA	3.3
37	DJ	84	ALA	3.3
35	CG	62	TRP	3.3
6	BF	39	LEU	3.3
14	BN	3	LYS	3.3
14	BN	48	LEU	3.3
53	CZ	31	GLN	3.3
14	BN	2	ALA	3.3
7	BG	45	SER	3.3
16	BP	77	GLU	3.3
34	CF	141	ILE	3.3
35	CG	45	HIS	3.3
36	DH	70	GLU	3.3
37	CJ	133	ALA	3.3
35	CG	107	LEU	3.3
34	CF	147	ASP	3.3
36	DH	66	ASN	3.3
46	CS	62	GLU	3.3
7	BG	108	ALA	3.3
13	AM	45	ILE	3.3
37	CJ	27	ALA	3.3
37	CJ	85	GLY	3.3
37	DJ	83	ALA	3.3
55	DA	1729	U	3.3
14	BN	51	LEU	3.3
49	CV	98	SER	3.3
1	AA	1016	A	3.3
31	CA	308	G	3.3
7	BG	69	VAL	3.3
2	AB	46	THR	3.3
37	DJ	33	VAL	3.3
1	BA	473	U	3.3

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Mol	Chain	Res	Type	RSRZ
31	CA	476	G	3.3
7	BG	39	ALA	3.3
20	BT	85	LYS	3.3
49	CV	49	VAL	3.3
1	BA	54	C	3.2
33	CE	104	ALA	3.2
19	BS	27	ASP	3.2
34	CF	96	MET	3.2
35	CG	126	PRO	3.2
37	DJ	37	GLU	3.2
36	CH	107	GLY	3.2
36	DH	63	ALA	3.2
37	CJ	135	SER	3.2
6	AF	97	THR	3.2
53	CZ	22	LEU	3.2
55	DA	1847	A	3.2
10	BJ	36	VAL	3.2
13	BM	113	ARG	3.2
47	CT	84	ARG	3.2
55	DA	2115	G	3.2
45	CR	71	GLN	3.2
13	BM	84	GLY	3.2
7	AG	45	SER	3.2
7	BG	66	LEU	3.2
1	BA	1441	A	3.2
13	BM	98	ARG	3.2
9	AI	19	VAL	3.2
43	CP	103	VAL	3.2
13	BM	13	LYS	3.2
54	DI	84	TYR	3.2
37	DJ	60	THR	3.2
20	BT	19	LYS	3.2
45	CR	73	GLY	3.2
31	CA	1044	C	3.2
9	AI	90	TYR	3.2
43	CP	29	HIS	3.2
7	BG	7	ILE	3.2
7	BG	111	ARG	3.2
23	C2	36	LEU	3.2
40	CM	142	ILE	3.2
36	CH	108	VAL	3.2
50	CW	27	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
30	CD	8	LYS	3.2
33	CE	10	SER	3.2
3	BC	159	GLY	3.2
10	BJ	22	THR	3.2
13	BM	28	THR	3.2
31	CA	1963	U	3.2
55	DA	546	U	3.2
1	BA	1002	G	3.2
13	BM	26	GLY	3.2
29	CC	249	GLY	3.2
43	CP	91	SER	3.2
35	CG	56	ASP	3.2
31	CA	2122	U	3.2
17	BQ	72	SER	3.2
24	C3	37	LYS	3.2
37	CJ	36	MET	3.2
18	AR	74	HIS	3.2
30	CD	41	ALA	3.2
34	CF	59	ALA	3.2
37	CJ	77	ALA	3.2
43	CP	90	VAL	3.2
36	CH	72	ILE	3.2
7	BG	60	GLU	3.2
55	DA	1175	A	3.2
51	CX	55	ARG	3.1
40	CM	108	ALA	3.1
22	C1	46	ASP	3.1
45	CR	91	ASP	3.1
1	AA	1302	C	3.1
3	BC	53	SER	3.1
37	DJ	34	ASN	3.1
7	BG	49	THR	3.1
20	BT	68	HIS	3.1
31	CA	1077	A	3.1
31	CA	2860	A	3.1
42	CO	116	VAL	3.1
1	BA	79	G	3.1
1	BA	204	G	3.1
31	CA	876	C	3.1
40	CM	138	ALA	3.1
22	C1	18	SER	3.1
33	CE	157	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
13	BM	102	THR	3.1
27	C0	7	ILE	3.1
43	CP	87	ILE	3.1
43	CP	93	ASP	3.1
50	CW	32	GLY	3.1
19	BS	41	PHE	3.1
29	CC	30	PHE	3.1
31	CA	548	G	3.1
2	BB	187	VAL	3.1
7	BG	73	VAL	3.1
34	CF	150	ARG	3.1
27	C0	24	LEU	3.1
13	BM	38	GLY	3.1
7	AG	57	SER	3.1
31	CA	335	C	3.1
23	C2	23	THR	3.1
24	C3	24	THR	3.1
37	CJ	70	VAL	3.1
19	BS	5	LEU	3.1
14	BN	43	ASN	3.1
14	BN	45	VAL	3.1
37	CJ	50	GLU	3.1
46	CS	14	VAL	3.1
31	CA	1075	C	3.1
35	CG	87	LEU	3.1
46	CS	37	GLU	3.1
35	CG	101	ASN	3.1
6	AF	61	LEU	3.1
7	AG	49	THR	3.1
41	CN	8	LYS	3.1
46	CS	92	TRP	3.1
55	DA	2108	A	3.1
1	BA	212	G	3.1
31	CA	1168	G	3.1
40	CM	134	ALA	3.1
50	CW	6	ALA	3.1
14	BN	9	ARG	3.1
1	BA	1201	A	3.1
2	BB	44	GLU	3.1
34	CF	149	VAL	3.1
36	DH	142	VAL	3.1
34	CF	84	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
36	CH	136	SER	3.1
43	CP	102	ARG	3.1
2	AB	32	PHE	3.1
46	CS	15	SER	3.1
31	CA	1873	G	3.1
31	CA	2801	G	3.1
34	CF	76	GLY	3.1
35	CG	122	THR	3.1
1	BA	1226	C	3.1
55	DA	1073	A	3.1
37	DJ	116	ASP	3.0
46	CS	55	ASP	3.0
34	CF	140	GLU	3.0
36	CH	110	VAL	3.0
53	CZ	32	ALA	3.0
1	BA	135	C	3.0
31	CA	53	A	3.0
55	DA	2164	C	3.0
55	DA	2169	A	3.0
1	BA	1025	U	3.0
5	BE	140	THR	3.0
31	CA	369	U	3.0
31	CA	1078	U	3.0
37	CJ	136	MET	3.0
7	BG	137	LYS	3.0
12	BL	113	ALA	3.0
16	BP	15	PRO	3.0
42	CO	120	GLU	3.0
47	CT	103	ILE	3.0
9	AI	128	SER	3.0
9	AI	63	LEU	3.0
19	AS	39	THR	3.0
35	CG	129	THR	3.0
34	CF	115	ARG	3.0
1	BA	86	G	3.0
7	BG	118	LEU	3.0
1	BA	843	U	3.0
9	BI	39	PHE	3.0
40	CM	117	THR	3.0
2	BB	21	ARG	3.0
33	CE	25	GLU	3.0
33	CE	193	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
14	BN	4	GLN	3.0
20	BT	6	SER	3.0
22	C1	34	SER	3.0
10	BJ	28	THR	3.0
31	CA	2165	C	3.0
31	CA	2175	C	3.0
1	BA	174	A	3.0
46	CS	12	HIS	3.0
10	BJ	71	LEU	3.0
20	BT	79	LEU	3.0
34	CF	56	ASP	3.0
30	CD	91	THR	3.0
35	CG	130	GLU	3.0
31	CA	228	C	3.0
31	CA	1015	U	3.0
31	CA	86	G	3.0
31	CA	1869	G	3.0
31	CA	2862	G	3.0
7	BG	130	ASN	3.0
9	BI	31	ASN	3.0
13	AM	36	ALA	3.0
20	BT	32	ILE	3.0
35	CG	17	VAL	3.0
19	AS	55	ARG	3.0
31	CA	646	U	3.0
34	CF	122	PHE	3.0
15	BO	26	GLU	3.0
9	AI	38	TYR	3.0
28	CB	117	G	3.0
37	CJ	123	GLU	3.0
46	CS	59	ILE	3.0
46	CS	38	VAL	3.0
6	BF	97	THR	3.0
13	BM	20	THR	3.0
9	AI	129	LYS	3.0
50	CW	12	GLN	3.0
14	BN	26	GLU	3.0
37	DJ	52	GLY	3.0
9	BI	6	TYR	3.0
13	BM	35	ALA	3.0
1	BA	1048	G	3.0
31	CA	81	G	3.0

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Mol	Chain	Res	Type	RSRZ
1	BA	1029	U	3.0
55	DA	2180	U	3.0
2	BB	210	VAL	3.0
7	BG	85	TYR	3.0
12	BL	117	TYR	3.0
30	CD	39	ASP	3.0
49	CV	11	VAL	3.0
1	BA	1005	A	3.0
35	CG	52	PHE	3.0
48	CU	59	ASN	3.0
13	BM	45	ILE	2.9
28	CB	98	G	2.9
34	CF	75	ALA	2.9
7	AG	118	LEU	2.9
33	CE	47	LYS	2.9
33	CE	140	ASP	2.9
35	CG	137	ASP	2.9
43	CP	88	LYS	2.9
22	C1	33	THR	2.9
37	CJ	25	GLY	2.9
43	CP	22	GLY	2.9
7	BG	134	ALA	2.9
36	CH	9	VAL	2.9
43	CP	74	VAL	2.9
20	BT	51	PHE	2.9
13	BM	46	SER	2.9
25	C4	28	ASN	2.9
37	DJ	90	SER	2.9
13	BM	27	LYS	2.9
1	BA	1004	A	2.9
3	BC	71	ALA	2.9
31	CA	1070	A	2.9
53	CZ	56	LEU	2.9
31	CA	2891	U	2.9
28	CB	116	G	2.9
40	CM	7	SER	2.9
31	CA	264	C	2.9
1	BA	1362	A	2.9
7	BG	70	ARG	2.9
36	CH	78	VAL	2.9
13	AM	41	GLU	2.9
31	CA	1072	C	2.9

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Mol	Chain	Res	Type	RSRZ
31	CA	1076	C	2.9
31	CA	501	A	2.9
1	BA	1240	U	2.9
9	AI	31	ASN	2.9
24	C3	26	ASN	2.9
33	CE	135	ALA	2.9
48	CU	76	ARG	2.9
17	BQ	69	LYS	2.9
39	CL	112	PHE	2.9
1	BA	69	G	2.9
7	BG	119	ARG	2.9
22	C1	5	GLN	2.9
40	CM	3	LEU	2.9
48	CU	67	VAL	2.9
1	AA	121	U	2.9
1	BA	459	A	2.9
16	AP	43	ALA	2.9
31	CA	2167	U	2.9
37	DJ	51	LYS	2.9
47	CT	98	LYS	2.9
51	CX	33	ALA	2.9
1	BA	1049	U	2.9
31	CA	1060	U	2.9
31	CA	1082	U	2.9
43	CP	32	PRO	2.9
48	CU	80	TRP	2.9
52	CY	49	LEU	2.9
28	CB	49	C	2.9
34	CF	145	LYS	2.9
35	DG	177	LYS	2.9
53	CZ	54	LYS	2.9
1	BA	468	A	2.9
31	CA	2861	U	2.9
37	DJ	85	GLY	2.9
40	CM	139	GLY	2.9
37	CJ	125	MET	2.9
48	CU	47	VAL	2.9
2	BB	133	GLU	2.9
16	BP	40	ASN	2.9
3	BC	192	THR	2.9
15	BO	25	THR	2.9
19	BS	79	THR	2.9

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Mol	Chain	Res	Type	RSRZ
31	CA	117	G	2.9
31	CA	2892	G	2.9
31	CA	1098	A	2.9
20	BT	82	GLN	2.9
18	AR	51	TYR	2.9
13	BM	66	GLU	2.9
34	CF	33	LYS	2.9
33	CE	24	ASN	2.9
48	CU	10	VAL	2.9
48	CU	24	MET	2.9
3	BC	193	TYR	2.9
10	BJ	86	ALA	2.9
7	BG	58	GLU	2.9
54	DI	72	LEU	2.9
7	BG	3	ARG	2.8
13	BM	104	THR	2.8
1	BA	213	G	2.8
31	CA	1047	G	2.8
43	CP	106	LEU	2.8
55	DA	613	A	2.8
34	CF	79	ILE	2.8
37	DJ	49	ILE	2.8
30	CD	59	ARG	2.8
1	AA	1286	U	2.8
31	CA	1729	U	2.8
31	CA	2160	C	2.8
16	BP	10	GLY	2.8
33	CE	154	ASP	2.8
46	CS	22	LEU	2.8
53	CZ	6	LEU	2.8
54	DI	124	ASP	2.8
16	BP	56	ARG	2.8
25	C4	37	ALA	2.8
31	CA	1059	G	2.8
38	CK	131	ASN	2.8
40	CM	130	GLY	2.8
1	AA	1037	C	2.8
13	AM	62	LYS	2.8
13	BM	58	ASP	2.8
31	CA	893	C	2.8
16	BP	80	LYS	2.8
36	DH	138	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
30	CD	90	PHE	2.8
55	DA	2117	A	2.8
15	BO	17	ARG	2.8
19	BS	33	THR	2.8
1	BA	1224	U	2.8
25	C4	41	LYS	2.8
34	CF	92	ARG	2.8
40	CM	5	THR	2.8
2	AB	30	PHE	2.8
40	CM	135	ILE	2.8
44	CQ	86	VAL	2.8
42	DO	125	ALA	2.8
31	CA	2117	A	2.8
34	CF	37	ASN	2.8
37	DJ	91	GLY	2.8
44	DQ	115	ASN	2.8
13	AM	39	ILE	2.8
43	CP	27	VAL	2.8
13	BM	11	ASP	2.8
31	CA	235	U	2.8
55	DA	2118	U	2.8
7	AG	110	LYS	2.8
37	CJ	48	SER	2.8
37	DJ	48	SER	2.8
20	BT	70	ASN	2.8
34	CF	99	PHE	2.8
37	CJ	112	THR	2.8
5	BE	125	ALA	2.8
9	BI	17	ALA	2.8
36	CH	12	LEU	2.8
22	C1	27	SER	2.8
31	CA	2300	C	2.8
2	BB	132	LYS	2.8
7	BG	143	ARG	2.8
20	BT	5	LYS	2.8
23	C2	44	ARG	2.8
7	BG	15	ASP	2.8
34	CF	107	ALA	2.8
35	CG	54	PRO	2.8
51	CX	59	LEU	2.8
35	CG	169	VAL	2.8
9	AI	28	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	BA	1003	G	2.8
28	CB	27	C	2.8
43	CP	25	ARG	2.8
25	C4	43	HIS	2.8
37	DJ	14	ALA	2.8
37	DJ	77	ALA	2.8
9	BI	126	GLN	2.8
31	CA	1174	U	2.8
48	DU	91	GLN	2.8
53	CZ	24	GLU	2.8
39	CL	21	CYS	2.8
13	AM	48	LEU	2.8
17	BQ	44	LEU	2.8
34	CF	58	ALA	2.8
43	CP	79	ALA	2.8
1	BA	201	G	2.8
31	CA	277	G	2.8
1	BA	609	A	2.8
1	BA	1067	A	2.8
7	BG	115	SER	2.8
19	BS	68	GLY	2.8
7	BG	56	LYS	2.8
13	AM	57	ARG	2.8
31	CA	1454	C	2.8
35	CG	43	VAL	2.8
46	CS	29	THR	2.8
53	CZ	7	ARG	2.8
49	CV	72	ILE	2.7
9	BI	68	LYS	2.7
16	BP	7	ALA	2.7
16	BP	38	PHE	2.7
20	BT	29	ARG	2.7
50	CW	13	GLY	2.7
55	DA	2176	A	2.7
16	BP	18	GLN	2.7
19	BS	28	LYS	2.7
43	CP	56	LYS	2.7
49	CV	52	LEU	2.7
9	BI	20	PHE	2.7
36	CH	47	PHE	2.7
36	DH	108	VAL	2.7
13	BM	33	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
40	CM	119	PRO	2.7
33	CE	150	THR	2.7
44	CQ	11	GLU	2.7
49	CV	66	GLN	2.7
37	DJ	106	LEU	2.7
31	CA	139	U	2.7
36	CH	142	VAL	2.7
48	CU	58	VAL	2.7
21	BU	2	PRO	2.7
34	CF	42	GLU	2.7
34	CF	69	LYS	2.7
37	DJ	97	LYS	2.7
51	CX	62	LYS	2.7
1	BA	460	A	2.7
30	CD	203	VAL	2.7
1	BA	67	C	2.7
19	BS	69	HIS	2.7
1	BA	108	G	2.7
7	BG	89	VAL	2.7
20	BT	63	ALA	2.7
31	CA	1055	G	2.7
31	CA	2107	G	2.7
48	CU	23	ALA	2.7
7	AG	48	GLU	2.7
13	AM	26	GLY	2.7
30	CD	44	GLY	2.7
43	CP	89	ASP	2.7
33	CE	186	VAL	2.7
22	C1	52	ARG	2.7
31	CA	1142	A	2.7
55	DA	2119	A	2.7
1	BA	153	C	2.7
7	AG	68	ASN	2.7
31	CA	1460	U	2.7
31	CA	2178	C	2.7
54	DI	32	GLY	2.7
13	BM	109	ARG	2.7
37	DJ	27	ALA	2.7
45	CR	90	ILE	2.7
50	CW	89	ILE	2.7
30	CD	55	LYS	2.7
31	CA	502	A	2.7

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Mol	Chain	Res	Type	RSRZ
1	BA	107	G	2.7
31	CA	1017	G	2.7
48	CU	62	VAL	2.7
13	BM	36	ALA	2.7
14	AN	25	ALA	2.7
31	CA	854	C	2.7
33	CE	128	ALA	2.7
37	CJ	41	ALA	2.7
13	AM	103	LYS	2.7
43	CP	30	ARG	2.7
50	CW	34	LYS	2.7
31	CA	1143	A	2.7
54	DI	26	VAL	2.7
55	DA	2151	U	2.7
31	CA	1407	G	2.7
34	CF	27	GLN	2.7
35	CG	135	GLY	2.7
36	DH	88	GLY	2.7
44	CQ	114	LEU	2.7
55	DA	2114	A	2.7
16	AP	39	PHE	2.7
34	CF	26	MET	2.7
43	CP	86	GLY	2.7
55	DA	1076	C	2.7
31	CA	361	G	2.7
30	CD	199	SER	2.6
34	CF	137	ILE	2.7
34	CF	91	LEU	2.6
1	BA	1035	A	2.6
1	BA	1235	U	2.6
30	CD	35	THR	2.6
55	DA	895	U	2.6
1	BA	90	C	2.6
1	BA	207	C	2.6
1	BA	210	C	2.6
1	BA	1028	C	2.6
20	BT	34	LYS	2.6
31	CA	357	C	2.6
31	CA	1531	C	2.6
33	CE	138	LEU	2.6
52	CY	35	SER	2.6
1	BA	1126	U	2.6

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Mol	Chain	Res	Type	RSRZ
30	CD	29	VAL	2.6
31	CA	355	U	2.6
40	CM	102	GLY	2.6
50	CW	67	GLY	2.6
33	CE	127	GLU	2.6
18	AR	68	LEU	2.6
31	CA	236	C	2.6
7	AG	129	GLU	2.6
22	C1	57	LYS	2.6
11	AK	15	GLN	2.6
14	BN	50	THR	2.6
31	CA	315	G	2.6
37	CJ	34	ASN	2.6
44	CQ	92	VAL	2.6
48	CU	68	LYS	2.6
1	BA	89	U	2.6
31	CA	1340	U	2.6
2	BB	57	LEU	2.6
13	AM	15	ALA	2.6
1	BA	250	A	2.6
48	CU	36	LYS	2.6
2	AB	221	VAL	2.6
9	AI	18	ARG	2.6
35	CG	72	LEU	2.6
17	AQ	53	CYS	2.6
31	CA	776	G	2.6
31	CA	1016	G	2.6
49	CV	73	PHE	2.6
53	CZ	44	LYS	2.6
5	AE	10	GLU	2.6
13	AM	6	GLY	2.6
34	CF	25	VAL	2.6
35	CG	79	VAL	2.6
31	CA	885	C	2.6
31	CA	1741	C	2.6
36	CH	41	LYS	2.6
1	BA	102	G	2.6
43	CP	28	VAL	2.6
27	C0	9	GLN	2.6
36	CH	133	GLN	2.6
37	CJ	30	GLN	2.6
14	BN	20	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
22	C1	6	ASN	2.6
1	BA	1303	C	2.6
31	CA	1170	C	2.6
34	CF	43	ALA	2.6
17	BQ	66	PRO	2.6
19	BS	42	PRO	2.6
1	BA	92	U	2.6
3	AC	190	HIS	2.6
52	CY	20	HIS	2.6
53	CZ	46	VAL	2.6
8	BH	2	SER	2.6
29	CC	251	GLN	2.6
41	CN	41	LEU	2.6
31	CA	85	G	2.6
31	CA	2668	G	2.6
27	C0	55	VAL	2.6
31	CA	550	C	2.6
31	CA	1606	C	2.6
51	CX	83	GLU	2.6
31	CA	850	U	2.6
7	BG	54	SER	2.6
15	BO	19	ALA	2.6
33	CE	191	ASP	2.6
35	CG	134	LYS	2.6
40	CM	85	VAL	2.6
54	DI	88	HIS	2.6
31	CA	611	C	2.6
1	BA	471	U	2.6
55	DA	2122	U	2.6
24	C3	45	SER	2.6
19	BS	58	VAL	2.6
8	BH	121	LEU	2.6
19	BS	15	LEU	2.6
2	BB	164	ILE	2.6
44	CQ	4	ILE	2.6
1	BA	186	C	2.6
33	CE	23	PHE	2.6
31	CA	2111	U	2.6
37	DJ	50	GLU	2.6
53	CZ	5	GLU	2.6
2	AB	225	ARG	2.6
7	AG	53	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
19	BS	51	VAL	2.6
24	C3	34	ARG	2.6
37	DJ	117	MET	2.6
12	BL	112	GLN	2.5
23	C2	53	LYS	2.5
1	BA	55	A	2.5
10	AJ	7	ARG	2.5
45	CR	30	ARG	2.5
55	DA	1090	A	2.5
31	CA	880	G	2.5
55	DA	1075	C	2.5
17	BQ	64	CYS	2.5
42	CO	62	ASN	2.5
19	BS	14	HIS	2.5
2	BB	139	ARG	2.5
35	CG	95	ARG	2.5
54	DI	92	ALA	2.5
24	C3	27	GLY	2.5
30	CD	166	GLY	2.5
54	DI	90	GLY	2.5
31	CA	596	U	2.5
31	CA	1539	U	2.5
30	CD	101	PHE	2.5
34	CF	172	ALA	2.5
46	CS	18	GLN	2.5
33	CE	32	VAL	2.5
14	BN	16	LEU	2.5
6	AF	62	MET	2.5
7	BG	37	SER	2.5
17	BQ	21	ILE	2.5
30	CD	96	ILE	2.5
31	CA	2796	U	2.5
45	CR	29	SER	2.5
7	BG	150	ALA	2.5
10	BJ	12	ALA	2.5
16	BP	58	ALA	2.5
36	CH	76	GLU	2.5
39	CL	89	ASN	2.5
42	CO	111	ALA	2.5
44	CQ	75	GLN	2.5
48	CU	84	TYR	2.5
31	CA	1171	G	2.5

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Mol	Chain	Res	Type	RSRZ
31	CA	1215	G	2.5
37	CJ	16	GLY	2.5
7	BG	106	GLU	2.5
54	DI	107	GLU	2.5
55	DA	1094	U	2.5
1	BA	1320	C	2.5
14	BN	47	LYS	2.5
31	CA	237	C	2.5
31	CA	332	A	2.5
35	CG	161	GLY	2.5
19	AS	78	ARG	2.5
1	BA	1305	G	2.5
6	AF	90	MET	2.5
49	CV	60	GLU	2.5
43	CP	82	ALA	2.5
35	CG	25	THR	2.5
1	BA	1145	A	2.5
30	CD	14	ILE	2.5
37	CJ	35	ILE	2.5
2	AB	131	LYS	2.5
9	BI	92	GLU	2.5
35	CG	138	LYS	2.5
14	AN	55	SER	2.5
38	CK	141	ASP	2.5
28	CB	24	G	2.5
42	CO	119	SER	2.5
7	AG	18	PHE	2.5
27	C0	44	ILE	2.5
31	CA	477	A	2.5
31	CA	1073	A	2.5
37	CJ	37	GLU	2.5
13	AM	3	ARG	2.5
13	BM	64	VAL	2.5
37	DJ	65	ARG	2.5
48	CU	61	LEU	2.5
51	CX	34	GLY	2.5
29	CC	272	SER	2.5
31	CA	895	U	2.5
16	BP	50	THR	2.5
28	CB	23	G	2.5
31	CA	1524	G	2.5
33	CE	173	THR	2.5

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Mol	Chain	Res	Type	RSRZ
23	C2	42	VAL	2.5
40	CM	131	ALA	2.5
42	CO	66	ALA	2.5
53	CZ	4	LYS	2.5
1	AA	4	U	2.5
1	BA	326	G	2.5
16	BP	54	LEU	2.5
19	AS	50	ALA	2.5
23	C2	46	HIS	2.5
44	CQ	19	SER	2.5
10	BJ	78	GLU	2.5
17	BQ	78	VAL	2.5
31	CA	2109	U	2.5
37	DJ	46	THR	2.5
43	CP	75	GLY	2.5
43	CP	50	ALA	2.5
46	CS	103	ALA	2.5
34	CF	109	PRO	2.5
46	CS	93	PHE	2.5
2	BB	208	ARG	2.5
33	CE	75	SER	2.5
36	CH	27	ARG	2.5
42	CO	96	ARG	2.5
1	BA	175	C	2.4
1	BA	1322	C	2.4
1	BA	461	A	2.4
31	CA	2766	A	2.4
40	CM	74	THR	2.4
34	CF	133	ARG	2.4
49	CV	48	PRO	2.4
24	C3	22	MET	2.4
1	BA	380	G	2.4
10	BJ	92	LEU	2.4
12	BL	93	VAL	2.4
49	CV	90	GLY	2.4
24	C3	23	ALA	2.4
34	CF	119	ALA	2.4
30	CD	28	GLU	2.4
9	BI	91	ASP	2.4
47	CT	82	MET	2.4
17	BQ	23	VAL	2.4
30	CD	50	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
51	CX	57	HIS	2.4
40	CM	140	GLY	2.4
15	AO	17	ARG	2.4
20	AT	2	ALA	2.4
36	DH	74	ALA	2.4
17	BQ	50	ASN	2.4
20	BT	80	THR	2.4
31	CA	1052	C	2.4
31	CA	1053	C	2.4
35	DG	101	ASN	2.4
19	AS	30	PRO	2.4
31	CA	1328	A	2.4
34	CF	74	VAL	2.4
43	CP	49	VAL	2.4
46	CS	51	VAL	2.4
47	CT	95	ARG	2.4
3	BC	50	ALA	2.4
20	BT	45	ALA	2.4
37	CJ	94	ASN	2.4
44	CQ	3	ASN	2.4
19	BS	23	VAL	2.4
42	CO	93	GLY	2.4
45	CR	117	LEU	2.4
48	CU	1	MET	2.4
31	CA	289	G	2.4
31	CA	2367	G	2.4
19	AS	25	SER	2.4
43	CP	107	ALA	2.4
47	CT	44	ALA	2.4
19	BS	65	GLU	2.4
35	CG	124	GLU	2.4
43	CP	60	GLU	2.4
45	CR	74	ILE	2.4
33	CE	164	LEU	2.4
34	CF	4	LEU	2.4
37	DJ	61	VAL	2.4
47	CT	36	LEU	2.4
9	AI	64	TYR	2.4
14	BN	23	LYS	2.4
37	DJ	64	ASP	2.4
31	CA	310	A	2.4
45	CR	25	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	AA	1015	G	2.4
1	AA	1127	G	2.4
1	BA	378	G	2.4
31	CA	597	G	2.4
31	CA	1074	G	2.4
39	CL	22	ILE	2.4
7	BG	68	ASN	2.4
7	BG	141	VAL	2.4
48	CU	50	LEU	2.4
13	AM	44	LYS	2.4
35	CG	100	GLY	2.4
41	CN	69	PRO	2.4
49	CV	17	LYS	2.4
1	BA	219	U	2.4
30	CD	176	ASP	2.4
31	CA	1864	U	2.4
1	BA	95	C	2.4
31	CA	1045	C	2.4
47	CT	96	ILE	2.4
36	CH	58	LEU	2.4
1	AA	1026	G	2.4
1	BA	251	G	2.4
29	CC	233	GLY	2.4
33	CE	199	MET	2.4
27	C0	23	THR	2.4
50	CW	37	PRO	2.4
30	CD	30	GLU	2.4
33	DE	7	ASP	2.4
36	CH	67	ALA	2.4
31	CA	87	U	2.4
1	BA	316	C	2.4
9	BI	40	GLY	2.4
13	AM	97	VAL	2.4
36	DH	82	SER	2.4
47	CT	105	VAL	2.4
48	CU	81	LYS	2.4
34	CF	77	PHE	2.4
1	BA	993	G	2.4
31	CA	307	G	2.4
36	DH	89	LYS	2.4
42	CO	52	ILE	2.4
5	BE	124	LEU	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
30	CD	84	LEU	2.4
35	CG	120	GLY	2.4
37	CJ	117	MET	2.4
1	BA	1460	C	2.4
10	AJ	5	ARG	2.4
1	AA	994	A	2.4
27	C0	48	ILE	2.4
7	BG	105	VAL	2.4
10	BJ	101	SER	2.4
3	AC	80	LYS	2.4
40	CM	136	GLU	2.4
1	BA	222	C	2.4
54	DI	127	ALA	2.4
2	BB	46	THR	2.4
2	BB	123	ASP	2.3
8	BH	90	ASP	2.3
35	CG	16	ASP	2.3
55	DA	1103	A	2.3
1	BA	1125	U	2.3
19	AS	24	GLU	2.3
30	CD	88	GLU	2.3
1	AA	1305	G	2.3
10	BJ	79	PRO	2.3
31	CA	2368	C	2.3
49	CV	69	ASN	2.3
13	BM	63	PHE	2.3
35	CG	78	GLY	2.3
19	AS	44	MET	2.3
51	CX	64	ASP	2.3
7	BG	47	LEU	2.3
16	BP	51	ARG	2.3
17	BQ	8	LEU	2.3
36	CH	4	ILE	2.3
51	CX	25	ARG	2.3
16	BP	13	LYS	2.3
31	CA	327	G	2.3
31	CA	1179	G	2.3
34	CF	64	LYS	2.3
49	DV	56	GLY	2.3
19	BS	78	ARG	2.3
30	CD	46	ARG	2.3
31	CA	2118	U	2.3

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Mol	Chain	Res	Type	RSRZ
34	CF	89	VAL	2.3
37	DJ	139	VAL	2.3
42	CO	84	GLY	2.3
50	CW	10	LYS	2.3
10	BJ	83	THR	2.3
1	AA	1020	G	2.3
1	BA	354	G	2.3
31	CA	930	G	2.3
48	CU	33	LYS	2.3
54	DI	120	ALA	2.3
27	C0	53	PHE	2.3
12	BL	14	ARG	2.3
9	AI	83	ILE	2.3
36	DH	64	ALA	2.3
48	CU	83	ALA	2.3
19	BS	38	SER	2.3
31	CA	1862	G	2.3
29	CC	180	GLU	2.3
35	CG	167	GLU	2.3
44	CQ	112	GLU	2.3
13	BM	83	LEU	2.3
19	BS	63	THR	2.3
23	C2	17	THR	2.3
14	BN	25	ALA	2.3
33	CE	121	VAL	2.3
33	CE	103	GLY	2.3
36	DH	139	PHE	2.3
44	CQ	30	VAL	2.3
8	AH	120	GLY	2.3
10	BJ	95	GLY	2.3
1	BA	1243	C	2.3
1	BA	1317	C	2.3
6	AF	98	GLU	2.3
28	CB	19	C	2.3
47	CT	6	LYS	2.3
54	DI	52	MET	2.3
1	BA	260	G	2.3
1	BA	388	G	2.3
28	CB	96	G	2.3
31	CA	180	G	2.3
31	CA	1018	U	2.3
41	CN	124	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
53	CZ	14	LEU	2.3
55	DA	1059	G	2.3
14	BN	44	ALA	2.3
16	BP	20	VAL	2.3
31	CA	514	A	2.3
36	DH	96	THR	2.3
2	AB	27	MET	2.3
13	BM	114	LYS	2.3
47	CT	101	SER	2.3
48	CU	21	SER	2.3
31	CA	1043	C	2.3
31	CA	1874	C	2.3
1	BA	1148	U	2.3
7	BG	91	VAL	2.3
17	BQ	83	VAL	2.3
28	CB	22	U	2.3
31	CA	328	U	2.3
36	CH	10	ALA	2.3
37	CJ	63	ALA	2.3
50	CW	65	VAL	2.3
34	CF	29	PRO	2.3
11	AK	97	ILE	2.3
19	AS	40	ILE	2.3
46	CS	98	ILE	2.3
1	AA	984	C	2.3
13	AM	60	VAL	2.3
15	BO	15	PHE	2.3
34	CF	55	ALA	2.3
35	CG	9	VAL	2.3
36	CH	144	VAL	2.3
9	AI	27	LYS	2.3
9	BI	22	LYS	2.3
27	C0	19	LYS	2.3
55	DA	898	C	2.3
9	AI	89	GLU	2.3
15	BO	14	GLU	2.3
35	CG	34	THR	2.3
54	DI	29	ASP	2.3
55	DA	2106	U	2.3
28	CB	73	A	2.3
31	CA	345	A	2.3
31	CA	1633	G	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
31	CA	1872	A	2.3
36	DH	84	ALA	2.3
43	CP	59	ALA	2.3
49	CV	76	ALA	2.3
31	CA	2166	U	2.3
31	CA	2795	C	2.3
1	BA	197	A	2.3
2	AB	4	VAL	2.3
19	AS	22	ALA	2.3
35	CG	174	ALA	2.3
36	CH	14	SER	2.3
36	CH	61	VAL	2.3
36	CH	100	ALA	2.3
39	CL	33	ALA	2.3
45	CR	118	ALA	2.3
1	BA	88	U	2.2
10	AJ	102	LEU	2.2
10	BJ	9	ARG	2.2
23	C2	22	THR	2.2
40	CM	94	THR	2.2
16	AP	4	ILE	2.2
9	AI	104	VAL	2.2
7	BG	57	SER	2.2
13	BM	61	ALA	2.2
37	CJ	124	ALA	2.2
45	DR	118	ALA	2.2
51	CX	61	ALA	2.2
7	BG	103	TRP	2.2
1	AA	205	A	2.2
13	BM	3	ARG	2.2
17	BQ	5	ILE	2.2
36	CH	77	THR	2.2
40	CM	121	THR	2.2
6	BF	10	VAL	2.2
46	CS	64	VAL	2.2
31	CA	2078	C	2.2
34	CF	98	GLU	2.2
37	CJ	15	ALA	2.2
55	DA	1870	C	2.2
19	AS	35	SER	2.2
35	CG	74	SER	2.2
33	CE	200	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	BA	172	A	2.2
39	CL	20	MET	2.2
12	BL	109	ASP	2.2
13	AM	82	ASP	2.2
2	BB	217	VAL	2.2
7	AG	2	PRO	2.2
19	AS	76	PRO	2.2
1	BA	1312	G	2.2
31	CA	1529	G	2.2
31	CA	2449	U	2.2
31	CA	2876	G	2.2
1	BA	1037	C	2.2
29	DC	272	SER	2.2
31	CA	2150	C	2.2
16	AP	16	PHE	2.2
17	BQ	17	MET	2.2
2	BB	31	ILE	2.2
11	AK	18	ASP	2.2
15	BO	21	ASP	2.2
17	AQ	83	VAL	2.2
1	AA	1332	A	2.2
10	BJ	80	THR	2.2
13	AM	115	PRO	2.2
20	BT	78	ASN	2.2
33	CE	101	TYR	2.2
35	CG	13	ALA	2.2
36	CH	74	ALA	2.2
43	CP	85	LYS	2.2
44	CQ	35	GLY	2.2
49	CV	16	GLY	2.2
49	CV	71	ALA	2.2
7	BG	50	LEU	2.2
1	BA	1020	G	2.2
31	CA	7	G	2.2
31	CA	68	G	2.2
31	CA	882	G	2.2
1	BA	1147	C	2.2
9	BI	11	ARG	2.2
46	CS	78	ARG	2.2
17	BQ	54	GLY	2.2
25	C4	36	LYS	2.2
7	BG	65	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
37	DJ	43	ASN	2.2
38	CK	78	THR	2.2
54	DI	2	ALA	2.2
30	CD	201	LEU	2.2
1	BA	96	U	2.2
31	CA	112	U	2.2
31	CA	894	U	2.2
31	CA	1108	U	2.2
10	AJ	76	ILE	2.2
42	CO	59	SER	2.2
46	CS	33	VAL	2.2
54	DI	105	LYS	2.2
7	AG	46	ALA	2.2
10	BJ	34	ALA	2.2
20	BT	81	ALA	2.2
28	CB	63	C	2.2
34	CF	126	GLY	2.2
53	CZ	8	GLU	2.2
11	BK	64	GLN	2.2
30	CD	132	ALA	2.2
43	CP	23	ALA	2.2
55	DA	2178	C	2.2
43	CP	104	GLN	2.2
1	BA	1146	A	2.2
1	BA	1286	U	2.2
2	AB	136	MET	2.2
15	BO	12	VAL	2.2
18	AR	21	ILE	2.2
31	CA	2833	U	2.2
43	CP	76	LYS	2.2
13	BM	67	GLY	2.2
40	CM	88	GLY	2.2
3	BC	144	LEU	2.2
27	C0	17	LEU	2.2
35	CG	118	PRO	2.2
51	CX	32	LEU	2.2
1	BA	455	G	2.2
31	CA	1455	G	2.2
31	CA	2852	G	2.2
14	BN	42	TRP	2.2
47	CT	7	HIS	2.2
31	CA	2904	U	2.2

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Mol	Chain	Res	Type	RSRZ
1	AA	1441	A	2.2
31	CA	101	A	2.2
43	CP	57	ALA	2.2
35	CG	18	LYS	2.2
41	CN	72	PRO	2.2
1	BA	1336	C	2.2
9	BI	21	ILE	2.2
11	AK	34	ILE	2.2
30	CD	189	VAL	2.2
31	CA	1319	C	2.2
49	CV	62	GLU	2.2
2	AB	17	GLY	2.2
13	BM	44	LYS	2.2
41	CN	116	ALA	2.2
50	DW	94	ALA	2.2
2	BB	88	ASP	2.2
31	CA	429	A	2.2
36	DH	86	ASP	2.2
55	DA	1057	A	2.2
13	AM	17	ILE	2.2
33	CE	131	THR	2.2
34	CF	68	THR	2.2
48	CU	28	ASN	2.2
28	CB	118	C	2.2
31	CA	1172	C	2.2
3	AC	189	ALA	2.2
18	AR	23	TYR	2.2
40	CM	141	LYS	2.2
46	CS	24	LYS	2.2
54	DI	3	LEU	2.2
27	C0	42	PRO	2.2
31	CA	45	G	2.2
31	CA	1530	G	2.2
14	BN	54	ASP	2.2
30	CD	9	VAL	2.2
30	CD	103	ASP	2.2
18	AR	48	ARG	2.2
31	CA	213	A	2.2
31	CA	2660	A	2.2
31	CA	2800	A	2.2
43	CP	20	GLU	2.2
36	DH	11	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
36	DH	68	ARG	2.2
37	DJ	118	THR	2.2
38	CK	83	GLY	2.2
1	BA	1237	C	2.1
31	CA	314	C	2.1
13	AM	21	SER	2.1
2	BB	186	ILE	2.1
9	BI	51	PRO	2.1
29	CC	244	PRO	2.1
31	CA	1058	U	2.1
33	CE	122	GLU	2.1
46	CS	52	PRO	2.1
34	CF	62	GLY	2.1
40	CM	70	LYS	2.1
1	BA	1297	G	2.1
18	BR	74	HIS	2.1
4	AD	189	SER	2.1
16	BP	45	GLU	2.1
16	BP	47	GLU	2.1
35	CG	69	ARG	2.1
35	CG	77	ILE	2.1
44	CQ	5	ILE	2.1
2	BB	12	ALA	2.1
2	BB	36	ASN	2.1
20	BT	47	ALA	2.1
51	DX	10	THR	2.1
26	C5	32	LYS	2.1
36	CH	109	GLU	2.1
1	BA	1325	C	2.1
29	CC	33	LEU	2.1
31	CA	61	C	2.1
31	CA	902	C	2.1
49	CV	57	GLY	2.1
43	CP	48	LEU	2.1
43	CP	108	ASP	2.1
11	BK	21	ALA	2.1
30	CD	182	ALA	2.1
35	CG	49	THR	2.1
37	CJ	114	ALA	2.1
41	CN	50	ARG	2.1
53	CZ	48	ARG	2.1
53	DZ	63	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
48	CU	31	VAL	2.1
53	CZ	59	GLU	2.1
54	DI	114	GLU	2.1
36	DH	107	GLY	2.1
54	DI	60	LEU	2.1
1	AA	89	U	2.1
22	C1	56	ALA	2.1
2	BB	42	ASN	2.1
2	BB	67	ILE	2.1
19	AS	21	LYS	2.1
37	DJ	103	ARG	2.1
1	BA	196	A	2.1
1	BA	1271	A	2.1
31	CA	474	G	2.1
31	CA	1236	G	2.1
35	CG	119	ALA	2.1
44	CQ	24	ASP	2.1
46	CS	28	ALA	2.1
31	CA	2245	U	2.1
36	DH	110	VAL	2.1
13	BM	55	THR	2.1
14	AN	24	ARG	2.1
16	AP	74	LEU	2.1
18	AR	55	LEU	2.1
37	DJ	81	LYS	2.1
42	CO	28	LEU	2.1
16	BP	48	GLU	2.1
24	C3	36	ALA	2.1
6	AF	42	TRP	2.1
31	CA	654	A	2.1
6	AF	63	ASN	2.1
8	BH	120	GLY	2.1
10	BJ	99	GLN	2.1
31	CA	2106	U	2.1
31	CA	1212	G	2.1
31	CA	2325	G	2.1
31	CA	2693	G	2.1
34	CF	39	GLY	2.1
46	CS	19	THR	2.1
51	CX	42	GLY	2.1
55	DA	2141	G	2.1
9	BI	64	TYR	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
16	AP	81	ALA	2.1
22	C1	24	ALA	2.1
39	CL	111	LYS	2.1
40	CM	91	ASP	2.1
1	BA	1212	U	2.1
24	C3	1	MET	2.1
27	C0	27	LEU	2.1
31	CA	1325	U	2.1
33	CE	17	THR	2.1
36	DH	77	THR	2.1
1	BA	352	C	2.1
1	BA	1228	C	2.1
9	AI	59	GLU	2.1
31	CA	1112	G	2.1
2	AB	14	VAL	2.1
7	BG	87	VAL	2.1
20	BT	58	VAL	2.1
26	C5	2	LYS	2.1
30	CD	7	LYS	2.1
36	DH	106	ALA	2.1
34	CF	12	VAL	2.1
7	BG	101	MET	2.1
9	AI	5	GLN	2.1
1	BA	91	U	2.1
7	BG	79	ARG	2.1
8	AH	108	LYS	2.1
31	CA	515	A	2.1
22	C1	16	ARG	2.1
48	CU	77	ARG	2.1
49	CV	47	LYS	2.1
34	CF	28	VAL	2.1
5	BE	92	SER	2.1
1	AA	1276	G	2.1
10	AJ	73	LEU	2.1
31	CA	881	G	2.1
1	AA	1025	U	2.1
7	BG	46	ALA	2.1
10	BJ	32	THR	2.1
30	CD	85	ALA	2.1
36	CH	25	TYR	2.1
37	DJ	74	PRO	2.1
40	CM	122	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	AB	157	LEU	2.1
10	AJ	8	ILE	2.1
19	AS	71	LEU	2.1
34	CF	61	SER	2.1
34	CF	166	GLY	2.1
49	CV	38	GLY	2.1
1	BA	931	C	2.1
1	BA	984	C	2.1
1	BA	1218	C	2.1
11	BK	112	ASP	2.1
31	CA	413	C	2.1
55	DA	1092	C	2.1
19	BS	81	ARG	2.0
37	CJ	97	LYS	2.0
39	CL	51	LYS	2.0
46	CS	48	LYS	2.0
31	CA	619	G	2.0
31	CA	1166	G	2.0
31	CA	2115	G	2.0
2	AB	134	ALA	2.0
1	BA	467	U	2.0
8	BH	55	THR	2.0
37	DJ	70	VAL	2.0
54	DI	54	VAL	2.0
17	BQ	61	ILE	2.0
30	CD	187	LEU	2.0
46	CS	101	ILE	2.0
2	BB	128	LYS	2.0
13	AM	11	ASP	2.0
53	CZ	47	ARG	2.0
1	BA	194	C	2.0
31	CA	1533	C	2.0
30	CD	75	ALA	2.0
34	CF	2	ALA	2.0
35	CG	48	ASN	2.0
37	CJ	101	ILE	2.0
1	BA	259	G	2.0
23	C2	25	LYS	2.0
31	CA	1534	U	2.0
39	CL	15	GLY	2.0
12	BL	110	ARG	2.0
19	BS	32	ARG	2.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
22	C1	38	HIS	2.0
34	CF	134	GLU	2.0
31	CA	1054	A	2.0
31	CA	1532	A	2.0
5	BE	110	ALA	2.0
29	CC	95	LEU	2.0
34	CF	47	LYS	2.0
36	CH	122	LEU	2.0
13	BM	93	ARG	2.0
50	CW	9	ARG	2.0
1	BA	842	U	2.0
1	BA	1017	U	2.0
31	CA	150	U	2.0
31	CA	2491	U	2.0
1	BA	953	G	2.0
1	BA	954	G	2.0
2	AB	44	GLU	2.0
7	AG	52	GLN	2.0
31	CA	1867	G	2.0
31	CA	2409	G	2.0
14	AN	22	ALA	2.0
34	CF	7	TYR	2.0
52	CY	78	TYR	2.0
42	CO	83	LEU	2.0
1	AA	1022	A	2.0
1	BA	78	A	2.0
31	CA	2108	A	2.0
35	CG	8	PRO	2.0
8	AH	3	MET	2.0
9	AI	9	THR	2.0
13	AM	104	THR	2.0
36	CH	45	GLU	2.0
46	CS	6	GLN	2.0
55	DA	1061	U	2.0
13	BM	43	VAL	2.0
36	CH	3	VAL	2.0
25	C4	40	ARG	2.0
43	CP	110	ALA	2.0
54	DI	118	ILE	2.0
1	BA	177	G	2.0
1	BA	1475	G	2.0
31	CA	214	G	2.0

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Mol	Chain	Res	Type	RSRZ
51	CX	26	PHE	2.0
1	AA	1492	A	2.0
28	CB	52	A	2.0
31	CA	1213	A	2.0
31	CA	2602	A	2.0
35	CG	6	LYS	2.0
48	CU	8	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	MA6	BA	1518	24/25	0.95	0.20	-	74,80,82,83	0
31	PSU	CA	2457	20/21	0.95	0.18	-	87,89,92,92	0
41	4D4	CN	81	12/13	0.94	0.22	-	90,96,114,114	0
12	D2T	AL	89	10/11	0.94	0.20	-	59,64,75,78	0
55	3TD	DA	1915	21/22	0.93	0.17	-	91,98,111,112	0
55	1MG	DA	745	24/25	0.99	0.17	-	18,25,33,38	0
55	6MZ	DA	1618	23/24	0.99	0.15	-	24,29,32,37	0
31	OMU	CA	2552	21/22	0.96	0.33	-	83,84,98,101	0
1	MA6	AA	1519	24/25	0.98	0.17	-	44,48,49,50	0
1	UR3	AA	1498	21/22	0.97	0.16	-	55,59,62,66	0
1	UR3	BA	1498	21/22	0.97	0.11	-	80,82,84,88	0
32	MEQ	DD	150[B]	10/11	0.99	0.19	-	18,24,29,30	10
31	1MG	CA	745	24/25	0.94	0.22	-	90,92,94,96	0
31	6MZ	CA	2030	23/24	0.93	0.18	-	81,86,89,90	0
31	PSU	CA	2580	20/21	0.96	0.16	-	83,91,93,93	0
1	2MG	BA	1207	24/25	0.90	0.20	-	140,147,149,151	0
1	2MG	AA	1516	24/25	0.97	0.15	-	50,54,57,58	0
1	5MC	AA	1407	21/22	0.97	0.14	-	50,55,58,61	0
32	MEQ	DD	150[A]	10/11	0.99	0.19	-	7,12,22,24	10
55	OMG	DA	2251	24/25	0.99	0.17	-	22,27,45,51	0
55	2MA	DA	2503	23/24	0.99	0.20	-	17,29,37,40	0
31	OMG	CA	2251	24/25	0.96	0.22	-	82,83,85,86	0
1	5MC	AA	967	21/22	0.97	0.17	-	80,86,94,96	0
31	2MA	CA	2503	23/24	0.89	0.20	-	90,100,103,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	5MU	DA	1939	21/22	0.99	0.21	-	31,36,39,44	0
1	2MG	BA	966	24/25	0.93	0.19	-	119,123,135,135	0
1	PSU	AA	516	20/21	0.98	0.13	-	75,79,82,82	0
55	5MC	DA	1962	21/22	0.98	0.18	-	33,44,47,50	0
55	OMC	DA	2498	21/22	0.99	0.18	-	15,24,25,29	0
31	5MC	CA	1962	21/22	0.96	0.25	-	81,88,89,92	0
1	5MC	BA	1407	21/22	0.93	0.18	-	86,95,98,102	0
55	H2U	DA	2449	20/21	0.99	0.18	-	25,28,29,32	0
55	6MZ	DA	2030	23/24	0.99	0.19	-	13,20,24,33	0
31	2MG	CA	1835	24/25	0.93	0.17	-	76,80,83,83	0
1	2MG	AA	1207	24/25	0.95	0.13	-	89,100,106,109	0
31	5MU	CA	1939	21/22	0.97	0.15	-	74,76,85,88	0
55	2MG	DA	2445	24/25	0.99	0.18	-	17,23,27,29	0
1	MA6	BA	1519	24/25	0.95	0.22	-	76,78,81,82	0
1	2MG	AA	966	24/25	0.96	0.15	-	76,84,94,94	0
55	PSU	DA	2604	20/21	0.98	0.17	-	33,39,50,51	0
31	PSU	CA	2504	20/21	0.94	0.17	-	76,87,89,93	0
55	PSU	DA	1911	20/21	0.97	0.14	-	66,80,82,83	0
55	PSU	DA	2580	20/21	0.99	0.17	-	20,24,29,32	0
1	G7M	BA	527	24/25	0.96	0.19	-	93,95,98,99	0
55	PSU	DA	2457	20/21	0.99	0.16	-	23,26,31,32	0
1	4OC	AA	1402	22/23	0.98	0.15	-	60,61,63,64	0
31	OMC	CA	2498	21/22	0.96	0.22	-	84,87,93,97	0
55	G7M	DA	2069	24/25	0.99	0.17	-	30,33,35,38	0
55	OMU	DA	2552	21/22	0.99	0.18	-	30,32,35,44	0
12	D2T	BL	89	10/11	0.90	0.30	-	92,99,108,108	0
1	2MG	BA	1516	24/25	0.93	0.16	-	66,73,79,81	0
31	2MG	CA	2445	24/25	0.93	0.27	-	74,80,84,85	0
31	PSU	CA	1911	20/21	0.93	0.21	-	104,121,124,125	0
31	5MU	CA	747	21/22	0.95	0.17	-	97,103,106,106	0
55	PSU	DA	2605	20/21	0.99	0.16	-	30,35,41,44	0
55	5MU	DA	747	21/22	0.99	0.16	-	24,31,35,40	0
55	2MG	DA	1835	24/25	0.97	0.19	-	43,49,53,53	0
1	4OC	BA	1402	22/23	0.96	0.16	-	78,79,81,82	0
55	PSU	DA	2504	20/21	0.99	0.18	-	33,36,37,40	0
55	PSU	DA	955	20/21	0.99	0.18	-	24,25,28,28	0
55	PSU	DA	1917	20/21	0.97	0.15	-	77,81,87,88	0
31	3TD	CA	1915	21/22	0.91	0.21	-	142,145,154,156	0
31	PSU	CA	955	20/21	0.95	0.17	-	85,87,92,92	0
1	MA6	AA	1518	24/25	0.98	0.17	-	41,46,49,51	0
31	PSU	CA	1917	20/21	0.89	0.24	-	120,123,132,132	0
1	PSU	BA	516	20/21	0.94	0.17	-	100,101,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	G7M	AA	527	24/25	0.97	0.14	-	58,70,72,74	0
55	PSU	DA	746	20/21	0.99	0.16	-	18,24,29,33	0
41	4D4	DN	81[B]	12/13	0.98	0.19	-	21,29,35,36	9
1	5MC	BA	967	21/22	0.93	0.24	-	115,124,127,128	0
31	6MZ	CA	1618	23/24	0.94	0.22	-	109,114,116,117	0
41	4D4	DN	81[A]	12/13	0.98	0.19	-	29,40,50,51	9
31	PSU	CA	746	20/21	0.95	0.13	-	86,98,100,101	0
31	G7M	CA	2069	24/25	0.95	0.18	-	80,84,87,88	0
31	PSU	CA	2605	20/21	0.94	0.17	-	82,84,87,88	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	PUT	AA	1674	6/6	0.69	0.63	50.77	112,117,121,123	0
59	PUT	DA	3198	6/6	0.71	0.61	40.79	102,102,104,105	0
61	PEG	D1	103	7/7	0.76	0.45	38.12	81,87,93,95	0
61	PEG	D3	102	7/7	0.70	1.25	37.43	88,94,99,99	0
56	MG	DA	3180	1/1	0.96	0.51	37.09	54,54,54,54	0
61	PEG	DA	3203	7/7	0.83	0.62	28.04	84,88,95,96	0
58	MPD	DA	3206	8/8	0.84	0.64	24.67	85,88,99,101	0
64	SPD	DA	3186	10/10	0.85	0.49	24.44	84,87,91,91	0
56	MG	DA	3175	1/1	0.77	0.42	22.30	97,97,97,97	0
56	MG	CA	3122	1/1	0.77	1.02	20.71	100,100,100,100	0
63	PGE	D3	101	10/10	0.65	0.81	20.55	105,111,114,114	0
57	PG4	DA	3196	13/13	0.87	0.93	18.33	90,94,96,97	0
61	PEG	DA	3220	7/7	0.80	0.35	17.44	136,137,139,139	0
59	PUT	DA	3223	6/6	0.81	0.66	17.00	118,122,122,123	0
56	MG	CA	3105	1/1	0.59	1.38	16.44	250,250,250,250	0
63	PGE	D1	102	10/10	0.70	0.69	16.41	113,119,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
58	MPD	DE	301	8/8	0.65	0.84	16.00	153,155,156,156	0
56	MG	CA	3039	1/1	0.80	1.16	15.94	252,252,252,252	0
63	PGE	DA	3216	10/10	0.92	0.41	15.20	68,72,83,84	0
59	PUT	DA	3224	6/6	0.78	0.37	14.20	50,53,55,56	0
59	PUT	DA	3215	6/6	0.79	0.42	14.05	83,90,96,98	0
58	MPD	DE	302	8/8	0.84	0.67	13.88	91,94,97,97	0
59	PUT	AA	1673	6/6	0.84	0.50	13.69	110,110,112,112	0
56	MG	DA	3129	1/1	0.97	0.28	13.67	64,64,64,64	0
56	MG	CA	3133	1/1	0.75	0.30	13.54	88,88,88,88	0
57	PG4	DS	202	13/13	0.82	0.43	13.37	67,78,83,83	0
59	PUT	DA	3221	6/6	0.88	0.38	13.26	65,71,74,75	0
65	1PE	DA	3205	16/16	0.86	0.33	12.89	77,84,87,88	0
61	PEG	DQ	201	7/7	0.75	0.78	12.68	92,94,96,97	0
57	PG4	DA	3218	13/13	0.90	0.35	12.20	90,94,98,99	0
56	MG	CA	3003	1/1	0.96	0.85	12.11	258,258,258,258	0
58	MPD	AA	1676	8/8	0.94	0.43	11.92	87,90,96,97	0
56	MG	DA	3128	1/1	0.95	0.35	11.84	54,54,54,54	0
63	PGE	DA	3219	10/10	0.91	0.35	11.67	85,88,91,91	0
56	MG	CA	3137	1/1	0.86	0.49	11.27	117,117,117,117	0
62	EDO	DA	3002	4/4	0.91	0.30	10.83	78,79,79,79	0
66	ACY	DA	3204	4/4	0.95	0.24	10.50	75,76,77,77	0
59	PUT	DA	3207	6/6	0.74	0.45	9.88	95,100,104,105	0
67	GUN	DA	3213	11/11	0.85	0.58	9.68	119,121,122,122	0
58	MPD	DA	3195	8/8	0.88	0.55	9.17	92,97,98,98	0
56	MG	CA	3026	1/1	0.84	0.68	9.16	129,129,129,129	0
58	MPD	DA	3004	8/8	0.79	0.36	8.80	106,109,119,121	0
58	MPD	DT	201	8/8	0.79	0.38	8.62	111,114,115,115	0
61	PEG	DA	3228	7/7	0.85	0.28	8.45	64,78,90,90	0
58	MPD	AA	1671	8/8	0.88	0.61	8.33	109,110,113,114	0
63	PGE	DS	201	10/10	0.79	0.46	8.24	87,98,101,102	0
57	PG4	AA	1670	13/13	0.84	0.32	8.16	74,86,104,104	0
57	PG4	BA	1642	13/13	0.86	0.42	8.10	77,87,100,100	0
56	MG	AA	1608	1/1	0.87	0.48	7.70	87,87,87,87	0
62	EDO	DA	3211	4/4	0.85	0.40	7.65	103,104,104,106	0
56	MG	BA	1612	1/1	0.81	0.45	7.11	201,201,201,201	0
56	MG	AA	1612	1/1	0.82	0.33	7.08	78,78,78,78	0
59	PUT	DA	3192	6/6	0.92	0.26	6.82	44,49,50,50	0
63	PGE	DU	101	10/10	0.88	0.35	5.44	71,82,92,93	0
58	MPD	DA	3209	8/8	0.88	0.42	5.43	90,94,98,98	0
63	PGE	DD	301	10/10	0.92	0.24	5.22	86,89,95,96	0
56	MG	DA	3039	1/1	0.98	0.23	5.15	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1642	1/1	0.86	0.32	5.04	126,126,126,126	0
61	PEG	AL	201	7/7	0.89	0.30	4.92	87,91,98,100	0
56	MG	BA	1627	1/1	0.94	0.38	4.71	142,142,142,142	0
64	SPD	DA	3226	10/10	0.94	0.23	4.66	37,46,63,65	0
64	SPD	DA	3208	10/10	0.84	0.23	3.65	112,117,118,119	0
59	PUT	DM	201	6/6	0.96	0.23	3.37	49,50,53,56	0
59	PUT	DA	3187	6/6	0.93	0.22	3.29	49,51,53,54	0
62	EDO	DA	3201	4/4	0.88	0.23	3.25	91,92,93,94	0
61	PEG	DL	201	7/7	0.88	0.25	3.14	73,79,80,80	0
56	MG	DA	3142	1/1	0.98	0.21	3.07	74,74,74,74	0
62	EDO	DA	3200	4/4	0.95	0.20	3.05	53,54,54,55	0
64	SPD	DA	3190	10/10	0.98	0.22	3.03	38,46,49,53	0
56	MG	DA	3126	1/1	0.91	0.22	2.14	83,83,83,83	0
57	PG4	DQ	202	13/13	0.93	0.29	1.95	66,71,76,78	0
63	PGE	DA	3189	10/10	0.94	0.17	1.84	42,45,49,49	0
65	1PE	DA	3188	16/16	0.95	0.18	1.75	47,60,87,91	0
56	MG	AA	1644	1/1	0.95	0.20	1.74	115,115,115,115	0
56	MG	BA	1643	1/1	0.95	0.21	1.53	105,105,105,105	0
56	MG	DD	302	1/1	0.97	0.21	1.48	41,41,41,41	0
56	MG	DA	3095	1/1	0.99	0.19	1.43	26,26,26,26	0
62	EDO	D1	101	4/4	0.92	0.18	1.32	61,62,64,66	0
58	MPD	DS	203	8/8	0.98	0.23	1.25	55,56,58,61	0
56	MG	DA	3026	1/1	0.99	0.21	1.01	33,33,33,33	0
56	MG	DA	3015	1/1	1.00	0.21	0.91	22,22,22,22	0
56	MG	CA	3153	1/1	0.96	0.22	0.49	58,58,58,58	0
56	MG	CA	3155	1/1	0.93	0.23	0.26	126,126,126,126	0
56	MG	CA	3080	1/1	0.92	0.28	0.10	143,143,143,143	0
56	MG	BA	1613	1/1	0.96	0.20	0.01	112,112,112,112	0
56	MG	DA	3025	1/1	0.98	0.19	-0.34	26,26,26,26	0
56	MG	CA	3089	1/1	0.96	0.19	-0.41	54,54,54,54	0
56	MG	CA	3099	1/1	0.92	0.25	-0.51	129,129,129,129	0
56	MG	CA	3009	1/1	0.88	0.17	-0.54	222,222,222,222	0
60	ZN	D5	101	1/1	0.99	0.15	-0.62	56,56,56,56	0
56	MG	CA	3102	1/1	0.93	0.14	-0.94	107,107,107,107	0
56	MG	AA	1657	1/1	0.98	0.18	-0.94	116,116,116,116	0
60	ZN	C5	101	1/1	0.93	0.09	-0.95	155,155,155,155	0
56	MG	CA	3100	1/1	0.96	0.17	-1.00	90,90,90,90	0
56	MG	CA	3061	1/1	0.75	0.16	-1.03	250,250,250,250	0
56	MG	AA	1661	1/1	0.96	0.17	-1.04	178,178,178,178	0
56	MG	CA	3019	1/1	0.84	0.16	-1.11	62,62,62,62	0
56	MG	CA	3027	1/1	0.98	0.15	-1.22	61,61,61,61	0
56	MG	DA	3019	1/1	1.00	0.17	-1.34	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3011	1/1	0.94	0.15	-1.34	72,72,72,72	0
56	MG	DA	3037	1/1	1.00	0.17	-1.35	29,29,29,29	0
56	MG	BA	1624	1/1	0.95	0.13	-1.43	157,157,157,157	0
56	MG	DA	3029	1/1	0.99	0.20	-1.47	48,48,48,48	0
56	MG	AA	1656	1/1	0.97	0.12	-1.61	95,95,95,95	0
56	MG	AA	1678	1/1	0.82	0.14	-1.63	59,59,59,59	0
56	MG	CA	3056	1/1	0.97	0.13	-1.74	66,66,66,66	0
56	MG	DA	3101	1/1	0.99	0.16	-1.78	22,22,22,22	0
56	MG	DA	3097	1/1	0.98	0.15	-1.82	106,106,106,106	0
56	MG	DA	3020	1/1	0.99	0.10	-1.89	42,42,42,42	0
56	MG	CA	3063	1/1	0.84	0.13	-1.93	103,103,103,103	0
56	MG	DA	3149	1/1	0.91	0.09	-1.99	123,123,123,123	0
56	MG	AA	1639	1/1	0.95	0.13	-2.05	122,122,122,122	0
56	MG	BA	1632	1/1	0.96	0.10	-2.07	85,85,85,85	0
56	MG	CB	201	1/1	0.84	0.07	-2.07	157,157,157,157	0
56	MG	CA	3018	1/1	0.98	0.11	-2.13	125,125,125,125	0
56	MG	AA	1677	1/1	0.98	0.08	-2.14	155,155,155,155	0
56	MG	CA	3037	1/1	0.96	0.15	-2.22	107,107,107,107	0
56	MG	BA	1610	1/1	0.94	0.08	-2.35	130,130,130,130	0
56	MG	CA	3103	1/1	0.96	0.11	-2.36	82,82,82,82	0
56	MG	BA	1608	1/1	0.97	0.17	-2.38	114,114,114,114	0
56	MG	AA	1663	1/1	0.96	0.17	-2.41	99,99,99,99	0
56	MG	CA	3020	1/1	0.99	0.16	-2.42	60,60,60,60	0
56	MG	CA	3013	1/1	0.98	0.17	-2.44	123,123,123,123	0
56	MG	CA	3041	1/1	0.99	0.08	-2.50	62,62,62,62	0
56	MG	DA	3094	1/1	0.96	0.14	-2.53	36,36,36,36	0
56	MG	DA	3112	1/1	0.99	0.15	-2.54	35,35,35,35	0
56	MG	BA	1614	1/1	0.80	0.11	-2.55	136,136,136,136	0
56	MG	CA	3101	1/1	0.98	0.09	-2.55	71,71,71,71	0
56	MG	BA	1617	1/1	0.94	0.12	-2.57	130,130,130,130	0
56	MG	BA	1620	1/1	0.98	0.10	-2.58	115,115,115,115	0
56	MG	DA	3012	1/1	1.00	0.14	-2.63	31,31,31,31	0
56	MG	AA	1659	1/1	0.93	0.09	-2.70	61,61,61,61	0
56	MG	CA	3144	1/1	0.98	0.05	-2.95	60,60,60,60	0
56	MG	AA	1611	1/1	0.93	0.12	-2.98	91,91,91,91	0
60	ZN	AB	301	1/1	0.96	0.07	-3.04	141,141,141,141	0
56	MG	BA	1615	1/1	0.98	0.10	-3.19	65,65,65,65	0
56	MG	AA	1668	1/1	0.99	0.11	-3.34	58,58,58,58	0
56	MG	DB	201	1/1	0.97	0.10	-3.35	56,56,56,56	0
56	MG	AA	1643	1/1	0.99	0.17	-3.37	69,69,69,69	0
56	MG	DA	3011	1/1	0.99	0.12	-3.45	20,20,20,20	0
56	MG	DA	3052	1/1	0.99	0.14	-3.49	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3152	1/1	1.00	0.12	-3.55	53,53,53,53	0
56	MG	DA	3031	1/1	0.99	0.16	-3.57	23,23,23,23	0
56	MG	DA	3033	1/1	1.00	0.17	-3.62	26,26,26,26	0
56	MG	CA	3094	1/1	0.93	0.08	-3.66	68,68,68,68	0
56	MG	BA	1605	1/1	0.92	0.08	-3.84	206,206,206,206	0
56	MG	CA	3052	1/1	0.97	0.11	-3.89	60,60,60,60	0
56	MG	DA	3045	1/1	0.98	0.14	-3.98	41,41,41,41	0
56	MG	CA	3024	1/1	0.94	0.07	-3.99	75,75,75,75	0
56	MG	DA	3001	1/1	0.99	0.13	-4.06	25,25,25,25	0
56	MG	DA	3096	1/1	0.97	0.13	-4.15	19,19,19,19	0
56	MG	DA	3068	1/1	0.99	0.16	-4.33	37,37,37,37	0
56	MG	DA	3024	1/1	0.99	0.14	-4.37	28,28,28,28	0
56	MG	DA	3063	1/1	0.99	0.16	-4.43	36,36,36,36	0
56	MG	CA	3054	1/1	0.86	0.09	-4.80	105,105,105,105	0
56	MG	CA	3030	1/1	0.98	0.07	-4.84	84,84,84,84	0
56	MG	BA	1602	1/1	0.81	0.07	-4.85	90,90,90,90	0
56	MG	AA	1648	1/1	0.98	0.05	-4.87	77,77,77,77	0
56	MG	BA	1626	1/1	0.88	0.06	-4.92	92,92,92,92	0
56	MG	CA	3040	1/1	0.97	0.07	-4.94	85,85,85,85	0
56	MG	DA	3092	1/1	0.99	0.13	-4.98	23,23,23,23	0
56	MG	AA	1631	1/1	0.98	0.06	-5.00	43,43,43,43	0
56	MG	DA	3103	1/1	0.98	0.15	-5.08	50,50,50,50	0
56	MG	CA	3051	1/1	0.99	0.08	-5.12	52,52,52,52	0
56	MG	AA	1653	1/1	0.99	0.08	-5.56	67,67,67,67	0
56	MG	CA	3088	1/1	0.99	0.06	-5.68	78,78,78,78	0
56	MG	CA	3031	1/1	0.76	0.09	-5.69	87,87,87,87	0
56	MG	DA	3162	1/1	0.98	0.11	-5.78	67,67,67,67	0
56	MG	DA	3114	1/1	1.00	0.17	-6.19	27,27,27,27	0
56	MG	BA	1622	1/1	0.99	0.07	-6.20	104,104,104,104	0
56	MG	AA	1637	1/1	0.99	0.08	-6.45	43,43,43,43	0
56	MG	DA	3111	1/1	0.99	0.14	-6.76	32,32,32,32	0
56	MG	DA	3137	1/1	0.96	0.06	-6.81	96,96,96,96	0
56	MG	CA	3086	1/1	0.98	0.05	-7.03	74,74,74,74	0
56	MG	DA	3086	1/1	1.00	0.11	-7.16	30,30,30,30	0
56	MG	CA	3044	1/1	0.92	0.07	-7.44	49,49,49,49	0
56	MG	DA	3099	1/1	0.96	0.09	-7.50	31,31,31,31	0
56	MG	DA	3049	1/1	0.98	0.12	-7.92	48,48,48,48	0
56	MG	DA	3066	1/1	0.99	0.08	-7.94	44,44,44,44	0
56	MG	DA	3073	1/1	0.99	0.06	-8.10	49,49,49,49	0
56	MG	DA	3060	1/1	0.99	0.10	-8.47	31,31,31,31	0
56	MG	AA	1646	1/1	0.99	0.06	-8.58	57,57,57,57	0
56	MG	DA	3006	1/1	0.99	0.09	-8.62	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1651	1/1	0.98	0.05	-8.96	68,68,68,68	0
56	MG	DA	3104	1/1	0.99	0.10	-9.20	37,37,37,37	0
56	MG	DA	3009	1/1	0.98	0.07	-9.23	82,82,82,82	0
56	MG	CA	3006	1/1	0.80	0.10	-9.56	144,144,144,144	0
56	MG	DA	3016	1/1	1.00	0.13	-9.98	13,13,13,13	0
56	MG	DA	3028	1/1	0.98	0.07	-10.41	83,83,83,83	0
56	MG	DA	3048	1/1	0.99	0.12	-10.78	36,36,36,36	0
56	MG	CA	3062	1/1	0.88	0.28	-	232,232,232,232	0
56	MG	CA	3014	1/1	0.64	0.16	-	161,161,161,161	0
56	MG	CA	3053	1/1	0.97	0.12	-	58,58,58,58	0
56	MG	CA	3045	1/1	0.87	0.12	-	110,110,110,110	0
56	MG	AA	1662	1/1	0.98	0.20	-	89,89,89,89	0
56	MG	AA	1665	1/1	0.95	0.27	-	123,123,123,123	0
56	MG	CA	3078	1/1	0.97	0.08	-	133,133,133,133	0
56	MG	CA	3112	1/1	0.92	0.24	-	65,65,65,65	0
56	MG	AA	1609	1/1	0.81	0.30	-	84,84,84,84	0
56	MG	AA	1607	1/1	0.98	0.63	-	90,90,90,90	0
56	MG	BA	1611	1/1	0.95	0.08	-	80,80,80,80	0
56	MG	CA	3047	1/1	0.64	0.69	-	272,272,272,272	0
61	PEG	DA	3202	7/7	0.81	0.56	-	87,88,91,91	0
57	PG4	DR	202	13/13	0.78	0.40	-	98,111,116,116	0
56	MG	AA	1622	1/1	0.76	1.22	-	112,112,112,112	0
56	MG	DA	3167	1/1	0.86	0.41	-	63,63,63,63	0
56	MG	CA	3124	1/1	0.69	0.30	-	156,156,156,156	0
56	MG	CA	3136	1/1	0.77	0.35	-	82,82,82,82	0
56	MG	BA	1621	1/1	0.97	0.17	-	29,29,29,29	0
56	MG	CA	3068	1/1	0.84	0.24	-	185,185,185,185	0
56	MG	BA	1625	1/1	0.90	0.07	-	235,235,235,235	0
56	MG	CA	3104	1/1	0.88	0.10	-	196,196,196,196	0
56	MG	DA	3007	1/1	0.98	0.13	-	77,77,77,77	0
56	MG	CA	3107	1/1	0.97	0.29	-	65,65,65,65	0
58	MPD	DN	201	8/8	0.72	0.45	-	91,96,102,102	0
56	MG	CA	3065	1/1	0.88	0.09	-	107,107,107,107	0
56	MG	DA	3177	1/1	0.90	0.47	-	80,80,80,80	0
56	MG	CA	3035	1/1	0.97	0.17	-	83,83,83,83	0
56	MG	DA	3121	1/1	0.98	0.30	-	64,64,64,64	0
56	MG	BA	1609	1/1	0.64	0.22	-	270,270,270,270	0
56	MG	CA	3084	1/1	0.96	0.24	-	181,181,181,181	0
56	MG	CA	3111	1/1	0.71	0.39	-	83,83,83,83	0
61	PEG	DP	201	7/7	0.74	0.72	-	108,109,109,110	0
56	MG	DA	3084	1/1	0.97	0.04	-	75,75,75,75	0
56	MG	AA	1635	1/1	0.98	0.13	-	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3184	1/1	0.92	0.26	-	74,74,74,74	0
56	MG	DA	3113	1/1	0.96	0.16	-	280,280,280,280	0
56	MG	CA	3043	1/1	0.85	0.07	-	90,90,90,90	0
56	MG	DA	3173	1/1	0.83	0.26	-	69,69,69,69	0
56	MG	BA	1616	1/1	0.70	0.27	-	185,185,185,185	0
56	MG	CA	3029	1/1	0.97	0.14	-	166,166,166,166	0
56	MG	DA	3078	1/1	0.98	0.11	-	32,32,32,32	0
56	MG	DA	3058	1/1	0.99	0.14	-	38,38,38,38	0
56	MG	CA	3154	1/1	0.16	0.70	-	152,152,152,152	0
56	MG	CA	3036	1/1	0.94	0.09	-	102,102,102,102	0
56	MG	DA	3057	1/1	0.99	0.23	-	30,30,30,30	0
56	MG	DA	3182	1/1	0.98	0.46	-	109,109,109,109	0
56	MG	CA	3005	1/1	0.85	1.23	-	235,235,235,235	0
56	MG	DA	3125	1/1	0.85	0.45	-	81,81,81,81	0
56	MG	CB	203	1/1	0.92	0.06	-	125,125,125,125	0
56	MG	DA	3136	1/1	0.86	0.33	-	87,87,87,87	0
56	MG	DA	3046	1/1	0.98	0.04	-	61,61,61,61	0
56	MG	DR	201	1/1	0.93	0.29	-	30,30,30,30	0
56	MG	CA	3113	1/1	0.58	0.55	-	90,90,90,90	0
56	MG	DA	3087	1/1	0.94	0.14	-	49,49,49,49	0
56	MG	DA	3176	1/1	0.93	0.41	-	92,92,92,92	0
58	MPD	DA	3193	8/8	0.90	0.33	-	89,91,93,93	0
56	MG	CA	3001	1/1	0.69	0.22	-	291,291,291,291	0
56	MG	AA	1649	1/1	0.99	0.05	-	57,57,57,57	0
56	MG	CA	3083	1/1	0.97	0.09	-	136,136,136,136	0
56	MG	DA	3232	1/1	0.98	0.23	-	30,30,30,30	0
56	MG	AA	1634	1/1	0.97	0.22	-	163,163,163,163	0
56	MG	DA	3118	1/1	1.00	0.12	-	45,45,45,45	0
56	MG	CA	3120	1/1	0.85	0.41	-	168,168,168,168	0
56	MG	DA	3107	1/1	0.99	0.17	-	25,25,25,25	0
56	MG	AA	1667	1/1	0.96	0.10	-	42,42,42,42	0
56	MG	DA	3181	1/1	0.78	0.44	-	85,85,85,85	0
56	MG	CA	3145	1/1	0.91	0.18	-	60,60,60,60	0
56	MG	CA	3098	1/1	0.98	0.07	-	91,91,91,91	0
56	MG	CA	3033	1/1	0.97	0.07	-	79,79,79,79	0
56	MG	CA	3064	1/1	0.94	0.48	-	274,274,274,274	0
56	MG	DA	3151	1/1	0.99	0.09	-	41,41,41,41	0
56	MG	CA	3143	1/1	0.93	0.22	-	104,104,104,104	0
56	MG	DB	208	1/1	0.92	0.30	-	56,56,56,56	0
56	MG	CA	3046	1/1	0.91	0.13	-	116,116,116,116	0
56	MG	AA	1615	1/1	0.92	0.45	-	81,81,81,81	0
56	MG	DA	3008	1/1	0.99	0.10	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3038	1/1	0.40	0.13	-	234,234,234,234	0
56	MG	CA	3117	1/1	0.97	0.35	-	76,76,76,76	0
56	MG	BA	1638	1/1	0.65	0.70	-	109,109,109,109	0
56	MG	CA	3076	1/1	0.80	0.15	-	163,163,163,163	0
56	MG	CA	3082	1/1	0.96	0.14	-	90,90,90,90	0
56	MG	DA	3133	1/1	0.80	0.29	-	68,68,68,68	0
56	MG	DA	3010	1/1	0.99	0.05	-	74,74,74,74	0
56	MG	CA	3081	1/1	0.99	0.12	-	82,82,82,82	0
56	MG	AA	1606	1/1	0.46	0.84	-	125,125,125,125	0
56	MG	BA	1633	1/1	0.92	0.38	-	163,163,163,163	0
62	EDO	DA	3003	4/4	0.80	0.51	-	97,98,98,98	0
56	MG	CA	3017	1/1	0.96	0.08	-	97,97,97,97	0
56	MG	DA	3080	1/1	0.99	0.06	-	50,50,50,50	0
56	MG	AA	1647	1/1	0.97	0.12	-	157,157,157,157	0
56	MG	DA	3115	1/1	0.99	0.10	-	81,81,81,81	0
56	MG	DA	3090	1/1	0.99	0.06	-	52,52,52,52	0
56	MG	AA	1618	1/1	0.93	0.81	-	83,83,83,83	0
56	MG	AA	1658	1/1	0.86	0.10	-	65,65,65,65	0
56	MG	AA	1645	1/1	0.96	0.11	-	61,61,61,61	0
56	MG	DA	3034	1/1	0.99	0.16	-	22,22,22,22	0
56	MG	AA	1624	1/1	0.90	0.61	-	107,107,107,107	0
56	MG	DA	3135	1/1	0.92	0.21	-	56,56,56,56	0
56	MG	DA	3123	1/1	0.96	0.13	-	78,78,78,78	0
56	MG	AA	1664	1/1	0.79	0.44	-	225,225,225,225	0
56	MG	DA	3134	1/1	0.94	0.15	-	68,68,68,68	0
56	MG	DA	3132	1/1	0.81	0.24	-	78,78,78,78	0
56	MG	CA	3025	1/1	0.96	0.08	-	88,88,88,88	0
56	MG	DA	3023	1/1	0.99	0.13	-	22,22,22,22	0
56	MG	DA	3158	1/1	0.74	0.61	-	75,75,75,75	0
56	MG	DA	3155	1/1	0.96	0.43	-	73,73,73,73	0
56	MG	DA	3088	1/1	0.99	0.11	-	36,36,36,36	0
56	MG	CA	3021	1/1	0.64	0.79	-	260,260,260,260	0
56	MG	DA	3109	1/1	0.97	0.17	-	34,34,34,34	0
56	MG	DA	3148	1/1	0.80	0.30	-	84,84,84,84	0
56	MG	DA	3018	1/1	0.99	0.10	-	69,69,69,69	0
56	MG	AA	1602	1/1	0.78	0.38	-	81,81,81,81	0
56	MG	CA	3042	1/1	0.99	0.12	-	87,87,87,87	0
56	MG	DA	3062	1/1	1.00	0.14	-	28,28,28,28	0
56	MG	AA	1620	1/1	0.87	0.30	-	67,67,67,67	0
59	PUT	DA	3214	6/6	0.85	0.30	-	71,79,82,85	0
56	MG	DA	3050	1/1	1.00	0.12	-	25,25,25,25	0
56	MG	CA	3131	1/1	0.74	0.31	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	PUT	DA	3225	6/6	0.95	0.21	-	61,62,70,72	0
56	MG	DB	207	1/1	0.96	0.66	-	84,84,84,84	0
56	MG	DA	3108	1/1	0.99	0.17	-	37,37,37,37	0
56	MG	AA	1627	1/1	0.82	0.40	-	83,83,83,83	0
56	MG	CA	3091	1/1	0.96	0.11	-	71,71,71,71	0
56	MG	AA	1614	1/1	0.59	0.84	-	117,117,117,117	0
56	MG	CA	3059	1/1	0.99	0.09	-	70,70,70,70	0
56	MG	DA	3067	1/1	0.97	0.16	-	26,26,26,26	0
56	MG	AA	1625	1/1	0.63	0.66	-	90,90,90,90	0
56	MG	CA	3121	1/1	0.93	0.15	-	60,60,60,60	0
56	MG	DA	3072	1/1	0.95	0.08	-	86,86,86,86	0
56	MG	DA	3055	1/1	0.99	0.09	-	40,40,40,40	0
56	MG	CA	3066	1/1	0.94	0.09	-	129,129,129,129	0
56	MG	DA	3032	1/1	0.97	0.20	-	47,47,47,47	0
62	EDO	DA	3210	4/4	0.86	0.27	-	88,88,89,89	0
56	MG	DA	3038	1/1	1.00	0.17	-	20,20,20,20	0
56	MG	CA	3016	1/1	0.97	0.54	-	150,150,150,150	0
56	MG	CB	202	1/1	0.98	0.05	-	100,100,100,100	0
56	MG	CA	3125	1/1	0.93	0.23	-	97,97,97,97	0
56	MG	DA	3172	1/1	0.95	0.22	-	57,57,57,57	0
56	MG	AA	1605	1/1	0.92	0.73	-	91,91,91,91	0
56	MG	DA	3146	1/1	0.93	0.80	-	80,80,80,80	0
56	MG	CA	3008	1/1	0.93	0.07	-	131,131,131,131	0
56	MG	DA	3064	1/1	0.92	0.20	-	243,243,243,243	0
56	MG	BA	1603	1/1	0.83	0.64	-	276,276,276,276	0
56	MG	DA	3043	1/1	0.99	0.18	-	13,13,13,13	0
56	MG	AA	1632	1/1	0.93	0.06	-	94,94,94,94	0
56	MG	BA	1640	1/1	0.84	0.32	-	118,118,118,118	0
56	MG	AA	1650	1/1	0.98	0.10	-	87,87,87,87	0
56	MG	CA	3060	1/1	0.25	0.40	-	194,194,194,194	0
56	MG	DA	3140	1/1	0.96	0.32	-	43,43,43,43	1
56	MG	DA	3119	1/1	0.98	0.14	-	82,82,82,82	0
56	MG	BA	1623	1/1	0.95	0.15	-	166,166,166,166	0
62	EDO	DA	3005	4/4	0.83	0.30	-	104,105,107,110	0
56	MG	AA	1619	1/1	0.63	0.60	-	90,90,90,90	0
56	MG	BA	1628	1/1	0.98	0.06	-	70,70,70,70	0
56	MG	CA	3114	1/1	0.82	0.29	-	51,51,51,51	0
56	MG	CA	3115	1/1	0.88	0.23	-	77,77,77,77	0
56	MG	CA	3007	1/1	0.67	0.31	-	216,216,216,216	0
56	MG	DA	3074	1/1	0.98	0.25	-	53,53,53,53	0
56	MG	DA	3231	1/1	0.99	0.06	-	46,46,46,46	0
56	MG	BA	1631	1/1	0.93	0.07	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1666	1/1	0.90	0.06	-	97,97,97,97	0
56	MG	BA	1619	1/1	0.98	0.12	-	70,70,70,70	0
63	PGE	DA	3227	10/10	0.94	0.28	-	81,90,107,109	0
56	MG	AA	1628	1/1	0.81	0.39	-	118,118,118,118	0
56	MG	DA	3053	1/1	0.99	0.12	-	22,22,22,22	0
56	MG	DB	205	1/1	0.88	0.47	-	73,73,73,73	0
56	MG	CA	3032	1/1	0.89	0.15	-	236,236,236,236	0
62	EDO	DB	210	4/4	0.86	0.29	-	95,95,96,97	0
66	ACY	DA	3194	4/4	0.94	0.20	-	92,93,94,94	0
56	MG	CA	3079	1/1	0.92	0.11	-	110,110,110,110	0
56	MG	CA	3055	1/1	0.60	0.16	-	260,260,260,260	0
56	MG	DA	3150	1/1	0.95	0.34	-	63,63,63,63	0
56	MG	CA	3015	1/1	0.97	0.17	-	48,48,48,48	0
56	MG	AA	1603	1/1	0.52	0.51	-	108,108,108,108	0
56	MG	CA	3022	1/1	0.71	0.41	-	170,170,170,170	0
56	MG	CA	3141	1/1	0.89	0.14	-	53,53,53,53	0
56	MG	DA	3069	1/1	0.99	0.15	-	42,42,42,42	0
56	MG	CA	3092	1/1	0.83	0.14	-	195,195,195,195	0
56	MG	DA	3082	1/1	0.97	0.13	-	173,173,173,173	0
62	EDO	DA	3197	4/4	0.95	0.26	-	52,57,59,60	0
58	MPD	DK	201	8/8	0.88	0.29	-	104,107,110,111	0
56	MG	DA	3141	1/1	0.98	0.19	-	57,57,57,57	0
56	MG	DA	3156	1/1	0.81	0.44	-	83,83,83,83	0
56	MG	CA	3074	1/1	0.95	0.25	-	131,131,131,131	0
56	MG	DA	3100	1/1	0.95	0.22	-	207,207,207,207	0
56	MG	CA	3138	1/1	0.96	0.05	-	74,74,74,74	0
56	MG	CA	3077	1/1	0.83	0.33	-	206,206,206,206	0
56	MG	DA	3059	1/1	0.99	0.13	-	27,27,27,27	0
56	MG	AA	1641	1/1	0.96	0.07	-	65,65,65,65	0
56	MG	CA	3085	1/1	0.97	0.07	-	56,56,56,56	0
56	MG	DA	3144	1/1	0.97	0.25	-	72,72,72,72	0
56	MG	CA	3087	1/1	0.96	0.08	-	65,65,65,65	0
56	MG	DA	3139	1/1	0.84	0.27	-	86,86,86,86	0
56	MG	CA	3150	1/1	0.86	0.97	-	89,89,89,89	0
56	MG	DA	3163	1/1	0.93	0.44	-	78,78,78,78	0
56	MG	BA	1637	1/1	0.81	0.77	-	87,87,87,87	0
56	MG	AA	1633	1/1	0.92	0.15	-	225,225,225,225	0
56	MG	BA	1606	1/1	0.85	0.22	-	273,273,273,273	0
56	MG	DA	3159	1/1	0.96	0.14	-	70,70,70,70	0
56	MG	DA	3030	1/1	0.99	0.10	-	55,55,55,55	0
56	MG	DA	3185	1/1	0.84	0.33	-	70,70,70,70	0
56	MG	CA	3142	1/1	0.92	0.13	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3017	1/1	0.97	0.12	-	60,60,60,60	0
61	PEG	DA	3229	7/7	0.88	0.33	-	79,83,88,88	0
56	MG	BA	1604	1/1	0.56	0.52	-	272,272,272,272	0
56	MG	DA	3164	1/1	0.93	0.24	-	62,62,62,62	0
56	MG	DA	3014	1/1	0.96	0.17	-	122,122,122,122	0
56	MG	DA	3130	1/1	0.92	1.05	-	68,68,68,68	0
56	MG	AA	1655	1/1	0.89	0.19	-	214,214,214,214	0
56	MG	DA	3127	1/1	0.89	0.24	-	60,60,60,60	0
56	MG	CA	3128	1/1	0.88	0.24	-	81,81,81,81	0
56	MG	CA	3148	1/1	0.94	0.45	-	50,50,50,50	1
56	MG	AA	1630	1/1	0.97	0.11	-	102,102,102,102	0
56	MG	DA	3230	1/1	0.99	0.05	-	53,53,53,53	0
56	MG	DA	3183	1/1	0.28	2.52	-	97,97,97,97	0
56	MG	AA	1604	1/1	0.77	0.34	-	66,66,66,66	0
56	MG	BA	1634	1/1	0.86	0.08	-	199,199,199,199	0
56	MG	DA	3081	1/1	0.98	0.25	-	130,130,130,130	0
56	MG	CA	3010	1/1	0.91	0.84	-	270,270,270,270	0
56	MG	CA	3058	1/1	0.97	0.09	-	87,87,87,87	0
56	MG	DA	3070	1/1	0.98	0.17	-	37,37,37,37	0
56	MG	CA	3130	1/1	0.80	0.22	-	72,72,72,72	0
56	MG	AA	1626	1/1	0.61	0.94	-	111,111,111,111	0
56	MG	CA	3093	1/1	0.90	0.09	-	72,72,72,72	0
56	MG	CA	3119	1/1	0.85	0.22	-	76,76,76,76	0
56	MG	CA	3134	1/1	0.50	0.61	-	107,107,107,107	0
56	MG	DA	3143	1/1	0.91	0.39	-	51,51,51,51	0
56	MG	CA	3118	1/1	0.97	0.23	-	47,47,47,47	0
56	MG	DA	3041	1/1	1.00	0.12	-	23,23,23,23	0
56	MG	DA	3116	1/1	0.98	0.09	-	40,40,40,40	0
56	MG	BA	1607	1/1	0.86	0.37	-	195,195,195,195	0
56	MG	DB	209	1/1	0.89	0.53	-	71,71,71,71	0
56	MG	CA	3067	1/1	0.86	0.77	-	278,278,278,278	0
56	MG	DA	3168	1/1	0.75	0.49	-	65,65,65,65	0
56	MG	DA	3178	1/1	0.86	0.68	-	89,89,89,89	0
56	MG	DA	3169	1/1	0.83	0.94	-	95,95,95,95	0
56	MG	CA	3146	1/1	0.92	0.24	-	149,149,149,149	0
56	MG	DA	3079	1/1	0.99	0.06	-	31,31,31,31	0
59	PUT	AA	1675	6/6	0.63	0.69	-	101,102,103,103	0
56	MG	CA	3108	1/1	0.90	0.18	-	65,65,65,65	0
56	MG	CA	3050	1/1	0.98	0.07	-	51,51,51,51	0
56	MG	DA	3027	1/1	1.00	0.10	-	43,43,43,43	0
56	MG	DA	3042	1/1	0.99	0.06	-	56,56,56,56	0
56	MG	CA	3049	1/1	0.93	0.13	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3110	1/1	0.99	0.09	-	32,32,32,32	0
56	MG	CA	3151	1/1	0.87	0.31	-	72,72,72,72	0
56	MG	DA	3056	1/1	0.98	0.13	-	151,151,151,151	0
56	MG	CA	3129	1/1	0.67	0.40	-	125,125,125,125	0
56	MG	CA	3126	1/1	0.39	0.39	-	107,107,107,107	0
56	MG	CA	3034	1/1	0.90	0.11	-	235,235,235,235	0
56	MG	DA	3157	1/1	0.83	0.15	-	69,69,69,69	0
56	MG	DB	203	1/1	0.99	0.12	-	34,34,34,34	0
56	MG	CA	3012	1/1	0.94	0.10	-	89,89,89,89	0
56	MG	DA	3161	1/1	0.93	0.16	-	119,119,119,119	0
59	PUT	AA	1672	6/6	0.82	0.36	-	79,82,85,85	0
56	MG	DA	3154	1/1	0.71	0.17	-	80,80,80,80	0
56	MG	DA	3153	1/1	0.98	0.19	-	33,33,33,33	0
56	MG	CA	3123	1/1	0.83	0.26	-	104,104,104,104	0
56	MG	AA	1621	1/1	0.80	0.34	-	69,69,69,69	0
56	MG	DA	3171	1/1	0.71	0.68	-	111,111,111,111	0
56	MG	AA	1623	1/1	0.77	0.40	-	77,77,77,77	0
56	MG	AA	1669	1/1	0.94	0.13	-	89,89,89,89	0
56	MG	DA	3138	1/1	0.92	0.21	-	72,72,72,72	0
56	MG	CA	3090	1/1	0.94	0.16	-	118,118,118,118	0
56	MG	DA	3071	1/1	1.00	0.11	-	50,50,50,50	0
56	MG	DA	3145	1/1	0.92	0.22	-	63,63,63,63	0
56	MG	BA	1639	1/1	0.82	0.28	-	103,103,103,103	0
56	MG	BA	1601	1/1	0.97	0.25	-	158,158,158,158	0
56	MG	CA	3152	1/1	0.67	0.39	-	158,158,158,158	0
56	MG	DA	3021	1/1	0.99	0.24	-	9,9,9,9	0
56	MG	AA	1601	1/1	0.86	1.09	-	86,86,86,86	0
56	MG	DA	3120	1/1	0.98	0.10	-	48,48,48,48	0
56	MG	DB	202	1/1	1.00	0.08	-	30,30,30,30	0
56	MG	CA	3072	1/1	0.95	0.66	-	274,274,274,274	0
56	MG	DA	3093	1/1	0.99	0.15	-	23,23,23,23	0
56	MG	CA	3116	1/1	0.72	0.51	-	79,79,79,79	0
56	MG	DA	3122	1/1	0.95	0.28	-	76,76,76,76	0
56	MG	AA	1610	1/1	0.92	0.27	-	85,85,85,85	0
56	MG	DA	3179	1/1	0.37	0.62	-	102,102,102,102	0
62	EDO	DB	211	4/4	0.88	0.32	-	98,99,99,100	0
56	MG	CA	3110	1/1	0.54	0.24	-	92,92,92,92	0
56	MG	DA	3047	1/1	0.99	0.07	-	61,61,61,61	0
56	MG	DA	3131	1/1	0.96	0.23	-	79,79,79,79	0
56	MG	AA	1636	1/1	0.89	0.17	-	110,110,110,110	0
56	MG	CA	3097	1/1	0.97	0.09	-	109,109,109,109	0
56	MG	CA	3075	1/1	0.54	2.38	-	238,238,238,238	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3135	1/1	0.68	0.29	-	81,81,81,81	0
56	MG	DA	3166	1/1	0.58	0.27	-	81,81,81,81	0
56	MG	DA	3089	1/1	0.98	0.16	-	32,32,32,32	0
56	MG	AA	1654	1/1	0.91	0.20	-	244,244,244,244	0
56	MG	CA	3071	1/1	0.93	0.21	-	146,146,146,146	0
56	MG	DA	3106	1/1	1.00	0.17	-	25,25,25,25	0
56	MG	DB	206	1/1	0.74	0.34	-	129,129,129,129	0
56	MG	CA	3004	1/1	0.96	0.07	-	83,83,83,83	0
56	MG	CA	3106	1/1	0.70	0.28	-	84,84,84,84	0
56	MG	BA	1629	1/1	0.98	0.55	-	144,144,144,144	0
56	MG	AA	1638	1/1	0.93	0.06	-	100,100,100,100	0
56	MG	DA	3165	1/1	0.91	0.14	-	72,72,72,72	0
56	MG	DA	3022	1/1	0.99	0.10	-	43,43,43,43	0
56	MG	DA	3102	1/1	0.98	0.16	-	29,29,29,29	0
56	MG	DA	3036	1/1	1.00	0.12	-	28,28,28,28	0
56	MG	DA	3160	1/1	0.94	0.55	-	57,57,57,57	0
56	MG	DA	3013	1/1	0.99	0.09	-	33,33,33,33	0
56	MG	CA	3048	1/1	0.85	0.09	-	97,97,97,97	0
56	MG	DA	3091	1/1	0.98	0.20	-	30,30,30,30	0
56	MG	BA	1630	1/1	0.41	0.15	-	271,271,271,271	0
56	MG	DA	3083	1/1	0.97	0.10	-	46,46,46,46	0
56	MG	BA	1618	1/1	0.95	0.10	-	106,106,106,106	0
56	MG	AA	1640	1/1	0.93	0.10	-	60,60,60,60	0
56	MG	DA	3051	1/1	0.98	0.14	-	46,46,46,46	0
56	MG	AA	1616	1/1	0.84	0.52	-	75,75,75,75	0
56	MG	AA	1652	1/1	0.99	0.21	-	30,30,30,30	0
56	MG	DA	3098	1/1	1.00	0.12	-	32,32,32,32	0
56	MG	AA	1617	1/1	0.68	0.39	-	101,101,101,101	0
56	MG	DA	3065	1/1	0.97	0.12	-	120,120,120,120	0
56	MG	CA	3156	1/1	0.89	0.22	-	210,210,210,210	0
56	MG	CA	3147	1/1	0.90	0.39	-	25,25,25,25	1
56	MG	CA	3057	1/1	0.85	0.16	-	121,121,121,121	0
56	MG	DA	3117	1/1	0.99	0.17	-	36,36,36,36	0
56	MG	DM	202	1/1	0.99	0.05	-	43,43,43,43	0
56	MG	CA	3028	1/1	0.73	0.22	-	277,277,277,277	0
56	MG	CA	3132	1/1	0.59	0.49	-	102,102,102,102	0
56	MG	CA	3096	1/1	0.98	0.05	-	97,97,97,97	0
56	MG	BA	1644	1/1	0.94	0.13	-	64,64,64,64	0
62	EDO	DA	3217	4/4	0.83	0.28	-	84,85,86,87	0
56	MG	CA	3095	1/1	0.95	0.11	-	68,68,68,68	0
56	MG	CA	3149	1/1	0.82	0.46	-	76,76,76,76	0
56	MG	DA	3061	1/1	0.99	0.08	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	BA	1641	1/1	0.70	0.14	-	94,94,94,94	0
56	MG	DA	3035	1/1	0.98	0.13	-	22,22,22,22	0
56	MG	DA	3076	1/1	0.97	0.09	-	39,39,39,39	0
56	MG	DA	3105	1/1	0.99	0.13	-	38,38,38,38	0
56	MG	DB	204	1/1	0.94	0.11	-	48,48,48,48	0
56	MG	DA	3077	1/1	1.00	0.16	-	42,42,42,42	0
56	MG	BA	1636	1/1	0.92	0.44	-	97,97,97,97	0
56	MG	DA	3147	1/1	0.95	0.25	-	95,95,95,95	0
56	MG	AA	1629	1/1	0.98	0.17	-	99,99,99,99	0
56	MG	CA	3127	1/1	0.77	0.14	-	87,87,87,87	0
56	MG	AA	1660	1/1	0.79	0.22	-	277,277,277,277	0
56	MG	DA	3170	1/1	0.71	0.53	-	106,106,106,106	0
56	MG	AA	1613	1/1	0.90	0.89	-	64,64,64,64	0
56	MG	CA	3070	1/1	0.84	0.08	-	79,79,79,79	0
56	MG	BA	1635	1/1	0.99	0.09	-	106,106,106,106	0
56	MG	CA	3073	1/1	0.90	0.21	-	175,175,175,175	0
56	MG	DA	3174	1/1	0.87	0.49	-	90,90,90,90	0
56	MG	CA	3109	1/1	0.92	0.24	-	63,63,63,63	0
58	MPD	DA	3212	8/8	0.88	0.28	-	83,85,86,90	0
56	MG	CA	3140	1/1	0.53	0.46	-	88,88,88,88	0
56	MG	DA	3124	1/1	0.85	1.07	-	49,49,49,49	0
59	PUT	DA	3191	6/6	0.92	0.24	-	48,54,57,59	0
56	MG	CA	3069	1/1	0.85	0.18	-	135,135,135,135	0
66	ACY	DA	3199	4/4	0.76	0.40	-	108,109,109,109	0
56	MG	DA	3044	1/1	0.99	0.13	-	29,29,29,29	0
56	MG	CA	3002	1/1	0.81	0.31	-	265,265,265,265	0
56	MG	CA	3023	1/1	0.73	0.18	-	245,245,245,245	0
56	MG	DA	3085	1/1	0.99	0.06	-	52,52,52,52	0
68	TRS	DA	3222	8/8	0.72	0.68	-	107,112,117,117	0
56	MG	DA	3040	1/1	0.99	0.10	-	20,20,20,20	0
56	MG	DA	3075	1/1	0.99	0.10	-	23,23,23,23	0
56	MG	DA	3054	1/1	0.95	0.17	-	190,190,190,190	0
56	MG	CA	3139	1/1	0.21	0.72	-	114,114,114,114	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.